STATISTICS FOR INDUSTRY AND TECHNOLOGY

Barry C. Arnold
N. Balakrishnan
José María Sarabia
Roberto Mínguez
Editors

Advances in Mathematical and Statistical Modeling

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Series Editor

N. Balakrishnan
McMaster University
Department of Mathematics and Statistics
1280 Main Street West
Hamilton, Ontario L8S 4K1
Canada

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Barry C. Arnold
N. Balakrishnan
José María Sarabia
Roberto Mínguez
Editors

Birkhäuser
Boston • Basel • Berlin

Barry C. Arnold
University of California Riverside
Dept. Statistics
Riverside CA 92521
USA
Barry.Arnold@ucr.edu

N. Balakrishnan
McMaster University
Dept. Mathematics & Statistics
Hamilton ON L8S 4K1
Canada
bala@mcmaster.ca
http://www.math.mcmaster.ca/bala

José María Sarabia
University of Cantabria
Dept. of Economics
Avenida de los Castros, s/n
39005 Santander
Spain
sarabiaj@unican.es
http://personales.unican.es/sarabiaj

Roberto Mínguez
University of Castilla-La Mancha
Dept. of Applied Mathematics
Canales y Puertos
13071 Ciudad Real
Spain
roberto.minguez@uclm.es
http://www.uclm.es/profesorado/robertominguez/homepage.htm

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This book is prepared as a tribute to Professor Enrique Castillo, who has contributed significantly to the fields of mathematics and engineering, and has nurtured numerous engineers and mathematicians.

ENRIQUE CASTILLO

Contents

Part V Extreme Value Theory

Part IX Discrete Distributions

Preface

Professor Enrique Castillo was born on October 17, 1946, in Santiago de Compostela, Spain. His parents, Mr. Enrique Castillo Latorre, an industrial engineer, and Mrs. Pastora Ron Noya, a school teacher, have four sons: María del Carmen, Enrique, María José, and Francisco.

This biographical summary includes Professor Castillo's family, education, and professional career and accomplishments, as well as the human side of Professor Castillo and his wife María del Carmen.

Family: Professor Castillo's own family started on July 17, 1970, when he got married to María del Carmen Sánchez Hidalgo. They now have five children: (1) María del Carmen, who was born in 1972 and now holds a Ph.D. Degree in Civil Engineering; (2) Enrique, who was born in 1973 and is now a civil engineer; (3) Eva, who was born in 1974 and is currently a school teacher specializing in English and special education; (4) Puri, who was adopted in 1978 and is now a hairdresser; and (5) Sergio, a child with a physical disability who was adopted in 1982.

Professor Castillo's family increased even further when his daughter Puri got married to José, his daughter Eva got married to Pepe, and his son Enrique got married to Gloria. Professor Castillo and his wife now have two granddaughters: Andrea and Irene.

Education: Initially Professor Castillo lived in Madrid and studied at the HH. Maristas School. He then attended the Polytechnical University of Madrid to study Civil Engineering. The third year he started working at a consulting engineering firm under the direction of Prof. Florencio del Pozo and was devoted to bridge design. Two years later he moved to another important consulting firm called Intecsa.

After getting his Bachelor of Science degree in Civil Engineering in 1969, he started his Ph.D. program of study with Professor Jiménez Salas, a member of the Spanish Academy of Sciences, in Geotechnics. Professor Salas then facilitated Professor Castillo's joining the Northwestern University's Geotechnical Program, with Professor Raymond Krizek, a member of the National Academy of Engineering in the United States of America.

In July 1970, Professor Castillo and María del Carmen travelled together to Chicago, where Professor Castillo started his Ph.D. Program at Northwestern University. Professor Castillo was the first person to go directly to the Ph.D. Program without going

through a Master's program in Geotechnics. He obtained the maximum grades and finished his Ph.D. degree in 1972 in record time (15 and one half months) at Northwestern University. He then returned to Spain in December 1972.

In 1973 he obtained a second Ph.D. degree in Geotechnics from the Polytechnical University of Madrid.

In 1974 he finished his Bachelor's of Science degree in Mathematics (in only one year he finished all the courses after some transfer of credits due to his degree in engineering).

Professional Career: In September 1973, he moved to Santander, Spain, and started teaching at the University of Santander (now University of Cantabria), changing from the Geotechnical field to the field of mathematics. In 1976 he became a Full University Professor in Algebra and Statistics. He has also served as the Head of the Department of Applied Mathematics (1975-1984), Vice Dean of the School of Civil Engineering (1975-1982), and Vice Rector of the University of Cantabria (1977-1978).

During the 1985-1986 academic year, Professor Castillo was invited by Professor Janos Galambos to spend a sabbatical year at Temple University with all his family. During this year, Professor Castillo wrote his first book on Extremes as well as some papers. In 2000-2001, he spent a year at the University of Castilla La Mancha in Ciudad Real, Spain, where he helped in the creation of the new School of Civil Engineers.

In 2006-2007 he spent another sabbatical year alternating between Santander and Ciudad Real to continue his collaboration. This time his job was more focused on research duties and on starting new research groups in several areas.

Professor Castillo has also visited several universities in Europe (e.g., ETH Zürich, Manchester University in the United Kingdom and Lorand Eotvos University in Budapest), USA (e.g., Northwestern, Temple and Cornell Universities), Argentina (e.g., San Juan University, the National University of Nordeste in Corrientes, the National University of Technology in Resistencia, and the National University of Misiones in Posadas), and the Catholic University of Valparaiso in Chile. He was also invited as a Distinguished Visiting Professor at the American University in Cairo, Egypt.

Professor Castillo has also been a member of several professional and honorary societies including the Spanish Academy of Engineering, the American Statistical Association, the International Statistical Institute, the American Mathematical Society, the Spanish Society of Civil Engineering, the Spanish Society of Numerical Methods for Engineering, and the Spanish Society of Operations Research, Statistics, and Informatics.

Teaching and Mentoring: Professor Castillo is an excellent teacher and an exemplary mentor who is genuinely interested in his students. His door is always open to his students. So far he has supervised 29 Ph.D. theses in Engineering, Mathematics, Statistics, Medicine and Economics. He has taught many courses in various fields such as Mathematics (e.g., Numerical and Symbolic Calculus, Functional Analysis, Functional Equations, and Optimization), Probability and Statistics (e.g., Statistical Inference, Time Series Analysis, Analysis of Variance and Experimental Design, Regression Analysis, Extreme Value Theory, Biostatistics, and Simulation), Computer Science (Data Bases, Multimedia and Authoring Languages, Expert Systems and Artificial Intelligence).

Research and Scholarly Activities: Professor Castillo is an extraordinary researcher and a prolific writer. One most amazing aspect is that Professor Castillo is an expert in so many different areas of science—from engineering to mathematics. He has published more than 165 papers in 95 different scientific journals, 137 papers in conference proceedings. He is also the author and co-author of 13 books in English (John Wiley & Sons (3), Springer-Verlag (5), Academic Press (1), Kluwer (1), Elsevier (2), and Marcel Dekker(1)) and 15 books in Spanish. Obviously, Professor Castillo's research record is outstanding and impressive. In recognition of his achievements, for example, he has been inducted to the Spanish Academy of Engineers and has been awarded the Doctor Honoris Causa by the University of Oviedo. His curriculum vitae does not actually reflect the scope, depth, and impact of his research and scholarly activities, but some details can be seen in his web site at http://personales.unican.es/castie/.

Scholarly Awards: Professor Castillo has received several awards in recognition of his extraordinary work. These include:

- Extraordinary Ph. D. Prize, Polytechnical University of Madrid (1973)
- Entrecanales Prize for the best Ph.D. Thesis in Geotechnics, Polytechnical University of Madrid (1974).
- Founding Member of the Spanish Royal Academy of Engineering (1994).
- Doctor Honoris Causa by the University of Oviedo, Spain (1999).
- Gold Medal of the University of Castilla La Mancha (2001)
- Silver Medal of Cantabria University (2005).

The Human Side: Last, but perhaps most important, is the human side of Professor Castillo and his wife, María del Carmen. For obvious reasons, this side cannot be seen in his professional resume. While engaging in all of his professional activities, Professor Castillo and his wife can find the time, resources, and kind hearts to help the poor and the needy out of the goodness of their hearts. For example, they have taken care of two homeless people, initiating the Informatics Chair in Dueso Penance Center, to help inmates in Spanish prisons, and, perhaps most important of all, adopting two disabled children: Puri, a three year-old, mixed-race girl in 1982, and Sergio, a four year-old with a mental disability as a result of maltreatment in 1986.

Professor Castillo also has a genuine interest in international collaboration and cooperation and in helping students, researchers, and scholars from various countries in the world. He is especially interested in helping people from underdeveloped countries (e.g., countries in Latin America and Africa).

Together with Melecio Agúndez and Jesús Flórez, he created the Theology Chair at the University of Cantabria. He also collaborated in a Master's Program at the University of Cantabria for South American students, but because some of them stay in Spain after finishing, he has been offering the courses in South America. Thus, he founded in collaboration with other professors from the University of Cantabria and the collaboration of the Castilla-La Mancha University, the Itinerant Master's Program in Informatics, to help universities without enough means to have this program.

This includes Northeast National University (Corrientes) and the Misiones National University (Posadas) in Argentina, and National University of Pilar (Pilar) and East National University (Ciudad del Este) in Paraguay, where he received the Pin of the University.

Ciudad Real
July 2007

Barry C. Arnold
N. Balakrishnan
José María Sarabia
Roberto Mínguez

List of Contributors

Barry C. Arnold
Department of Statistics
University of California, Riverside
United States of America
barry.arnold@ucr.edu

N. Balakrishnan
Department of Mathematics and Statistics
McMaster University, Canada
bala@mcmaster.ca

Piero Baraldi
Department of Nuclear Engineering
Polytechnic of Milan, Italy
piero.baraldi@polimi.it

Eric Beutner
Institute of Statistics
RWTH Aachen University
Germany
beutner@stochastik.rwth-aachen.de

Jean-Philippe Boucher
Institute of Actuarial Sciences
Université Catholique de Louvain
Belgium
boucher@stat.ucl.ac.be

Carmen Castillo
Department of Civil Engineering
University of Castilla-La Mancha
Spain
MariaCarmen.Castillo@uclm.es

Eduardo W.V. Chaves
Department of Applied Mechanics and Engineering Design
University of Castilla-La Mancha
Spain
Eduardo.Vieira@uclm

Antonio S. Cofiño Gonzalez
C.M.T. de Cantabria y Asturias
Instituto Nacional de Meteorología
Spain
antonio.cofino@unican.es

Antonio J. Conejo
Department of Electrical Engineering
University of Castilla-La Mancha
Spain
Antonio.Conejo@uclm.es

Pedro Corcuera
Department of Applied Mathematics and Computational Sciences
University of Cantabria, Spain
pedro.corcuera@unican.es

Ulf Cormann
Department of Mathematics
University of Siegen, Germany
ulf.cormann@web.de

Carles M. Cuadras
Department of Statistics
University of Barcelona
Spain
ccuadras@ub.edu

Michel Denuit
Institute of Actuarial Sciences
Université Catholique de Louvain
Belgium
denuit@stat.ucl.ac.be

Fernando Escobedo
Department of Building and Civil Engineering
University of Castilla-La Mancha
Spain
fernando.escobedo@uclm.es

M. Isabel Fraga Alves
Department of Statistics and Operations Research
Faculty of Sciences of the University of Lisbon
Portugal
isabel.alves@fc.ul.pt

Pedro Galeano
Department of Statistics and Operations Research
University of Santiago de Compostela
Spain
pgaleano@usc.es

Akemi Gálvez
Department of Applied Mathematics and Computational Sciences
University of Cantabria
Spain
akemigt@hotmail.com

Giulio Gola
Department of Nuclear Engineering
Polytechnic of Milan
Italy
giulio.gola@polimi.it

M. Ivette Gomes
Department of Statistics
University of Lisbon
Portugal
ivette.gomes@fc.ul.pt

Patricia Gómez
Department of Applied Mathematics and Computational Sciences
University of Cantabria
Spain
gomezp@unican.es

Emilio Gómez-Deniz
Department of Quantitative Methods in Economics
University of Las Palmas de Gran Canaria
Spain
egomez@dmc.ulpgc.es

Montserrat Guillén
Department of Econometrics
University of Barcelona
Spain
mguillen@ub.edu

José M. Gutiérrez
Department of Applied Mathematics and Computer Sciences
University of Cantabria
Spain
gutierjm@unican.es

Ali S. Hadi
Department of Mathematics
American University in Cairo
Egypt
ahadi@aucegypt.edu

Dong-hoon Han
Department of Mathematics and Statistics
McMaster University
Canada
hand2@mcmaster.ca

Pedro J. Hernández
Department of Quantitative and Informatics Methods
Polytechnical University of Cartagena
Spain
pedroj.hernandez@upct.es

Sixto Herrera
Department of Applied Mathematics and Computer Sciences
University of Cantabria
Spain
sixto.herrera@alumnos.unican.es

Andrés Iglesias
Department of Applied Mathematics and Computational Sciences
University of Cantabria
Spain
andres.iglesias@unican.es

Daniel Jeske
Department of Statistics
University of California
United States of America
daniel.jeske@ucr.edu

Udo Kamps
Institute of Statistics
RWTH Aachen University
Germany
udo.kamps@rwth-aachen.de

Dimitris Karlis
Department of Statistics
Athens University of Economics and Business
Greece
karlis@aueb.gr

Adrienne Kemp
School of Mathematics and Statistics
University of St. Andrews
United Kingdom
awk@st-and.ac.uk

David Kemp
School of Mathematics and Statistics
University of St. Andrews
United Kingdom
cdk@st-and.ac.uk

Beatriz Lacruz
Department of Statistical Methods
University of Zaragoza
Spain
lacruz@unizar.es

Nirian Martín
Department of Statistics and Operations Research III
Complutense University of Madrid
Spain
nirian@estad.ucm.es

María Luisa Menéndez
Department of Applied Mathematics
Technical University of Madrid
Spain
ml.menendez@upm.es

Roberto Mínguez
Department of Applied Mathematics
University of Castilla-La Mancha
Spain
Roberto.Minguez@uclm.es

Jorge Navarro
Department of Statistics and Operations Research
University of Murcia
Spain
jorgenav@um.es

Claudia Neves
Department of Mathematics
University of Aveiro
Portugal
claudia@mat.ua.pt

Leandro Pardo
Department of Statistics and Operations Research I
Complutense University of Madrid
Spain
lpardo@mat.ucm.es

Julio A. Pardo
Department of Statistics and Operations Research I
Complutense University of Madrid
Spain
julio_pardo@mat.ucm.es

María del Carmen Pardo
Department of Statistics and Operations Research I
Complutense University of Madrid
Spain
mcapardo@mat.ucm.es

Marta Pascual
Department of Economics
University of Cantabria
Spain
pascualm@unican.es

Nicola Pedroni
Department of Nuclear Engineering
Polytechnic of Milan
Italy
nicolapedroni@gmail.com

Daniel Peña
Department of Statistics
Carlos III University of Madrid
Spain
dpena@est-econ.uc3m.es

Dinis Pestana
Department of Statistics
University of Lisbon
Portugal
dinis.pestana@fc.ul.pt

S. James Press
Department of Statistics
University of California at Riverside
United States of America
jpress@ucr.edu

Rosa Eva Pruneda
Department of Mathematics
University of Castilla-La Mancha
Spain
rosa.pruneda@uclm.es

Jaime Puig-Pey
Department of Applied Mathematics and Computational Sciences
University of Cantabria
Spain
puigpeyj@unican.es

Rolf-Dieter Reiss
Department of Mathematics
University of Siegen
Germany
reiss@stat.math.uni-siegen.de

Ligia Rodrigues
Department of Mathematics
Polytechnical Institute of Tomar
Portugal
ligia@aim.estt.ipt.pt

José Rodríguez
Department of Applied Mathematics and Computational Sciences
University of Cantabria
Spain
jose.rodriguezp@unican.es

Daniel San Martín Segura
Department of Applied Mathematics and Computational Sciences
University of Cantabria
Spain
sanmartind@unican.es

Lee Sang Eun
Department of Statistics
Kyonggi University, Korea
sanglee62@kyonggi.ac.kr

Jose María Sarabia
Department of Economics
University of Cantabria
Spain
sarabiaj@unican.es

María Sarabia
Department of Business Administration
University of Cantabria
Spain
sarabiam@unican.es

Key-Il Shin
Department of Statistics
Hankuk University of Foreign Studies
Korea
keyshin@hufs.ac.kr

Cristina Solares
Department of Applied Mathematics
University of Castilla-La Mancha
Spain
Cristina.Solares@uclm.es

José María Ureña
Department of Geography, City and Regional Planning
University of Cantabria
Spain
urenaj@unican.es

Clara Viseu
Department of Mathematics
Polytechnical Institute of Coimbra
Portugal
cviseu@iscac.pt

Ishay Weissman
Faculty of Industrial Engineering and Management
Technion - Israel Institute of Technology
Israel
ieriw01@ie.technion.ac.il

Evdokia Xekalaki
Department of Statistics
Athens University of Economics and Business
Greece
exek@aueb.gr

Qihao Xie
Department of Mathematics and Statistics
McMaster University, Canada
xiegi@math.macmaster.ca

Enrico Zio
Department of Nuclear Engineering
Polytechnic of Milan, Italy
enrico.zio@polimi.it

List of Tables

List of Figures

Part I

Distribution Theory and Applications

1

Enrique Castillo's Contributions to Conditional Specification

Barry C. Arnold

Department of Statistics, University of California, Riverside

Abstract: Enrique Castillo and his coworkers have made extensive contributions to our understanding of conditionally specified distributions. In addition to the development of a broad panoply of models, careful development of efficient appropriate inference procedures has been provided. A survey of this corpus of work is provided. Enrique's skills in stochastic modelling, simulation, graphical presentation, optimization and creative approaches to estimation and inference have found opportunities to be manifested in this aspect of his research career.

Keywords and phrases: Conditional densities, compatibility, near compatibility

1.1 Introduction

A bivariate density function will be said to be conditionally specified if its corresponding families of conditional densities (of X given Y and of Y given X) are either specifically prescribed or are postulated to be members of given parametric families of densities.

The classical example of this phenomenon is the class of bivariate densities with normal conditionals. For this we require that for each $y \in \mathbb{R}$, the conditional density of X given $Y = y$ should be a normal density with mean $\mu_1(y)$ and standard deviation $\sigma_2(y)$ (i.e., the conditional mean and variance are functions of y). In addition it is postulated that for each $x \in \mathbb{R}$, the conditional density of Y given $X = x$ is a normal density with mean $\mu_2(x)$ and standard deviation $\sigma_2(x)$. Such densities will be said to be of the normal conditionals form. Interest in such densities dates back at least to Bhattacharyya (1943). He discussed such distributions in the context of determining sufficient additional conditionals to guarantee that a model with normal conditionals should be a classical bivariate normal model.

In 1987, a joint paper by Enrique Castillo and Janos Galambos provided a complete characterization of the form of all normal conditionals densities (Castillo and Galambos, 1987). The solution was attractively simple. The class of normal conditionals densities formed an 8 parameter exponential family of densities. This opened the way for the development of appropriate inference procedures. However the high dimensionality of

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the parameter space meant that considerable creativity was required on the part of Enrique and other researchers in order to implement effective estimation strategies.

We may ask why Castillo and Galambos were able to completely resolve the issue of identifying the precise nature of the class of all normal conditionals densities. It is remarkable that Bhattacharrya 44 years earlier had come very close to identifying the solution. He provided a quite general form of densities with normal conditionals. However he did not verify that his model included all possible normal conditionals densities, nor did he discuss necessary constraints on the parameters in his model to ensure that it would represent a proper (integrable) density. Castillo and Galambos tied up all the loose ends.

The solution involves setting up and solving a functional equation – a problem that was naturally attractive to Castillo given his great interest in and understanding of functional equations. In the normal conditionals case it turned out that the functional equation in question was a special case of a classical functional equation dating back to the beginning of the twentieth century. Castillo and Galambos solved the equation independently of the earlier work but the subsequent recognition of its relation to more general fundamental equations opened up wide avenues for extension of the normal conditionals ideas to encompass a broad spectrum of conditionally specified models. We will document some of these developments in the present paper. It should be remarked that the field is far from exhausted. Many questions remain open. For example even if we restrict attention to the natural extension of the normal-conditionals model to 3 dimensions, the complete specification of the natural parameter space is not readily available.

Castillo to a much broader class of distributions, but also he has considered difficult questions involving partial and/or imprecise conditional specification. The most extensive discussion of material related to Castillo's work on conditional specification may be found in the book (Arnold et al., 1999) and the more recent survey article (Arnold et al., 2001a). Reference to current issues of *Math. Reviews* will reveal continued extensions and further contributions by Enrique, his coworkers and other researchers attracted to this fascinating field of inquiry.

1.2 Conditionals in Given Exponential Families

It is natural to begin the discussion by considering the question of when two families of conditional densities are compatible in the sense that there exists a joint density with the prescribed conditional densities as its conditional densities. Assume that (X, Y) is a random vector that has a joint density with respect to some product measure $\mu_1 \times \mu_2$ on $S(X) \times S(Y)$, where $S(X)$ denotes the set of possible values of X and $S(Y)$ the set of possible values of Y. For example, one variable could be discrete and the other absolutely continuous with respect to Lebesgue measure. The marginal, conditional and joint densities are denoted by $f_X(x), f_Y(y), f_{X|Y}(y|x), f_{X,Y}(x, y)$ and the sets of possible values $S(X)$ and $S(Y)$ can be finite, countable or uncountable.

In all our examples μ_1 and μ_2 correspond to either one-dimensional Lebesgue measure or to counting measure on some finite or countably infinite set. Nevertheless it is

good to keep in mind that natural extensions to more general measure spaces can be readily accommodated.

Consider two candidate families of conditional densities $a(x,y)$ and $b(x,y)$. We ask when is it true that there will exist a joint density for (X,Y) such that

$$f_{X|Y}(x|y) = a(x,y), \quad x \in S(X),\ y \in S(Y)$$

and

$$f_{Y|X}(y|x) = b(x,y), \quad s \in S(X),\ y \in S(Y).$$

If such a density exists we will say that a and b are compatible families of conditional densities.

A simple resolution to this problem was documented in Arnold and Press (1989). A joint density $f_{X,Y}(x,y)$ with $a(x,y)$ and $b(x,y)$ as its conditional densities will exist if and only if:

(i) $\{(x,y) : a(x,y) > 0\} = \{(x,y) : b(x,y) > 0\} = N$, say, and

(ii) There exist functions $u(x)$ and $v(y)$ such that for every $(x,y) \in N$,

$$\frac{a(x,y)}{b(x,y)} = u(x)v(y) \tag{1.1}$$

where $u(x)$ is integrable.

Careful discussion of the possible uniqueness of such a joint density $f_{X,Y}(x,y)$ may be found in Arnold et al. (1999, 2001a).

Most statistical applications involve a parametric formulation of possible models. With this in mind, it is appropriate to extrapolate from the precise compatibility question just described, to discuss the case in which the conditional densities are not completely specified but are postulated to belong to given parametric families of densities.

Consider a k-parameter family of densities in $\mathbb{R}$ with respect to μ_1 denoted by $\{f_1(x;\underline{\theta}) : \underline{\theta} \in \Theta\}$, where $\Theta \subset \mathbb{R}^k$. Also consider a second l-parameter family of densities $\{f_2(y;\underline{\tau}) : \underline{\tau} \in T\}$, where $T \subset \mathbb{R}^l$. We wish to identify, if possible, all of the joint densities for a random variable (X,Y) which have all their conditional densities given by f_1 and f_2. Thus, we require that for every $y \in S(Y)$ we have

$$f_{X|Y}(x|y) = f_1(x;\underline{\theta}(y)) \tag{1.2}$$

and for every $x \in S(X)$ we have

$$f_{Y|X}(y|x) = f_2(y;\underline{\tau}(x)) \tag{1.3}$$

for certain functions $\underline{\theta} : S(Y) \to \Theta$ and $\underline{\tau} : S(X) \to T$. If (1.2) and (1.3) are to hold, there must exist marginal densities for X and Y (f_X and f_Y) such that

$$f_Y(y) f_1(x;\underline{\theta}(y)) = f_X(x) f_2(y;\underline{\tau}(x)) \ \forall x \in S(X),\ y \in S(Y). \tag{1.4}$$

Our problem then is to solve the functional equation (1.4) for the functions $f_X(x)$, $f_Y(y)$, $\underline{\theta}(y)$ and $\underline{\tau}(x)$, given the families of densities f_1 and f_2. An expert on functional equations will be especially equipped to resolve such issues. Enter Castillo.

It must be remarked that just writing down a functional equation leaves us a long way from solving it. Only for special cases of f_1 and f_2, will (1.4) be amenable to solution. However the choices of f_1 and f_2 in which solution is feasible are quite varied and include many examples commonly discussed in the statistical literature. For example, the case in which f_1 and f_2 are quite general exponential families is readily solvable. This of course includes the normal conditionals model as a prototypical case.

Let $\{f_1(x;\underline{\theta}) : \underline{\theta} \in \Theta\}$ denote an l_1-parameter exponential family of densities with respect to μ_1 on $S(X)$, i.e.,

$$f_1(x;\underline{\theta}) = r_1(x)\beta_1(\underline{\theta}) \exp\left\{\sum_{i=1}^{l_1} \theta_i q_{1i}(x)\right\}. \tag{1.5}$$

Here $\Theta \subset \mathbb{R}^{l_1}$ is the natural parameter space (all $\underline{\theta}$'s such that (1.5) is integrable) and the q_{1i}'s are linearly independent. Consider also a second l_2-parameter exponential family of densities with respect to μ_2 on $S(Y)$.

$$f_2(y;\underline{\tau}) = r_2(y)\beta_2(\underline{\tau}) \exp\left\{\sum_{j=1}^{l_2} \tau_j q_{2j}(y)\right\}. \tag{1.6}$$

The class of all bivariate densities with conditionals in the families (1.5) and (1.6) may then be shown to be itself an exponential family of densities. Specifically we have the following result of Arnold and Strauss (1991).

Theorem 1. *Let $f(x,y)$ be a bivariate density whose conditional densities satisfy*

$$f(x|y) = f_1(x;\underline{\theta}(y))$$

$$f(y|x) = f_2(y:\underline{\tau}(x))$$

for some function $\underline{\theta}(y)$ and $\underline{\tau}(x)$ where f_1 and f_2 are defined in (1.5) and (1.6). It follows that $f(x,y)$ is of the form

$$f(x,y) = r_1(x)r_2(y)\exp\{\underline{q}^{(1)}(x)M\underline{q}^{(2)}(y)'\}, \tag{1.7}$$

in which

$$\underline{q}^{(1)}(x) = (q_{10}(x), q_{11}(x), q_{12}(x), \ldots, q_{1l_1}(x)),$$

$$\underline{q}^{(2)}(y) = (q_{20}(y), q_{21}(y), q_{22}(y), \ldots, q_{2l_2}(y)),$$

where $q_{10}(x) = q_{20}(y) \equiv 1$ and M is a matrix of parameters of appropriate dimensions [i.e., $(l_1+1)\times(l_2+1)$] subject to the requirement that

$$\int_{S(X)}\int_{S(Y)} f(x,y)d\mu_1(x)d\mu_2(y) = 1.$$

For convenience we can partition the matrix M as follows:

$$M = \begin{pmatrix} m_{00} & \vert & m_{01} & \cdots & m_{0l_2} \\ -- & + & -- & -- & -- \\ m_{10} & \vert & & & \\ \cdots & \vert & & \tilde{M} & \\ m_{l_1 0} & \vert & & & \end{pmatrix}. \tag{1.8}$$

Note that the case of independence is included; it corresponds to the choice $\tilde{M} \equiv 0$.

The proof of this result consists of writing the joint density of (X, Y) as a product of a marginal and a conditional density in two ways to obtain the relation

$$r_1(x)r_2(y)\exp\left[\sum_{j=0}^{l_2}\tau_j(x)q_{2j}(y)\right] = r_1(x)r_2(y)\exp\left[\sum_{i=0}^{l_1}\theta_i(y)q_{li}(x)\right], \tag{1.9}$$

where we have defined

$$\tau_0(x) = \log[g(x)\beta_2(\underline{\tau}(x))/r_1(x)],$$
$$\theta_0(y) = \log[h(y)\beta_1(\underline{\theta}(y))/r_2(y)].$$

Cancelling $r_1(x)r_2(y)$ from both sides of (1.9) we reduce to an equation whose solution is given directly by the following classical theorem.

Theorem 2 (Stephanos (1904); Levi-Civita (1913); Suto (1914)). *All solutions of the equation*

$$\sum_{i=1}^{r} f_i(x)\phi_i(y) = \sum_{j=1}^{s} g_j(y)\psi_j(x),\ x \in S(X),\ y \in S(Y), \tag{1.10}$$

where $\{\phi_i\}_{i=1}^r$ *and* $\{\psi_j\}_{j=1}^s$ *are given systems of linearly independent functions, are of the form*

$$\underline{f}(x) = C\underline{\phi}(x)$$

and

$$\underline{g}(y) = D\underline{\phi}(y).$$

where $D = C'$.

For details on this and related functional equations see Castillo and Ruiz-Cobo (1992).

Using the notation of Theorem 1, the totality of bivariate densities with normal conditionals are those of the form

$$f_{X,Y}(x,y) = \exp\left\{(1, x, x^2)\begin{pmatrix} m_{00} & m_{01} & m_{02} \\ m_{10} & m_{11} & m_{12} \\ m_{20} & m_{21} & m_{22} \end{pmatrix}\begin{pmatrix} 1 \\ y \\ y^2 \end{pmatrix}\right\} \tag{1.11}$$

subject to the constraint that the m_{ij}'s be chosen such that (1.11) is integrable.

The conditional expectations and variances are

$$E[Y|x] = -\frac{m_{01} + m_{11}x + m_{21}x^2}{2(m_{02} + m_{12}x + m_{22}x^2)}, \tag{1.12}$$

$$\mathrm{Var}[Y|x] = -\frac{1}{2(m_{02} + m_{12}x + m_{22}x^2)}, \tag{1.13}$$

$$E[X|y] = -\frac{m_{10} + m_{11}y + m_{12}y^2}{2(m_{20} + m_{21}y + m_{22}y^2)}, \tag{1.14}$$

$$\mathrm{Var}[X|y] = -\frac{1}{2(m_{20} + m_{21}y + m_{22}y^2)}. \tag{1.15}$$

Densities of the form (1.11), the normal conditionals densities, form an 8 parameter exponential family. The coefficient m_{00} is a normalizing constant, determined by the other m_{ij}'s to ensure that the density integrates to 1.

Sufficient conditions for integrability of (1.11) are that the m_{ij}'s satisfy one of the following two sets of conditions:

$$\text{(I)} \quad m_{22} = m_{21} = m_{12} = 0,\ m_{20} < 0,\ m_{02} < 0 \text{ and } m_{11}^2 < 4m_{02}m_{20}, \tag{1.16}$$

$$\text{(II)} \quad m_{22} < 0,\ 4m_{22}m_{02} > m_{12}^2,\ 4m_{22}m_{20} > m_{21}^2. \tag{1.17}$$

Case I corresponds to classical bivariate normal densities. In the non-Gaussian case (i.e., when (1.17) holds) the regression functions are non-linear and consequently they can intersect more than once. It follows that the corresponding joint densities can be bimodal or even trimodal!

Theorem 1 provides a simple specification of the form of joint densities with conditionals in prescribed exponential families. However the determination of the natural parameter space for the joint density is frequently a non-trivial exercise. The reader is referred to Castillo and Galambos (1989) for discussion of the constraints on the m_{ij}'s appearing in (1.7) necessary to ensure integrability when the conditional densities are in the normal and the gamma family.

Of course if the supports of X and Y are bounded then no constraints are required on the m_{ij}'s to ensure integrability. See Arnold and Sen Gupta (2004) for such an example, involving circular normal (or von Mises) conditional densities.

1.3 Conditionals in Given Non-Exponential Families

Recall again the key functional equation (1.4) for determining all bivariate densities with conditionals in parametric families (1.2) and (1.3), i.e.,

$$f_Y(y)f_1(x;\underline{\theta}(y)) = f_X(x)f_2(y;\tau(x)),\ x \in S(X), y \in S(Y).$$

As we have seen, cases in which f_1 and f_2 are exponential families of densities yield a simple solution of this functional equation using the Stephanos-Levi-Civita-Suto theorem. Enrique Castillo and coworkers identified several other choices for f_1 and f_2 that were not exponential families but that lent themselves to straightforward solutions of the functional equation (1.4). The list of such models includes

(i) Pareto conditionals. Suppose that

$$f_1(x;\alpha,\sigma) = \frac{\alpha}{\sigma}(1+\frac{x}{\sigma})^{-(\alpha+1)}\ I(x>0). \tag{1.18}$$

Suppose that $\alpha > 0$ is fixed and we seek all densities with conditionals of X given Y and of Y given X in the family (1.18). Upon setting up the corresponding functional equation (1.4) and transforming it to form (1.10) we readily identify the desired class of densities to be of the form

$$f_{X,Y}(x,y) \propto \frac{1}{(\lambda_{00}+\lambda_{10}x+\lambda_{01}y+\lambda_{11}xy)^{\alpha+1}} \tag{1.19}$$

for suitable choices of $\lambda_{00}, \lambda_{10}, \lambda_{01}$ and λ_{11} (chosen to ensure non-negativity and integrability).

(ii) Cauchy conditionals. The Cauchy density is of the form

$$f_X(x;\mu,\sigma) = [\pi\sigma(1+(\frac{x-\mu}{\sigma})^2)]^{-1}, \quad x \in \mathbb{R} \tag{1.20}$$

where $\mu \in \mathbb{R}$ and $\sigma \in \mathbb{R}^+$. The by-now-familiar functional equation route leads to the following class of bivariate densities with Cauchy conditionals

$$f_{X,Y}(x,y) \propto [(1,x,x^2)M(1,y,y^2)']^{-1} \tag{1.21}$$

where the m_{ij}'s are chosen to ensure non-negativity and integrability of the density.

See Arnold et al. (1999) for a more extensive list of examples. Notably absent from the list in which solution is obtainable is the case of logistic conditionals. To identify the general class of bivariate densities with all conditionals in the logistic family one would need to solve the following innocuous looking functional equation:

$$\phi(y)\cosh(\frac{x-\mu_1(y)}{2\sigma_1(y)}) = \varphi(x)\cosh(\frac{y-\mu_2(x)}{2\sigma_2(x)}). \tag{1.22}$$

It is possible to solve (1.22) in the trivial case in which $\sigma_1(y) = \sigma_1$ and $\sigma_2(x) = \sigma_2$, but even Enrique is not able to solve the general equation.

1.4 Truncated and Weighted Distributions

Many cases in which it is possible to identify all bivariate densities with conditionals in families f_1 and f_2 also allow for straightforward resolution of the problem in which the conditionals are required to be members of truncated and/or weighted versions of f_1 and f_2. See Arnold et al. (2005) for details on this.

1.5 A Digression on Improper Models

There are situations in which improper models are judged to be useful. For example in Bayesian inference settings it is not uncommon to use improper priors. In such a setting both sets of conditional densities (the likelihood and the posterior density) are proper but one marginal (the prior) and the joint density are improper.

If one wishes to use fiducial inference techniques, analogous problems arise. For example if $X \sim N(\mu,1)$, then the fiducial distribution of μ, having observed $X = x$, will be $\mu \sim N(x,1)$. Interpreting these as conditional densities we have $X|\mu \sim N(\mu,1)$ and $\mu|X = x \sim N(x,1)$. No integrable joint density for (X,μ) will exist with these conditional densities. Here too the improper model may be deemed to be still useful

for inference purposes. Several other instances of improper models, many in the context of fatigue models, are discussed in Castillo et al. (1985) and Castillo (1988).

1.6 Characterizations of Classical Models Via Conditional Specifications

Bhattacharyya's (1943) introduction of models with normal conditionals was motivated by a search for characterizations of the classical bivariate normal model beginning with assumptions about the families of conditional densities of a bivariate density. He and, subsequently, Castillo and Galambos (1989) investigated what additional conditions, besides normal conditionals, were needed to characterize the classical model. In addition to normal conditionals, any one of the following properties is sufficient to guarantee a classical bivariate normal distribution for (X, Y).

(i) $\text{var}(X|Y) = y) = c \in \mathbb{R}^+$
(ii) $\text{var}(Y|X) = x) = c \in \mathbb{R}^+$
(iii) $\lim_{y\to\infty} y^2 \text{ var}(X|Y = y) = \infty$
(iv) $\lim_{x\to\infty} x^2 \text{ var}(Y|X = x) = \infty$
(v) $E(Y|X = x) = ax + b$ with $a \neq 0$
(vi) $E(X|Y = y) = ay + b$ with $a \neq 0$.

Each of these conditions is sufficient to guarantee that $m_{22} = 0$ in (1.11) and consequently that the model is of the classical bivariate normal type.

It is of course possible to define a k-variate joint density with normal conditionals and to investigate how such distributions are related to classical k-variate normal densities. For discussion of such issues see Arnold et al. (1994b,c).

Parallel discussion of the multivariate Pareto model may be found in Arnold et al. (1994a).

1.7 Back to the Bayesian Scenario

The usual setting for Bayesian inference involves data $\underline{X}$ whose distribution is described by a family of densities $\{f(\underline{x};\underline{\theta}) : \theta \in \Theta\}$ where $\Theta \subset \mathbb{R}^k$. A suitable prior density is selected for $\underline{\theta}$ and attention is focused on the posterior density of $\underline{\theta}$, i.e., $f(\underline{\theta}|\underline{x})$. Typically a prior density for $\underline{\theta}$, say $f(\underline{\theta})$, is selected to approximately reflect prior beliefs about $\underline{\theta}$ and to be of such a form as to ensure that the resulting posterior density $f(\underline{\theta}|\underline{x})$ is analytically tractable, or at least is of a such a nature that permits easy simulation.

Conditionally specified distributions can, in many cases, be shown to provide convenient conjugate prior families in settings where the parameter space is of dimension greater than 1. Discussion of such conditionally conjugate priors may be found in Arnold et al. (1997, 1998a,b). For normal data with unknown mean μ and unknown precision $\tau(= 1/\sigma^2)$, a joint prior with normal and gamma conditionals is suggested.

With such a prior, the posterior density of (μ, τ) given $\underline{X} = \underline{x}$ (given the data) is again found to have normal and gamma conditionals. Simulation of realizations from such a density is readily accomplished using a simple Gibbs sampler routine.

In principle, the conditional specification approach can be used in a variety of multiparameter settings, which may be troublesome from a classical viewpoint (see e.g., Arnold et al. (1999), p. 322–3).

1.8 Inference for Conditionally Specified Models

The typical conditionally specified multivariate model will include many parameters and an awkward normalizing constant that is often not available in analytic form. Some ingenuity is required to fit such models and to perform routine inference (estimation and hypothesis testing).

Typically the awkward normalizing constant only appears in the joint and marginal densities. It does not appear in the conditional densities. In view of this, Arnold and Strauss (1988) (and earlier, Besag (1974)) suggested maximizing the so-called pseudo-likelihood (or conditional likelihood function). Thus we choose values of $\underline{\Theta}$ to maximize

$$PL(\underline{\theta}) = \prod_{i=1}^{n} f_{X|Y}(x_i|y_i;\underline{\theta}) f_{Y|X}(y_i|x_i;\underline{\theta}). \tag{1.23}$$

Estimates obtained in this way are consistent and asymptotically normal and sometimes remarkably efficient.

Several alternative estimation strategies have been proposed. For example, Moschopoulos and Staniswallis (1994) utilize Poisson regression programs to deal with discrete and/or grouped data from distributions with conditionals in exponential families. Several variations on the method of moments have been proposed. A promising recent proposal is that of Arnold et al. (2001b), who utilize an extension of a well known lemma of Charles Stein to develop systems of equations suitable for estimation via the method of moments.

1.9 Incomplete and Imprecise Conditional Specification

Rather than having precise knowledge of all the conditional distributions of a given bivariate model, it may well be the case that only partial and/or imprecise knowledge is available about some features of the bivariate distribution. In such a situation we naturally seek a joint distribution that is compatible with the given information or, failing that, one which is in some sense minimally incompatable. In this section we will restrict attention to finite discrete models.

Thus we consider a bivariate random variable (X, Y) where X has possible values $1, 2, \ldots, I$ and Y has possible values $1, 2, \ldots, J$. We consider first the case where full

conditional information is available, i.e., we suppose that two candidate conditional distribution matrices are given

$$A = (a_{ij})$$
$$B = (b_{ij})$$

both of dimension $I \times J$. In these matrices

$$a_{ij} = P(X = i|Y = j)$$
$$b_{ij} = P(Y = j|X = i).$$

The columns of A sum to 1 and the rows of B sum to 1. We say A and B are compatible if there exists

$$P = (p_{ij})$$

with $p_{ij} \geq 0 \ \forall i, j$ and $\sum_{ij} p_{ij} = 1$ such that

$$a_{ij} = p_{ij}/p_{\cdot j} \ \forall i, j$$

and

$$b_{ij} = p_{ij}/p_{i\cdot} \ \forall i, j$$

(here $p_{i\cdot} = \sum_j p_{ij}$ and $p_{\cdot j} = \sum_j p_{ij}$). The interpretation is that

$$p_{ij} = P(X = i, Y = j)$$

where (X, Y) has conditional distributions given by A and B. A discrete version of criterion (1.1) is available. Thus A and B are compatible if

(i) $a_{ij} \neq 0$ iff $b_{ij} \neq 0$ (i.e., same incidence matrix) and
(ii) there exist vectors $\underline{\tau}$ and $\underline{\eta}$ such that

$$\tau_i b_{ij} = \eta_j a_{ij} \ \forall i, j. \tag{1.24}$$

(Except for normalization $\underline{\tau}$ and $\underline{\eta}$ corresponds to marginal densities for X and Y).

There are other compatibility criteria available. For example under the assumption that $a_{ij}b_{ij} > 0 \ \forall i, j$, A and B are compatible if any one of the following conditions is true.

(i) all cross product ratios of A are equal to the corrresponding cross product ratios of B.
(ii) A and B have identical uniform marginal representations (obtained by successive row and column adjustments; iterative proportional fitting).
(iii) The matrix C with elements $c_{ij} = a_{ij}/b_{ij}$ is of rank one.

If, instead, we make no assumptions about the incidence sets of A and B then we can phrase our search for a corresponding matrix P as one involving non-negative solutions of systems of linear equations.

Three formulations are possible:

(I) Seek $P = (p_{ij})$ such that

$$p_{ij} - a_{ij}(\sum_i p_{ij}) = 0 \ \forall i, j$$

$$p_{ij} - b_{ij}(\sum_j p_{\cdot j}) = 0 \ \forall i, j$$

and

$$p_{ij} \geq 0 \ \forall i, j.$$

(II) Seek two vectors $\underline{\tau}$ and $\underline{\eta}$ such that

$$\eta_j a_{ij} - \tau_i b_{ij} = 0 \ \forall i, j$$

$$\sum_i \tau_i = 1$$

$$\sum_j \eta_j = 1$$

and

$$\tau_i \geq 0 \ \forall i, \quad \eta_j \geq 0 \ \forall j.$$

These vectors $\underline{\tau}$ and $\underline{\eta}$ are in fact appropriate marginal distributions for a compatible distribution P which can be obtained from $\underline{\tau}$ and B (or from $\underline{\eta}$ and A).

(III) Seek one vector $\underline{\tau}$ such that

$$a_{ij} \sum_{i'} \tau_{i'} b_{i'j} - \tau_i b_{ij} = 0 \ \forall i, j$$

$$\sum_i \tau_i = 1$$

and

$$\tau_i \geq 0 \ \forall i.$$

This vector $\underline{\tau}$ will be an appropriate marginal distribution for a compatible distribution P.

All three methods can be viewed as linear programming problems. From this viewpoint method III, involving fewer constraints and fewer unknowns, would appear to be the most attractive alternative. In all three cases an algorithm provided by Castillo et al. (1999) can be used to identify the class of all possible solutions.

Of course there is no guarantee that the given matrices will be compatible. This will be especially true if A and B represent subjective evaluations of conditional probabilities since subjective probability assessments are notorious for disobeying the rules of probability! It thus seems better to restate (I), (II) and (III) in such a way that instead of seeking a solution to the given equations we seek values of the unknowns that are minimally incompatible with the given conditional information. In this way, if a solution exists we will find it, but if it does not, we will have at hand a compromise that comes close to having the desired properties.

In this spirit, Arnold et al. (2001c) introduced the concepts of ϵ-compatiblity and η-compatibility. The idea of ϵ-compatibility for formulation I is as follows:

For a fixed $\delta > 0$ seek P such that

$$|p_{ij} - a_{ij} \sum_i p_{ij}| \leq \delta \ \forall i, j$$

$$|p_{ij} - b_{ij} \sum_j p_{ij}| \leq \delta \ \forall i, j$$

$$\sum_i \sum_j p_{ij} = 1$$

and

$$p_{ij} \geq 0 \ \forall i, j.$$

Then try and pick δ as small as possible to satisfy this.

This can be viewed as a linear programming problem with objective functions $f(\underline{p}, \delta) = \delta$ to be minimized. If the minimum value of this objective function is ϵ, we say that A and B are ϵ-compatible. If A and B are incompatible, but are ϵ-compatible, any ϵ-compatible solution could be taken as a minimally incompatible one. Analogous versions of ϵ-compatibility are availble for formulations (II) and (III).

The idea of η-compatibility arises when one tries to interpret the meaning of the quantity ϵ in an epsilon compatible distribution. It does not give us a bound on the difference between the given conditional probabilities (the a_{ij}'s and b_{ij}'s) and the conditional probabilities associated with the minimally incompatible matrix P. The η-compatibility criterion does provide such a bound.

For it, we modify formulation I in terms of the differences between the conditional distributions of P and the given matrices A and B. Thus for a fixed λ we seek a matrix P such that

$$\left| \frac{p_{ij}}{\sum_i p_{ij}} - a_{ij} \right| \leq \lambda, \quad \forall i, j$$

$$\left| \frac{p_{ij}}{\sum_j p_{ij}} - b_{ij} \right| \leq \lambda, \quad \forall i, j$$

$$\sum_i \sum_j p_{ij} = 1$$

and

$$p_{ij} \geq 0, \quad \forall i, j.$$

We then try to pick λ as small as possible to satisfy the above constraints. We will say that A and B are η-compatible if the smallest possible satisfactory value of λ is η. In this context η does indeed represent the maximal deviation between the conditional probabilities of the optimal choice of P (the minimally incompatible P) and the corresponding elements of A and B. The problem is no longer a linear programming problem but is readily resolved using, for example, the GAMS system described in Castillo et al. (2001).

Of course other distance measures can be used to quantify the discrepency between the conditional probabilities determined by P and the corresponding elements A and B. A survey of such approaches may be found in Arnold et al. (1999), Chap. 2.

In many situations only partial or imprecise information is provided about the distribution of (X, Y). This information may come in the form of marginal and/or conditional probabilities or marginal and/or conditional expected values. We begin by considering partial but precise information. Suppose that we are provided with information of the following kind regarding the distribution of (X, Y).

$$\begin{aligned}
&\text{(i)} \ P((X,Y) \in A_i) = \delta_i, i = 1, 2, \ldots, n_1 \text{ for specified subsets} \\
&\quad A_i \text{ of } I \times J \\
&\text{(ii)} \ P(X,Y) \in B_i | (X,Y) \in C_i) = \eta_i, \text{ for specified sets } B_i \text{ and} \\
&\quad C_i, i = 1, 2, \ldots, n_2 \\
&\text{(iii)} \ E(\epsilon_i(X,Y)) = \zeta_i, i = 1, 2, \ldots, n_3 \text{ for specified functions} \\
&\quad \epsilon_1, \epsilon_2, \ldots, \epsilon_{n_3} \\
&\text{(iv)} \ E(\varphi_i(X,Y) | \phi_i(X,Y) = \lambda_i) = w_i, \text{ for specified functions} \\
&\quad \varphi_i, \phi_i \text{ and constants } \lambda_i, i = 1, 2, \ldots, n_4
\end{aligned} \tag{1.25}$$

All of these requirements can be stated in terms of linear equalities that the elements of P (the p_{ij}'s) must satisfy. For example

$$P((X,Y) \in B_i | (X,Y) \in C_i) = \eta_i$$

is equivalent to

$$\sum_{(i,j) \in B_i \cap C_i} p_{ij} - \eta_i \sum_{(i,j) \in C_i} p_{ij} = 0.$$

Consequently if we rewrite the matrix P as a vector $\underline{p}$ of dimension $I \times J$, all the given information can be summarized in a statement of the form

$$A\underline{p} = \underline{b} \tag{1.26}$$

where A, a matrix of dimension $M \times (I \times J)$),and $\underline{b}$ are known. We will thus seek non-negative solutions to (1.26) (the constant $\sum_i \sum_j p_{ij} = 1$ can be included in the formulation of the matrix A in (1.26)). Techniques for solving such systems and for identifying all possible solutions are available in Castillo et al. (1999).

However, when A has many rows (i.e., when many pieces of information are provided), especially when the information is subjectively determined, it is unlikely that any non-negative solution $\underline{p}$ exists for (1.26). Here once more it is appropriate to seek a minimally incompatible non-negative vector $\underline{p}$ (probably insisting that the elements in the vector sum exactly to 1). Consequently we can state that we are searching for a vector $\underline{p}$ to satisfy

$$A\underline{p} \approx \underline{b}$$

with $\underline{p} \geq \underline{0}$ and $\sum_{k=1}^{I \times J} p_k = 1$.

As objective functions we might consider using one of the following:

$$d_1(A\underline{p}, \underline{b}) = \sum_{i=1}^{M} (A_{(i)}\underline{p} - b_i)^2$$

or

$$d_2(A\underline{p}, \underline{b}) = \sum |A_{(i)}\underline{p} - b_i| \tag{1.27}$$

or

$$d_3(A\underline{p}, \underline{b}) = \max |A_{(i)}\underline{p} - b_i|.$$

Use of the third objective function in (1.27) can be reformulated in the sense of ϵ-compatibility as follows.

We will say that $\underline{p}$ is ϵ-compatible with the system of equation (1.25) if ϵ is the smallest value of δ such that the system

$$|A_{(\cdot)}\underline{p} - b_i| < \delta \quad i = 1, 2, \ldots, I \times J$$

has a solution with $p_i \geq 0$ and $\underline{p}'\underline{1} = 1$. But this again is just a linear programming problem with objective function δ.

In practice we are likely to be given bounds rather than precise values for the quantities in (1.25). Thus our information about the distribution of (X, Y) is likely to be of the form:

(i) $\delta_i' \leq P((X,Y) \in A_i) \leq \delta_i'', i = 1, \ldots, n_1$ for specified sets $A_1, \ldots, A_{n_1}$.

(ii) $\tau_i' \leq P((X,Y) \in B_i | (X,Y) \in C_i) \leq \tau_i'', i = 1, \ldots, n_2$ for specified sets $B_1, \ldots, B_{n_2}$ and $C_1, \ldots, C_{n_2}$. (1.28)

(iii) $\xi_i' \leq E(\epsilon_j(X,Y)) \leq \xi_i'', i = 1, \ldots, n_3$ for specified functions $\epsilon_1, \ldots, \epsilon_{n_3}$.

(iv) $w_i' \leq E(\varphi_i(X,Y) | \phi_i(X,Y) = \lambda_i) \leq w_i'', i = 1, \ldots, n_4$ for specified functions $\varphi_1, \ldots, \varphi_{n_4}, \phi_1, \ldots, \phi_{n_4}$ and specified constants $\lambda_1, \ldots, \lambda_{n_4}$.

All of the constraints in (1.28) can be rewritten as equivalent linear inequality constraints on the p_{ij}'s). Again we arrange the elements of P (the p_{ij}'s) in a single column vector $\underline{p}$. We will be able to phrase our problem as a search for a vector $\underline{p}$ satisfying

$$D\underline{p} \leq \underline{b} \tag{1.29}$$

where D and $\underline{b}$ are known. Of course (1.29) is not guaranteed to have a solution so that we may search for an ϵ-compatible solution where ϵ is the smallest value of δ such that

$$D\underline{p} \leq \underline{b} + \delta\underline{1}. \tag{1.30}$$

has a solution. Once again, we are faced with a straightforward linear programming problem and reference to Castillo et al. (1999) will enable us to identify all appropriate solutions to this problem.

To conclude this section, we will mention the existence of a straightforward technique for identifying all possible compatible matrices P when precise partial information is available about A and B (the conditional probability matrices). We will utilize the concept of rank one completion. A positive matrix P will be of rank one if it is expressible in the form $\underline{a}'\underline{b}$ for two vectors $\underline{a} > \underline{0}$ and $\underline{b} > \underline{0}$ (equivalently if all cross product ratios are equal to 1). The compatibility result (1.1) can be rephrased in terms of such matrices. We have that A and B will be compatible if $\{(i,j) : a_{ij} > 0\} = \{(i,j) : b_{ij} > 0\}$ and if there exists a positive matrix C of rank one such that

$$c_{ij} = a_{ij}/b_{ij} \quad \forall (i,j) \text{ with } c_{ij} > 0.$$

C is said to be a rank one completion of the incomplete matrix with (i,j)'th entry equal to a_{ij}/b_{ij}, for those (i,j)'s for which $a_{ij} > 0$.

If instead we have only partial information about the a_{ij}'s and b_{ij}'s we can formally fill out an $I \times J$ matrix C by putting in $c_{ij} = a_{ij}/b_{ij}$ for any (i,j) for which positive values are provided for both a_{ij} and b_{ij}, putting in $c_{ij} = a_{ij}/x_{ij}$ if only a positive value of a_{ij} is provided, putting in $c_{ij} = y_{ij}/b_{ij}$ if only a positive value of b_{ij} is provided and finally putting $c_{ij} = z_{ij}$ for any (i,j) for which neither a positive value for a_{ij} or for b_{ij} was provided. Our matrix C thus involves several unknown x_{ij}'s, y_{ij}'s and z_{ij}'s. We then will need to write the conditions necessary for C to be a positive matrix of rank one in terms of these unknown x_{ij}'s, y_{ij}'s and z_{ij}'s and solve. In this fashion all compatible joint probability distribution matrices can be identified. Some examples and further discussion may be found in Arnold et al. (2004).

1.10 Future Prospects

The bibliography of this paper contains a fairly complete catalog of Enrique Castillo's work on problems related to conditional specification. The field has been mined extensively but there still exist many intriguing open questions. Many more opportunities exist for Castillo to utilize his extensive skills as a developer of algorithms as a linear algebra expert, as a modeller, simulator, optimizer and master of graphical display.

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2

The Polygonal Distribution

Dimitris Karlis[1] and Evdokia Xekalaki[2]

[1] Department of Statistics, Athens University of Economics and Business
[2] Department of Statistics, Athens University of Economics and Business
Department of Statistics, University of California, Berkeley

Abstract: The triangular distribution, although simpler than the beta distribution both for mathematical treatment and for natural interpretation, has not been widely used in the literature as a modelling tool. Applications of this distribution as an alternative to the beta distribution appear to be limited in financial contexts and specifically in the assessment of risk and uncertainty and in modelling prices associated with trading single securities. One of the basic reasons is that it can have only a few shapes. In this paper, a new class of distributions stemming from finite mixtures of the triangular distribution is introduced. Their polygonal shape makes them appealing for modelling purposes since they can be used as simple approximations to several distribution functions. Properties of these distributions are studied and parameter estimation is discussed. Further, the distributions arising when using the triangular distribution instead of the beta distribution as the mixing distribution in the case of two well-known beta mixtures, the beta-binomial and the beta-negative binomial distribution, are examined.

Keywords and phrases: Triangular distribution, binomial mixtures, negative binomial mixtures, triangular-binomial distribution

2.1 Introduction

The probability density function (pdf) of the triangular distribution is given by

$$f(x \mid \theta) = \begin{cases} \frac{2x}{\theta}, & 0 \le x \le \theta \\ \frac{2(1-x)}{1-\theta}, & \theta \le x \le 1 \\ 0, & \text{elsewhere} \end{cases} \tag{2.1}$$

with "0/0" interpreted as 1. The above definition restricts the random variable X in the interval $[0, 1]$. One can define in a similar manner triangular distributions in a finite

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interval $[\alpha, \beta]$ by considering the transformation $Y = \frac{X-\alpha}{\beta-\alpha}$. From (2.1), one can see that the density is linearly increasing in the interval $[0, \theta)$ and linearly decreasing in the interval $[\theta, 1]$ (θ is the mode of the distribution). The distribution is not symmetric except for the case $\theta = 1/2$. The parameter θ is allowed to take the values 0 and 1, using the appropriate part of the definition given in (2.1). More details about the triangular distribution can be found in van Dorp and Kotz (2004) and the references therein. Johnson (1997) and Johnson and Kotz (1999) refocused interest in the triangular distribution, which appeared to have been ignored as a modeling tool over the last decades, one of the most probable basic reasons being that it can have only a few shapes.

In this paper, a new class of distributions is introduced stemming from finite mixtures of the triangular distribution. Contrary to the triangular distribution, the members of this class have a shape flexibility that makes them appealing for modeling purposes. Because of their shape, which is polygonal, these distributions are termed in the sequel polygonal distributions.

The paper is organized as follows. Following a brief presentation of the triangular distribution in Section 2.2, the polygonal distribution is defined as a finite mixture of triangular component distributions in Section 2.3. Properties of it and estimation are discussed. In Section 2.4, mixture distributions arising when using the triangular as an approximation to a beta mixing distribution are examined. In particular, the cases of beta mixtures of binomial and negative binomial distributions are considered. The paper concludes with some remarks in Section 2.5.

2.2 The Triangular Distribution

We briefly review some properties of the triangular distribution that can have potential use in the context of polygonal distributions.

The triangular distribution consists of two parts that are truncated forms of the $Beta(\alpha, \beta)$ distribution with density

$$f(x) = \frac{1}{B(\alpha,\beta)} x^{\alpha-1}(1-x)^{\beta-1}, \quad 0 \le x \le 1, \quad \alpha, \beta > 0, B(\alpha,\beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}. \quad (2.2)$$

In particular, the first part is a tail truncated $Beta(2, 1)$ distribution, while the second part a head truncated $Beta(1, 2)$ distribution, both truncated at θ. The triangular distribution also arises as the distribution of the mean of two uniform random variables.

The $s-th$ simple moment of the distribution is given by

$$\mu_s = \frac{2(1-\theta^{s+1})}{(s+1)(s+2)(1-\theta)}. \quad (2.3)$$

The above expression holds for not necessarily integer values of s, which enables computation of non-integral moments of a triangular variate.

Noting that $1 - \theta^{s+1} = (1-\theta)\sum_{i=0}^{s} \theta^i$, for integer $s \ge 0$, simple moments can be rewritten as

$$\mu_s = \frac{2\sum_{i=0}^{s} \theta^i}{(s+1)(s+2)}, \qquad s = 1, 2, \ldots \tag{2.4}$$

and can be computed recursively using

$$\mu_{s+1} = \frac{2\theta^{s+1}}{(s+2)(s+3)} + \left(\frac{s+1}{s+3}\right)\mu_s \tag{2.5}$$

for $s = 0, 1, \ldots$ with $\mu_0 = 1$. It can easily be verified that

$$E(X) = \frac{(1+\theta)}{3} \qquad \text{and} \qquad Var(X) = \frac{(1-\theta+\theta^2)}{18}$$

implying that the mean ranges from 1/3 to 2/3 and the variance becomes minimum at $\theta = 0.5$. It holds also that the first inverse moment has the form

$$\mu_{-1} = E(X^{-1}) = \frac{-2\log(\theta)}{(1-\theta)},$$

and that the second inverse moment does not exist since the corresponding integral diverges.

Random variate generation from the triangular distribution is simple via the inversion method. Finally, ML estimation is described in Johnson and Kotz (1999) and van Dorp and Kotz (2004). Note that since the ML estimate is necessarily one of the observations, it suffices to evaluate the likelihood at all the observations to locate the maximum. Some references about the triangular distribution can be found in Johnson and Kotz (1999) and van Dorp and Kotz (2004).

2.3 The Polygonal Distribution

Let $f_j(x \mid \theta_j),\ j = 1, 2, \ldots, k$ be the probability densities of k independent triangular variables on $[0, 1]$ with parameters $\theta_j,\ j = 1, \ldots, k$. A broad family of distributions stemming from these densities with interesting properties arises from a mixture of them defined by the probability density function

$$f_k(x) = \sum_{j=1}^{k} p_j f_j(x \mid \theta_j) \tag{2.6}$$

with mixing proportions $\{p_j\}_{j=1}^{k}$ satisfying $p_j > 0$, $1 \le j \le k$ and $\sum_{j=1}^{k} p_j = 1$.

This distribution has a polygonal form with at most k points of inflection. Some members of the family of distributions are depicted in figure 2.1. Observe that the densities are piecewise linear, a feature that offers great flexibility as far as shape is concerned. The probability density function defined by (2.6) and (2.1) can take shapes which are not common in other distributions. For example, a 2-polygonal distribution with $p = 0.5$ and $\theta_1 = 0.25, \theta_2 = 0.75$ is flat over the interval $(0.25, 0.75)$, having a

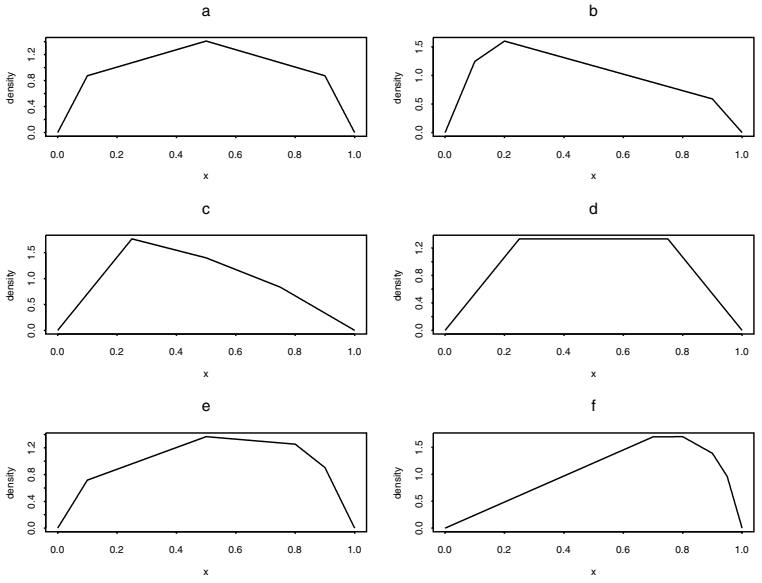

Figure 2.1. Examples of polygonal distributions. The depicted densities correspond to the following choices of parameter values: (a) $p_1 = p_2 = p_3 = 1/3$ and $\theta_1 = 0.1, \theta_2 = 0.5, \theta_3 = 0.9$, (b) $p_1 = 0.4, p_2 = 0.4, p_3 = 0.2$ and $\theta_1 = 0.1, \theta_2 = 0.2, \theta_3 = 0.9$, (c) $p_1 = 0.8, p_2 = 0.1, p_3 = 0.1$ and $\theta_1 = 0.25, \theta_2 = 0.5, \theta_3 = 0.25$, (d) $p_1 = p_2 = 0.5$ and $\theta_1 = 0.25, \theta_2 = 0.75$, (e) $p_1 = p_2 = p_3 = p_4 = 1/4$ and $\theta_1 = 0.1, \theta_2 = 0.5, p_3 = p_4 = 1/4$ and $\theta_1 = 0.7, \theta_2 = 0.8, \theta_3 = 0.9, \theta_4 = 0.95$

modal interval, rather than a mode. When components are close together and their number becomes larger and larger, the density approaches a smooth curve.

In the sequel, the distribution with k triangular components defined above is interchangeably referred to as the k-polygonal distribution or as the polygonal distribution. We also assume for simplicity that its components are ordered with respect to the values of their parameters θ_i.

The mean and variance of the polygonal distribution are given by

$$E(X) = \frac{1}{3} + \frac{1}{3}\sum_{j=1}^{k} p_j\theta_j \qquad \text{and}$$

$$Var(X) = \frac{1}{6} - \frac{1}{18}\sum_{j=1}^{k} p_j\theta_j + \frac{1}{6}\sum_{j=1}^{k} p_j{\theta_j}^2 - \frac{1}{9}\left(\sum_{j=1}^{k} p_j\theta_j\right)^2,$$

respectively. It can be seen that the mean lies in the interval $(1/3, 2/3)$.

Monotonicity It can be easily verified that the polygonal distribution has always a unique mode. This is supported by the fact that the segments of its density function over the intervals (θ_j, θ_{j+1}) given by

$$f_k(x) = \sum_{i=j+1}^{k} p_i\frac{2x}{\theta_i} + \sum_{i=1}^{j} p_i\frac{2(1-x)}{(1-\theta_i)}, \quad j = 0, \ldots, k, \quad \theta_0 = 0; \quad \theta_{k+1} = 1 \tag{2.7}$$

have derivatives given by

$$f_k'(x) = 2\left(\sum_{i=j+1}^{k} \frac{p_i}{\theta_i} - \sum_{i=1}^{j} \frac{p_i}{(1-\theta_i)}\right). \tag{2.8}$$

Hence, the derivative of $f_k(x)$ is constant in each interval (θ_j, θ_{j+1}). It starts from a positive value, implying that the density is increasing in the first interval and, since in (2.8) at each interval a negative quantity replaces a positive one, continues to be increasing, but with a smaller and smaller slope over the following subintervals. As a result, the derivative corresponding to any of the sub-intervals is smaller than the derivative of the preceding sub-interval. The mode of the distribution occurs at the interval where the derivative becomes negative for the first time.

The position of the mode depends on the mixing proportions and it is not easy to be determined for general k. However, the mode is necessarily one of the $\theta's$ or a modal interval from θ_j to θ_{j+1}. For the mode of the 2-polygonal distribution, in particular, the following result holds

Proposition 1. *For a 2-polygonal distribution if* $p_1 > \frac{1-\theta_1}{\theta_2-\theta_1+1}$, *the mode is located at the point* θ_1, *otherwise, the mode is located at the point* θ_2 . *When* $p_1 = \frac{1-\theta_1}{\theta_2-\theta_1+1}$ *the distribution has a modal interval (the interval* (θ_1, θ_2)*) instead of a mode.*

For a proof, note that in accordance with the above, the density of the distribution is increasing in the first interval and decreasing in the third interval. Hence, the mode will be located at θ_1 or at θ_2 according as the derivative of the density over the second interval (θ_1, θ_2) given by $f_k'(x) = 2\left(\frac{p_2}{\theta_2} + \frac{p_1}{(1-\theta_1)}\right)$ is negative or positive; equivalently, according as p_1 exceeds or is exceeded by $\frac{1-\theta_1}{\theta_2-\theta_1+1}$. Note that if $p_1 = \frac{1-\theta_1}{1-\theta_1+\theta_2}$, the derivative $f_k'(x)$ equals 0, and thus the distribution has a modal interval from θ_1 to θ_2, where the density takes a constant value. Such a distribution will have a trapezoidal shape. Note that letting $\theta_1 \to 0$, while $\theta_2 \to 1$, the distribution tends to a uniform distribution.

2.3.1 Estimation

ML estimation can be carried out using the finite mixture representation via an EM algorithm. This comprises the following steps.

Step 1 (E-step): Given the current values for the parameters, say ${\theta_j}^{old}$ and ${p_j}^{old}$, $j = 1, \ldots, k$, calculate

$$w_{ij} = \frac{{p_j}^{old} f(x_i \mid {\theta_j}^{old})}{f_k(x_i)},$$

where $f(x \mid \theta)$ and $f_k(x)$ are given in (2.1) and (2.6) respectively.

Step 2 (M-step): For each component j, $j = 1, \ldots, k$ update p_j by

$$p_j^{new} = \sum_{i=1}^{n} w_{ij}/n,$$

then update θ_j by solving $L_j(\theta) = \sum_{i=1}^{n} w_{ij} \log f(x_i \mid \theta)$.

The maximization can be easily carried out, since the solution is one of the observations and thus evaluating L_j at all the observations suffices to locate the maximum. Note that w_{ij}'s do not depend on the estimate and hence the monotonicity of the likelihood holds as in Johnson and Kotz (1999).

2.4 The Polygonal Distribution as a Mixing Density

This section looks at the polygonal distribution as a mixing distribution in mixtures of discrete distributions $\{p_\theta(x); x = 0, 1, \ldots, m\}, m \in Z^+ \cup \{0\}$ with parameter $\theta \in (0, 1)$. These can obviously be seen as finite mixtures of triangular mixtures on θ of $p_\theta(\cdot)$ due to the associative property of finite mixtures. This is particularly appealing in the context of applications since then one can focus on triangular mixtures that are of a simpler structure. The application potential of the triangular and hence the polygonal distribution, is particularly enhanced in the area of mixtures by Johnson's (1997) result, which shows that any beta distribution can always be closely approximated by a triangular distribution.

In the remainder of this section we discuss the distributions to which two well known beta mixtures, the beta-binomial and the beta-negative binomial, are converted when the beta form of their mixing density is transitioned to a triangular form.

2.4.1 The binomial–triangular distribution

The binomial distribution is a prominent member of the family of discrete distributions. Mixtures of the binomial distribution with respect to the parameter p have been considered in the literature. Such mixtures have probability functions of the form

$$P(X = x) = \binom{n}{x} \int_0^1 p^x (1-p)^{n-x} dG(p), \qquad x = 0, 1, \ldots, n. \tag{2.9}$$

Note that $G(p)$ denotes a generic mixing distribution that can be either a finite step distribution giving positive probabilities at only a finite number of points or a continuous distribution. Some identifiability problems arise for small values of n (see, for example, Follmann and Lambert (1991)). The distribution is identifiable only up to the first n moments of the mixing distribution.

The beta-binomial (B-B) is the best known member of the family of binomial mixture distributions. It arises when the parameter p follows a beta distribution (see, for example, Tripathi and Gurland (1994) and the references therein). Only a few other binomial mixtures have been developed, mainly due to numerical difficulties (see Alanko and Duffy (1996), Horsnell (1957), Brooks et al. (1997)).

Assume that the parameter p has a triangular distribution given in (2.1). Then the resulting probability function is given by

$$P(X = x) = 2 \binom{n}{x} \left(\frac{1}{\theta} \int_0^\theta p^{x+1} (1-p)^{n-x} dp + \frac{1}{1-\theta} \int_\theta^1 p^x (1-p)^{n-x+1} dp \right). \tag{2.10}$$

Both integrals are in fact incomplete beta integrals (see Abramowitz and Stegun (1974)) defined as $B_x(\alpha,\beta) = \int_0^x t^{\alpha-1}(1-t)^{\beta-1}dt$. Using the representation

$$I_x(\alpha,\beta) = \frac{B_x(\alpha,\beta)}{B(\alpha,\beta)},$$

with $I_x(\alpha,\beta) = 1 - I_{1-x}(\beta,\alpha)$ and $I_x(\alpha,\beta) = xI_x(\alpha-1,\beta) + (1-x)I_x(\alpha,\beta-1)$, and after tedious algebraical manipulations one can write the probability function of the binomial-triangular (B-T) distribution as

$$P(X=x) = 2\binom{n}{x}(\theta^{-1}B_\theta(x+2,n-x+1) + \\ + (1-\theta)^{-1}B(x+1,n-x+2) + (1-\theta)^{-1}B_\theta(x+1,n-x+2)).$$

This probability function is quite awkward for calculations as it involves incomplete beta functions. One can improve by considering recurrence relationships for beta integrals and incomplete beta integrals. A simpler method can be used for calculating the probabilities, based on a finite series representation of the probability mass function.

Sivaganesan and Berger (1993) showed that for a general $G(p)$ the resulting mixed binomial distribution can be written as

$$P(X=k) = \sum_{j=k}^{n} h(j,k)E(p^j), \qquad k=0,1,\ldots,n, \tag{2.11}$$

where $h(j,k) = (-1)^{j-k}\frac{n!}{k!(j-k)!(n-j)!}$ for $j \geq k$ and 0 if $j < k$, $E(p^r)$ denotes the $r-th$ simple moment of the mixing distribution. For the case of the triangular distribution, we obtain

$$P(X=k) = \sum_{j=k}^{n} h(j,k)\frac{2\sum_{i=0}^{j}\theta^i}{(j+1)(j+2)}, \qquad k=0,1,\ldots,n. \tag{2.12}$$

Computationally, this form is particularly convenient,since the coefficients $h(j,k)$ can be easily computed recursively using

$$h(0,0) = 1, \qquad h(j+1,j+1) = \frac{n-j}{j+1}h(j,j), \quad j=0,1,\ldots,n \text{ and}$$

$$h(j+1,k) = -\frac{n-j}{j-k+1}h(j,k), \qquad j=k=,\ldots,n-1,$$

while the moments of the triangular distribution can be derived recursively. Evaluation of the probability function using the above form is easy and inexpensive. Even for large values of n near 200, no overflows were encountered for the entire range of values of θ.

A graphical comparison of the resulting distribution to the B-B distribution with the same mean and variance indicates a close agreement (see figure 2.2).

The mean and the variance of the B-T distribution are given by

$$E(X) = nE(p) = \frac{n(1+\theta)}{3} \quad \text{and} \quad Var(X) = \frac{n(n+3)}{18} - \frac{n(n-3)\theta(1-\theta)}{18},$$

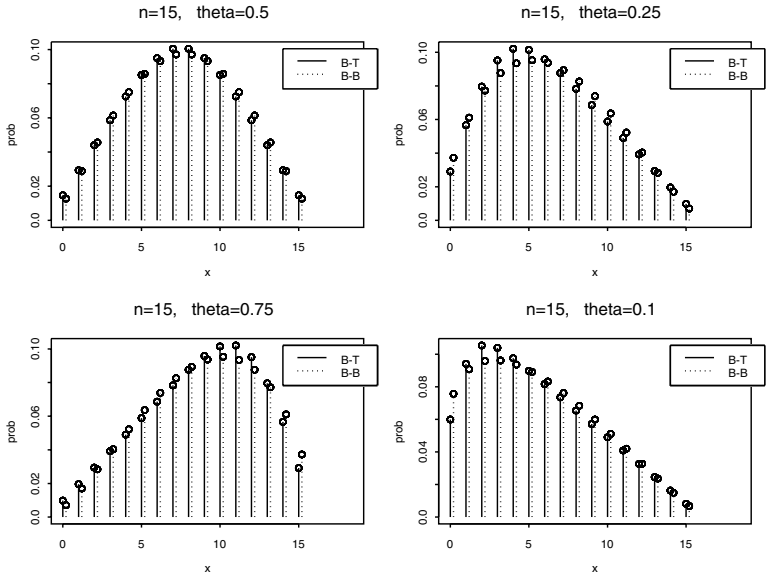

Figure 2.2. Plots of the probability function of the B-T distribution for $n = 15$ and $\theta = 0.5, 0.25, 0.75, 0.1$ superimposed by plots of the B-B with the same mean and variance

respectively. Note that there is a symmetry analogous to that existing in the case of the simple binomial distribution. So if X follows a B-T distribution with parameter θ, then $Y = 1 - X$ follows a B-T distribution with parameter $1 - \theta$.

The simple moments can be derived easily from the simple moments of the binomial distribution. It holds, in particular, that the simple moments of the B-T distribution are given by

$$\mu_r = 2\sum_{j=0}^{r} \frac{S(r,j)n!}{(n-r)!} \frac{\sum_{i=0}^{j} \theta^i}{(j+1)(j+2)},$$

where $S(r, j)$ denote the Stirling numbers of the second kind .

Moment estimates of the parameter θ can be obtained through equating the mean with the sample mean. This yields the unbiased estimator $\hat{\theta} = 3n^{-1}\bar{x} - 1$, which leads to parameter estimates whenever $\bar{x}$ is in the range $(n/3, 2n/3)$. The variance of the moment estimator is given by $Var(\hat{\theta}) = \frac{9}{n^2}\frac{Var(X)}{N}$, where N denotes the sample size.

From (2.12), we can see that the probability function is a polynomial with respect the parameter θ. The same is true for the likelihood. Direct maximization is not easy because of the sum involved in the probability function, but grid search is not prohibitive since we have only one parameter distribution in a limited range of values.

2.4.2 An application

As an application of the B-T distribution illustrating a notable closeness to the B-B distribution, consider the data in table 2.1. The data refer to the numbers of courses

taken by a class of 65 students from the first year of the Department of Statistics of Athens University of Economics. The students enrolled in this class attended 8 courses during the first year of their study. The total numbers of successful examinations (including resits) were recorded. For this data set, $n = 8$ and $\bar{x} = 5.2$.

The binomial distribution with $\hat{p} = 0.65$ provided a very poor fit. This was expected since it would not be reasonable to consider the probability of success p to be constant for all the students. Considering the students as having different probability of success according to their ability would be more natural.

Assuming that the probability of success varies according to a triangular distribution, the B-T distribution was fitted to the data. The moment estimate of θ was found to be 0.95. The likelihood was maximized at $\hat{\theta} = 1$. The maximized loglikelihood was -134.85. Assuming a beta distribution for p and fitting the data by the B-B distribution with parameter estimates $\hat{\alpha} = 1.825$ and $\hat{\beta} = 0.968$, yielded a maximized loglikelihood of -134.76. It is evident that the improvement of the loglikelihood from the B-T model to the B-B model is very small, taking into account that one parameter is added. The fits as judged by the χ^2 goodness of fit test give some indication of the closeness of the B-T distribution to the B-B distribution

Sivaganesan and Berger (1993) showed that for a general $G(p)$ the resulting posterior expectation of θ can be obtained as

$$E(\theta \mid X = k) = \frac{\sum_{j=k}^{n} h(j,k) E(p^{j+1})}{P(X = k)}, \qquad k = 0, 1, \ldots, n,$$

where $P(X = k)$ is given in (2.11), and it can be useful for Bayesian approaches, beyond the well known case of a conjugate Beta prior distribution. The values of $E(\theta \mid x)$ given in table 2.1 are indicative of a linear behavior, which is not in general true, and it is due to the value of θ estimated to be equal to 1.

Table 2.1. Data concerning the number of passed courses for a class of 65 students at the Dept. of Statistics, Athens University of Economics ($n = 8$). (The asterisk indicates grouped cells)

x	observed	expected			$E(\theta \mid x)$
		BB	BT	Binomial	
0	1	1.80	1.45	0.01*	0.1818
1	4	3.28	2.89	0.22*	0.2727
2	4	4.65	4.35	1.41*	0.3636
3	8	5.97	5.78	5.25	0.4545
4	9	7.25	7.23	12.18	0.5455
5	6	8.51	8.67	18.10	0.6364
6	8	9.78	10.12	16.82	0.7273
7	12	11.11	11.56	8.92	0.8182
8	13	12.65	12.97	2.08	0.9091
χ^2		1.45	3.15	105.4	
df		6	7	5	
p-value		0.96	0.88	0.00	

2.4.3 The negative binomial–triangular distribution

The triangular distribution can be also used as the mixing distribution for some other discrete distributions, having a parameter defined in the interval $[0, 1]$. Such examples are the geometric and the negative binomial distributions. The negative binomial distribution has probability function given by

$$P(X = x) = \frac{\Gamma(\alpha + x)}{\Gamma(\alpha)x!} p^{\alpha}(1-p)^{x}, \qquad x = 0, 1, \ldots, n, \alpha > 0, 0 \leq p \leq 1. \tag{2.13}$$

Mixtures of the negative binomial distribution with respect the parameter p can be developed by allowing the parameter p to vary according to some distribution $G(p)$. Such a mixture has probability function of the form

$$P(X = x) = \frac{\Gamma(\alpha + x)}{\Gamma(\alpha)x!} \int_0^1 p^{\alpha}(1-p)^{x} dG(p), \qquad x = 0, 1, \ldots, n. \tag{2.14}$$

The literature on mixtures of the negative binomial is rather sparse. Note that one can define mixtures with respect to either of the parameters α and p. Allowing $G(p)$ to have a $beta(\alpha, \beta)$ form, the generalized Waring distribution arises (see for example, Xekalaki (1983)).

Expanding $(1-p)^x$ in (2.14), one obtains that

$$\int_0^1 p^{\alpha}(1-p)^{x} dG(p) = \int_0^1 p^{\alpha} \sum_{k=0}^{x} \binom{x}{k} (-1)^{x-k} p^{x-k} dG(p) =$$

$$= \int_0^1 \sum_{k=0}^{x} \binom{x}{k} (-1)^{x-k} p^{\alpha+x-k} dG(p)$$

$$= \sum_{k=0}^{x} \binom{x}{k} (-1)^{x-k} \int_0^1 p^{\alpha+x-k} dG(p) = \sum_{k=0}^{x} \binom{x}{k} (-1)^{x-k} E(p^{\alpha+x-k}),$$

thus leading to

$$P(X = x) = \frac{\Gamma(\alpha + x)}{\Gamma(\alpha)x!} \sum_{k=0}^{x} \binom{x}{k} (-1)^{x-k} E(p^{\alpha+x-k}).$$

In other words, the probability density function can be written as a finite series of non-integral moments of the mixing distribution.

Assuming a triangular distribution as a mixing distribution, one obtains the negative binomial-triangular distribution with probability function given by

$$P(X = x) = \frac{\Gamma(\alpha + x)}{\Gamma(\alpha)x!} \sum_{k=0}^{x} \binom{x}{k} \frac{(-1)^{x-k} 2(1 - \theta^{\alpha+x-k+1})}{(\alpha + x - k + 1)(\alpha + x - k + 2)(1 - \theta)}.$$

The above formula can be used for calculating the probability function. A similar scheme as the one proposed for the binomial-triangular distribution is applicable. However, since now the values of x are not restricted in a finite range, minor anomalies may

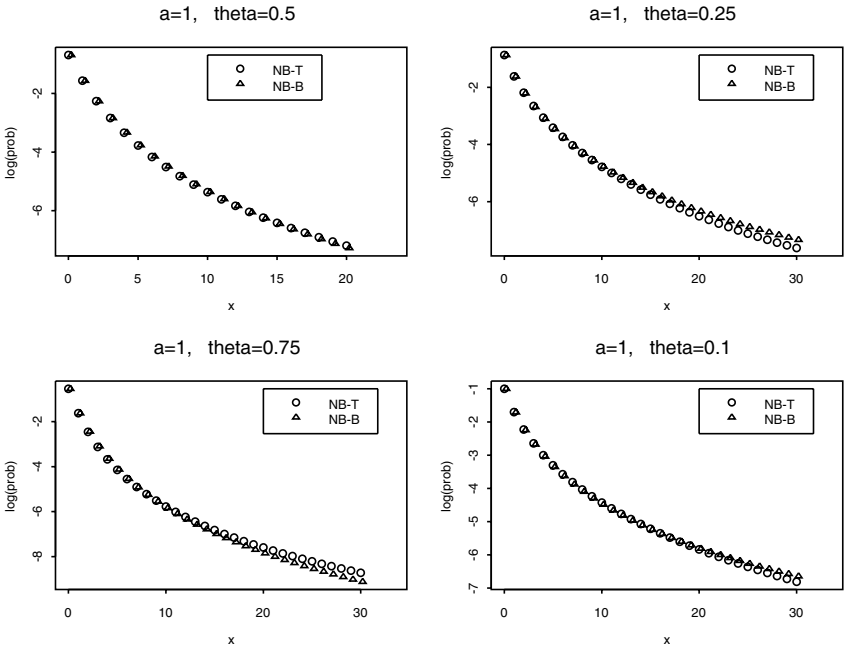

Figure 2.3. Plots of the probability function in log scale of the NB-T distribution for $\alpha = 1$ and $\theta = 0.5, 0.25, 0.75, 0.1$ superimposed by plots of the Generalized Waring (NB-B) distribution with the same mean

be found at the tail. Alternatively, the probability function can be written via incomplete beta functions in a similar manner as for the simple binomial case.

From figure 2.3, there appears a close agreement between the NB-T distribution and the NB-B (Generalized Waring) distribution with the same mean for $\alpha = 1$ and different values of θ.

Setting $\alpha = 1$, a geometric-triangular mixture is obtained. Now the moments used are of integral order and thus the recursive relationships for the moments of the triangular distribution can be used. Similar is the case when the Pascal distribution is considered.

The mean of the negative binomial-triangular distribution is

$$E(X) = \int_0^1 \frac{\alpha(1-p)}{p} g(p)dp = \alpha E(p^{-1}) - \alpha = \alpha \left(\frac{-2\log(\theta)}{1-\theta} - 1 \right).$$

Since $0 \leq \theta \leq 1$, it holds that $E(X) > \alpha$ for every value of θ. The variance does not exist, since it involves the second inverse moment of the triangular distribution which does not exist. The distribution exhibits a very long tail.

Note that mixtures of the negative binomial distribution with respect to the parameter p are in fact mixtures of the Poisson distribution, with mixing distribution a gamma mixture. For example, the negative binomial-triangular distribution defined

above is a Poisson mixture with mixing distribution the mixture of a Gamma density with a triangular mixing density.

2.5 Discussion

A new class of distributions has been introduced stemming from the triangular distribution. Their polygonal shape offers them an appealing application potential and enhances their plausibility as modelling tools in areas ranging from risk analysis assessment, where its simplest member, the triangular distribution has been used, to developing envelope functions for rejection algorithms in simulation studies and as approximations to the beta distributions.

A notable feature is that the members of this family have always one mode (or modal interval), and the number of angles of the polygon depicting their density depends on the number of triangular components used in their finite mixture representation. In this sense, the polygonal distribution generalizes the trapezoidal distribution studied by van Dorp and Kotz (2003)

Finally, one may expand the definition of polygonal distributions beyond the interval $[0, 1]$ over a more general interval $[\alpha, \beta]$ using the transformation $y = \frac{x-\alpha}{\beta-\alpha}$. Alternatively, one may expand the polygonal distribution to the positive real line by the transformation $y = \frac{x}{1-x}$.

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3

Conditionally Specified Models: New Developments and Applications

José María Sarabia[1], María Sarabia[2], and Marta Pascual[1]

[1] Department of Economics, University of Cantabria, Spain
[2] Department of Business Administration, University of Cantabria, Spain

Abstract: In recent years, an important part of Enrique Castillo's research work has been focused on statistical applications of models with conditional specification. The present paper introduces some new developments and applications of these kinds of models to be studied in the near future. Firstly, some new and some old bivariate discrete distributions specified by conditionals are presented. Models of bivariate distributions where one of the conditional distributions is discrete and the other one is continuous have important applications in risk theory and actuarial statistics. In this sense, some of these mixture models are proposed. Distributions for modelling bivariate income distributions are reviewed. Certain conditionally specified densities are also shown to provide convenient flexible conjugate prior families in certain multiparameter Bayesian settings. We propose prior distributions for inference with incomplete count data and in certain hurdle models. Finally, we describe the construction of flexible bivariate continuous distributions based on specification of some prescribed conditional hazard functions.

Keywords and phrases: Bivariate discrete distributions, compatibility, income distributions, hurdle models, conjugate priors, conditional hazard functions

3.1 Introduction

In recent years, an important part of Enrique Castillo's research work has been focused on statistical applications of models with conditional specification. From his pioneer work on conditional distributions presented in 1985 in the "Conference on Weighted Distributions" held at Penn. State University, and published later in Castillo and Galambos (1987a,b, 1989) important advances have taken place. Part of the work about models with conditional specification can be found in Arnold et al. (1992, 1999, 2001) and in Kotz et al. (2000). The present paper introduces some new developments and applications of this kind of models to be studied in a near future.

The paper is organized as follows. In Section 3.2 some new and some old bivariate discrete distributions specified by conditionals are presented. Models of bivariate

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distributions where one of the conditional distributions is discrete and the other one is continuous have important applications in risk theory and actuarial statistics. Some of these mixture models are introduced in Section 3.3. Bivariate income distributions with conditional specification are reviewed in Section 3.4. Certain conditionally specified densities are also shown to provide convenient flexible conjugate prior families in certain multiparameter Bayesian settings. We propose prior distributions for inference with incomplete count data and in certain hurdle models in Section 3.5. Finally in Section 3.6, we describe the construction of flexible bivariate continuous distributions based on specification of some prescribed conditional hazard functions.

3.2 Bivariate Power Conditionals Distribution

The purpose of this section is to study a new class of bivariate discrete distribution called bivariate power conditionals distribution. The first bivariate power conditionals distributions were described by Arnold and Strauss (1991), and they included the bivariate Poisson, binomial and geometric conditionals distribution.

3.2.1 Bivariate Poisson conditionals distribution

The bivariate Poisson conditionals distribution has the following joint density,

$$\Pr(X = x, Y = y) = k(\lambda_1, \lambda_2, \lambda_3)\frac{\lambda_1^x}{x!}\frac{\lambda_2^y}{y!}\lambda_3^{xy}, \quad x, y = 0, 1, 2, \ldots \tag{3.1}$$

with $\lambda_1, \lambda_2 > 0$ and $0 < \lambda_3 \leq 1$. The conditional distribution of X given y is $\mathcal{P}o(\lambda_1\lambda_3^y)$ and Y given x is $\mathcal{P}o(\lambda_2\lambda_3^x)$. If $\lambda_3 = 1$, X and Y are independent and if $0 < \lambda_3 < 1$, X and Y are negatively correlated with correlation coefficient range $\rho(X, Y) \in (-1, 0)$. The marginal distributions of (3.1) are,

$$\Pr(X = x) = k\frac{\lambda_1^x}{x!}\exp(\lambda_2\lambda_3^x), \quad x = 0, 1, 2, \ldots$$
$$\Pr(Y = y) = k\frac{\lambda_2^y}{y!}\exp(\lambda_1\lambda_3^y), \quad y = 0, 1, 2, \ldots$$

which are not Poisson except in the independence case. If we denote $(Z)^k = Z(Z - 1)\cdots(Z - (k - 1))$ we have,

$$E[(X)^r(Y)^s] = \lambda_1^r\lambda_2^s\lambda_3^{rs}\frac{k(\lambda_1, \lambda_2, \lambda_3)}{k(\lambda_1\lambda_3^s, \lambda_2\lambda_3^r, \lambda_3)}.$$

The cross-moments can be written as,

$$E(X^rY^s) = \frac{E(Z_1^rZ_2^s\lambda_3^{Z_1Z_2})}{E(\lambda_3^{Z_1Z_2})},$$

where Z_1 and Z_2 are independent Poisson random variables with parameters λ_1 and λ_2 respectively. Wesolowski (1996) has characterized this distribution using a conditional distribution and the other conditional expectation.

3.2.2 Bivariate binomial conditionals distribution

The bivariate binomial conditionals distribution has the following joint density

$$\Pr(X=x,Y=y)=k\binom{n_1}{x}p_1^x(1-p_1)^{n_1-x}\binom{n_2}{y}p_2^y(1-p_2)^{n_2-y}r^{xy}, \qquad (3.2)$$

where $x=0,1,\ldots,n_1$ and $y=0,1,\ldots,n_2$, $0<p_1,p_2<1$ and $r>0$. The conditional distributions of (3.2) are,

$$X|Y=y\sim\mathcal{B}in\left(n_1,\tilde{p}_1=\frac{p_1r^y}{1-p_1(1-r^y)}\right),$$
$$Y|X=x\sim\mathcal{B}in\left(n_2,\tilde{p}_2=\frac{p_2r^x}{1-p_2(1-r^x)}\right).$$

The case $r=1$ corresponds to independence, and the correlation is positive if $r>1$ and negative if $r<1$ and is not limited. This is an important property required in practical situations. The marginal distribution are respectively,

$$\Pr(X=x)=k\binom{n_1}{x}p_1^x(1-p_1)^{n_1-x}\left[1-p_2(1-r^x)\right]^{n_2},\ x=0,1,\ldots,n_1,$$
$$\Pr(Y=y)=k\binom{n_2}{y}p_2^y(1-p_2)^{n_2-y}\left[1-p_1(1-r^y)\right]^{n_1},\ y=0,1,\ldots,n_2.$$

The cross-moments are given by,

$$E(X^rY^s)=\frac{E(Z_1^rZ_2^sr^{Z_1Z_2})}{E(r^{Z_1Z_2})},$$

where Z_1 and Z_2 are independent binomial random variables with parameters (n_1,p_1) and (n_2,p_2) respectively.

3.2.3 A general class

The class of power series distributions includes many of the common distributions. A distribution is said to be a power series distribution if its probability mass function can be written in the form,

$$\Pr(X=x)=\frac{a(x)\theta^x}{\eta(\theta)},\ \ x=0,1,2,\ldots;\theta>0, \qquad (3.3)$$

where $a(x)>0$ and $\eta(\theta)=\sum_{x=0}^{\infty}a(x)\theta^x<\infty$. The most bivariate discrete distribution with conditionals of the form (3.3), takes the form,

$$\Pr(X=x,Y=y)=\frac{1}{\eta(\underline{\theta})}\,a_1(x)a_2(y)\theta_1^x\theta_2^y\theta_3^{xy},\ \ x,y=0,1,2,\ldots,$$

where η^{-1} is the normalizing constant, $\theta_i>0$, $i=1,2,3$ and the case $\theta_3=1$ corresponds to the independent model. Properties of this distribution and estimation methods have been studied by Sarabia et al. (2006).

3.3 Mixture Conditional Models with Applications to Actuarial Statistics

Mixture conditional distributions are distributions where one of the conditional distributions is discrete and the other one is continuous. These models have important applications in risk theory in the classical collective model (Sarabia et al. (2004) and Sarabia and Guillén (2006)).

As an important model, we ask for the most general bivariate distribution (X, N) whose conditional distributions $X|N$ and $N|X$ are log-normal and Poisson respectively, that is,

$$X|N = n \sim \mathcal{LN}(\mu(n), \sigma^2(n)), \tag{3.4}$$
$$N|X = x \sim \mathcal{P}o(\lambda(x)), \tag{3.5}$$

where $\mu(n) : N \to R$, $\sigma(n) : N \to R^+$ and $\lambda(x) : R^+ \to R^+$ are unknown functions. We have the following theorem.

Theorem 1. *The most general bivariate distribution with conditional distributions (3.4) and (3.5) is given by,*

$$f(x, n; M) = (xn!)^{-1} \exp\{u_x^\top M v_n\}, \;\; x > 0; \; n = 0, 1, 2, \ldots, \tag{3.6}$$

where the vectors u_x and v_n are given by,

$$u_x = (1 \; , \; \log x \; , \; \log^2 x)^\top$$
$$v_n = (1 \; , \; n)$$

and $M = \{m_{ij}\}$, $i = 0, 1, 2$, $j = 0, 1$ is a parameter matrix. The parameter m_{00} is the normalizing constant and must be satisfy $\sum_n \int f(x, n; M)dx = 1$. The parameters $\{m_{ij}\}$ must be selected to satisfy $\int_x f(x, n; M)dx < \infty$ or $\sum_n f(x, n; M) < \infty$.

Expanding equation (3.6), the following bivariate density is obtained,

$$f(x, n; M) = (xn!)^{-1} \exp\{m_{00} + m_{10} \log x + m_{20} \log^2 x + m_{01} n + m_{11} n \log x + m_{21} n \log^2 x\}, \;\; x > 0; \; n = 0, 1, \ldots,$$

where $m_{20} < 0$ and $m_{21} \leq 0$. The conditional parameters are given by,

$$\mu(n) = -\frac{m_{10} + m_{11} n}{2(m_{20} + m_{21} n)},$$
$$\sigma^2(n) = -\frac{1}{2(m_{20} + m_{21} n)},$$

and

$$\lambda(x) = \exp(m_{01} + m_{11} \log x + m_{21} \log^2 x).$$

The marginal distributions are,

$$f_X(x; M) = x^{-1} \exp\{m_{00} + m_{10} \log x + m_{20} \log^2 x + \lambda(x)\}, \;\; x > 0,$$

and

$$f_N(n;M) = \frac{\sqrt{2\pi}e^{m_{00}}}{n!\sqrt{-2(m_{20}+m_{21}n)}} \exp\left\{-\frac{(m_{10}+m_{11}n)^2}{2(m_{20}+m_{21}n)}\right\},\ n=0,1,\ldots$$

3.4 Bivariate Income Distributions

A recent application of these kinds of distributions is the specification of bivariate income distributions. The list of bivariate income distributions is very limited and many times reduces to the bivariate lognormal distribution. Unfortunately this distribution presents some shortcomings; for instance, the range of the correlation coefficient is limited and is more narrowed than the normal case. As an alternative to this model, Sarabia et al. (2006) have proposed bivariate distributions with lognormal conditionals, where the joint pdf is given by

$$f(x,y;\underline{\delta},M) = (x-\delta_1)^{-1}(y-\delta_2)^{-1}\exp\left\{-u_{\delta_1}(x)^\top M\ u_{\delta_2}(y)\right\}, \tag{3.7}$$

if $x>\delta_1$, $y>\delta_2$ and $u_{\delta_i}(\cdot)$ denotes the vector

$$u_{\delta_i}(z) = (1\ ,\ \log(z-\delta_i)\ ,\ [\log(z-\delta_i)]^2)^\top,\ \ i=1,2,$$

and $M=\{m_{ij}\}$ is a 3×3 matrix of parameters. This new distribution is very broad and contains as a particular case the classical bivariate lognormal distribution. The properties of (3.7), as well as an application with real data, can be found in Sarabia et al. (2006).

Other relevant models correspond to bivariate distributions with Pareto conditionals. The first model was proposed by Arnold (1987), where classical Pareto distribution is considered. This model was extended in Arnold et al. (1993a) to distributions with generalized Pareto conditionals, according to the hierarchy of Pareto distributions introduced by Arnold (1983).

3.5 Flexible Conjugate Prior Families

An important application of the models with conditional specification is the specification of conjugate prior distributions in a Bayesian framework. This methodology has been used for the Bayesian estimation of the parameters of classical distributions (see Arnold et al. (1993b, 1998a) and Sarabia et al. (2005)) and in the Bayesian estimation of ratios of gamma scale parameters (Arnold et al. (1998b) and Moschopoulos and Sha (2005)). In this section we propose two new applications.

3.5.1 Hurdle count data models: Bayesian analysis

Hurdle models were introduced by Mullahy (1986) and are useful in econometrics because of their interpretation as a two-stage decision process. These models allow individuals below and above the hurdle to have different statistical behavior. The common hurdle count data is hurdle at zero, in which case the outcome is a reparametized zero-modified distribution (see Johnson et al. (2005)).

Suppose that α and $1-\alpha$ are the probabilities of failing and crossing the hurdle. Let as assume also that the conditional distribution of nonzero observations is a zero-truncated distribution for which the probabilities are $\{p_x\}$, $x = 0, 1, 2, \ldots$ Then the hurdle model has probabilities,

$$\begin{aligned} &\Pr(X = 0) = \alpha, \\ &\Pr(X = x) = \frac{(1-\alpha)p_x}{1-p_0}, \quad x = 1, 2, \ldots \end{aligned}$$

Assume that $\{p_x\}$ belongs to the power series distribution with pmf $p_x = \eta(\theta)^{-1} a(x)\theta^x$, $x = 0, 1, 2, \ldots$ In consequence, we obtain the hurdle model,

$$\Pr(X = 0) = \alpha, \tag{3.8}$$

$$\Pr(X = x) = \frac{(1-\alpha)a(x)\theta^x}{\eta(\theta) - a(0)}, \quad x = 1, 2, \ldots \tag{3.9}$$

If we take a random sample $X_1, \ldots, X_n$ from (3.8)-(3.9), we obtain the likelihood,

$$\ell(\alpha, \theta; \underline{X}) \propto \alpha^{n_0}(1-\alpha)^{n-n_0}[\eta(\theta) - a(0)]^{-(n-n_0)}\theta^{\sum_{X_i \geq 1} X_i},$$

where n_0 denotes the zero frequency. Bayesian analysis requires the specification of prior distribution for the parameters α and θ. We want a conjugate prior distribution with dependence between parameters. Then, if θ is known, a conjugate prior for α is the classical beta distribution and if α is known, a conjugate prior for α is $\pi(\theta) \propto \theta^{b-1}[\eta(\theta) - a(0)]^{-c}$, and we will denote $\theta \sim \mathcal{PC}(b, c)$. In consequence, we look for the most general bivariate distribution with conditionals,

$$\alpha|\theta \sim \mathcal{B}(p(\theta), q(\theta)), \tag{3.10}$$

$$\theta|\alpha \sim \mathcal{PC}(b(\alpha), c(\alpha)), \tag{3.11}$$

where $p(\cdot)$, $q(\cdot)$, $b(\cdot)$ and $c(\cdot)$ are unknown functions. The most general bivariate distribution satisfying (3.10) and (3.11) is given by

$$\pi(\alpha, \theta; M) = [\alpha(1-\alpha)]^{-1} \exp\left\{u^\top M v\right\},$$

where $u = (1, \log\alpha, \log(1-\alpha))^\top$ and $v = (1, \log\theta, \log[\eta(\theta) - a(0)])^\top$. The hurdle Poisson, binomial and geometric are tractable models and can be used in practical applications.

3.5.2 Estimating with incomplete count data

The second application corresponds to estimating with incomplete count data. Assume that x_t is an homogeneous Poisson process $\mathcal{P}o(\lambda t)$, where t is a time interval, λ is

unknown and x_t is unobservable. Let us suppose the available sample information is variable y_t, which is an unknown proportion of x_t. In practice, x_t might represent the number of violent crimes in a given period of time t or the number of accidents caused by the customers of a given insurance company during time t. The data y_t might be the actual number of reported violent crimes or the claims to the company. These are standard situations in criminology and actuarial statistics.

Assuming that the number of incidents x_t that are reported independently of each other with probability θ, the same for all incidents, a possible model might be

$$f(x_t|\lambda) = \frac{(\lambda t)^{x_t}}{x_t!}\exp(-\lambda t), \quad x_t = 0, 1, 2, \ldots$$
$$f(y_t|x_t, \theta) = \binom{x_t}{y_t}\theta^{y_t}(1-\theta)^{x_t - y_t}, \quad y_t = 0, 1, \ldots, x_t,$$

where $\lambda > 0$ and $0 < \theta < 1$. Well known probabilistic computations led to

$$f(y_t|\lambda, \theta) = \frac{(\lambda\theta t)^{y_t}}{y_t!}\exp(-\lambda\theta t).$$

Then, the number of reported counts conditional on (λ, θ) is Poisson distributed with parameter $\lambda\theta t$. This likelihood is unable to distinguish among the pairs (λ, θ) with the same product. We need the specification of a prior for the pair (λ, θ). Moreno and Girón (1998) have proposed a prior distribution assuming independency between parameters. However, a conjugate prior distribution with dependence between parameters can be specified as in the previous section. Now, λ given θ is a gamma distribution and θ given λ a truncated gamma distribution.

3.6 Conditional Hazard Functions

In this section we describe the construction of bivariate continuous distribution (X, Y) based on the specification of conditional hazard functions. We consider several possibilities.

A first possibility is by conditioning on events of the form $\{X = x\}$, that is

$$X|Y = y \sim \lambda_1(x|y),$$
$$Y|X = x \sim \lambda_2(y|x),$$

where $\lambda_1(x|y)$ and $\lambda_2(y|x)$ are the conditional hazard functions. This problem has been studied by Balakrishnan et al. (2004) and led to the joint probability density function $f_{X,Y}(x, y)$.

A second possibility is by conditioning on events of the form $\{X > x\}$ in the next way

$$\Pr(X > x|Y > y) = \exp[-\alpha_1(y)\Lambda_1(x)],$$
$$\Pr(Y > y|X > x) = \exp[-\alpha_2(x)\Lambda_2(y)],$$

where $\Lambda_i(x)$, $i = 1, 2$ are the integrated hazard functions (which are known) and $\alpha_i(z) : R^+ \to R^+$, $i = 1, 2$ are unknown functions. The solution to this problem given in terms of the joint survival function is

$$\Pr(X > x, Y > y) = \exp[-\alpha_1\Lambda_1(x) - \alpha_2\Lambda_2(y) - \alpha_{12}\Lambda_1(x)\Lambda_2(y)].$$

For this model the bivariate hazard function $\lambda(x, y) = f(x, y)/\Pr(X > x, Y > y)$ is

$$\lambda(x, y) = \lambda_1(x)\lambda_2(y)[\gamma_0 + \gamma_1\Lambda_1(x) + \gamma_2\Lambda_2(y) + \gamma_{12}\Lambda_1(x)\Lambda_2(y)],$$

where $\lambda_i(x) = \Lambda_i'(x)$, $i = 1, 2$ $\gamma_0 = \alpha_1\alpha_2 + \alpha_{12}$, $\gamma_i = \alpha_i\alpha_{12}$, $i = 1, 2$ and $\gamma_{12} = \alpha_{12}^2$. Assume now linear conditional hazard functions of the form,

$$\lambda_1(x|y) = \alpha_{11}(y) + 2\alpha_{12}(y)x,$$
$$\lambda_2(y|x) = \alpha_{21}(x) + 2\alpha_{22}(x)y,$$

and conditioning on events of the form $\{X > x\}$. Then we obtain the joint survival function

$$\begin{aligned}\Pr(X > x, Y > y) = \ & \exp(a_{10}x + a_{01}y + a_{11}xy + a_{20}x^2 + a_{02}y^2 \\ & + a_{12}xy^2 + a_{21}x^2y + a_{22}x^2y^2),\end{aligned}$$

where we need some constraints about the parameters a_{ij}. More flexible bivariate survival functions can be obtained using mixture hazard function proposed by Shaked (1977) with the specification

$$\Pr(X > x|Y > y) = \exp\left[-\alpha_{11}(y)\Lambda_{11}(x) - \alpha_{12}(y)\Lambda_{12}(x)\right],$$
$$\Pr(Y > y|X > x) = \exp\left[-\alpha_{21}(x)\Lambda_{21}(y) - \alpha_{22}(x)\Lambda_{22}(y)\right].$$

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4

Modelling of Insurance Claim Count with Hurdle Distribution for Panel Data

Jean-Philippe Boucher[1], Michel Denuit[1], and Montserrat Guillén[2]

[1] Institut des Sciences Actuarielles, Université Catholique de Louvain, Belgium
[2] Department of Econometrics RFA-IREA, University of Barcelona, Spain

Abstract: The aim of the paper is to propose a new model for panel data. In a recent paper, the authors showed that the hurdle model is an interesting alternative to Poisson and Negative Binomial for the analysis of the number of claims reported by an insured driver. We generalize the hurdle model to account for longitudinal data under the assumption that covariates are time independent. Predictive distributions are shown to be easily computed analytically, as well as future premiums that can be calculated using the classical credibility theory.

Keywords and phrases: Count data, panel data, hurdle distribution, predictive distribution, credibility

4.1 Introduction

The basis for insurance agreements is risk-sharing between individuals, so that each one contributes economically to constitute a fund that is used to re-establish the wealth of the one that suffers a loss. This is the principle of mutualization. In automobile insurance, for example, when an accident occurs, the responsible driver is liable for the damages caused to others, but since third-party liability automobile insurance is compulsory in most countries, the insurance company takes up the economic compensation for losses. If accident occurrence were completely hazardous and the insured risk was the same (i.e., they all share the same characteristics), all insureds would agree to pay the same price (premium) to sign an insurance contract. Risk factors come into play because there exists a heterogeneity in risk exposure due to the vehicle, the driver, the mileage or even the geographical location.

The aim of statistics in insurance is to predict future claims conditional on risk factors. Claims amounts (or economic compensations to be paid) are more difficult to predict than claiming frequency (the number of accidents for a given period of time). Nowadays, panel data that contain information on the number of claims reported by insureds each year (or month) together with their characteristics, are the main source of information for insurers to derive models that should be used to estimate the expected

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number of claims conditional on the information on the risk covariates. The number of individuals is usually very large, compared to the time framework for which information is available. Covariates (i.e., the risk characteristics) may change over time and insureds are also free to cancel an insurance contract to go to a competitor.

In this paper we discuss models suitable to this situation. We also show the practical difficulties of applying them in practice and illustrate with real data examples from the Spanish insurance market. We note that the kind of data that we present here are central in insurance and quantitative risk management, but they are also very frequent in many other microeconomic problems. Some examples from different contexts are: repeated purchase of products made by a consumer, number of visits to doctors, number of patents written by an industry.

We especially want to stress that our contribution is in the way we address the excess-of-zeros phenomenon that is common in this kind of data sets.

4.1.1 Data used

In this paper, we worked with a sample of the automobile portfolio of a major company operating in Spain. Only private use cars have been considered in this sample. The panel data contains information from 1991 until 1998. Our sample contains 15,179 policyholders that stay in the company for seven complete periods, resulting in 106,253 insurance contracts. We have 5 exogeneous variables (see table 4.1) that are kept in the panel plus the yearly number of accidents. For every policy we have the initial information at the beginning of the period and the total number of claims at fault that took place within this yearly period. The average claim frequency of the portfolio is 6.8412%.

To analyse these data, we make the following assumption: All covariates used are the ones observed at the beginning of year 1. Thus, all regressors can be seen as time independent. Nevertheless, this assumption is not so restricting as it might seem. Indeed, the majority of the time dependent covariates that are used in insurance involve the age of the insured or the length of stay in the company. These variables do not evolve randomly in time since the change can already be known in advance. Other covariates can also change in time, such as the city or the type of vehicle of the driver but this kind of major change often involves the creation of another policy.

In this paper, the exogenous variables shown in table 4.1 are used to model the parameters of the distributions. The characteristics of the insureds are expressed through some functions $h(\beta_0 + x_i'\beta)$, where β_0 is the intercept, $\beta' = (\beta_1, ..., \beta_p)$ is a vector of regression parameters for explanatory variables $x_i = (x_{i,1}, ..., x_{i,p})$.

Table 4.1. Exogenous variables

Variable	Description
v1	equals 1 for women and 0 for men
v2	equals 1 if the client was in the company between 3 and 5 years
v3	equals 1 if the client was in the company for more than 5 years
v4	equals 1 if the insured is 30 years old or younger
v5	equals 1 if power is larger or equal to 5500 cc

4.2 Cross Section versus Panel Data

Usually, data are analysed by cross-sectional analysis, where each observation, here each annual a contract, is considered to be mutually independent. Thus, in this situation, we worked with $N \times T$ independent observations. However, it is clear that insurance data is a repetition of one-year contract for an insured, where some dependence over contracts of the same insured exists. Longitudinal data (or panel data) consists of repeated observations of individual units that are observed over time. Each individual is assumed to be independent, but correlation between observation of the same individual is permitted. This fact must be regarded as an advantage and must be used in the construction of frequency models.

4.2.1 Modelling

There exist many models that imply time dependence, but the most popular way of dealing with these data is the use of a common individual term (Hausman et al., 1984) that affects all contracts of the same insured. To illustrate, this random effects model can represent individual specificities not captured by the covariates, such as swiftness of reflexes, aggressiveness behind the wheel, consumption of drugs, etc. Given the insured-specific random effect term θ_i, the annual claim numbers $N_{i,1}, N_{i,2}, \ldots, N_{i,T}$ are independent. The joint probability function of $N_{i,1}, ..., N_{i,T}$ is thus given by

$$\begin{aligned} &\Pr[N_{i,1} = n_{i,1}, ..., N_{i,T} = n_{i,T}] \qquad (4.1)\\ &= \int_0^\infty \Pr[N_{i,1} = n_{i,1}, ..., N_{i,T} = n_{i,T}|\theta_i] g(\theta_i) d\theta_i \\ &= \int_0^\infty \left(\prod_{t=1}^{T} \Pr[N_{i,t} = n_{i,t}|\theta_i] \right) g(\theta_i) d\theta_i. \qquad (4.2) \end{aligned}$$

Many conditional distributions for the random variables $N_{i,t}$ can be chosen as well as a distribution for the random effect θ_i, as we will see in the following sections.

Endogeneous regressors and fixed effects

In linear regression, correlation between the regressors and the random effect term leads to inconsistency of the estimated parameters (Mundlak (1978), or for a general overview, Hsiao (2003)). The same problem exists for the count data regression when $E[\theta|x_i] \neq E[\theta]$ Mullahy (1997), and it leads to biased estimates of parameters. In insurance, correlation between regressors and error term is often present (Boucher and Denuit, 2006) and may be caused by omitted variables that are correlated with the included ones.

As noted in Winkelmann (2003), consistent estimates may be found if corrections are made to the standard estimation procedures. However, as shown by Boucher and Denuit (2006), for insurance applications, standard methods of estimation can still be used. Indeed, the resulting estimates of parameters, while being biased, represent the

apparent effect on the frequency of claim, which is the real interest when the correlated omitted variables cannot be used in classification.

4.3 Poisson Distribution

4.3.1 Overview

Commonly, the starting point for the modelling of the number of reported claims is the Poisson distribution:

$$f_{N_{i,t}}(n_{i,t}) = \frac{\lambda_i^{n_{i,t}} e^{-\lambda_i}}{n_{i,t}!} \tag{4.3}$$

where covariates are included in the model by the parameter $\lambda_i = \exp(x_i'\beta)$ (Dionne and Vanasse, 1989). The Poisson distribution is equidispersed since its mean and variance are both equal to λ_i. Because the Poisson distribution has some severe drawbacks that limit its use, other distributions can be used, such as zero-inflated or hurdle models (Boucher et al., 2007), which is analyzed in the next section.

4.3.2 Panel data

To generalize the Poisson distribution for panel data, an individual random effect term θ_i is added to its mean parameter. Formally, we can express the classic Poisson random effects model as:

$$N_{i,t}|\theta_i \sim Poisson(\theta_i\lambda_i), \quad i = 1, ..., N \;\; t = 1, ..., T$$

where i represents an insured and t his covered period. As for the heterogeneity models of the cross-sectionnal model (Boucher et al., 2007), many possible distribution for the random effects can be chosen. The use of a gamma heterogeneity is a natural possibility because it can express the joint distribution in a closed form since the gamma is conjugated to the Poisson distribution. Formally, the joint distribution of the number of claims, when the heterogeneity term follows a gamma distribution of mean 1 and variance α, is equal to (Hausman et al., 1984):

$$\begin{aligned} Pr(n_{i,1}, ..., n_{i,T}) = &\left[\prod_{t=1}^{T} \frac{(\lambda_i)^{n_{i,t}}}{n_{i,t}!}\right] \frac{\Gamma(\sum_{i=1}^{T} n_{i,t} + 1/\alpha)}{\Gamma(1/\alpha)} \left(\frac{1/\alpha}{T\lambda_i + 1/\alpha}\right)^{1/\alpha} \\ &\times (T\lambda_i + 1/\alpha)^{-\sum_{i=1}^{T} n_{i,t}} \end{aligned} \tag{4.4}$$

This distribution is known as a Multinomial Negative Binomial or negative multinomial, which has been often applied (see Chapter 36 of Johnson et al. (1996), for an overview). Note that this distribution can also be seen as the generalization of the bivariate Negative Binomial of Marshall and Olkin (1990). For this distribution, $E[N_{i,t}] = \lambda_i$ and $Var[N_{i,t}] = \lambda_i + \alpha\lambda_i^2$, so overdispersion can be accounted. Maximum likelihood estimations of parameters and variances of these estimates are straightforward.

The generalization of the Negative Multinomial to other kinds of Multivariate Negative Binomial distributions can also be done. If we suppose that the random effects are following a gamma distribution with both parameters equal to λ_i^{1-k}/α, the joint distribution can be expressed as:

$$Pr(n_{i,1},...,n_{i,T}) = \left[\prod_{t=1}^{T}\frac{(\lambda_i)^{n_{i,t}}}{n_{i,t}!}\right]\frac{\Gamma(\sum_{i=1}^{T}n_{i,t}+\lambda_i^{1-k}/\alpha)}{\Gamma(\lambda_i^{1-k}/\alpha)} \times\left(\frac{\lambda_i^{1-k}/\alpha}{T\lambda_i+\lambda_i^{1-k}/\alpha}\right)^{\lambda_i^{1-k}/\alpha}(T\lambda_i+\lambda_i^{1-k}/\alpha)^{-\sum_{i=1}^{T}n_{i,t}}, \tag{4.5}$$

where $k = 1$ is the standard negative multivariate distribution (MVNB2), $k = 0$ is the multivariate NB1 equivalence (MVNB1). The variable k can also be numerically estimated, which can be used to construct a method of discriminating between the MVNB2 and the MVNB1 models. This method, used by Boucher et al. (2007) is based on the creation of a hypermodel, where the additional parameter, here the random variable k, is used to test whether MVNB2 or MVNB1 is statistically the better by doing a simple confidence interval. Expressed in its general form, the MVNBk distribution has the following moments:

$$\begin{aligned} E[N_{i,t}] &= E[E[N_{i,t}|\theta_i]] \\ &= \lambda_i \end{aligned} \tag{4.6}$$

$$\begin{aligned} Var[N_{i,t}] &= E[Var[N_{i,t}|\theta_i]] + Var[E[N_{i,t}|\theta_i]] \\ &= \lambda_i + \alpha\lambda_i^{k+1} \end{aligned} \tag{4.7}$$

$$\begin{aligned} Cov[N_{i,t}, N_{i,t+j}] &= Cov[E[N_{i,t}|\theta_i], E[N_{i,t+j}|\theta_i]] + E[Cov[N_{i,t}, N_{i,t+j}|\theta_i]] \\ &= Cov[\lambda_i\theta_i, \lambda_i\theta_i] + 0 \\ &= \alpha\lambda_i^{k+1}, \quad j > 0 \end{aligned} \tag{4.8}$$

As for the cross-sectional data, other distributions can be chosen to model the random effects, such as the Inverse Gaussian or the LogNormal distributions, which result in distributions having the same form for the two first moments, distinctions found using higher moments. Note that the MVNB2 and MVNB1 models are nested to the Poisson distribution in the case when $\alpha \to 0$.

4.4 Hurdle Models

4.4.1 Overview

Because the vast majority of the insureds reports less than 2 claims per year, Boucher et al. (2007) proposed to model the number of reported claims by two different processes. Firstly, a dichotomic distribution to differentiate insureds with and without

claim. Secondly, another process that precises, conditionally on having reported at least one time, the number of reported claims. The distribution that uses two processes to determine the number of reported claims can be driven by the same explanatory variables, which may be interpreted differently depending on the process involved. This kind of modelling looks like the double modelling of the amount of claims, where the limited costs and the excess-of-loss costs (costs above a certain value) are modelized separately.

The most popular distribution implying the assumption that the data come from two separate processes is the hurdle count models that were introduced by Mullahy (1986). The hurdle model is characterized by the process below the hurdle and the one above. Obviously, the most widely used hurdle model is the one that sets the hurdle at zero. Formally, the hurdle-at-zero model is expressed as:

$$P(N_i = n_i) = \begin{array}{ll} f_1(0) & \text{for } n_i = 0 \\ \frac{1-f_1(0)}{1-f_2(0)} f_2(n_i) = \Phi f_2(n_i) & \text{for } n_i = 1, 2, ... \end{array} \tag{4.9}$$

The variable Φ can be interpreted as the probability of crossing the hurdle, or more precisely in case of insurance, the probability to report at least one claim. Clearly, the model collapses to f if $f_1 = f_2 = f$. Expected values and variance of this hurdle model are expressed as:

$$E[N_i] = \frac{1 - f_1(0)}{1 - f_2(0)} \sum_{k=0}^{\infty} k f_2(k) \tag{4.10}$$

$$Var[N_i] = \Phi \sum_{k=1}^{\infty} k^2 f_2(k) - [\Phi \sum_{k=1}^{\infty} k^2 f_2(k)]^2, \tag{4.11}$$

where $\Phi = (1 - f_1(0))/(1 - f_2(0))$. Consequently, the model can be over or underdispersed, depending on the values of the parent processes. Many possibilites exist for the choice of the processes f_1 and f_2. Nested models where f_1 and f_2 come from the same distribution, such as the Poisson distribution (Mullahy, 1986) or the Negative Binomial (Pohlmeier and Ulrich, 1995), which is by far the most popular hurdle model (Winkelmann, 2000), are possible. However, non-nested models (Grootendorst (1995), (Gurmu, 1998), or Winkelmann (2003)) can also be used. These models do not nest with a standard count distributions such as the Poisson or the NB types, but are overlapping Vuong (1989) since models can be equivalent for certain parameter restrictions.

Estimation of the parameters by maximum likelihood is easy. The log-likelihood function of a hurdle model can be expressed as:

$$\begin{aligned} \ell = & \sum_{i=1}^{n} I_{(n_i=0)} \log(f_1(0; \theta_1)) + I_{(n_i>0)} \log(1 - f_1(0; \theta_1)) \\ & + \sum_{i=1}^{n} I_{(n_i>0)} \log(f_2(n_i; \theta_1)/(1 - f_2(0; \theta_i)) \end{aligned} \tag{4.12}$$

The hurdle model is interesting because it allows us to estimate the parameters by two separate steps. Indeed, the zero-part parameters can be estimated using MLE on the first part of the loglikelihood equation while the other parameters only use the second part, only composed with non-zero elements. This characteristic of the model is very useful to save computer time in the estimation.

Unobserved heterogeneity

To add some uncertainty due to the absence of important classification variables, an heterogeneity term can be added to the distribution. The standard approach is to integrate the heterogeneity prior to the conversion into a hurdle model:

$$\hat{f}_1(n_i) = \int f_1(n_i|\theta) g_1(\theta) d\theta \tag{4.13}$$

$$\hat{f}_2(n_i) = \int f_2(n_i|\theta) g_2(\theta) d\theta \tag{4.14}$$

$$P(N_i = n_i) = \begin{cases} \hat{f}_1(0) & \text{for } n_i = 0 \\ \frac{1-\hat{f}_1(0)}{1-\hat{f}_2(0)} \hat{f}_2(n_i) & \text{for } n_i = 1, 2, ... \end{cases} \tag{4.15}$$

However, as noted by Santos Silva (2003), it seems more natural to estimate the heterogeneity on the positive part and on the zero part of the model. Formally,

$$P(N_i = n_i) = \begin{cases} \int f_1(0|\theta) g_1(\theta) d\theta & \text{for } n_i = 0 \\ \left(\int (1 - f_1(0|\theta)) g_1(\theta) d\theta\right) \left(\int \frac{f_2(n_i|\theta)}{1-f_2(0|\theta)} g_2(\theta) d\theta\right) & \text{for } n_i = 1, 2, ... \end{cases} \tag{4.16}$$

Conceptually, models (4.15) and (4.16) differ in interpretation. As noted in Santos Silva (2003) and reviewed in Winkelmann (2003), the zero and positive processes of the hurdle model are evaluated separately and possesses their own heterogeneity. Consequently, model (4.16) seems to be more intuitive since we avoid the step of needing to compute $\int f_2(0|\theta) g_2(\theta) d\theta$ although the zeros are supposed to be generated by another process.

When a heterogeneity term is chosen for model (4.16), closed expression can be found using a transformation. Indeed, a new random variable $n_i* = n_i - 1$ can be used to model the second part of the hurdle model with standard count models, such as a Poisson distribution or other variations.

Model interpretation

The hurdle models are quite popular for modelling health care demands. Indeed, it is generally accepted that the demand for certain types of health care services depends on two processes: the decisions of the individual and the one of the health care provider (Stoddart and Barer (1981), Pohlmeier and Ulrich (1995), Mullahy (1997), Santos Silva and Windmeijer (2001)). Consequently, conditionally on certain assumptions, the use of a hurdle model is intuitive, and the parameters can have a structural interpretation.

Many direct applications of this model can be used for insurance data, such as the amount of coverage implied for a claim, the number of injured people or the number of implicated third parties. Such modellings using separate processes are appropriate since these processes are not the same as the one that drives the number of accidents.

However, beside these specific examples, such modelling can also have a natural interpretation for the number of reported claims. Indeed, since there exists a reluctance from some insureds to report their accident since they would lose their good bonus-malus rating, we can suppose that the behavior of the insureds is not the same when they already have reported a claim.

4.4.2 Panel data

The hurdle model can be directly generalized to panel data using the transformation $n_i^* = n_i - 1$:

$$P(N_{i,1},...,N_{i,t}) = \int \prod_t f_1(0|\theta_{i,1})^{I_{(n_{i,t}=0)}} \left(1 - f_1(0|\theta_{i,1})\right)^{1-I_{(n_{i,t}=0)}} g_1(\theta_{i,1}) d\theta_{i,1} \times \int \prod_t f_2^*(n_{i,t}^*|\theta_{i,2})^{1-I_{(n_{i,t}=0)}} g_2(\theta_{i,2}) d\theta_{i,2}. \tag{4.17}$$

As for the cross-sectional data, the hurdle model is interesting because it allows us to estimate the parameters on two separate steps. The transformation of the positive part allows us to fit the data using standard Poisson random effects models seen in Section 4.3, where the mean variable can be expressed as $\gamma_i = \exp(x_i\delta)$. For the zero-part of the model, instead of using the classic Poisson parametrization approach that results in a complicated form for the joint distribution expression, a more intuitive model could be the use of a Bernouilli distribution where the parameter is beta distributed to account for the invidual specificities.

Using a Bernouilli-Beta combination for the zero part, the joint distribution of the variable $Z_{i,t}$, which can take values of 0 or 1, is well known and can be expressed as:

$$\begin{aligned} P(Z_{i,1},...,Z_{i,t}) &= \int \prod_t \theta_i^{z_{i,t}} (1-\theta_i)^{1-z_{i,t}} \frac{\Gamma(a_i+b)}{\Gamma(a_i)\Gamma(b)} \theta_i^{a_i-1} (1-\theta_i)^{b-1} \, d\theta_i \\ &= \frac{\Gamma(a_i+b)}{\Gamma(a_i)\Gamma(b)} \frac{\Gamma(\sum_t z_{i,t} + a_i)\Gamma(T - \sum_t z_{i,t} + b)}{\Gamma(T + a_i + b)} \end{aligned} \tag{4.18}$$

The covariates can be included in the model as $a_i = \exp(x_i\beta)$. Having the upper part modeled with the transform random variable n_i^* and basing the computations on equations (4.10) and (4.11), the complete hurdle model involves the following moments:

$$\begin{aligned} E[N_{i,t}] &= \frac{a_i}{a_i+b} \sum_{j=0}^{\infty} (1+j) f_{n_i^*}(j) \\ &= \frac{a_i}{a_i+b}(1+\gamma_i) && (4.19) \\ E[N_{i,t}^2] &= \frac{b}{a_i+b} \sum_{j=0}^{\infty} (1+j)^2 f_{n_i^*}(j) \\ &= \frac{a_i}{a_i+b}\left[1 + 3\gamma_i + \alpha\gamma_i^{k+1} - \gamma_i^2\right] && (4.20) \\ Var[N_{i,t}] &= E[N_{i,t}^2] - E[N_{i,t}]^2 && (4.21) \\ Cov[N_{i,t}, N_{i,t+j}] &= (1+\gamma_i)^2 \frac{a_i b}{(a_i+b+1)(a_i+b)^2} \\ &\quad + \frac{\gamma_i^{k+1}}{\alpha}\left(\frac{a_i b}{(a_i+b+1)(a_i+b)^2} + \left(\frac{a_i}{a_i+b}\right)^2\right), \quad j > 0. && (4.22) \end{aligned}$$

4.5 Predictive Distribution

For the Poisson and the hurdle models for panel data, at each insured period, the random effects θ_i and p_i can be updated for past claims experience, revealing some individual information. Formally, the predictive distribution can be found using the following development:

$$\begin{aligned}\Pr[n_{i,T+1}|n_{i,1},...,n_{i,T}] &= \frac{\Pr(n_{i,1},...,n_{i,T+1})}{\Pr(n_{i,1},...,n_{i,T})} = \frac{\int \Pr(n_{i,1},...,n_{i,T+1},\theta_i)d\theta_i}{\int \Pr(n_{i,1},...,n_{i,T},\theta_i)d\theta_i} \\ &= \int \Pr(n_{i,T+1}|\theta_i)\left(\frac{\Pr(n_{i,1},...,n_{i,T}|\theta_i)g(\theta_i)}{\int \Pr(n_{i,1},...,n_{i,T}|\theta_i)g(\theta_i)d\theta_i}\right)d\theta_i \\ &= \int \Pr(n_{i,T+1}|\theta_i)\left(\frac{[\prod_t \Pr(n_{i,t}|\theta_i)]\,g(\theta_i)}{\int [\prod_t \Pr(n_{i,t}|\theta_i)]\,g(\theta_i)d\theta_i}\right)d\theta_i \\ &= \int \Pr(n_{i,T+1}|\theta_i)g(\theta_i|n_{i,1},...,n_{i,T})d\theta_i, \end{aligned} \tag{4.23}$$

where $g(\theta_i|n_{i,1},...,n_{i,T})$ is the *a posteriori* distribution of the random effects θ_i, reflecting the past claims experience of insured i. If this *a posteriori* distribution can be expressed in closed form, moments of the predictive distribution can be found easily by conditioning on the random effects θ_i.

4.5.1 Poisson

As it is well known, we found that the a *posteriori* distribution of the random effect term is also a Gamma distribution having parameters equal to $T\lambda_i + \lambda_i^{(1-k)}/\alpha$ and $\sum_t^T n_{i,t} + \lambda_i^{(1-k)}/\alpha$. The two first moments of the predictive distributions are equaled to:

$$E[N_{i,t+1}|N_{i,1},...,N_{i,t}] = \lambda_i \frac{\sum_t^T n_{i,t} + \lambda_i^{(1-k)}/\alpha}{T\lambda_i + \lambda_i^{(1-k)}/\alpha} \tag{4.24}$$

$$Var[N_{i,t+1}|N_{i,1},...,N_{i,t}] = \lambda_i \frac{\sum_t^T n_{i,t} + \lambda_i^{(1-k)}/\alpha}{T\lambda_i + \lambda_i^{(1-k)}/\alpha} + \lambda_i^2 \frac{\sum_t^T n_{i,t} + \lambda_i^{(1-k)}/\alpha}{(T\lambda_i + \lambda_i^{(1-k)}/\alpha)^2}. \tag{4.25}$$

We see that the future premium only depends on the sum of the number of reported claims. Additionally, we observe that the premium of insured i goes to its average number of reported claims if the number of insured periods goes large. For models where the variable k is different than 1, the variance of the heterogeneity distribution depends on characteristics of the insureds. Then, the impact on a premium of having a claim is more important for low variance heterogeneity and thus, premium modifications for negative composants of λ_i are more severe.

4.5.2 Hurdle

The same development can be done for the two processes of the hurdle distribution, since the panel hurdle model can be expressed as:

$$P(N_{i,1},...,N_{i,t}) = \int \prod_t f_1(0|p_i)^{z_{i,t}} \left(1 - f_1(0|p_i)\right)^{1-z_{i,t}} g(p_i)dp_i \times \int \prod_t f_2^*(n_{i,t}^*|\theta_i)^{1-I_{(n_{i,t}=0)}} h(\theta_i)d\theta_i. \tag{4.26}$$

Because the two processes can be analyzed separately, the *a posteriori* distribution of the random effect term of the first process can be found as follows:

$$\begin{aligned} g[p_i|z_{i,1},...,z_{i,T}] &\propto p_i^{\sum_t^T z_{i,t}}(1-p_i)^{T-\sum_t^T z_{i,t}} \frac{\Gamma(a_i+b)}{\Gamma(a_i)\Gamma(b)} p_i^{a-1}(1-p_i)^{b-1}dp_i \\ &\propto p_i^{\sum_t^T z_{i,t}+a_i-1}(1-p_i)^{T-\sum_t^T z_{i,t}+b-1}dp_i. \end{aligned}$$

From which, we can see that it is beta distributed with parameters $\sum_t^T z_{i,t} + a_i$ and $T - \sum_t^T z_{i,t} + b$. For the first part of the distribution, the expected value of the predicted distribution is then calculated as:

$$E[z_{i,T+1}|z_{i,1},...,z_{i,T}] = \frac{\sum_t^T z_{i,t} + a_i}{T + b + a_i} \tag{4.27}$$

The second process $N_i^* = N_i - 1$ of the hurdle distribution is following a MVNB distribution. Then, the *a posteriori* distribution of the random effect term can be found using the same development as Section 4.5.1, and thus the expected value of the second process is equal to:

$$\begin{aligned} E[n_{i,J+1}|n_{i,J+1} > 0, n_{i,1},...,n_{i,J}] &= 1 + E[N_{i,J+1}^* = n_{i,J+1}^*|n_{i,1},...,n_{i,J}] \\ &= 1 + \gamma_i \frac{\sum_t^J n_{i,t} + \gamma_i^{(1-k)}/\alpha}{J\gamma_i + \gamma_i^{(1-k)}/\alpha}, \end{aligned} \tag{4.28}$$

where J is equaled to the number of insured period where the insured has reported at least one claim. Combining equations (4.27) and (4.28) leads to the predictive expected value of the count distribution, while the variance of the model can be computed using equations (4.11) and (4.21):

$$E[n_{T+1}|n_1,...,n_T] = \frac{\sum_t^T z_{i,t} + a_i}{T + b + a_i} \left(1 + \gamma_i \frac{\sum_t^J n_{i,t} + \gamma_i^{(1-k)}/\alpha}{J\gamma_i + \gamma_i^{(1-k)}/\alpha}\right) \tag{4.29}$$

$$\begin{aligned} E[n_{T+1}^2|n_1,...,n_T] = \frac{\sum_t^T z_{i,t} + a_i}{T + a_i + b} \Bigg[& 1 + 3\gamma_i \frac{\sum_t^J n_{i,t} + \gamma_i^{(1-k)}/\alpha}{J\gamma_i + \gamma_i^{(1-k)}/\alpha} \\ & + \gamma_i^2 \frac{\sum_t^J n_{i,t} + \gamma_i^{(1-k)}/\alpha}{(J\gamma_i + \gamma_i^{(1-k)}/\alpha)^2} - \left(\gamma_i \frac{\sum_t^J n_{i,t} + \gamma_i^{(1-k)}/\alpha}{J\gamma_i + \gamma_i^{(1-k)}/\alpha}\right)^2 \Bigg]. \end{aligned} \tag{4.30}$$

As opposed to the Multivariate Negative Binomial models, the future premium not only depends on the sum of reported claims, but also on the number of insured periods without claim. Additionally, when the insured period goes to infinite, the premium of the insured does not converge to the average number of reported claims, but on the product of two limited values: the average number of time periods with at least one claim and the average of the number of reported claims greater or equal to one.

4.5.3 Linear credibility

Predictive and *a posteriori* distributions used Bayesian theory and are strongly related to credibility theory (Bühlmann (1967), Bühlmann and Straub (1970), Hachemeister (1975), Jewell (1975)). Linear credibility is a theory used to obtain a premium based on a weighted average of past experience and *a priori* premium, such as:

$$P_{T+1} = Z\bar{n}_{i,t} + (1 - Z) \times P_0, \tag{4.31}$$

where $\bar{n}_{i,t} = \sum_{t=1}^{T} \frac{n_{i,t}}{T}$, P_{T+1} is the predictive premium a time $T + 1$, P_0 is the a *priori* premium and $n_{i,t}$ is the number of reported claim for insured i at period t. The coefficient Z, that gives weight to the two components, is the value that minimizes the squared error of the predictive value (Bühlmann, 1967) which corresponds to:

$$Z = \frac{Cov(\bar{N}_{i,t}, N_{n+1})}{Var(N_i^*)}.$$

The linear credibility model gives exact results only for conjugated distributions Jewell (1975), such as the Poisson with gamma random effects or Bernoulli with Beta parameters. Then, using standard results of the credibility theory, it is possible to obtain the same premium as the one obtained in equation (4.29).

4.6 Insurance Application

The models seen in the preceding sections can be used to calculate the impact of the covariates on the number of reported claims, but can also be used to calculate *a priori* premiums or predictive premiums of the frequency part of an insurance premium. The amount of claims is the other part of a standard insurance premium. The *a priori* premium represents the premium that a new insured must paid to be covered. By opposition, the predictive premium is the premium of the other insureds, that depends on the experience of each insured.

4.6.1 Estimations

Applications of the Poisson and the hurdle models on our insurance data lead to the results shown in table 4.2 for the models based on Poisson generalization, while tables 4.3 and 4.4 refer to the hurdle model since it can be decomposed in two parts.

For the Multivariate Negative Binomial models, the estimated parameters are quite the same for all models. Not surprisingly, we see that women exhibit fewer claims than

Table 4.2. Multivariate negative binomial models

Parameter	MVNB2	MVNB1	MVNBk
b0	−2.6600 (0.0352)	−2.6635 (0.0341)	−2.6646 (0.0337)
b1	0.1087 (0.0409)	0.1170 (0.0387)	0.1166 (0.0380)
b2	−0.1805 (0.0327)	−0.1731 (0.0314)	−0.1684 (0.0326)
b3	−0.2103 (0.0370)	−0.2068 (0.0358)	−0.2022 (0.0368)
b4	0.0471 (0.0346)	0.0599 (0.0329)	0.0613 (0.0324)
b5	0.0990 (0.0316)	0.0931 (0.0305)	0.0904 (0.0305)
α	0.8832 (0.0432)	0.0610 (0.0031)	0.0339 (0.0426)
k	. .	. .	−0.2188 (0.4682)
LogLike	26,703.0	26,699.4	26,699.3

men, while new insureds in the company seem to have a worse loss experience than older clients. In the presence of other covariates, we can also see that young drivers exhibit a better claim experience, but it is not statistically significant. To finish, we observe that insureds with powerful vehicles suffer more accidents than other drivers. A look at the p-values of the parameters implying time dependence between contracts of the same insured leads to the conclusion that it improves the model. However, more statistical tests must be done to conclude that the introduction of this term improves the Poisson models since it cannot be negative, and the tested hypothesis is on the boundary of the parameter space. Indeed, when a parameter is bounded by the H_0 hypothesis, the estimate is also bounded and the asymptotic normality of the MLE no longer hold under H_0.

By comparison of the log-likelihoods, we see that the form of the random effects do not really modify the fitting of the data. The confidence interval implied by the k variable of MVNBk model concludes that the MVNB2 and the MVNB1 are both accepted.

For the hurdle models, we have to notice that the parameters obtained cannot be compared directly to the ones obtained with the multivariate negative binomial distributions since they do have the same impact on the expected value (See equations (4.19) and (4.6)). However, by the sign of the estimated parameters of the zero-part of the hurdle model (table 4.3), we can reach the same conclusions as the ones done with the MVNB distribution for the probability to report at least one claim in a time period. As opposed to the Poisson generalization models, the time dependence assumption cannot be analyed directly with this parametrization.

The parameters of table 4.4 allow us to observe what kinds of insureds are most likely to report a high number of claim in a single time period. The result is a little bit strange since only the insureds that were in the company between 3 and 5 years at the beginning of the study are statistically better than the others. The α parameter seems to be quite significant and the k variable seems to favor the MVNB2 distribution, even if its confidence interval accepts both models.

4.6.2 Premiums

Difference between models can be analyzed through the mean and the variance of some insured profiles. Several profiles have been selected and are described in table 4.5. The first profile is classified as a good driver, while the last one usually exhibits bad loss

Table 4.3. Hurdle models: Zero part

Parameter	Beta
b0	0.3066 (0.0682)
b1	0.1298 (0.0401)
b2	−0.1726 (0.0325)
b3	−0.2124 (0.0370)
b4	0.0616 (0.0341)
b5	0.0975 (0.0315)
b	19.9640 (1.2279)
Loglike.	24,637.9

Table 4.4. Hurdle Models: Positive part

Parameter	MVNB2	MVNB1	MVNBk
b0	−2.3688 (0.0525)	−2.3695 (0.0524)	−2.3687 (0.0526)
b2	−0.1951 (0.0933)	−0.1922 (0.0933)	−0.1953 (0.0935)
α	0.8122 (0.2070)	0.0718 (0.0183)	0.6955 (4.7872)
k	. .	. .	0.9359 (2.8422)
Loglike.	2,050.80	2,050.85	2,050.80

experience. The other profile is medium risk. The results are given in table 4.6. This table shows that the expected values of all profiles are quite the same for the 4 models studied. The biggest differences lie in the variance values, where the hurdle models exhibit higher values.

Table 4.7 shows the predictive premiums of the 2^{nd} profile for MVNB2 and hurdle-MVNB2 (chosen arbitrarily between available models), which depends on the sum of reported claims and on the number of insured periods with at least one reported claim ($t = T - T_0$). To illustrate, we selected a loss experience of 10 years, but other situations can be easily illustrated since equations (4.24) and (4.29) are simple to use.

Interesting conclusions can be done from the analysis of predictive premiums. Indeed, we can see that the number of insured periods with a claim have a greater impact on the next year's premium than the total number of reported claims. Indeed, the

Table 4.5. Profiles analyzed

Profile Number	Kind of Profile	v1	v2	v3	v4	v5
1	Good	0	0	1	0	0
2	Average	1	1	0	0	0
4	Bad	1	0	0	1	1

Table 4.6. *A priori* premiums

	1^{st} Profile		2^{nd} Profile		3^{rd} Profile	
Models	Mean	Variance	Mean	Variance	Mean	Variance
MVNB2	0.0567	0.0595	0.0651	0.0688	0.0902	0.0974
MVNB1	0.0567	0.0601	0.0659	0.0699	0.0911	0.0966
H. Be-MVNB2	0.0570	0.0667	0.0659	0.0753	0.0911	0.1065
H. Be-MVNB1	0.0570	0.0667	0.0659	0.0753	0.0911	0.1065

Table 4.7. Predictive premiums

		Sum of claims						
Models	t	0	1	2	3	4	10	20
PG2	.	0.0413	0.0778	0.1143	0.1509	0.1874	0.4064	0.7715
H. PG2	0	0.0448	.	.	.	.	.	
	1	.	0.0790	0.0833	0.0876	0.0920	0.1180	0.5067
	2	.	.	0.1128	0.1187	0.1246	0.1598	0.5345
	3	.	.	.	0.1465	0.1538	0.1972	0.5623
	4	.	.	.	.	0.1800	0.2309	0.5901
	10	.	.	.	.	.	0.3786	0.7570
	20	.	.	.	.	.	0.7393	1.0351

premium increases only by 16.4% if the insured reports 4 claims instead of one in a single insured period. On the other hand, if the insured reports his 4 claims on 4 different time periods instead of only one, his premium increases by more than 95%. For insureds who reported 1 claim or less, the hurdle model offers a discount that is smaller than the MVNB model. For higher claims reporters, we can see that the hurdle model exhibits a wide panel of premium values that go from 0.3 to 1.8 times the MVNB's premiums.

4.7 Conclusion

The behavior of the insureds toward their bonus-malus scheme seems to influence their probability to report a claim. Models such as the hurdle distribution use this feature to model the number of reported claims and provide good fitting. The generalization of the Hurdle model to panel data can be done directly and shows interesting properties, such as the discrimination of the insureds depending on the number of reported claims and the number of insured periods without claim. The choice of the best distribution describing our data must be supported by specification tests for nested or non-nested models and should be the subject of further analysis. There is also a general feeling in the insurance industry that drivers have either good claiming behavior (never claim) or a bad claiming behavior (claim a lot). Indeed many marketing strategies are designed to capture good customers and let the bad drivers go to the competitor. This paper shows that this classification must go a little beyond where the number of insured periods without claim has some importance.

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5

Distance-Based Association and Multi-Sample Tests for General Multivariate Data

Carles M. Cuadras

Department of Statistics, University of Barcelona, Spain

Abstract: Most multivariate tests are based on the hypothesis of multinormality. But often this hypothesis fails, or we have variables that are non quantitative. On the other hand we can deal with a large number of variables. Defining probabilistic models with mixed data is not easy. However, it is always possible to define a measure of distance between two observations. We prove that the use of distances can provide alternative tests for comparing several populations when the data are of general type. This approach is illustrated with three real data examples. We also define and study a measure of association between two data sets and make a Bayesian extension of the so-called distance-based discriminant rule.

Keywords and phrases: Statistical distances, multivariate association, discriminant analysis, MANOVA, ANOQE, permutation test, large data sets

5.1 Introduction

Let $\Omega = \{\omega_1, \omega_2, ..., \omega_n\}$ be a finite set with n individuals. Let $\delta_{ii'} = \delta(\omega_i, \omega_{i'}) = \delta(\omega_{i'}, \omega_i) \geq \delta(\omega_i, \omega_i) = 0$ a distance or dissimilarity function defined on Ω. We suppose that the $n \times n$ distance matrix $\mathbf{\Delta} = (\delta_{ii'})$ is Euclidean. Then there exists a configuration $\mathbf{x}_1, \ldots, \mathbf{x}_n \in R^p$, with $\mathbf{x}_i = (x_{i1}, \ldots, x_{ip})'$, $i = 1, \ldots, n$, such that

$$\delta_{ii'}^2 = \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 = (\mathbf{x}_i - \mathbf{x}_{i'})'(\mathbf{x}_i - \mathbf{x}_{i'}). \tag{5.1}$$

These coordinates constitute an $n \times p$ matrix $\mathbf{X} = (x_{ij})$ such that the Euclidean distance between two rows i and i' equals $\delta_{ii'}$.

A way of obtaining $\mathbf{X}$ from $\mathbf{\Delta}$ is as follows. Compute $\mathbf{A} = -\frac{1}{2}\mathbf{\Delta}^{(2)}$and $\mathbf{G} = \mathbf{HAH}$, where $\mathbf{\Delta}^{(2)} = (\delta_{ii'}^2)$ and $\mathbf{H} = \mathbf{I}_n - n^{-1}\mathbf{1}_n\mathbf{1}_n'$ is the centering matrix. Then $\mathbf{\Delta}$ is Euclidean with dimension p =rank($\mathbf{G}$) if and only if $\mathbf{G} \geq \mathbf{0}$. The spectral decomposition $\mathbf{G} = \mathbf{U}\mathbf{\Lambda}^2\mathbf{U}'$ gives $\mathbf{X} = \mathbf{U}\mathbf{\Lambda}$. Thus $\mathbf{G} = \mathbf{X}\mathbf{X}'$ and the relation between $\mathbf{\Delta}^{(2)}$ and $\mathbf{G}$ is given by $\mathbf{\Delta}^{(2)} = \mathbf{1}\mathbf{g}' + \mathbf{g}\mathbf{1}' - 2\mathbf{G}$, where the $n \times 1$ vector $\mathbf{g}$ contains the diagonal entries

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in $\mathbf{G}$. Note that if $\mathbf{S} = (s_{ii'})$ is a similarity matrix and we define the squared distance $\delta^2_{ii'} = s_{ii} + s_{i'i'} - 2s_{ii'}$, then $\mathbf{G} = \mathbf{HSH}$.

Matrices $\mathbf{X}$ and $\mathbf{U}$ contain the principal and standard coordinates, respectively. This method is called classic multidimensional scaling or principal coordinate analysis (Cox and Cox (1994); Gower (1966); Mardia et al. (1979)).

Classic multivariate inference is mainly based on the hypothesis of normality. But often this hypothesis fails or we have non-quantitative variables. On the other hand, we can deal with a large number of variables. The main aim of this paper is to present two distance-based methods, on the basis of general data (quantitative, qualitative, binary, nominal, mixed), for comparing several populations. This distance-based approach extends some results by Cuadras and Fortiana (2004) and is in the line of Cuadras (1989, 1992), Cuadras and Arenas (1990), Cuadras et al. (1996, 1997a,b), Rao (1982) and Liu and Rao (1995). See Arenas and Cuadras (2002) for a general perspective.

Firstly, let us comment on some distance-based aspects of multivariate association and discrimination.

5.2 Multivariate Association

Suppose that we have two data sets $\mathcal{D}_1$ and $\mathcal{D}_2$ on the same Ω. The task of associating $\mathcal{D}_1$ and $\mathcal{D}_2$ has been well studied when two quantitative data matrices are available. Thus, if $\mathbf{X}$ and $\mathbf{Y}$ are two centered data matrices of orders $n \times p$ and $n \times q$, Escoufier (1973) introduced the generalized correlation

$$\mathrm{RV}(\mathbf{X}, \mathbf{Y}) = \mathrm{tr}(\mathbf{S}_{12}\mathbf{S}_{21}) / \sqrt{\mathrm{tr}(\mathbf{S}_{11}^2)\mathrm{tr}(\mathbf{S}_{22}^2)},$$

where $\mathbf{S}_{11} = \mathbf{X}'\mathbf{X}, \mathbf{S}_{22} = \mathbf{Y}'\mathbf{Y}, \mathbf{S}_{12} = \mathbf{X}'\mathbf{Y}, \mathbf{S}_{21} = \mathbf{Y}'\mathbf{X}$. This correlation is quite related to the Procrustes statistics (Cox and Cox, 1994)

$$\mathrm{R}^2 = 1 - \{\mathrm{tr}(\mathbf{X}'\mathbf{Y}\mathbf{Y}'\mathbf{X})^{1/2}\}^2 / \{\mathrm{tr}(\mathbf{X}'\mathbf{X})\mathrm{tr}(\mathbf{Y}'\mathbf{Y})\}.$$

Yanai et al. (2006) employ determinants of rectangular matrices to introduce a measure $\mathrm{Re}(\mathbf{X}, \mathbf{Y})$ of association, where

$$\mathrm{Re}(\mathbf{X}, \mathbf{Y})^2 = \det \begin{bmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Y} \\ \mathbf{Y}'\mathbf{X} & \mathbf{Y}'\mathbf{Y} \end{bmatrix} / [\det(\mathbf{X}'\mathbf{X}) \det(\mathbf{Y}'\mathbf{Y})].$$

We have $\mathrm{RV}(\mathbf{X}, \mathbf{Y}) = 1$, $\mathrm{R}^2 = \mathrm{Re}(\mathbf{X}, \mathbf{Y})^2 = 0$ if $\mathbf{X} = \mathbf{TY}$ ($\mathbf{T}$ orthogonal) and $\mathrm{RV}(\mathbf{X}, \mathbf{Y}) = 0$, $\mathrm{R}^2 = \mathrm{Re}(\mathbf{X}, \mathbf{Y})^2 = 1$ if $\mathbf{X}'\mathbf{Y} = \mathbf{0}$.

Next, let us show that we can use principal coordinates to define association with general data when a distance function is available. In this case, we may obtain $\mathbf{X}, \mathbf{Y}$ by considering a distance between observations, which provides the $n \times n$ distance matrices $\boldsymbol{\Delta}_x$ and $\boldsymbol{\Delta}_y$. By spectral decomposition of the corresponding inner product matrices $\mathbf{G}_x = \mathbf{U}\boldsymbol{\Lambda}_x^2\mathbf{U}'$, $\mathbf{G}_y = \mathbf{V}\boldsymbol{\Lambda}_y^2\mathbf{V}'$, we can obtain the standard coordinates $\mathbf{U}, \mathbf{V}$ and the principal coordinates $\mathbf{X} = \mathbf{U}\boldsymbol{\Lambda}_x, \mathbf{Y} = \mathbf{V}\boldsymbol{\Lambda}_y$.

We define the *association* between $\mathcal{D}_1$ and $\mathcal{D}_2$ by

$$\eta^2(\mathcal{D}_1, \mathcal{D}_2) = \det(\mathbf{U}'\mathbf{V}\mathbf{V}'\mathbf{U}). \tag{5.2}$$

For the sake of simplicity, we write $\eta^2(\mathbf{X}, \mathbf{Y})$.

This association coefficient satisfies the following properties:

1. $0 \leq \eta^2(\mathbf{X}, \mathbf{Y}) = \eta^2(\mathbf{Y}, \mathbf{X}) \leq 1$.
2. $\eta^2(\mathbf{X}, \mathbf{Y}) = \det(\mathbf{X}'\mathbf{Y}\mathbf{Y}'\mathbf{X})/[\det(\mathbf{X}'\mathbf{X})\det(\mathbf{Y}'\mathbf{Y})]$.
3. $\eta^2(\mathbf{X}, \mathbf{Y})$ does not depend on the configuration matrices $\mathbf{X}, \mathbf{Y}$.
4. If $\mathbf{y}$ is a vector and $\mathbf{X}$ is a matrix, both quantitative, then $R^2(\mathbf{y}, \mathbf{X}) = \eta^2(\mathbf{y}, \mathbf{X})$, where R is the multiple correlation coefficient.
5. If $r_j, j = 1, \cdots, q$ are the canonical correlation coefficients between $\mathbf{X}$ and $\mathbf{Y}$, then

$$\eta^2(\mathbf{X}, \mathbf{Y}) = \prod_{j=1}^{q} r_j^2.$$

We outline the proof. Write $\mathbf{W} = \mathbf{U}\mathbf{V}'$, where the columns of $\mathbf{U}$ and $\mathbf{V}$ are orthonormal. Then 1) follows from $0 \leq \det(\mathbf{W}\mathbf{W}') = \det(\mathbf{W}'\mathbf{W}) \leq 1$. As $\mathbf{\Lambda}_x, \mathbf{\Lambda}_y$ are diagonal, 2) reduces to $\det(\mathbf{U}'\mathbf{V}\mathbf{V}'\mathbf{U})$. Similarly, if $\mathbf{S}$ and $\mathbf{T}$ are $p \times p$ nonsingular matrices, then $\eta^2(\mathbf{X}, \mathbf{Y}) = \eta^2(\mathbf{X}\mathbf{S}, \mathbf{Y}\mathbf{T})$. In particular $\mathbf{S}$ and $\mathbf{T}$ can be orthogonal matrices and $\mathbf{X}\mathbf{S}, \mathbf{Y}\mathbf{T}$ define the same distance matrices $\mathbf{\Delta}_x, \mathbf{\Delta}_y$. To prove 4), note that $\mathbf{\Lambda}_x/\sqrt{n}$ contains the standard deviations of the columns of $\mathbf{X} = \mathbf{U}\mathbf{\Lambda}_x$. If $\mathbf{y} = \sqrt{n}s_y\mathbf{v}$ and $\mathbf{r} = \Lambda_x^{-1}\mathbf{X}'\mathbf{y}s_y^{-1}$ is the vector of simple correlations between $\mathbf{y}$ and $\mathbf{X}$, as $\mathbf{R}_{xx} = \mathbf{I}$, then:

$$\begin{aligned} R^2(\mathbf{y}, \mathbf{X}) &= \mathbf{r}'\mathbf{R}_{xx}^{-1}\mathbf{r} \\ &= s_y^{-2}\mathbf{y}'\mathbf{X}\mathbf{\Lambda}_x^{-1}\mathbf{\Lambda}_x^{-1}\mathbf{X}'\mathbf{y} \\ &= \mathbf{v}'\mathbf{U}\mathbf{U}'\mathbf{v}. \end{aligned}$$

Finally, the canonical correlations satisfy $\det(\mathbf{R}_{xy}\mathbf{R}_{yy}^{-1}\mathbf{R}_{yx} - r_j^2\mathbf{R}_{xx}) = 0$, with $\mathbf{R}_{xx} = \mathbf{R}_{yy} = \mathbf{I}$ and $\mathbf{R}_{xy} = \mathbf{R}'_{yx} = \mathbf{U}'\mathbf{V}$ and 5) follows.

The association measure (5.2) is similar to the measure used in Arenas and Cuadras (2004) for studying the agreement between two representations of the same data. This measure can be computed using only distances and is given by

$$\theta(\mathbf{X}, \mathbf{Y}) = 2[1 - \mathrm{tr}(\mathbf{G}_{xy})/\mathrm{tr}(\mathbf{G}_x + \mathbf{G}_y)],$$

where $\mathbf{G}_{xy} = \mathbf{G}_x + \mathbf{G}_y - (\mathbf{G}_x^{1/2}\mathbf{G}_y^{1/2} + \mathbf{G}_y^{1/2}\mathbf{G}_x^{1/2})/2$. Normalizing $\mathbf{G}_x, \mathbf{G}_y$ to $\mathrm{tr}(\mathbf{G}_x) = \mathrm{tr}(\mathbf{G}_y) = \mathrm{tr}(\mathbf{\Lambda}_x^2) = \mathrm{tr}(\mathbf{\Lambda}_y^2) = 1$, this measure reduces to

$$\theta(\mathbf{X}, \mathbf{Y}) = \mathrm{tr}(\mathbf{U}\mathbf{\Lambda}_x\mathbf{U}'\mathbf{V}\mathbf{\Lambda}_y\mathbf{V}').$$

5.2.1 Example of multivariate association

Is there a relation between trade and science? table 5.1 is a matrix reporting trade and scientific relations between 10 countries. The lower triangle contains 1 if significant trade occurred between two countries, 0 otherwise. The diagonal and upper triangle contains, for every pair of countries, the number of papers (mathematics and statistics, period 1996-2002) published in collaboration. Thus, Spain published 8597 papers without collaboration, 692 collaborating with USA, 473 with France, etc. The upper matrix $\mathbf{Q}$ is standardized to $\mathbf{S} = \mathbf{D}^{-1}\mathbf{Q}$, where $\mathbf{D} = \mathrm{diag}(\mathbf{S})$. Thus $\mathbf{S}$ has ones in the diagonal.

Table 5.1. Trade (1 if significant, 0 otherwise) and scientific relation (number of papers of mathematics and statistics in collaboration during 1996-2002) among ten countries

	USA	Spa	Fra	U.K.	Ital	Ger	Can	Jap	Chi	Rus
USA	63446	692	2281	2507	1642	2812	2733	1039	1773	893
Spain	1	8597	473	347	352	278	163	69	104	177
France	1	1	17155	532	916	884	496	269	167	606
U.K.	1	1	1	12585	490	810	480	213	339	365
Italy	0	1	1	0	13197	677	290	169	120	512
Germany	1	1	1	1	1	16588	499	350	408	984
Canada	1	0	0	1	0	0	7927	228	601	204
Japan	1	0	0	0	0	0	1	20001	371	193
China	1	0	0	0	0	0	1	1	39140	64
Russia	0	0	0	0	0	0	0	0	1	18213

The lower matrix is transformed to a matrix of similarities using the Jaccard coefficient, as explained in Cox and Cox (1994), p. 73. Then we obtain the spectral decomposition $\mathbf{G} = \mathbf{HSH}$ for each similarity matrix, and considering all principal dimensions (i.e., nine), we get $\eta^2(\mathcal{D}_1, \mathcal{D}_2) = 0.0816$. This coefficient reveals a weak association between trade and science.

5.3 The Proximity Function

Let $\mathbf{X}$ be a random vector with pdf $f(\mathbf{x})$ with respect to a suitable measure and support S. Since the results below can be generalized easily, we may suppose the Lebesgue measure. If δ is a distance or dissimilarity function between the observations of $\mathbf{X}$, we define the *geometric variability* of $\mathbf{X}$ with respect to δ as

$$V_\delta(\mathbf{X}) = \frac{1}{2}\int_{S\times S} \delta^2(\mathbf{x},\mathbf{y})\, f(\mathbf{x})\, f(\mathbf{y})\, d\mathbf{x}d\mathbf{y}. \tag{5.3}$$

The *proximity function* of an observation $\mathbf{x}$ to the population Π represented by $\mathbf{X}$ is defined by

$$\phi^2_\delta(\mathbf{x},\Pi) = \int_{S\times S} \delta^2(\mathbf{x},\mathbf{y}) f(\mathbf{y}) d\mathbf{y} - V_\delta(\mathbf{X}). \tag{5.4}$$

Suppose that $\psi : S \to L$ is a representation of S in a Euclidean (or separable Hilbert) space L such that $\delta^2(\mathbf{x},\mathbf{y}) = ||\psi(\mathbf{x}) - \psi(\mathbf{y})||^2$. The interest of $V_\delta(\mathbf{X})$ and $\phi^2_\delta(\mathbf{x})$ comes from the following properties:

1. We can interpret $V_\delta(\mathbf{X})$ as a generalized variance and $\phi^2_\delta(\mathbf{x})$ as the squared distance from $\mathbf{x}$ to an ideal mean of $\mathbf{X}$:

$$\begin{aligned} V_\delta(\mathbf{X}) &= E||\psi(\mathbf{X})||^2 - ||E(\psi(\mathbf{X})||^2, \\ \phi^2_\delta(\mathbf{x},\Pi) &= ||\psi(\mathbf{x}) - E(\psi(\mathbf{X}))||^2. \end{aligned} \tag{5.5}$$

In fact, if δ is the ordinary Euclidean distance, then $V_\delta(\mathbf{X}) = \mathrm{tr}(\mathbf{\Sigma})$.

2. If we transform the distance: $\widetilde{\delta}^2 = a\delta^2 + b$, then $\widetilde{V}_\delta = aV_\delta + b/2$ and $\widetilde{\phi}^2_\delta = a\phi^2_\delta + b/2$.
3. If $\delta^2 = \delta^2_1 + \delta^2_2$ then $\phi^2_\delta = \phi^2_{\delta_1} + \phi^2_{\delta_2}$.
4. By suitable choices of a, b we may transform δ and generate the probability density

$$f_\delta(\mathbf{x}) = \exp(-\phi^2_\delta\,(\mathbf{x},\Pi)).$$

Then:

$$I(f||f_\delta) = V_\delta\,(\mathbf{X}) - H(f) \geq 0,$$

where $I(f||f_\delta)$ is the Kullback-Leibler divergence and $H(f)$ is the Shannon entropy.
5. Given g populations $\Pi_1, \ldots, \Pi_g$, where $\mathbf{X}$ has pdf $f_k(\mathbf{x})$ when $\mathbf{x}$ comes from Π_k, we can allocate an individual $\omega \in \Pi_1 \cup \cdots \cup \Pi_g$ by using the distance-based (DB) discriminant rule (Cuadras et al., 1997b):

$$\text{allocate } \omega \text{ to } \Pi_i \text{ if } \quad \phi^2_\delta\,(\mathbf{x},\Pi_i) = \min_{1\leq k\leq g}\{\phi^2_\delta\,(\mathbf{x},\Pi_k)\}.$$

5.4 The Distance-based Bayes Allocation Rule

Here we extend the above rule. Suppose that $\Pi_1, \ldots, \Pi_g$ have probabilities "a priori" $P(\Pi_j) = q_j$, with $\sum q_j = 1$. The DB discriminant rule is equivalent to the Bayes rule by using the dissimilarity

$$\delta^2(\mathbf{x},\mathbf{y}) = \log[f_j(\mathbf{x})f_j(\mathbf{y})] + 2\log q_j \qquad \text{if } \mathbf{x},\mathbf{y} \text{ comes from } \Pi_j.$$

Then $\phi^2_\delta\,(\mathbf{x},\Pi_j) = \log f_j(\mathbf{x}) + \log q_j$ and the Bayes rule

$$\text{allocate } \omega \text{ to } \Pi_i \text{ if } \quad q_i f_i(\mathbf{x}) = \max_{1\leq k\leq g}\{q_k f_k(\mathbf{x})\},$$

is equivalent to the DB rule

$$\text{allocate } \omega \text{ to } \Pi_i \text{ if } \quad \log f_i(\mathbf{x}) + \log q_i = \min_{1\leq k\leq g}\{\log f_k(\mathbf{x}) + \log q_k\}.$$

However, the DB rule has interest when we can define a proper distance between observations without using the pdf. For example, suppose that Π_j is multivariate normal $N_p(\mu_j, \mathbf{\Sigma})$. The Mahalanobis distance $M^2(\mathbf{x},\mathbf{y}) = (\mathbf{x}-\mathbf{y})'\mathbf{\Sigma}^{-1}\,(\mathbf{x}-\mathbf{y})$ between observations provides $V_M = p$ and $\phi^2_M = (\mathbf{x}-\mu_j)'\mathbf{\Sigma}^{-1}(\mathbf{x}-\mu_j)$.

By adding an additive constant

$$\widetilde{M}^2(\mathbf{x},\mathbf{y}) = (\mathbf{x}-\mathbf{y})'\mathbf{\Sigma}^{-1}(\mathbf{x}-\mathbf{y}) - 4\log q_j \qquad \text{if } \mathbf{x},\mathbf{y} \text{ comes from } \Pi_j,$$

then $\widetilde{\phi}^2_M\,(\mathbf{x},\Pi_j) = (\mathbf{x}-\mu_j)'\Sigma^{-1}(\mathbf{x}-\mu_j) - 2\log q_j$, and the DB rule

$$\text{allocate } \omega \text{ to } \Pi_i \text{ if } \quad d(\mathbf{x},\mu_i,q_i) = \min_{1\leq k\leq g}\{d(\mathbf{x},\mu_k,q_k)\},$$

where $d(\mathbf{x},\mu_j,q_j) = (\mathbf{x}-\mu_j)'\mathbf{\Sigma}^{-1}(\mathbf{x}-\mu_j) - 2\log q_j$, is equivalent to the Bayes discriminant rule.

5.5 Multivariate Multiple-Sample Tests

The comparison of several populations can be approached under parametric models. A non-parametric general method, which extends that of Cuadras and Fortiana (2004) is next proposed.

Suppose that $\mathcal{D}_1, \ldots, \mathcal{D}_g$ are $g \geq 2$ independent data sets coming from the populations $\Pi_1, \ldots, \Pi_g$. These data can be general (quantitative, qualitative, nominal, mixed). We wish to test

$$H_0 : \Pi_1 = \cdots = \Pi_g.$$

Under H_0 all data come from the same underlying distribution.

First, we assume that, by means of a distance function between observations, we can obtain the intra-distance matrices $\boldsymbol{\Delta}_{11}, \ldots, \boldsymbol{\Delta}_{gg}$, and the inter-distance matrices $\Delta_{12}, \ldots, \Delta_{g-1g}$. Thus we have the $n \times n$ super-distance matrix

$$\boldsymbol{\Delta} = \begin{bmatrix} \boldsymbol{\Delta}_{11} & \cdots & \boldsymbol{\Delta}_{1g} \\ \vdots & \ddots & \vdots \\ \boldsymbol{\Delta}_{g1} & \cdots & \boldsymbol{\Delta}_{gg} \end{bmatrix},$$

where Δ_{ij} is $n_i \times n_j$.

Next, we compute, via principal coordinate analysis, the matrices $\mathbf{G}$ and $\mathbf{X}$ such that $\mathbf{G} = \mathbf{X}\mathbf{X}'$. We write the full $\mathbf{X}$ as

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \vdots \\ \mathbf{X}_g \end{bmatrix}.$$

The Euclidean distances between the rows of $\mathbf{X}_i$ and $\mathbf{X}_{i'}$ give $\boldsymbol{\Delta}_{ii'}$. Thus the matrices $\mathbf{X}_1, \ldots, \mathbf{X}_g$ may represent the g quantitative data sets, which can be compared for testing H_0.

5.5.1 Partitioning the geometric variability

The rows $\mathbf{x}_1, \ldots, \mathbf{x}_n$ of any $N \times p$ multivariate data matrix $\mathbf{X}$ satisfy

$$\sum_{i=1}^{N} \sum_{i'=1}^{N} (\mathbf{x}_i - \mathbf{x}_{i'})(\mathbf{x}_i - \mathbf{x}_{i'})' = 2N \sum_{i=1}^{N} (\mathbf{x}_i - \overline{\mathbf{x}})(\mathbf{x}_i - \overline{\mathbf{x}})', \tag{5.6}$$

where $\overline{\mathbf{x}} = N^{-1} \sum_{i=1}^{N} \mathbf{x}_i$ is the vector of means.

Now suppose g data matrices $\mathbf{X}_1, \ldots, \mathbf{X}_g$, where each $\mathbf{X}_i$ has order $n_i \times p$. Recall the identity $\mathbf{T} = \mathbf{B} + \mathbf{W}$, with

$$\begin{aligned} \mathbf{B} &= \sum_{k=1}^{g} n_k (\overline{\mathbf{x}}_k - \overline{\mathbf{x}})(\overline{\mathbf{x}}_k - \overline{\mathbf{x}})', \\ \mathbf{W} &= \sum_{k=1}^{g} \sum_{i=1}^{n_k} (\mathbf{x}_{ki} - \overline{\mathbf{x}}_k)(\mathbf{x}_{ki} - \overline{\mathbf{x}}_k)', \\ \mathbf{T} &= \sum_{k=1}^{g} \sum_{i=1}^{n_k} (\mathbf{x}_{ki} - \overline{\mathbf{x}})(\mathbf{x}_{ki} - \overline{\mathbf{x}})', \end{aligned}$$

where $n = n_1 + \cdots + n_g$, $\mathbf{x}'_{ki}$ is a row of $\mathbf{X}_k$ with vector of means $\overline{\mathbf{x}}_k$ and $\overline{\mathbf{x}}$ is the overall mean. Matrices $\mathbf{T}, \mathbf{B}, \mathbf{W}$ are the total, between samples and within samples, respectively.

From (5.6) we obtain:

$$\begin{aligned}
\mathbb{T} &= \textstyle\sum_{k,h=1}^{g} \sum_{i,i'=1}^{n_k,n_h} (\mathbf{x}_{ki} - \mathbf{x}_{hi'})(\mathbf{x}_{ki} - \mathbf{x}_{hi'})' \\
&= 2n \textstyle\sum_{k=1}^{g} \sum_{i=1}^{n_k} (\mathbf{x}_{ki} - \overline{\mathbf{x}})(\mathbf{x}_{ki} - \overline{\mathbf{x}})', \\
\mathbb{B} &= \textstyle\sum_{k,h=1}^{g} n_k n_h (\overline{\mathbf{x}}_k - \overline{\mathbf{x}}_h)(\overline{\mathbf{x}}_k - \overline{\mathbf{x}}_h)' \\
&= 2n \textstyle\sum_{k=1}^{g} n_k (\overline{\mathbf{x}}_k - \overline{\mathbf{x}})(\overline{\mathbf{x}}_k - \overline{\mathbf{x}})', \\
\mathbb{W}_k &= \textstyle\sum_{i,i'=1}^{n_k} (\mathbf{x}_{ki} - \mathbf{x}_{ki'})(\mathbf{x}_{ki} - \mathbf{x}_{ki'})' \\
&= 2n_k \textstyle\sum_{i=1}^{n_k} (\mathbf{x}_{ki} - \overline{\mathbf{x}}_k)(\mathbf{x}_{ki} - \overline{\mathbf{x}}_k)',
\end{aligned}$$

which shows the following identity concerning matrices built with differences between observations and between means:

$$\mathbb{T} = \mathbb{B} + n \sum_{k=1}^{g} n_k^{-1} \mathbb{W}_k, \tag{5.7}$$

where $\mathbb{T}, \mathbb{B}$ and $\mathbb{W}_k$ are $p \times p$ matrices.

We can partition the variability in a similar way. The *geometric variability* of an $n \times n$ distance matrix $\mathbf{\Delta} = (\delta_{ii'})$, with related inner product matrix $\mathbf{G}$, is defined by

$$V_\delta = \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{i'=1}^{n} \delta_{ii'}^2 = \mathrm{tr}(\mathbf{G})/n,$$

where $\delta_{ii'}^2 = (\mathbf{x}_i - \mathbf{x}_{i'})'(\mathbf{x}_i - \mathbf{x}_{i'})$. V_δ is the sampling version of (5.3).

By taking traces in (5.7) we obtain

$$\mathrm{tr}(\mathbb{T}) = \mathrm{tr}(\mathbb{B}) + n \sum_{k=1}^{g} n_k^{-1} \mathrm{tr}(\mathbb{W}_k).$$

We write this identity as

$$V_\delta(\text{total}) = V_\delta(\text{between}) + n^{-1} \sum_{k=1}^{g} n_k V_\delta(\text{within } k). \tag{5.8}$$

5.5.2 Tests with principal coordinates

The above identities (5.7) and (5.8) can be used for comparing populations. Given g independent data sets $\mathcal{D}_1, \ldots, \mathcal{D}_g$, we may obtain the super-distance matrix $\mathbf{\Delta}$ and the principal coordinates $\mathbf{X}_1, \ldots, \mathbf{X}_g$. Then we can obtain $\mathbb{B}$ and $\mathbb{T}$ and compute two statistics for testing H_0:

a) $\gamma_1 = \det(\mathbb{T} - \mathbb{B}) / \det(\mathbb{T})$,

b) $\gamma_2 = V_\delta(\text{between}) / V_\delta(\text{total})$.

Both statistics lie between 0 and 1. Small values of γ_1 and large values of γ_2, respectively, give evidence to the alternative hypothesis. Note that $\gamma_2 = \mathrm{tr}(\mathbb{B})/\mathrm{tr}(\mathbb{T})$ is

a statistic based on quadratic entropy, and it is used in ANOQE (analysis of quadratic entropy), a generalization of ANOVA (analysis of variance) proposed by C. R. Rao in several papers. Also note that the distribution of γ_1 is Wilks if the populations are multivariate normal with the same covariance matrix and we choose the ordinary Euclidean distance between observations.

Except for multinormal data and a few other distributions, the sample distribution of γ_1 and γ_2 is unknown. The asymptotic distribution involves sequences of nuisance parameters, which were found for very specific distances and distributions (see Cuadras and Fortiana (1995); Cuadras and Lahlou (2000); Cuadras et al. (2006)). Liu and Rao (1995) derives the bootstrap distribution of V_δ(between). Indeed, the use of resampling methods, as described in Flury (1997), may overcome this difficulty.

5.5.3 Tests with proximity functions

Another test, which avoids resampling procedures, can be derived by using proximity functions and non-parametric statistics. First note that, with quantitative data and Mahalanobis distances, the proximity functions are

$$\phi^2_\delta(\mathbf{x},\Pi_k) = (\mathbf{x}-\mu_k)'\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\mu_k), \quad k=1,\ldots,g.$$

These functions are equal under $H_0 : \mu_1 = \cdots = \mu_g$.

Suppose in general that $\mathbf{x}_{11},\ldots,\mathbf{x}_{1n_1}$ represent the n_1 observations coming from Π_1 and ω is a new individual with coordinates $\mathbf{x}$. The sampling counterpart of the proximity function (5.4) is

$$\widehat{\phi}^2_1(\mathbf{x}) = \frac{1}{n_1}\sum_{i=1}^{n_1}\delta^2(\mathbf{x},\mathbf{x}_{1i}) - V_\delta(\text{within } 1),$$

where $\delta(\omega,\omega_{1i}) = \delta(\mathbf{x},\mathbf{x}_{1i})$. Note that we *do not need* to find the $\mathbf{x}$'s vectors.

We similarly obtain $\widehat{\phi}^2_2(\mathbf{x})$, etc. However, under H_0 all the population proximity functions are the same, see (5.5). Thus, we may work with the full proximity function

$$\widehat{\phi}^2(\mathbf{x}) = \frac{1}{n}\sum_{k=1}^{g}\sum_{i=1}^{n_k}\delta^2(\mathbf{x},\mathbf{x}_{ki}) - V_\delta(\text{total}).$$

If $a_{ki} = \widehat{\phi}^2(\mathbf{x}_{ki}) = ||\mathbf{x}_{ki}-\overline{\mathbf{x}}||^2$, where $\mathbf{x}_{ki}$ comes from Π_k, we obtain the proximity values (computed using only distances) for each population:

$$\Pi_1 : a_{11},\ldots,a_{1n_1};\ \cdots\ ;\ \Pi_g : a_{g1},\ldots,a_{gn_g}.$$

Under H_0 the a_{ki} follows (approximately) the same distribution. Then a Kruskal-Wallis test can be performed to accept or reject H_0. This test is based on

$$H = \left(\frac{12}{n(n+1)}\right)\sum_{k=1}^{g}\frac{R_k^2}{n_k} - 3(n+1),$$

where the n values a_{ki} are arranged and R_k is the sum of the ranks for the values in Π_k. This statistic H is asymptotically chi-square with $g-1$ d.f.

Note that this test may not work for equidistant populations, e.g., for $g = 3$ populations with vectors of means forming an equilateral triangle, as the vertices are equidistant to the center. In particular, for $g = 2$ the present test based on H is not an efficient one. In this case one can invoke the procedure in Cuadras and Fortiana (2004), which is based on Mann-Whitney-Wilcoxon comparisons of proximity values.

5.5.4 Multivariate dispersion

We have compared means rather than dispersions. For distance-based tests comparing multivariate dispersions with two samples, see Cuadras and Fortiana (2004), who studied the significance of the ratios $V_\delta(\mathbf{X})/V_\delta(\mathbf{Y})$ of geometric variabilities. Anderson (2006) approached the multi-sample case by performing an extension of Levene's test on Euclidean distances or general dissimilarities.

5.5.5 Examples of multi-sample tests

We consider three real data sets covering the quantitative, mixed and nominal cases. The first data set is the well-known Fisher Iris data with $p = 4$ quantitative variables, $g = 3$ species and $n_k = 50$. We use the city-block distance. The student mixed data is taken from Mardia et al. (1979), p. 294. We only consider $g = 3$ groups with $n_1 = 25$, $n_2 = 117, n_3 = 26$. There is a quantitative variable and a qualitative variable and we use the distance $\delta_{ij} = \sqrt{1 - s_{ij}}$, where s_{ij} is Gower's similarity coefficient for mixed variables (Gower and Legendre, 1986). The DNA data, used in (Cuadras et al., 1997b), consists of sequences of length 360 base pairs taken from a segment of mitochondrial DNA for a set of 120 individuals belonging to $g = 4$ human groups, with $n_1 = 25, n_2 = 41, n_3 = 37, n_4 = 17$ individuals. Since the data are large strings of ACGT, the standard methods fail miserably, whereas the DB approach provides a solution. Table 5.2 describes data and distances used.

We obtain the randomization distribution of γ_1 and γ_2 for $N' = 10000$ partitions into subsets of sizes $n_1, \ldots, n_g$ and estimate the P-values. In contrast, note that the statistic H can be obtained without resampling.

Table 5.3 reports the results obtained. There are significant differences among Iris species, Student groups and DNA groups. It is worth noting that using the Euclidean distance for Iris data would give $\gamma_1 = 0.0234$, which under normality and H_0 is distributed as Wilks $\Lambda(4, 147, 2)$.

Finally, we test the performance of this method by comparing three artificial populations. Suppose the bivariate normal populations $N_2(c\mathbf{1}, \mathbf{\Sigma})$, $N_2(2c\mathbf{1}, \mathbf{\Sigma})$, $N_2(3c\mathbf{1}, \mathbf{\Sigma})$. We simulate samples of sizes $n_1 = n_2 = n_3$ for $c = 0$ and $c = 1$, respectively. We then choose the Euclidean distance, compute the Wilks statistic, the exact and the empirical P-values after $N = 10000$ permutations. The results, summarized in table 5.4, show that the conclusions (to accept H_0 for $c = 0$, to reject H_0 for $c = 1$) at level of significance $\alpha = 0.05$ are the same.

We conclude that this distance-based approach may provide multi-sample tests when the traditional test based on multinormality is inappropriate (quantitative non-multinormal data) or impossible (nominal data, mixed data, more variables than observations).

Table 5.2. Features and sizes of data sets used to illustrate three distance-based multisample tests

Data	Type	Groups	Sizes	Distance
Iris	Quantitative	3	$50 + 50 + 50 = 150$	City-block
Students	Mixed	3	$25 + 117 + 26 = 168$	Gower
DNA	Nominal	4	$25 + 41 + 37 + 17 = 120$	Matching

Table 5.3. Some results of three distance-based multisample tests on real data

Data	γ_1	$P-$value	γ_2	$P-$value	H	d.f.	$P-$value
Iris	0.0000	0.000	0.6287	0.000	95.237	2	0.000
Students	0.5788	0.008	0.0424	0.003	7.820	2	0.020
DNA	0.0071	0.000	0.7800	0.000	27.49	3	0.000

Table 5.4. Distance-based comparison of three (simulated) bivariate normal populations using the Euclidean distance

$c = 0$				$c = 1$			
		Exact	Empirical			Exact	Empirical
Size	Wilks	P-value	P-value	Size	Wilks	P-value	P-value
3	0.3364	0.203	0.221	3	0.2243	0.086	0.078
5	0.7609	0.538	0.527	5	0.1835	0.001	0.001
10	0.8735	0.465	0.470	10	0.4608	0.000	0.000

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Part II

Probability and Statistics

6

Empirical Bayes Assessment of the Hyperparameters in Bayesian Factor Analysis

S. James Press[1], Key-Il Shin[2], and Lee Sang Eun[3]

[1] Department of Statistics, University of California, Riverside
[2] Department of Statistics, Hankuk University of Foreign Studies, Korea
[3] Associate Professor, Department of Statistics, Kyonggi University, Korea

Abstract: Bayesian Factor Analysis was introduced by Press and Shigemasu (1989) (PS). For Bayesian analysis, the prior distribution permits the analyst to identify the model by bringing prior information about the model to bear. In PS, it was assumed that the parameters of the prior distribution, the hyperparameters, were known, or would be readily assessable from a preliminary principal components analysis. In this study, we provide an empirical Bayes (EB) way of assessing the hyperparameters from the current data, and we show, using the AIC and BIC criteria, that it improves upon the suggested assessment method of the PS model.

Keywords and phrases: Empirical Bayes, hyperparameters, Bayesian Factor Analysis, AIC criterion, BIC criterion

6.1 Introduction

The Bayesian Factor Analysis model (BFA) was introduced by Press and Shigemasu (1989) (PS) to provide a Bayesian model for explaining underlying relationships among a set of variables in terms of a few linear subsets. It had the advantages over classical factor analysis models of having a unique solution, and of permitting the analyst to bring prior information to bear on the solution in a constructive and flexible way. As in all Bayesian inference approaches for the Bayesian paradigm to work it is necessary to pre-specify complete prior distributions for the unknown parameters of the model. PS suggested that to implement their approach it might be useful to carry out a preliminary principal components analysis on the (same) data, to achieve preliminary ideas of what numerical values might be likely and appropriate for completely specifying the prior distributions of some of the unknown model parameters for beginning the BFA modeling. Ad hoc procedures for determining preliminary likely numerical values for the remaining model parameter prior distributions were invoked as well. Since the prior distributions that resulted from this approach were determined from the same data set, the approach was called "empirical Bayesian," rather than strictly Bayesian. That empirical Bayesian approach was illustrated in an example in PS.

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Hyashi (1997) adopted a frequentist approach to assessing numerical values for the parameters of the BFA model. Shera (2000), and Shera and Ibrahim (1998) proposed elicitation methods for implementing the required values for the model parameters. Lee (1994), and Lee and Press (1998) studied the robustness of the BFA model to variations in the model parameters. Rowe (1998) extended the BFA model to correlated data vectors.

In this paper we introduce a new empirical Bayesian approach to assessing the BFA model parameters for situations in which not much is known, a priori, about them. Of course for more informative situations in which more information is available about the BFA model parameters, perhaps from previous studies, or from theory, that additional information should be used to structure the prior distributions (see, e.g., Press (2003), Chapter 15; or Press (2005)).

The format of the paper is as follows. The original PS–BFA model is reviewed, in outline form, in Section 6.2. The procedures currently being proposed for numerically assessing the likely values of the parameters of the prior distributions of the BFA model are presented in Section 6.3. In Section 6.4 we show how to estimate the parameters of the BFA model in terms of the parameters of the prior distributions assessed in Section 6.3. Section 6.5 provides a numerical example (suggested originally in PS). In Section 6.5, for the case in which not much is known a priori about the model parameters, there is a comparison of two methods for assessing likely numerical values for the parameters of the model: (a) the method suggested in PS; and (b) the currently proposed empirical Bayes (EB) method. The paper culminates in Section 6.6 with a comparison of methods and a summary.

6.2 The BFA Model

In this section, to make this paper self-contained, we outline the basic model of BFA. Define the p-variate observation vectors $(x_1, \cdots, x_n) \equiv X'$ on N objects. The means are assumed to have been subtracted out, so that $E(X) = 0$. The BFA model is:

$$x_{j\,(p\times 1)} = \Lambda_{(p\times m)} f_{j\,(m\times 1)} + \epsilon_{j\,(p\times 1)}, j = 1, \ldots, N, m < p$$

where Λ denotes a matrix of constants called the factor loading matrix; f_j denotes the factor score vector for subject j, $F' \equiv (f_1, \ldots, f_N)$; $\epsilon_j' s$ are assumed to be mutually uncorrelated and normally distributed as $N(0, \Psi)$, independent of F, for Ψ, a symmetric positive definite matrix, i.e, $\Psi > 0$.

Note that Ψ is not assumed to be diagonal, as it would be in classical factor analysis, although $E(\Psi)$ will be taken to be diagonal. That is, while Ψ is not assumed to be diagonal, it is taken to be diagonal on the average. So we can write the probability law of x_j as:

$$L(x_j|\Lambda, f_j, \Psi) = N(\Lambda f_j, \Psi)$$

where $L()$ denotes probability law. Now combine results for all observations and adopt an independent prior for all of the factor score vectors, F. We adopt the generalized natural conjugate family of prior distributions for $\Lambda, \Psi, F)$ and take the joint pdf

$$p(\Lambda, F, \Psi) = p_1(\Lambda|\Psi)p_2(\Psi)p_3(F),$$

where:

$$p_1(\Lambda|\Psi) \propto |\Psi|^{-m/2} exp\{(-1/2)tr(\Lambda - \Lambda_0)H(\Lambda - \Lambda_0)'\Psi^{-1}\}, \tag{6.1}$$

and

$$p_2(\Psi) \propto |\Psi|^{-\nu/2} exp\{(-1/2)tr\Psi^{-1}B\}, \tag{6.2}$$

with B a diagonal matrix and $H > 0$, a positive definite matrix. Thus, we assume that Ψ^{-1} follows a Wishart distribution and (ν, B) are hyperparameters to be assessed. Moreover, we assume that $(\Lambda|\Psi)$ is normally distributed, a priori, and (Λ_0, H) are hyperparameters to be assessed. Thus, the hyperparameters of the BFA problem are, so far: (Λ_0, H, ν, B).

6.3 Assessing the Hyperparameters

In this section we make a distinction between "estimation of parameters" of the basic BFA model, and assessment of hyperparameters, that is, determining likely values for the parameters of the prior distributions.

We note that $E(\Psi) = (\nu - 2p - 2)^{-1}B, \quad \nu > 2p + 2$. Now we need to assess the hyperparameters (Λ_0, H, ν, B).

6.3.1 Assessment of Λ_0

We define the $p \times p$ covariance matrix, $\Sigma > 0$:

$$\Sigma = Var(x_j|\Lambda, \Psi) = Var(\Lambda f_j|\Lambda, \Psi) + \Psi$$

where Λ and f_j are assumed to be independent of ϵ, and $\epsilon \sim N(0, \Psi), \Psi > 0$.

We have independent data vectors, $(x_1, \cdots, x_N), x_j : (p \times 1), j = 1, ..., N$.

An estimate of Σ by sample covariance matrix is $N^{-1}\sum_{j=1}^{N} x_j x_j'$. Also, we assume, without loss of generality, that f_j is distributed $N(0, I)$.

Then since:

$$Var(\Lambda f_j|\Lambda, \Psi) = \Lambda[Var(f_j|\Lambda, \Psi)]\Lambda' = \Lambda\Lambda',$$

we have

$$\Sigma = \Lambda\Lambda' + \Psi, \Psi > 0. \tag{6.3}$$

Since Σ is positive and symmetric we can write it as:

$$\Sigma = \Gamma D_\theta \Gamma',$$

where Γ denotes an orthogonal matrix of latent vectors of Σ, so that $\Gamma\Gamma' = I$, $D_\theta = diag(\theta_1, ...\theta_p)$, and the $\theta_j' s$ are the (positive) latent roots of $\Sigma, \theta_1 \geq \theta_2 \geq ... \geq \theta_p > 0$.

Now drop the smallest latent roots and the latent vectors corresponding to them and leave only the m(=number of factors in BFA)largest latent roots and the m latent vectors corresponding to them. Next define the diagonal matrices:

$$\bar{D}_{(m\times m)} = diag(\theta_1, ..., \theta_m), \underline{\mathrm{D}} = diag(\theta_{m+1}, ..., \theta_p).$$

Now if we define $\Lambda_{0(p\times m)} = \bar{\Gamma}_{p\times m}\bar{D}^{1/2}$, where $\bar{\Gamma}_{p\times m}$ denotes the column orthogonal matrix of latent vectors corresponding to the m largest latent roots, we can say approximately that:

$$\Sigma \approx \Lambda_0\Lambda_0'$$

Since Σ has been estimated from the data, we can assess $\Lambda_0 = \bar{\Gamma}_{p\times m}\bar{D}^{1/2}$ from the data as well.

We now assume that Λ_0 has been assessed.

6.3.2 Assessment of minimal ν

If we assume that little is known about ν, we can take it to be its minimum possible value, in order for the prior mean of Ψ to exist. Since $(E(\Psi) = (\nu - 2p - 2)^{-1}B$, we must have $\nu > 2p + 2$. So assess ν to be: $\nu^* \approx 2p + 3$.

6.3.3 Assessment of B

Since $E(\Psi) = \frac{B}{\nu-2p-2}$, $\nu > 2p+2$ and B is diagonal, we have $E(\Psi) = B/(\nu-2p-2) = B$ with $\nu = 2p + 3$. Therefore in order to assess the B, we need to have an approximation of $E(\Psi)$.

Now from the equation (3), we have

$$\Sigma = \Lambda\Lambda' + \Psi, \Psi > 0.$$

By taking $\Psi \approx \Psi^* = \Sigma - \Lambda_0\Lambda_0'$, we have as an approximation, $E(\Psi) \approx E(\Psi^*) \approx \Psi^*$. So that Ψ^* can be used as $E(\Psi)$.

Now let $\Psi^* = (\Psi^*_{ij})$ and $B = (b_{ij})$. Hence we can assess $b_{ii} = \Psi^*_{ii}$ and $b_{ii} = 0$ for $i \neq j$.

6.3.4 Assessment of H

Now we need to assess the scale matrix, H. Let $\lambda = Vec(\Lambda) = (\lambda_1', ..., \lambda_m')'$. Then the prior distribution for $(\lambda|\Psi)$ is $\mathrm{N}(\lambda_0, H^{-1} \otimes \Psi)$. Since $Var(\lambda|\Psi) = H^{-1} \otimes \Psi$ we have $Var(\lambda) = H^{-1} \otimes E(\Psi)$, and $Cov[(\lambda_i, \lambda_j)|\Psi] = H^{-1}_{ij}\Psi$. Therefore we have:

$$Cov[(\Psi^{-1/2}\lambda_i, \Psi^{-1/2}\lambda_j)|\Psi] = Cov(\Psi^{-1/2}\lambda_i, \Psi^{-1/2}\lambda_j) = H^{-1}_{ij}I_p. \tag{6.4}$$

Let $\Delta = (\Psi^{-1/2}\Lambda)' = (\delta_{1(m\times 1)}, \cdots, \delta_{p(m\times 1)})$. Then from the equation(4) we can see that δ_i are independent. Therefore we have $Cov[(\delta_i, \delta_j)|\Psi] = Cov[\delta_i, \delta_j] = 0$ for $i \neq j$ and $Cov[(\delta_i, \delta_i)|\Psi] = Cov[\delta_i, \delta_i] = H^{-1}, i = 1, \cdots, p$.

Since we can assume $\Lambda_0 \approx \Lambda$ from Section 6.3.1 and Ψ^* is defined in Section 6.3.3, $Cov[\delta_i, \delta_i]$ can be evaluated as $Cov[\delta_i^*, \delta_i^*]$ where $\Delta^* = (\Psi^{*-1/2}\Lambda_0)' = (\delta_1{}^*, \cdots, \delta_p{}^*)$.

Then we can assess $H^{-1} = Var(\delta_i) \approx p^{-1}\sum_{i=1}^p(\delta_i^* - \bar{\delta}^*)(\delta_i^* - \bar{\delta}^*)'$ where $\bar{\delta}^* = p^{-1}\sum_{i=1}^p \delta_i^*$. Now we have assessed the H.

6.3.5 Iterative computation of the hyperparameters

Up to this point we proposed a new way of assessing the hyperparameters : (Λ_0, ν, B, H). Based on the theory of Section 6.3.4, the steps of the simulation algorithm for assessment of Λ_0, ν, B, H from the data are as follows:

Step 1: Variance-covariance matrix, Σ, is evaluated from the data and we get the initial values of Λ_0 from Σ and call it as $\Lambda_0^{(1)}$. Also, we denote the covariance matrix Σ of the original data by $\Sigma^{(1)}$ and finally we have $\Psi^{(1)} = \Sigma^{(1)} - \Lambda_0^{(1)}\Lambda_0^{(1)'}$ as the initial values of Ψ.

Step 2: Define $\Psi^{(2)} = diag(\Psi^{(1)})$ and calculate $\Sigma^{(2)} = \Sigma^{(1)} - \Psi^{(2)}$. From $\Sigma^{(2)}$ we can get $\Lambda_0^{(2)}$: $\Sigma^{(2)} = \Lambda_0^{(2)}\Lambda_0^{(2)'}$.

Step 3: Calculate the differences of $\Lambda_0^{(1)}$ and $\Lambda_0^{(2)}$ and also $\Psi^{(1)}$ and $\Psi^{(2)}$: call them as $dif_\lambda = \Lambda_0^{(1)} - \Lambda_0^{(2)}$ and $dif_\Psi = \Psi^{(1)} - \Psi^{(2)}$. And calculate the $dif_\lambda^2 = dif_\lambda dif_\lambda'$ and $dif_\Psi^2 = dif_\Psi dif_\Psi'$ and in order to see the convergence of the matrix, the determinant or trace of dif_λ^2 and dif_Ψ^2 are evaluated.

Step 4: Repeat steps 1 through 3 until the determinant or trace of dif_λ^2 and dif_Ψ^2 are small enough to be convergent. Then take $\Lambda_0^{(i)}$ and $\Psi^{(i)}$ as the converged values.

Step 5: At this point if we do have the convergent values, then take $\Lambda_0^{(i)}$ as the assessed values of hyperparameter, Λ_0 and for $\Psi^{(i)}$, since $\Psi > 0$, we only take the positive diagonal elements in matrix $\Psi^{(i)}$, which means if $\Psi_{ii}^{(i)} < 0$ then replace them to the '0's' and call it as Ψ^*.

Step 6: After assessing the hyperparameter, Λ_0, we can get the convergent value of Ψ^* and then B and H can be assessed.

For assessing the B, we take the diagonal elements of Ψ^* and make the diagonal matrix. For H, calculate the variance-covariance matrix of $\Delta^* = (\Psi^{*-1/2}\Lambda_0)'$.

Now we have assessed all four hyperparameters.

6.4 Bayesian Estimation of Λ, F, Ψ

After assessing the hyperparameters, Bayesian estimators of factor analysis are obtained.

From the basic model in Section 6.2, combining the likelihood $L(x_j|\Lambda, f_j, \Psi) = N(\Lambda f_j, \Psi)$, and priors distribution $p(\Lambda, F, \Psi) = p_1(\Lambda|\Psi)p_2(\Psi)p_3(F)$, using Bayes' theorem, the joint posterior density of the parameters becomes

$$p(\Lambda, F, \Psi|X) \propto p_3(F)|\Psi|^{(N+m+\nu)/2} exp[(-1/2)tr(\Psi^{-1}G)] \tag{6.5}$$

where $G = (X - F\Lambda')'(X - F\Lambda') + (\Lambda - \Lambda_0)H(\Lambda - \Lambda_0)' + B$.

Now integrating the equation(5) with respect to Ψ using Inverted Wishart density, gives the marginal posterior density of (Λ, F):

$$p(\Lambda, F|X) \propto \frac{p_3(F)}{|R_F + (\Lambda - \Lambda_F)Q_F(\Lambda - \Lambda_F)'|^{\gamma/2}} \tag{6.6}$$

where

$$\begin{aligned} Q_F &= H + F'F \\ R_F &= X'X + B + \Lambda_0 H \Lambda_0' - (X'F + \Lambda_0 H) Q_F^{-1} (X'F + \Lambda_0 H)' \\ \Lambda_F &= (X'F + \Lambda_0 H)(H + F'F)^{-1} \\ \gamma &= N + m + \nu - p - 1. \end{aligned}$$

Integrating the Eqn. (6) with respect to Λ using the normalizing constant of the matrix T-distribution gives the marginal posterior density of F:

$$p(F|X) \propto \frac{p_3(F)|H + F'F|^{(\gamma - m - p)/2}}{|A + (F - \hat{F})'(I_N - XW^{-1}X')(F - F')|^{\gamma - m)/2}} \tag{6.7}$$

where

$$\begin{aligned} \hat{F} &= (I_N - XW^{-1}X')^{-1} XW^{-1} \Lambda_0 H \\ W &= X'X + B + \Lambda_0 H \Lambda_0' \\ A &= H - H\Lambda_0' H^{-1} \Lambda_0 H - (H' \Lambda_0' W^{-1} X')(I_N - XW^{-1}X')(XW^{-1}\Lambda_0 H). \end{aligned}$$

Now consider the case in which very little is known a priori about F. As an approximation we take:

$$p_3(F) \propto K = constant. \tag{6.8}$$

Note that if there is substantive prior information about F available, it should be incorporated at this point as an informative prior distribution. Because $F'F = \sum_1^N f_j f_j'$, by the law of large numbers, for large N, $|H + F'F|$ in Eqn. (7) behaves increasingly as if it were a constant, so that because the numerator of Eqn. (7) becomes approximately constant, $p(F|X)$ follows approximately a matrix T distribution. Since $p(F|X)$ is approximately a matrix T-distribution, in large samples, the estimator of factor score matrix, $\hat{F}$, is:

$$\hat{F} = (I_N - XW^{-1}X')^{-1} XW^{-1} \Lambda_0 H.$$

Now using the marginal posterior distribution of (Λ, F), and F, the conditional distribution of $(\Lambda|F)$ becomes the matrix T distribution. So the estimator of Λ, $\hat{\Lambda} = E(\Lambda|\hat{F}, X)$(see Eqns. (7) and (8)) is :

$$\hat{\Lambda} = \Lambda_F = (X'\hat{F} + \Lambda_0 H)(H + \hat{F}'\hat{F})^{-1}$$

Lastly, for estimator of the disturbance covariance, $\hat{\Psi}$, using the joint posterior of (Λ, F, Ψ) and the marginal posterior of (Λ, F), the conditional density of $(\Psi|\Lambda, F, X)$ is obtained as the kernel of the Inverted Wishart distribution:

$$p(\Psi|\hat{\Lambda}, \hat{F}, X) \propto \frac{exp[(-1/2) tr \Psi^{-1} \hat{G}]}{|\Psi|^{(N + mp + \nu)/2}},$$

where $\hat{G} = [(X - \hat{F}\hat{\Lambda}')'(X - \hat{F}\hat{\Lambda}') + (\hat{\Lambda} - \Lambda_0)H(\hat{\Lambda} - \Lambda_0)' + B]$.

Therefore, using the property of Inverted Wishart distribution, $\hat{\Psi}$ is:

$$\hat{\Psi} = \frac{\hat{G}}{(N + mp + \nu + 2p - 2)}.$$

6.5 Example

There are 48 applicants for a certain job, and they have been scored on 15 variables regarding their acceptability. They are shown in table 6.1.

The correlation matrix for the 15 variables is given in (6.9). We assume the sample size of 48 is large enough to estimate the mean well enough for it to be ignored after subtracting it out. So we have data with p, the number of variables, equal to 15, and sample size, N is 48 and hyperparameter ν becomes 33.

$$\begin{pmatrix}
1 & 0.24 & 0.04 & 0.31 & 0.11 & 0.23 & -0.09 & 0.27 & 0.55 & 0.38 & 0.29 & 0.39 & 0.37 & 0.47 & 0.59 \\
0.24 & 1 & 0.12 & 0.38 & 0.42 & 0.38 & 0.33 & 0.48 & 0.14 & 0.32 & 0.55 & 0.48 & 0.51 & 0.29 & 0.38 \\
0.04 & 0.12 & 1 & 0.00 & 0.01 & 0.08 & -0.02 & 0.05 & 0.27 & 0.10 & 0.04 & 0.21 & 0.29 & -0.32 & 0.14 \\
0.31 & 0.38 & 0.00 & 1 & 0.29 & 0.49 & 0.64 & 0.35 & 0.14 & 0.37 & 0.35 & 0.47 & 0.61 & 0.68 & 0.33 \\
0.11 & 0.42 & 0.01 & 0.29 & 1 & 0.80 & 0.37 & 0.82 & 0.03 & 0.69 & 0.84 & 0.70 & 0.67 & 0.47 & 0.27 \\
0.23 & 0.38 & 0.08 & 0.49 & 0.80 & 1 & 0.35 & 0.82 & 0.16 & 0.69 & 0.76 & 0.88 & 0.78 & 0.53 & 0.42 \\
-0.09 & 0.33 & -0.02 & 0.64 & 0.37 & 0.35 & 1 & 0.22 & -0.13 & 0.23 & 0.19 & 0.32 & 0.40 & 0.43 & 0.02 \\
0.27 & 0.48 & 0.09 & 0.35 & 0.82 & 0.82 & 0.22 & 1 & 0.24 & 0.81 & 0.85 & 0.77 & 0.74 & 0.55 & 0.55 \\
0.55 & 0.14 & 0.27 & 0.14 & 0.03 & 0.16 & -0.13 & 0.24 & 1 & 0.37 & 0.20 & 0.36 & 0.36 & 0.22 & 0.69 \\
0.38 & 0.32 & 0.10 & 0.37 & 0.69 & 0.69 & 0.23 & 0.81 & 0.37 & 1 & 0.77 & 0.70 & 0.78 & 0.60 & 0.65 \\
0.29 & 0.55 & 0.04 & 0.35 & 0.84 & 0.76 & 0.19 & 0.85 & 0.20 & 0.77 & 1 & 0.77 & 0.77 & 0.55 & 0.44 \\
0.38 & 0.48 & 0.21 & 0.47 & 0.70 & 0.88 & 0.32 & 0.77 & 0.36 & 0.70 & 0.77 & 1 & 0.87 & 0.53 & 0.58 \\
0.37 & 0.51 & 0.29 & 0.61 & 0.69 & 0.78 & 0.40 & 0.74 & 0.36 & 0.78 & 0.77 & 0.87 & 1 & 0.55 & 0.58 \\
0.47 & 0.29 & -0.32 & 0.68 & 0.47 & 0.53 & 0.43 & 0.55 & 0.22 & 0.60 & 0.55 & 0.53 & 0.55 & 1 & 0.40 \\
0.59 & 0.38 & 0.14 & 0.33 & 0.27 & 0.42 & 0.02 & 0.55 & 0.65 & 0.69 & 0.44 & 0.58 & 0.58 & 0.40 & 1
\end{pmatrix} \tag{6.9}$$

Now we postulate a model with 4 factors. This choice was based on a principal components analysis in PS. (It could also be based upon Press and Shigemasu, 1999, which depends upon maximizing the posterior probability for the number of factors. For other related considerations, see Press (2003), Section 15.4. For assessing the hyperparameters, Λ_0, B, H, we calculate dif_λ^2 defined in step 3 and we use 10^{-5} for the convergence criterion. Based on the theory developed in Section 6.3, we construct the prior factor loading matrix, Λ_0, as:

Table 6.1. Names of variables

(1)	Form of letter application	(9)	Experience
(2)	Appearance	(10)	Drive
(3)	Academic ability	(11)	Ambition
(4)	Likeability	(12)	Grasp
(5)	Self-Confidence	(13)	Potential
(6)	Lucidity	(14)	Keenness to join
(7)	Honesty	(15)	Suitability
(8)	Salesmanship		

$$\Lambda_0 = \begin{pmatrix} 1.2156598 & 1.368708 & 0.4871069 & -0.426764 \\ 1.0354062 & -0.119182 & 0.0970379 & 0.2503054 \\ 0.2435675 & 0.4451025 & -0.415397 & 1.2921365 \\ 1.6258524 & -0.384803 & 1.9589576 & 0.4214353 \\ 1.8354735 & -1.008388 & -0.615048 & -0.187176 \\ 2.6963778 & -0.838522 & -0.308678 & 0.2103994 \\ 0.845824 & -1.023012 & 1.1766185 & 0.5283349 \\ 3.0477339 & -0.495849 & -0.860623 & -0.457604 \\ 1.3548248 & 2.4374048 & 0.0292391 & 0.1732282 \\ 2.4643022 & 0.1602599 & -0.351122 & -0.330044 \\ 2.5364329 & -0.5565 & -0.694222 & -0.342439 \\ 2.652991 & -0.098857 & -0.199276 & 0.5173438 \\ 2.9141746 & -0.096444 & 0.1490095 & 0.8369568 \\ 1.8579476 & -0.199453 & 1.317401 & -1.176095 \\ 2.2337726 & 1.8324691 & 0.0205074 & -0.087512 \end{pmatrix} \tag{6.10}$$

For assessing the H, we rearrange the elements of the converged matrix Ψ with following condition:

$$\Psi^* = \max[0, \psi_{ii}]$$

as suggested in Section 6.3.5.

This condition gives all the diagonal elements of Ψ^* nonnegative values. Then we have the assessed value of H as following:

$$H = \begin{pmatrix} 0.5067606 & 0.2322973 & 0.037914 & 0.6931582 \\ 0.2322973 & 0.1237675 & 0.0164664 & 0.3167849 \\ 0.037914 & 0.0164664 & 0.0181701 & 0.0329019 \\ 0.6931582 & 0.3167849 & 0.0329019 & 0.979064 \end{pmatrix}$$

Now we take the diagonal element from Ψ as the assessed values of B:

$$B = \text{diag}(\ 0.0,\ 0.0,\ 0.0108292,\ 0.0041514,\ 0.0,\ 0.0,\ 0.0,\ 0.0006516,\ 0.0201611,\ 0.000117,\ 0.0,\ 0.0,\ 0.0,\ 0.0,\ 0.0)$$

Using the above values, Bayesian estimators of factor loading matrix, $\hat{\Lambda}$, factor score matrix, $\hat{F}$, and disturbance covariance matrix, $\hat{\Psi}$ are evaluated.

$$\hat{\Lambda} = \begin{pmatrix} 1.2156905 & 1.3757201 & 0.4894049 & -0.416805 \\ 1.0353308 & -0.117702 & 0.0932766 & 0.2552337 \\ 0.1967339 & 0.2948986 & -0.446953 & 1.0743623 \\ 1.6011882 & -0.283249 & 1.564739 & 0.1383427 \\ 1.8360166 & -1.012591 & -0.615524 & -0.196882 \\ 2.696299 & -0.8396 & -0.311727 & 0.2094949 \\ 0.8454201 & -1.022951 & 1.1652667 & 0.53644 \\ 2.9551617 & -0.470779 & -0.616943 & -0.383953 \\ 1.2976032 & 1.8499437 & 0.0348762 & 0.0338488 \\ 2.4360767 & 0.1225104 & -0.159646 & -0.259586 \\ 2.5361934 & -0.556489 & -0.692031 & -0.349217 \\ 2.6528884 & -0.098004 & -0.204808 & 0.5186247 \\ 2.914977 & -0.095403 & 0.1408729 & 0.8450765 \\ 1.8637007 & -0.200152 & 1.3506358 & -1.19945 \\ 2.2369999 & 1.8537076 & 0.016734 & -0.074800 \end{pmatrix} \tag{6.11}$$

$$\hat{\Psi} = \begin{pmatrix}
2.44 & 0.19 & 0.14 & 0.07 & 0.31 & 0.21 & -0.13 & -0.27 & -0.06 & -0.40 & 0.22 & 0.17 & -0.03 & 0.17 & -0.88 \\
0.19 & 2.34 & -0.01 & 0.06 & 0.04 & -0.60 & 0.16 & 0.27 & -0.21 & -0.58 & 0.60 & -0.17 & -0.20 & -0.23 & 0.33 \\
0.14 & -0.01 & 1.97 & 0.17 & 0.02 & -0.16 & -0.14 & 0.10 & 0.63 & 0.23 & 0.08 & -0.07 & 0.13 & 0.03 & -0.19 \\
0.07 & 0.06 & 0.17 & 1.76 & -0.09 & 0.16 & -0.02 & -0.10 & -0.14 & -0.40 & 0.13 & -0.21 & 0.01 & -0.06 & 0.11 \\
0.31 & 0.04 & 0.02 & -0.09 & 0.33 & -0.21 & 0.38 & -0.05 & 0.11 & 0.06 & -0.21 & -0.18 & -0.08 & -0.03 & 0.14 \\
0.21 & -0.60 & -0.16 & 0.16 & -0.21 & 1.35 & -0.36 & 0.20 & -0.09 & -0.28 & -0.58 & 0.53 & -0.34 & -0.03 & 0.07 \\
-0.13 & 0.16 & -0.14 & -0.02 & 0.38 & -0.36 & 1.24 & 0.08 & 0.20 & 0.20 & -0.07 & -0.17 & -0.41 & -0.09 & 0.73 \\
-0.27 & 0.27 & 0.10 & -0.10 & -0.05 & 0.20 & 0.08 & 1.72 & -0.17 & 0.40 & -0.05 & -0.17 & -0.11 & -0.13 & 0.37 \\
-0.06 & -0.21 & 0.63 & -0.14 & 0.12 & -0.09 & 0.20 & -0.17 & 4.22 & -0.09 & -0.14 & 0.03 & -0.04 & 0.02 & 0.06 \\
-0.40 & -0.58 & 0.23 & -0.40 & 0.06 & -0.28 & 0.20 & 0.40 & -0.09 & 1.82 & 0.00 & -0.49 & 0.22 & -0.01 & 0.17 \\
0.22 & 0.60 & 0.08 & 0.13 & -0.21 & -0.58 & -0.07 & -0.05 & -0.14 & 0.00 & 0.86 & -0.13 & 0.24 & 0.08 & -0.34 \\
0.17 & -0.17 & -0.07 & -0.21 & -0.18 & 0.53 & -0.17 & -0.17 & 0.03 & -0.49 & -0.13 & 0.92 & -0.28 & 0.14 & -0.30 \\
-0.03 & -0.20 & 0.13 & 0.01 & -0.08 & -0.34 & -0.41 & -0.11 & -0.04 & 0.22 & 0.24 & -0.28 & 0.40 & 0.07 & -0.37 \\
0.17 & -0.23 & 0.03 & -0.06 & -0.03 & -0.03 & -0.09 & -0.13 & 0.02 & -0.01 & 0.08 & 0.14 & 0.07 & 0.09 & -0.25 \\
-0.88 & 0.33 & -0.19 & 0.11 & 0.14 & 0.07 & 0.73 & 0.37 & 0.06 & 0.17 & -0.34 & -0.30 & -0.37 & -0.25 & 1.03
\end{pmatrix} \tag{6.12}$$

$$\hat{F} = \begin{pmatrix}
0.5441119 & 0.6121569 & -0.986808 & -1.656711 \\
1.180791 & 0.1915586 & -0.199083 & -0.825082 \\
0.8565437 & 0.3306071 & -0.532051 & -1.484819 \\
-0.0074 & 0.1591623 & 0.7745533 & 0.9676632 \\
0.1633761 & 0.8873184 & 1.9044676 & 1.3122201 \\
0.1791155 & -0.155316 & 0.349929 & 0.4845764 \\
1.1382553 & 0.7975967 & -0.003819 & -0.459641 \\
1.3531862 & 0.5427265 & -0.021557 & -0.920193 \\
1.2465876 & 0.8386423 & 0.2274794 & -0.728583 \\
1.109129 & 0.3049835 & -2.658699 & 0.7621033 \\
0.6789187 & -0.267292 & -3.080943 & 0.8047847 \\
0.9233149 & -0.329226 & -1.829764 & 1.6162558 \\
-0.057269 & 0.7222003 & 1.4465467 & 0.6517656 \\
-0.077143 & 0.8046151 & 0.4349906 & 0.9132892 \\
-0.430252 & 0.2933901 & 1.1405053 & 1.7845993 \\
0.7391632 & 0.2710406 & 0.0197922 & 0.0320599 \\
0.4398294 & 0.4832092 & -0.700655 & -1.277928 \\
-0.294351 & -0.75315 & -0.934673 & -1.809066 \\
-0.2832 & -0.270987 & -1.151171 & -1.016825 \\
0.8940261 & -0.170256 & 0.706032 & -0.02676 \\
0.5532025 & -0.308019 & -0.11882 & 1.0152528 \\
1.1506597 & -0.1616 & 0.9177135 & -0.716883 \\
1.2600069 & -0.367189 & 1.0147419 & -0.528007 \\
1.094753 & -0.059829 & 1.6709679 & -0.132859 \\
-0.786572 & -0.224953 & 1.4536752 & 0.6537053 \\
-0.365028 & 0.7222023 & 0.514206 & 0.4977748 \\
0.0349953 & -1.471733 & -0.02288 & 1.0073119 \\
-1.665609 & -0.671037 & -0.131229 & -2.001258 \\
-1.824617 & 0.3396818 & -0.826088 & -2.884954 \\
-0.745062 & -1.503162 & 0.5527005 & -1.825148 \\
-0.446436 & -1.143044 & 0.8753072 & -1.461364 \\
-0.436669 & -1.48905 & 0.5516333 & 0.9144677 \\
-0.584531 & -1.722635 & 0.4429568 & 0.4194087 \\
-1.375633 & -0.302196 & 1.0135947 & -0.194345 \\
-1.514796 & 0.44609 & 1.4289122 & -0.087323 \\
-0.354099 & -0.299241 & 1.3206915 & 0.6385668 \\
-0.0962 & -1.867837 & -1.995435 & 0.0627968 \\
0.0768491 & -1.805829 & -1.539933 & -0.703392 \\
1.4847705 & 0.5994364 & 0.9189217 & -0.210801 \\
1.5543793 & 0.5475245 & 0.4757133 & -0.483608 \\
-1.449395 & 3.5870505 & -1.232841 & 0.1074385 \\
-1.473696 & 3.8333912 & -1.656083 & -0.041145 \\
-1.051058 & 1.6094415 & 0.357348 & 0.3107456 \\
0.6096896 & -0.559059 & -0.956751 & -0.0294 \\
0.0594285 & 0.1061082 & 0.4312686 & 2.1533067 \\
0.3210613 & -0.395968 & 0.3595921 & 2.6231925 \\
-2.160527 & -1.396556 & -0.309572 & 0.9049762 \\
-2.166602 & -1.334971 & -0.415383 & 0.8678303
\end{pmatrix} \tag{6.13}$$

6.6 Method Comparison and Summary

Bayesian Factor Analysis (BFA) was proposed originally to provide a means for introducing prior information into a factor analysis problem in a formal way, and because of the frequent occurrence of improper solutions in maximum likelihood factor analysis caused by over-parameterization of the model. However, carefully assessing prior information is always an issue. Therefore, in this paper, we proposed an empirical Bayes (EB) procedure for assessing the hyperparameters in BFA. Bayesian estimates of the factor loading matrix, Λ, factor score matrix, F, and the disturbance covariance matrix, Ψ, were calculated by using the EB method for assessing the hyperparameters proposed in Section 6.3. Below, we compare the advantages and disadvantages of the proposed empirical Bayes(EB) method with those of PS.

In the EB method, the Bayesian estimate of the factor loading matrix, $\hat{\Lambda}$, becomes pretty much the same as the hyperparameter, $\hat{\Lambda}_0$, because $\hat{\Lambda}|\Psi$ is assumed to have a normal distribution with mean Λ_0 . For the same reason, PS gives equivalent results, but in the PS case, instead of assessing Λ_0 from data, we take its value as known, so $\hat{\Lambda}$ is closer to Λ_0 than for $\hat{\Lambda}_{PS}$. These results are predictable because Bayesian estimates are represented by a weighted average of data and prior information. It is of course not surprising that Bayesian estimates depend on the information we include in the prior. That is, both estimates, $\hat{\Lambda}$ and $\hat{\Lambda}_{PS}$ are similar to the assessed hyperparameter, Λ_0.

We compared the two models for assessing the hyperparameters based upon how well the model fits the data. In order to compare the suggested models we calculate the AIC (Akaike Information Criterion) and the BIC (Bayesian Information Criterion) criteria.

- AIC = -2 log (maximized likelihood) + 2 (number of free, independent, parameters);
- BIC = -2 log (maximized marginal likelihood) + (log n)(number of free parameters, including hyperparameters).

We find the results shown in table 6.2: Thus, for either criterion, the EB approach yields the smaller value (better model fit to the data), and so is deemed superior. Of course our showing that EB results in better outcomes than PS for one example doesn't prove a point, but it is suggestive.

Table 6.2. Model fit criteria

	AIC Criterion	BIC Criterion
PS Model	1088.16	1573.54
EB Model	822.37	1567.51

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Part III

Order Statistics and Analysis

7

Negative Mixtures, Order Statistics, and Systems

Jorge Navarro[1] and Pedro J. Hernández[2]

[1] Department of Statistics and Operations Research, University of Murcia, Spain
[2] Department of Quantitative and Informatics Methods, Polytechnical University of Cartagena, Spain

Abstract: This paper shows the relationship between mixtures, order statistics and coherent systems with possibly dependent components. These relationships are used to obtain reliability properties of order statistics and systems. The results are illustrated through a series of examples.

Keywords and phrases: Mixtures, order statistics, coherent systems, k-out-of-n systems, hazard rate

7.1 Introduction

The mixtures are common models in statistics. In reliability the mixtures are used to represent populations with different kinds of units (e.g., units with or without manufacturing defects). Sometimes, these models lead to distributions with bathtub shaped hazard (failure) rate functions (see Navarro and Hernandez (2004) and Wondmagegnehu et al. (2005)).

The negative mixtures are mixtures with some negative weights. Some properties and characterizations for these kind of mixtures were given in Everitt and Hand (1981), Wu and Lee (1998, 1999), Wu (2001, 2002) and Navarro and Ruiz (2004). In practice, they arise in several situations. For example, they are used to define new families of distributions in Bartholomew (1969), Botta et al. (1987) and in Harris et al. (1992). Baggs and Nagaraja (1996) and Navarro and Shaked (2006) used them to represent the distributions of order statistics and coherent systems. They can also be used to obtain the distribution of the MLEs of exponential parameters under step-stress models (see Balakrishnan and Qihao Xie (2007a,b) and Balakrishnan et al. (2007)) or progressively censored order statistics (see Kamps and Cramer (2001) and Balakrishnan and Cramer (2006)).

The coherent systems are very important in reliability and survival theories (see, e.g., Barlow and Proschan (1975)). The series, the parallel and, in general, the k-out-of-n systems are particular cases of coherent systems. The lifetime of a k-out-of-n system can be represented by the $(n-k+1)$th order statistics $X_{n-k+1:n}$ associated with the

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lifetimes $X_1, X_2, \ldots, X_n$ of the components. In particular, the series and the parallel systems are represented by the extreme order statistics $X_{1:n}$ and $X_{n:n}$, respectively. Several properties of coherent systems have been obtained when the components are independent (see, e.g., Barlow and Proschan (1975), Lillo et al. (2001) and Boland and Samaniego (2004)). Also, when the components are dependent, some properties were obtained in Baggs and Nagaraja (1996), Navarro et al. (2005), Franco and Vivo (2006), Navarro and Shaked (2006) and Navarro and Rychlik (2007).

The purpose of this paper is to show the relationships between mixtures, order statistics and coherent systems and to use these relationships and known properties for mixtures to obtain new properties for order statistics and systems. The results are illustrated through a series of examples.

The paper is organized as follows. Section 7.2 shows the relationships between mixtures, order statistics and coherent systems. In Section 7.3 some properties for order statistics and coherent systems are obtained using known properties of mixtures. The results are illustrated in Section 6.4 using the well known bridge structure and different distributions for the components.

Throughout the paper, 'increasing' stands for 'non-decreasing' and 'decreasing' stands for 'non-increasing.'

7.2 Relationships between Mixtures and Systems

Let $(X_1, X_2, \ldots, X_n)$ be a random vector representing a random sample or the lifetimes of n (possibly dependent) components in a system. Then the corresponding order statistics $X_{1:n}, X_{2:n}, \ldots, X_{n:n}$ represent the lifetimes of k-out-of-n systems (i.e., systems which work when at least k components work). In particular, $X_{1:n} = \min(X_1, X_2, \ldots, X_n)$ and $X_{n:n} = \max(X_1, X_2, \ldots, X_n)$ represent the lifetimes of series and parallel systems, respectively.

In general, the lifetime T of a coherent system can be written as $T = \phi(X_1, X_2, \ldots, X_n)$ where ϕ is called the structure function (see Barlow and Proschan (1975), p. 12). The series, the parallel and, in general, the k-out-of-n systems are coherent systems. A set $P \subseteq \{1, 2, \ldots, n\}$ is a minimal path (cut) set of a coherent system (or a structure function ϕ) if the system works (fails) when all the components in P work (fail). A minimal path (cut) set is a minimal set of elements whose functioning (failure) insures the functioning (failure) of the system. For example, the minimal path sets of a k-out-of-n system are all the sets with k-elements. In particular, the minimal path (cut) sets of the parallel (series) system with n components are $\{1\}, \{2\}, \ldots, \{n\}$ and the unique minimal path (cut) set of the series (parallel) system with n components is $\{1, 2, \ldots, n\}$.

Barlow and Proschan (1975), p. 12, proved that the lifetime of a coherent system $T = \phi(X_1, X_2, \ldots, X_n)$ with minimal path sets $P_1, P_2, \ldots, P_m$ and minimal cut sets $C_1, C_2, \ldots, C_s$ can be written as

$$T = \max_{1 \le j \le m} \min_{i \in P_j} X_i = \min_{1 \le j \le s} \max_{i \in C_j} X_i. \tag{7.1}$$

If we represent the lifetime of the series system with components in the set P by $Y_P = \min_{i \in P} X_i$ and the lifetime of the parallel system with components in the set P

by $Z_P = \max_{i\in P} X_i$, then (7.1) can be written as

$$T = \max_{1\le j\le m} Y_{P_j} = \min_{1\le j\le s} Z_{C_j}. \tag{7.2}$$

Thus, using the inclusion-exclusion formula, the reliability (survival) function $R_T(t) = \Pr(T \ge t)$ of system T can be written as

$$R_T(t) = \Pr\left(\max_{1\le j\le m} Y_{P_j} \ge t\right) = \Pr\left(\bigcup_{1\le j\le m}(Y_{P_j} \ge t)\right)$$
$$= \sum_{j=1}^{m} \Pr\left(Y_{P_j} \ge t\right) - \sum_{i<j} \Pr(Y_{P_j\cup P_i} \ge t) + \ldots + (-1)^{m+1} \Pr(Y_{P_1\cup P_2\cup\ldots\cup P_m} \ge t).$$

Hence it is a negative mixture (i.e., a mixture with some negative weights) of the reliability functions of series systems with components in the union of its minimal path sets. Note that the unions of the minimal path sets are path sets. This representation can be traced to Agrawal and Barlow (1984) (see also Navarro and Shaked (2006) or Navarro et al. (2007)). For example, if $n = 2$ the reliability function $R_{2:2}$ of the two-components parallel system can be written as

$$R_{2:2}(t) = R_1(t) + R_2(t) - R_{1:2}(t)$$

where R_1 and R_2 are the reliability functions of the components (i.e., series systems with one component) and $R_{1:2}$ is the reliability function of the two-components series system. This relationship was used in Baggs and Nagaraja (1996) and Franco and Vivo (2006) to obtain properties for the parallel system based on properties of series systems and negative mixtures.

Analogously, the distribution function $F_T(t) = \Pr(T \le t)$ of system T can be written as

$$F_T(t) = \Pr\left(\min_{1\le j\le s} Z_{C_j} \le t\right) = \Pr\left(\bigcup_{1\le j\le s}(Z_{C_j} \le t)\right)$$
$$= \sum_{j=1}^{s} \Pr\left(Z_{C_j} \le t\right) - \sum_{i<j} \Pr(Z_{C_i\cup C_j} \le t) + \ldots + (-1)^{s+1} \Pr(Z_{C_1\cup C_2\cup\ldots\cup C_s} \le t)$$

for all t. Hence it is a negative mixture of the distribution functions of parallel systems with components in the union of its minimal cut sets.

In practice, a relevant case is when the joint distribution $F(x_1, x_2, \ldots, x_n)$ of $(X_1, X_2, \ldots, X_n)$ is exchangeable, that is, when

$$(X_1, X_2, \ldots, X_n) =_{st} (X_{\sigma(1)}, X_{\sigma(2)}, \ldots, X_{\sigma(2)})$$

for any permutation σ, where $=_{st}$ denotes equality in law. Note that this case includes the case of independent and identically distributed (i.i.d.) components. If F is exchangeable and P is a set with i elements, then $Y_P =_{st} X_{1:i}$ and $Z_P =_{st} X_{i:i}$. Hence, the reliability function of the system T can be written as

$$R_T(t) = \sum_{j=1}^{n} \alpha_i R_{1:i}(t) \tag{7.3}$$

where $\alpha_1, \alpha_2, \ldots, \alpha_n$ are some (unique) real numbers which only depend on the path sets (or the structure function) of the system, satisfying $\sum_{j=1}^{n} \alpha_i = 1$. The vector

$(\alpha_1, \alpha_2, \ldots, \alpha_n)$ is called the minimal signature of the system in Navarro et al. (2007). Analogously, the distribution function of the system can be written as

$$F_T(t) = \sum_{j=1}^{n} \beta_i F_{i:i}(t) \tag{7.4}$$

where $\beta_1, \beta_2, \ldots, \beta_n$ are some (unique) real numbers which only depend on the cut sets (or the structure function) of the system, satisfying $\sum_{j=1}^{n} \beta_i = 1$. The vector $(\beta_1, \beta_2, \ldots, \beta_n)$ is called the maximal signature of the system in Navarro et al. (2007). Note that if the components are i.i.d. then $R_{1:i}(t) = R^i(t)$ and $F_{i:i}(t) = F^i(t)$, where R and F are the common reliability and distribution functions of the components, respectively.

In particular, if the joint distribution is exchangeable, the reliability function $R_{n-k+1:n}$ of the order statistic $X_{n-k+1:n}$ which represents the lifetime of the k-out-of-n system can be written as

$$R_{n-k+1}(t) = \sum_{j=k}^{n} (-1)^{j-k} \binom{n}{j} \binom{j-1}{k-1} R_{1:j}(t) \tag{7.5}$$

or as

$$R_{n-k+1}(t) = \sum_{j=n-k+1}^{n} (-1)^{j-n+k-1} \binom{n}{j} \binom{j-1}{n-k} R_{j:j}(t) \tag{7.6}$$

(see David and Nagaraja (2003), p. 46). These expressions can be used to compute the minimal and maximal signatures of k-out-of-n systems.

For example, the minimal and maximal signatures of the 2-out-of-4 system whose lifetime is $X_{3:4}$ are $(0, 6, -8, 3)$ and $(0, 0, 4, -3)$, respectively. Hence, its distribution is a negative mixture of three series system distributions or two parallel system distributions. The minimal and maximal signatures of all the coherent systems with three or four components can be seen in Navarro and Shaked (2006) and Navarro et al. (2007).

7.3 Properties of Mixtures and Systems

This section shows how known properties of mixtures can now be applied to order statistics and coherent systems using the representations given in the preceding section.

We say that a distribution function F is generalized (finite) mixture of the distribution functions $F_1, F_2, \ldots, F_n$ if

$$F(t) = \sum_{i=1}^{n} p_i F_i(t) \tag{7.7}$$

for all t, where $p_1, p_2, \ldots, p_n$ are some real numbers such that $\sum_{i=1}^{n} p_i = 1$. If all the weights $p_1, p_2, \ldots, p_n$ are positive, then F is a positive or usual mixture. In this case, the right hand side (RHS) of (7.7) always defines a distribution function. If some weights

are negative, then we say that F is a negative mixture. In this case the (RHS) of (7.7) does not necessarily define a proper distribution function. However, note that we will assume that F in (7.7) is a distribution function. Also note that this is always true when F is the distribution of an order statistic or a coherent system.

The hazard or failure rate function is a very useful tool to describe the aging process of components and systems. The hazard function of a random variable X with density function f and reliability function R is defined by $h(t) = f(t)/R(t)$ for t such that $R(t) > 0$. By convention, $h(t) = \infty$ when $R(t) = 0$. It is also used to define the hazard (failure) rate order ($X \leq_{hr} Y$ if $h_X \geq h_Y$) and the IFR and DFR classes.

The negatives mixtures have properties similar to that of positive mixtures. However, in general, the properties are not the same. For example, it is well known that the positive mixtures of DFR (i.e., decreasing failure (hazard) rate function) distributions are also DFR. However, this property is not true for negative mixtures. Actually, we have that a negative mixture of an IFR (increasing failure rate) distribution with a positive weight and DFR distributions with negative weights, is IFR (see Navarro and Hernandez (2006)Navarro and Hernandez (2006)).

In general it is difficult to determine the shape of the hazard rate of a mixture even if we know the shape of the hazard rates of the members of the mixture. The following property shows that, under some assumptions, the limiting behaviour of the hazard rate of a generalized mixture is equivalent to that of the best (in the hazard rate order) member of the mixture when $t \to \infty$. This result is included in Navarro and Hernandez (2006)Navarro and Hernandez (2006) (see also Navarro and Shaked (2006)). For completeness we provide the proof in the appendix.

Theorem 1. *Let F be a distribution function satisfying (7.7) for absolutely continuous distributions $F_1, F_2, \ldots, F_n$ such that $F_i(t) < 1$ for all t, and for weights $p_1, p_2, \ldots, p_n$ such that $p_i \neq 0$ and $\sum_{i=1}^{n} p_i = 1$. Let h be the hazard rate function associated to F and let h_i be the hazard rate function associated to F_i, for $i = 1, 2, \ldots, n$. If*

$$\liminf_{t\to\infty} \frac{h_i(t)}{h_1(t)} > 1 \tag{7.8}$$

and

$$\limsup_{t\to\infty} \frac{h_i(t)}{h_1(t)} < \infty \tag{7.9}$$

for $i = 2, 3, \ldots, n$, then $p_1 > 0$ and

$$\lim_{t\to\infty} \frac{h(t)}{h_1(t)} = 1. \tag{7.10}$$

Moreover, condition (7.9) can be replaced by the weaker condition

$$\lim_{t\to\infty} \frac{f_i(t)}{f_1(t)} = 0 \tag{7.11}$$

for $i = 2, 3, \ldots, n$, where $f_i(t) = F_i'(t)$ for $i = 1, 2, \ldots, n$.

Now, we obtain a similar property for coherent systems using the representation of their distributions as negative mixtures of the distributions of the series systems obtained using their path sets.

Theorem 2. *Let T be the lifetime of a coherent system with minimal path sets $P_1, P_2, \ldots, P_m$. Let h_T be the hazard rate function associated to T and let h_P be the hazard rate function associated to the series system $Y_P = \min_{i \in P} X_i$. If*

$$\liminf_{t \to \infty} \frac{h_P(t)}{h_{P_1}(t)} > 1 \tag{7.12}$$

and

$$\limsup_{t \to \infty} \frac{h_P(t)}{h_{P_1}(t)} < \infty \tag{7.13}$$

for all path set P, $P \neq P_1$, then

$$\lim_{t \to \infty} \frac{h_T(t)}{h_{P_1}(t)} = 1.$$

Moreover, condition (7.13) can be replaced by the weaker condition

$$\lim_{t \to \infty} \frac{f_P(t)}{f_{P_1}(t)} = 0 \tag{7.14}$$

for all path set P, $P \neq P_1$, where f_P is the density function of the series system Y_P.

The proof is easy. Note that the tail behaviour of the hazard rate of a coherent system is equivalent to that of the hazard rate of the tail-best series system obtained from its minimal path sets. Also note that the series systems are not necessarily hr-ordered (see Navarro and Shaked (2006)) and hence we need to check (7.12) and (7.13) for any path set P. However, if the components are independent and $P = \cup_{j \in J} P_j$ for $J \subseteq \{1, 2, \ldots, m\}$, then $h_P(t) = \sum_{j \in J} h_{P_j}(t) \geq h_{P_j}(t)$ for all $j \in J$. Therefore, if the components are independent, then (7.12) can be replaced by

$$\liminf_{t \to \infty} \frac{h_{P_i}(t)}{h_{P_1}(t)} > 1 \tag{7.15}$$

for $i = 2, 3, \ldots, n$. Analogously, (7.13) can be replaced by

$$\limsup_{t \to \infty} \frac{h_{P_1 \cup P_2 \cup \ldots \cup P_m}(t)}{h_{P_1}(t)} < \infty. \tag{7.16}$$

In particular, if the joint distribution of the lifetimes of the components is exchangeable, from (7.3) and Theorem 1 we have the following result.

Theorem 3. *Let T be the lifetime of a coherent system with components having exchangeable joint distribution. Let $(0, \ldots, 0, \alpha_i, \alpha_{i+1}, \ldots, \alpha_j, 0, \ldots, 0)$, where $1 \leq i \leq j \leq n$, be the minimal signature associated to T and let h_T be the hazard rate function associated to T. If*

$$\liminf_{t \to \infty} \frac{h_{1:k}(t)}{h_{1:i}(t)} > 1 \tag{7.17}$$

and

$$\limsup_{t \to \infty} \frac{h_{1:k}(t)}{h_{1:i}(t)} < \infty \tag{7.18}$$

for $k = i+1, i+2, \ldots, j$, then

$$\lim_{t\to\infty} \frac{h_T(t)}{h_{1:i}(t)} = 1.$$

Moreover, condition (7.18) can be replaced by the weaker condition

$$\lim_{t\to\infty} \frac{f_{1:k}(t)}{f_{1:i}(t)} = 0 \tag{7.19}$$

for $k = i+1, i+2, \ldots, j$.

In particular, if the components are i.i.d. with common hazard rate function h then

$$\lim_{t\to\infty} \frac{h_{1:k}(t)}{h_{1:i}(t)} = \lim_{t\to\infty} \frac{kh(t)}{ih(t)} = \frac{k}{i}. \tag{7.20}$$

Hence (7.17) and (7.18) hold for $k = i+1, i+2, \ldots, j$, and then

$$\lim_{t\to\infty} \frac{h_T(t)}{h(t)} = i.$$

For example, if $T = X_{n-k+1:n}$ is the lifetime of a k-out-of-n system with i.i.d. components with common hazard rate function h, from (7.5), we have

$$\lim_{t\to\infty} \frac{h_{n-k+1:n}(t)}{h(t)} = k$$

for $k = 1, 2, \ldots, n$. In particular, for the parallel systems we have

$$\lim_{t\to\infty} \frac{h_{k:k}(t)}{h(t)} = 1$$

for $k = 1, 2, \ldots, n$.

Unfortunately, in general, Theorem 1 cannot be applied to the representation of a coherent system in terms of the parallel systems obtained from its cut sets since the tail-behaviour of the hazard rate of a parallel system is equivalent to that of the hazard rate of the tail-best component in the hazard rate order. Hence (7.8) does not hold. For example, if the system has i.i.d. components, then

$$\lim_{t\to\infty} \frac{h_{k:k}(t)}{h_{i:i}(t)} = 1$$

for $k = 1, 2, \ldots, n$ and Theorem 1 cannot be applied to representation (7.4) since (7.8) does not hold.

7.4 The Bridge Structure

In this section we analyze the tail behaviour of the hazard rate of a system having the bridge structure given in figure 7.1 (see also Barlow and Proschan (1975), p. 9). Its minimal path sets are $P_1 = \{1, 4\}$, $P_2 = \{2, 5\}$, $P_3 = \{1, 3, 5\}$ and $P_4 = \{2, 3, 4\}$.

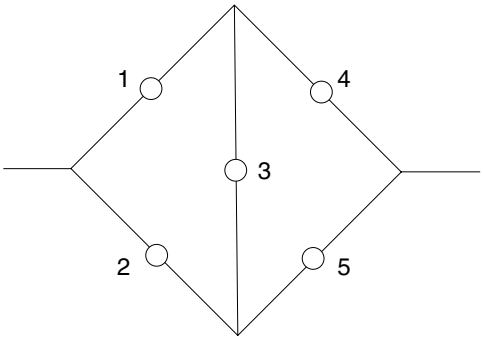

Figure 7.1. Bridge structure

Therefore, the reliability function R_T of the system can be computed from the following negative mixture:

$$R_T(t) = R_{\{1,4\}}(t) + R_{\{2,5\}}(t) + R_{\{1,3,5\}}(t) + R_{\{2,3,4\}}(t) + 2R_{\{1,2,3,4,5\}}(t)$$
$$-R_{\{1,2,3,4\}}(t) - R_{\{1,3,4,5\}}(t) - R_{\{1,2,4,5\}}(t) - R_{\{1,2,3,5\}}(t) - R_{\{2,3,4,5\}}(t)$$

In particular, if the lifetimes of the components have an exchangeable joint distribution, then

$$R_T(t) = 2R_{1:2}(t) + 2R_{1:3}(t) - 5R_{1:4}(t) + 2R_{1:5}(t),$$

that is, its minimal signature is $(0, 2, 2, -5, 2)$.

Therefore, if the components are i.i.d. with common hazard function h, then using the results given in the preceding section we obtain

$$\lim_{t\to\infty} \frac{h_T(t)}{h(t)} = 2,$$

where h_T is the hazard rate of the system.

If the components are independent and satisfy the proportional hazard (PHR) model, i.e., their hazard rate functions h_i satisfy $h_i(t) = \lambda_i h(t)$ for $i = 1, 2, \ldots, 5$, where h is a hazard rate function, then

$$\lim_{t\to\infty} \frac{h_T(t)}{h(t)} = \lambda,$$

where $\lambda = \min(\lambda_1 + \lambda_4, \lambda_2 + \lambda_5, \lambda_1 + \lambda_3 + \lambda_5, \lambda_2 + \lambda_3 + \lambda_4)$. Note that if $\lambda_1 + \lambda_4 = \lambda_2 + \lambda_5 < \lambda_1 + \lambda_3 + \lambda_5 < \lambda_2 + \lambda_3 + \lambda_4$, then (7.15) does not hold. However, note that, in this case, Theorem 1 can be applied to the representation

$$R_T(t) = 2R_{\{1,4\}}(t) + R_{\{1,3,5\}}(t) + R_{\{2,3,4\}}(t) + 2R_{\{1,2,3,4,5\}}(t)$$
$$-R_{\{1,2,3,4\}}(t) - R_{\{1,3,4,5\}}(t) - R_{\{1,2,4,5\}}(t) - R_{\{1,2,3,5\}}(t) - R_{\{2,3,4,5\}}(t)$$

and then $\lim_{t\to\infty} h_T(t)/h(t) = \lambda_1 + \lambda_4$.

If the components have different distributions, the best tail behaviour of the hazard rate of the system is obtained by placing the best components in positions 1 and 4 (or

in 2 and 5), i.e., when $\lambda_1 < \lambda_4 < \lambda_i$ for $i = 2, 3, 5$. However, the initial behaviour could be different.

If the component lifetimes have the Farlie-Gumbel-Morgenstern (FGM) distribution with exponential marginals; that is, the joint reliability (survival) function of $(X_1, X_2, \ldots, X_5)$ is given by

$$R(x_1, x_2, \ldots, x_5) = e^{-\sum_{i=1}^{5} \lambda_i x_i} \big(1 + \alpha \prod_{i=1}^{5} (1 - e^{-\lambda_i x_i})\big)$$

for $x_i \geq 0$, $i = 1, 2, \ldots, 5$, where $|\alpha| \leq 1$, then it is easy to see that the hazard function h_P of the series system Y_P is given by $h_P(t) = \sum_{i \in P} \lambda_i$ for all $P \subset \{1, 2, \ldots, 5\}$. However, if $P = \{1, 2, \ldots, 5\}$, then a straightforward computation yields

$$h_{\{1,2,..,5\}}(t) = \sum_{i=1}^{5} \lambda_i - \frac{\alpha \sum_{i=1}^{5} \left(e^{-\lambda_i t} \prod_{j \neq i} (1 - e^{-\lambda_j t})\right)}{1 + \alpha \prod_{i=1}^{5} (1 - e^{-\lambda_i t})}.$$

Note that $\lim_{t \to \infty} h_{\{1,2,..,5\}}(t) = \sum_{i=1}^{5} \lambda_i$. Therefore, Theorem 3 applies to T and hence $\lim_{t \to \infty} h_T(t) = \min(\lambda_1 + \lambda_4, \lambda_2 + \lambda_5, \lambda_1 + \lambda_3 + \lambda_5, \lambda_2 + \lambda_3 + \lambda_4)$ and T has an asymptotic exponential distribution.

Figure 7.2 shows all the options of hazard rate functions of a system with a bridge structure and components having a FGM joint distribution with parameters $\alpha = 0.5$ and $\lambda_i = 1, 1, 2, 2, 2$ for $i = 1, 2 \ldots, 5$. Note that the limits of the hazard rate functions of the systems are 2 or 3 and that the tail-best option is obtained by placing the best components at positions 1 and 4 (or equivalently at 2 and 5). Also note that this is also the best option for all t. The worst option is obtained by placing the best component at position 3 (the 'bridge').

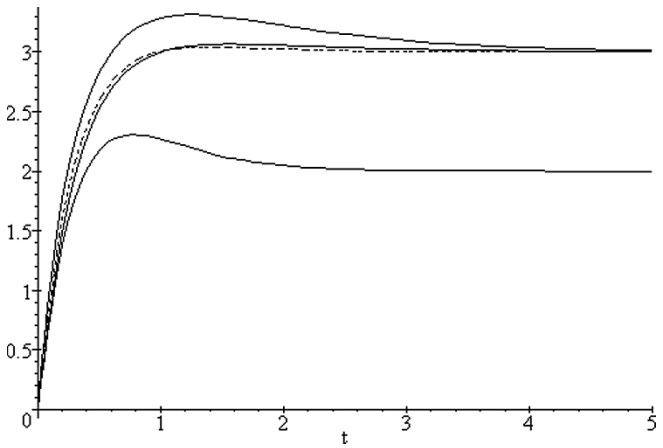

Figure 7.2. Hazard rate function of a system with a bridge structure and joint FGM distribution with parameters $\alpha = 0.5$ and $\lambda_1 = \lambda_2 = 1$ and $\lambda_3 = \lambda_4 = \lambda_5 = 2$ (dashed line), $\lambda_1 = \lambda_3 = 1$ and $\lambda_2 = \lambda_4 = \lambda_5 = 2$ (continuous line at the top), $\lambda_1 = \lambda_4 = 1$ and $\lambda_2 = \lambda_3 = \lambda_5 = 2$ (continuous line at the bottom) and $\lambda_1 = \lambda_5 = 1$ and $\lambda_2 = \lambda_3 = \lambda_4 = 2$

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Appendix

PROOF OF THEOREM 1. Let $\varepsilon > 0$ be such that $\liminf_{t\to\infty} h_i(t)/h_1(t) > 1+\varepsilon$ for $i = 2, 3, \ldots, n$. Then there exists a t_i such that

$$h_i(t) - h_1(t) > \varepsilon h_1(t)$$

for all $t \geq t_i$ and for $i = 2, 3, \ldots, n$. So, if $R_i = 1 - F_i$, for $t \geq t_i$ we have

$$\begin{aligned}
\frac{R_i(t)}{R_1(t)} &= \exp\left\{ -\int_{-\infty}^{t} (h_i(x) - h_1(x))\, dx \right\} \\
&= \exp\left\{ -\int_{-\infty}^{t_i} (h_i(x) - h_1(x))\, dx \right\} \exp\left\{ -\int_{t_i}^{t} (h_i(x) - h_1(x))\, dx \right\} \\
&\leq \frac{R_i(t_i)}{R_1(t_i)} \cdot \exp\left\{ -\varepsilon \int_{t_i}^{t} h_1(x)\, dx \right\} \\
&= \frac{R_i(t_i)}{R_1(t_i)} \left(\frac{R_1(t)}{R_1(t_i)} \right)^{\varepsilon}.
\end{aligned}$$

Letting $t \to \infty$, we obtain $\lim_{t\to\infty} R_i(t)/R_1(t) = 0$ for $i = 2, 3, \ldots, n$.

Then, note that

$$\frac{R(t)}{R_1(t)} = \left(p_1 + \sum_{i=2}^{n} p_i \frac{R_i(t)}{R_1(t)} \right).$$

Therefore,

$$\lim_{t\to\infty} \frac{R(t)}{R_1(t)} = p_1 \geq 0 \tag{7.21}$$

and hence $p_1 > 0$, since $p_1 \neq 0$.

Moreover, note that

$$\frac{h(t)}{h_1(t)} = \frac{R_1(t)}{R(t)} \left(p_1 + \sum_{i=2}^{n} p_i \frac{h_i(t) R_i(t)}{h_1(t) R_1(t)} \right). \tag{7.22}$$

By assumption (7.9), $h_i(t)/h_1(t)$ is bounded and as $\lim_{t\to\infty} R_i(t)/R_1(t) = 0$ for $i = 2, 3, \ldots, n$ and $\lim_{t\to\infty} R_1(t)/R(t) = p_1^{-1} > 0$, we have (7.10).

Finally, we note that, from (7.22), condition (7.9) can be replaced by (7.11) since $h_i(t)R_i(t) = f_i(t)$. ■

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8

Models of Ordered Data and Products of Beta Random Variables

Eric Beutner and Udo Kamps

Institute of Statistics, RWTH Aachen University, Germany

Abstract: Generalized order statistics provide a unified approach to a variety of models of random variables arranged in ascending order of magnitude with different interpretations and statistical applications. An extension to a more general family of models of ordered random variables is proposed. Intermediate or fractional order statistics turn out to be a particular sub-model. Their joint density may also be described as ordered Dirichlet distribution.

Keywords and phrases: Beta distribution, Dirichlet distribution, ordered Dirichlet distribution, generalized order statistics, intermediate order statistics, fractional order statistics

8.1 Introduction

Generalized order statistics have been introduced as a unifying distribution theoretical set-up for models of ordered random variables, such as order statistics and record values (Kamps, 1995). Alternatively, generalized order statistics may be defined via products of random variables with power function distributions (see Definition 1 below). It turned out that this approach has some advantages when studying properties of generalized order statistics. In what follows we consider products of beta random variables. Let $Beta(a, b)$ denote the beta distribution with parameters $a > 0, b > 0$ and density

$$g(x) = \frac{x^{a-1}(1-x)^{b-1}}{B(a,b)}, \quad 0 < x < 1,$$

where $B(a, b)$ is the beta function.

Definition 1. *(Cramer and Kamps, 2003) Let F be some distribution function, $\gamma_1, \ldots, \gamma_n$ be positive numbers and $B_1, \ldots, B_n$ be independent random variables with $B_j \sim Beta(\gamma_j, 1)$, $1 \leq j \leq n$. Then the random variables*

$$X_*^{(r)} = F^{-1}(1 - \prod_{j=1}^{r} B_j), \quad 1 \leq r \leq n,$$

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are called generalized order statistics (based on F and $\gamma_1, \ldots, \gamma_n$), where F^{-1} denotes the quantile function of F.

This definition of generalized order statistics may be extended to consider the random variables $W_1, \ldots, W_n$ defined by

$$W_r = F^{-1}(1 - \prod_{j=1}^{r} B_j), \quad 1 \le r \le n, \tag{8.1}$$

where $B_1, \ldots, B_n$ are independent random variables, each with a beta distribution with parameters α_i and β_i, $1 \le i \le n$.

It is well known that spacings of generalized order statistics based on an exponential distribution with distribution function $F(x) = 1 - e^{-\lambda x}$, $\lambda > 0$, are independent. This also holds for the random variables $W_r, 1 \le r \le n$, defined by (8.1) since $W_r = -\frac{1}{\lambda} \sum_{j=1}^{r} \log B_j$, which implies that $W_r - W_{r-1} = -\frac{1}{\lambda} \log B_r$. Moreover, $W_r - W_{r-1}$ has a log-beta distribution (cf. Johnson et al. (1994), p. 247)) with density

$$f^{W_r - W_{r-1}}(x) = \frac{\lambda}{B(\alpha_r, \beta_r)} e^{-\lambda \alpha_r x} (1 - e^{-\lambda x})^{\beta_r - 1}. \tag{8.2}$$

In Mathai (1993), p. 84, the density function of a product of independent beta variables is given which directly leads to a representation of the distribution function of W_r.

Lemma 1. *For $r = 1, \ldots, n$, the distribution function of W_r is given by*

$$F^{W_r}(w) = 1 - \prod_{j=1}^{r} \frac{\Gamma(\alpha_j + \beta_j)}{\Gamma(\alpha_j)} \times \int_0^{1-F(w)} G_{r,r}^{r,0}\left(x \,\middle|\, \begin{matrix} \alpha_1 + \beta_1 - 1, \ldots, \alpha_r + \beta_r - 1 \\ \alpha_1 - 1, \quad \ldots, \quad \alpha_r - 1 \end{matrix} \right) dx, \tag{8.3}$$

where $G_{r,r}^{r,0}$ denotes Meijer's G-function.

Intermediate or fractional order statistics are contained in this setup by a particular choice of the distribution parameters α_i and β_i. Papadatos (1995) introduced intermediate order statistics $(U_{(\tilde{a}_1)}, \ldots, U_{(\tilde{a}_r)})$ from the uniform distribution on $(0, 1)$ of order $\tilde{a}_1, \ldots, \tilde{a}_r$, where $r \in \{1, \ldots, n\}$ and $1 \le \tilde{a}_1 < \ldots < \tilde{a}_r \le n$, by their joint density

$$f(u_1, \ldots, u_r) = \frac{\Gamma(n+1)}{\Gamma(a_1) \cdot \Gamma(\tilde{a}_2 - \tilde{a}_1) \cdot \ldots \cdot \Gamma(n + 1 - \tilde{a}_r)} \times u_1^{\tilde{a}_1 - 1} \cdot (u_2 - u_1)^{\tilde{a}_2 - \tilde{a}_1 - 1} \cdot \ldots \cdot (u_r - u_{r-1})^{\tilde{a}_r - \tilde{a}_{r-1} - 1} (1 - u_r)^{n - \tilde{a}_r}, \quad 0 < u_1 < \ldots < u_r < 1. \tag{8.4}$$

In the particular case $\tilde{a}_i = i$, $1 \le i \le r$, we obtain the joint density of the first r order statistics. Intermediate order statistics from an arbitrary distribution function F are then obtained via quantile transformation. The structure of intermediate order statistics coincides with so-called fractional order statistics defined by Stigler (1977) (see also David and Nagaraja (2003), p. 21). The connection of intermediate order statistics to (8.1) is illustrated by means of an ordered Dirichlet distribution.

8.2 Intermediate Order Statistics and the Ordered Dirichlet Distribution

Following Connor and Mosimann (1969) or James (1972), the Dirichlet distribution can be introduced as follows.

Definition 2. *The nonnegative random vector* $(Y_1, \ldots, Y_n)$ *with* $\sum_{i=1}^{n} Y_i < 1$ *has a Dirichlet distribution with parameter vector* $(a_1, \ldots, a_n, b_n)$, $a_i > 0, 1 \le i \le n$, $b_n > 0$ *if*

(i) the ratios $Y_1, \frac{Y_2}{1-Y_1}, \ldots, \frac{Y_n}{1-Y_1-\ldots-Y_{n-1}}$ *are independent, and*
(ii) each ratio is beta distributed, the i-th ratio with parameters a_i *and* b_i*, satisfying* $b_{i-1} = a_i + b_i$ *for all* $i = 2, \ldots, n$.

An alternative definition which is equivalent to the one given above is the following (see Kotz et al. (2000)).

Definition 3. *Let* $X_1, \ldots, X_{n+1}$ *be independent random variables with* $X_j \sim \Gamma(a_i, 1)$, $1 \le j \le n+1$, *where* $\Gamma(a, 1)$ *denotes the gamma distribution with parameters* $a > 0$ *and 1, and density*

$$f(x) = \frac{x^{a-1}e^{-x}}{\Gamma(a)}, \quad 0 < x < \infty.$$

The distribution of the random vector

$$(Y_1, \ldots, Y_n) = \left(\frac{X_1}{\sum_{j=1}^{n+1} X_j}, \ldots, \frac{X_n}{\sum_{j=1}^{n+1} X_j} \right)$$

is called Dirichlet distribution.

Closely related to the Dirichlet distribution is the ordered Dirichlet distribution.

Definition 4. *Let* $(Y_1, \ldots, Y_n)$ *be Dirichlet distributed with parameter vector* $(a_1, \ldots, a_n, b_n)$. *The distribution of the random vector*

$$(Z_1, \ldots, Z_n) = (Y_1, Y_1 + Y_2, \ldots, Y_1 + Y_2 + \ldots + Y_n) \tag{8.5}$$

is called ordered Dirichlet distribution with parameter vector $(a_1 \ldots, a_n, b_n)$.

The joint density

$$\begin{aligned} f(z_1, \ldots, z_n) = {} & \tfrac{\Gamma(a_1+\ldots+a_n+b_n)}{\Gamma(a_1)\cdot\ldots\cdot\Gamma(a_n)\cdot\Gamma(b_n)} z_1^{a_1-1} \cdot (z_2 - z_1)^{a_2-1} \\ & \cdot \ldots \cdot (z_n - z_{n-1})^{a_n-1}(1 - z_n)^{b_n-1}, \; 0 < z_1 < \ldots < z_n < 1 \end{aligned} \tag{8.6}$$

of $Z = (Z_1, \ldots, Z_n)$ may be found in Wilks (1962), p. 182.

Putting $n = r$, $a_j = \tilde{a}_j - \tilde{a}_{j-1}$, $1 \le j \le n$, $\tilde{a}_0 = 0$, and $b_n = n+1-\tilde{a}_r$ it follows from (8.4) and (8.6) that intermediate order statistics from the uniform distribution have an ordered Dirichlet distribution. The next lemma shows that the ordered Dirichlet distribution can be obtained by products of beta random variables.

Lemma 2. *Let $B_1, \ldots, B_n$ be independent random variables with $B_j \sim Beta(a_j, b_j)$, $a_j, b_j > 0, 1 \leq j \leq n$, where the parameters satisfy the conditions*

$$b_{j-1} = a_j + b_j, \;\; 2 \leq j \leq n.$$

Then the random vector $X = (X_1, \ldots, X_n)$ defined by

$$X_r = 1 - \prod_{j=1}^{r}(1 - B_j), \;\; 1 \leq r \leq n, \tag{8.7}$$

is ordered Dirichlet distributed with parameter vector $(a_1, \ldots, a_n, b_n)$.

Proof. From Definition 2 it follows that the joint distribution of the random variables

$$Y_1 = B_1, \qquad Y_r = B_r \prod_{j=1}^{r-1}(1 - B_j), \;\; 2 \leq r \leq n,$$

where $B_1, \ldots, B_n$ are independent and $B_i \sim Beta(a_i, b_i)$, $1 \leq i \leq n$, with $b_{i-1} = a_i + b_i$, $i = 2, \ldots, n$, is a Dirichlet distribution. Using that

$$\sum_{j=1}^{r}\left(\prod_{k=1}^{j-1}(1 - B_k)\right) B_j = 1 - \prod_{j=1}^{r}(1 - B_j), \;\; r = 1, \ldots, n,$$

(by convention $\prod_{\emptyset} = 1$) we obtain from Definition 4 that the random variables $X_r = \sum_{j=1}^{r} Y_j = 1 - \prod_{j=1}^{r}(1 - B_j)$, $r = 1, \ldots, n$, have an ordered Dirichlet distribution. This proves the assertion. ∎

Lemma 2 implies that intermediate order statistics from the uniform distribution on $(0, 1)$ may be constructed via products of independent beta variates.

Corollary 1. *Let $(U_{(\tilde{a}_1)}, \ldots, U_{(\tilde{a}_r)})$ be intermediate order statistics from the uniform distribution on $(0, 1)$ of order $\tilde{a}_1, \ldots, \tilde{a}_r$ where $1 \leq \tilde{a}_1 < \ldots < \tilde{a}_r \leq n$. Then*

$$U_{(\tilde{a}_j)} \stackrel{d}{=} 1 - \prod_{k=1}^{j} B_k \stackrel{d}{=} \tilde{B}_j, \;\; 1 \leq j \leq r, \tag{8.8}$$

where $B_1, \ldots, B_r$ are independent and $B_i \sim Beta(n - \tilde{a}_i + 1, \tilde{a}_i - \tilde{a}_{i-1})$, $1 \leq i \leq r$, $\tilde{a}_0 = 0$, and $\tilde{B}_j \sim Beta(\tilde{a}_j, n - \tilde{a}_j + 1)$, $1 \leq j \leq r$. Here $\stackrel{d}{=}$ denotes equality in distribution.

Proof. Using Lemma 2 and noticing that $1 - Beta(\alpha, \beta) \sim Beta(\beta, \alpha)$ and $Beta(\alpha_1, \beta_1) \cdot Beta(\alpha_2, \beta_2) \sim Beta(\alpha_2, \beta_1 + \beta_2)$ if $\alpha_1 = \alpha_2 + \beta_2$ we obtain 8.8. ∎

The marginal distribution of $U_{(\tilde{a}_j)}$ may also be obtained from (8.3), since plugging in the particular choice of α_i and β_i leads to

$$\begin{aligned} & G_{j,j}^{j,0}\left(x \;\middle|\; \begin{matrix} n, & n - \tilde{a}_1, \ldots, n - \tilde{a}_{j-1} \\ n - \tilde{a}_1, & n - \tilde{a}_2, \ldots, n - \tilde{a}_j \end{matrix}\right) \\ = \; & G_{1,1}^{1,0}\left(x \;\middle|\; \begin{matrix} n \\ n - \tilde{a}_j \end{matrix}\right) \stackrel{Mathai(1993,\, p.\, 130)}{=} \frac{1}{\Gamma(\tilde{a}_j)} x^{n - \tilde{a}_j}(1 - x)^{\tilde{a}_j - 1}. \end{aligned}$$

In the introduction we mentioned that intermediate and fractional order statistics coincide. Stigler (1977) introduced fractional order statistics by means of the finite dimensional distributions of a Dirichlet process. From his definition it follows at once that fractional order statistics have an ordered Dirichlet distribution. We propose to use the term fractional order statistics since the term intermediate order statistics already has a different meaning (cf. David and Nagaraja (2003), p. 311).

8.3 Properties of Fractional Order Statistics

The above representation allows both an easy derivation as well as some extensions of known properties of fractional order statistics. Recall that fractional order statistics $(X_{(\tilde{a}_1)}, \ldots, X_{(\tilde{a}_r)})$ from an arbitrary distribution function F are defined by

$$(X_{(\tilde{a}_1)}, \ldots, X_{(\tilde{a}_r)}) = (F^{-1}(U_{(\tilde{a}_1)}), \ldots, F^{-1}(U_{(\tilde{a}_r)})), \tag{8.9}$$

where $(U_{(\tilde{a}_r)}, \ldots, U_{(\tilde{a}_r)})$ are fractional order statistics from the uniform distribution on $(0, 1)$.

Corollary 2. *Let $X_{(\tilde{a}_j)} = F^{-1}(U_{(\tilde{a}_j)})$ be a fractional order statistic, $j \in \{1, \ldots, r\}$. Then*

(i) $X_{(\tilde{a}_j)} \sim F^{-1}(Z)$, where $Z \sim Beta(\tilde{a}_j, n - \tilde{a}_j + 1)$.
(ii) $P(X_{(\tilde{a}_j)} \leq F^{-1}(p)) = I_p(\tilde{a}_j, n - \tilde{a}_j + 1)$, if F is continuous in $F^{-1}(p)$, where I_p denotes the incomplete beta function
$I_p(a, b) = \frac{1}{B(a,b)} \int_0^p x^{a-1}(1-x)^{b-1} dx$.

Proof. This is an immediate consequence of Corollary 1 and (8.9). ■

For the special case $r = 1$, Corollary 2 (i) and (ii) is stated in Papadatos (1995) in (2.5) and Theorem (3.1), respectively.

Since fractional order statistics can be represented by products of beta random variables, an easy proof of the following theorem is possible representing a fractional order statistic as a stochastic convex combination of its neighbours.

Theorem 1. *(Jones, 2003) Let $U_{(\tilde{a}_1)}, U_{(\tilde{a}_2)}, U_{(\tilde{a}_3)}$ be fractional order statistics with $\tilde{a}_1 = j$, $\tilde{a}_2 = j + c$, $\tilde{a}_3 = j + 1$, $0 < c < 1$, $1 \leq j \leq n - 1$, and $C \sim Beta(c, 1 - c)$ independent of the $U's$. Then*

$$U_{(\tilde{a}_2)} \stackrel{d}{=} (1 - C)U_{(\tilde{a}_1)} + CU_{(\tilde{a}_3)}.$$

Proof. By definition $U_{(\tilde{a}_1)} \sim Beta(j, n+1-j), U_{(\tilde{a}_2)} \sim Beta(j+c, n+1-j-c), U_{(\tilde{a}_3)} \sim Beta(j + 1, n - j)$. From Corollary 1 and its proof we have

$$U_{(\tilde{a}_1)} \stackrel{d}{=} 1 - B_1 \text{ and } U_{(\tilde{a}_3)} \stackrel{d}{=} 1 - B_1 B_2 B_3$$

where $B_1 \sim Beta(n - j + 1, j), B_2 \sim Beta(n - j - c + 1, c)$ and $B_3 \sim Beta(n - j, 1 - c)$. Noticing that

$$\begin{aligned}(1-C)U_{(\tilde{a}_1)} + CU_{(\tilde{a}_3)} &= (1-C)(1-B_1) + C(1-B_1B_2B_3)\\ &= 1 - B_1(1-C(1-B_2B_3))\end{aligned}$$

the result follows directly since $B_2B_3 \sim Beta(n-j,1)$, $C(1-B_2B_3) \sim Beta(c, n-j+1-c)$ and $1 - B_1 \cdot Beta(n-j+1-c,c) \stackrel{d}{=} U_{(\tilde{a}_2)}$. ■

Let $X_{1,n}, \ldots, X_{n,n}$ denote the order statistics from a sample of size n from the exponential distribution. Then $Y_1 = X_{1,n}, \ldots, Y_n = X_{n,n} - X_{n-1,n}$ are independent and again exponentially distributed (cf. David and Nagaraja (2003), p. 18). The following corollary is an immediate consequence of (8.2) and Corollary 1, and shows that spacings of fractional order statistics based on an exponential distribution may be exponentially distributed.

Corollary 3. *Let $(X_{(\tilde{a}_1)}, \ldots, X_{(\tilde{a}_r)})$ be fractional order statistics of order $\tilde{a}_1, \ldots, \tilde{a}_r$ from an exponential distribution with $\tilde{a}_j - \tilde{a}_{j-1} = 1$, $2 \leq j \leq r$. Then $Y_1 = X_{(\tilde{a}_2)} - X_{(\tilde{a}_1)}, \ldots, Y_{r-1} = X_{(\tilde{a}_r)} - X_{(\tilde{a}_{r-1})}$ are independent and again exponentially distributed.*

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9

Exact Inference and Optimal Censoring Scheme for a Simple Step-Stress Model Under Progressive Type-II Censoring

Qihao Xie, N. Balakrishnan, and Dong-hoon Han

Department of Mathematics and Statistics. McMaster University, Canada

Abstract: In reliability and life-testing experiments, the researcher is often interested in the effects of extreme or varying stress factors such as temperature, voltage and load on the lifetimes of experimental units. Step-stress test, which is a special class of accelerated life-tests, allows the experimenter to increase the stress levels at fixed times during the experiment in order to obtain information on the parameters of the life distribution more quickly than under normal operating conditions. In this article, we consider a simple step-stress model under the exponential distribution when the available data are progressively Type-II censored. We derive the maximum likelihood estimators (MLEs) of the parameters assuming a cumulative exposure model with lifetimes being exponentially distributed. The exact distributions of the MLEs of parameters are obtained through the use of conditional moment generating functions. We then construct confidence intervals for the parameters using these exact distributions, asymptotic distributions of the MLEs and the parametric bootstrap methods, and assess their performance through a Monte Carlo simulation study. Next, we investigate optimal progressive censoring schemes as well as optimal time for change of stress level based on the simple step-stress model. Finally, we present two examples to illustrate all the methods of inference discussed here.

Keywords and phrases: Accelerated testing, bootstrap method, conditional moment generating function, coverage probability, cumulative exposure model, exponential distribution, maximum likelihood estimation, optimal censoring scheme, order statistics, step-stress models, tail probability, progressive type-II censoring

9.1 Introduction

The accelerated life-testing (ALT) experiments have found importance in reliability and survival analysis. Such experiments allow the experimenter to obtain adequate life data for the product under accelerated stress conditions, which cause the products to fail more quickly than under the normal operating conditions. Some key references in the area of accelerated testing include Nelson (1990), Meeker and Escobar (1998), and

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Bagdonavicius and Nikulin (2002). A special class of the ALT is called *step-stress testing*, which allows the experimenter to choose one or more stress factors in a life-testing experiment. Stress factors can include humidity, temperature, vibration, voltage, load or any other factor that directly affects the life of the products. In such a step-stress testing experiment, n identical units are placed on an initial stress level s_0 under a m-step-stress model, and only the successive failure times are recorded. The stress levels are changed to $s_1, \ldots, s_m$ at the pre-fixed times $\tau_1 < \cdots < \tau_m$, respectively. The most common model used to analyse these times-to-failure data is the "cumulative damage" or "cumulative exposure" model.

In many situations, the experimenter might not always obtain complete information on failure times for all experimental units. In many situations the removal of units from the experiment is pre-planned and intentional in order to save time and cost, or to free up testing facilities for other experiments. Conventional Type-I and Type-II censoring schemes result in censoring only at the end of the experiment, and they do not allow removal of units during the experiment. For this reason, we consider here the *Progressive Type-II Censoring Scheme*, which allows the experimenter to remove units from a life-test at various stages during the experiment. The concept of *Progressive Censoring* was first introduced by Herd (1956). Cohen (1963, 1966, 1991), Nelson (1982), Cohen and Whitten (1988), Balakrishnan and Cohen (1991), Balakrishnan and Aggarwala (2000), Balasooriya et al. (2000), and Ng et al. (2002, 2004) have all discussed inferential procedures based on progressively censored samples. One may refer to Balakrishnan (2007) for a recent overview of various developments relating to progressive censoring. A progressively Type-II censored sample is observed as follows. n identical units are placed on a life-testing experiment, and r and R_k $(k = 1, \ldots, r-1)$ are fixed in advance. At the time of the first failure, R_1 of the $n-1$ surviving units are randomly removed from the experiment; at the time of the second failure, R_2 of the $n-2-R_1$ surviving units are randomly removed from the experiment, and so on; the test continues until the r^{th} failure occurs at which time all the remaining $R_r = n - r - R_1 - \cdots - R_{r-1}$ surviving units are removed. If $R_1 = \cdots = R_r = 0$, then $n = r$ which corresponds to the complete sample situation. If $R_1 = \cdots = R_{r-1} = 0$, then $R_r = n - r$ which corresponds to the conventional Type-II right censoring scheme.

We consider here a simple step-stress model with only two stress levels when the failure time are progressively Type-II censored. This model has been studied extensively in the literature. DeGroot and Goel (1979) proposed the tampered random variable model and discussed optimal tests under a Bayesian framework. Nelson (1980) proposed the cumulative exposure model, while Miller and Nelson (1983) and Bai et al. (1989) discussed the determination of optimal time at which to change the stress level from s_0 to s_1. Bhattacharyya and Zanzawi (1989) proposed the tampered failure rate model, which assumes that the effects of changing stress level is to multiply the initial failure rate function by a factor subsequent to the change times. Madi (1993) generalized this tampered failure rate model from the simple step-stress model (case $m = 1$) to the multiple step-stress model (case $m \geq 2$). Khamis and Higgins (1998) discussed the same generalization under the Weibull distribution. Xiong (1998) and Xiong and Milliken (1999) considered inference under the assumption of exponential lifetimes. They assumed that the mean life of an experimental units is a log-linear function of the stress level, and developed inference for the two parameters of the corresponding log-linear link function. Watkins (2001) argued that it is preferable to work with the original exponential parameters even though the log-linear link function provides a

simple reparametrization. Balakrishnan et al. (2007) derived the exact conditional distributions of the MLEs under the exponential distribution when the data are Type-II censored. Gouno and Balakrishnan (2001) reviewed the developments on step-stress accelerated life-tests. Gouno et al. (2004) discussed inference for step-stress models under the exponential distribution when the available data are progressively Type-I censored. While Balakrishnan et al. (2007) developed the exact inference for a simple step-stress model under the exponential distribution in the presence of time constraint, Balakrishnan and Xie (2007a,b) handled the cases when the available samples are Type-I and Type-II hybrid censored in this setup.

In this paper, we consider a simple step-stress model with two stress levels based on the exponential distribution when the available data are progressively Type-II censored. The model is discussed in detail in Section 9.2. Due to the form of the time constraint, the MLEs of the unknown parameters do not always exist. We then derive the conditional MLEs, and their joint conditional moment generating functions (CMGF) and their joint conditional distributions, and then discuss their properties in Section 9.3. In Section 9.4, we discuss the exact method of constructing conditional confidence intervals (CIs) for the unknown parameters as well as the asymptotic method and the bootstrap methods. Monte Carlo simulation results are presented in Section 9.5. In Section 9.6, we discuss optimal progressive censoring schemes through the "variance optimality" and "mean squared error optimality" as well as the determination of the optimal time at which to change the stress level. Finally, we present two illustrative examples and some concluding remarks in Sections 9.7 and 9.8, respectively.

9.2 Model Description and MLEs

Suppose that the data come from a cumulative exposure model, and we consider a simple step-stress model based on progressive Type-II censoring with only two stress levels s_0 and s_1. The lifetime distributions at s_0 and s_1 are assumed to be exponential with failure rates θ_1 and θ_2, respectively. The probability density function (PDF) and cumulative distribution function (CDF) are given by

$$f_k(t;\theta_k) = \frac{1}{\theta_k}\exp\big\{-t/\theta_k\big\}, \quad t \geq 0, \quad \theta_k > 0, \quad k = 1,2 \tag{9.1}$$

and

$$F_k(t;\theta_k) = 1 - \exp\big\{-t/\theta_k\big\}, \quad t \geq 0, \quad \theta_k > 0, \quad k = 1,2, \tag{9.2}$$

respectively. We then have the cumulative exposure distribution (CED) $G(t)$ as

$$G(t) = \begin{cases} G_1(t) = F_1(t;\theta_1) & \text{if } 0 < t < \tau \\ G_2(t) = F_2\Big(t - \big(1 - \frac{\theta_2}{\theta_1}\big)\tau;\theta_2\Big) & \text{if } \tau \leq t < \infty \end{cases}, \tag{9.3}$$

where $F_k(\cdot)$ is as given in (9.2). The corresponding PDF is

$$g(t) = \begin{cases} g_1(t) = \frac{1}{\theta_1}\exp\big\{-\frac{1}{\theta_1}t\big\} & \text{if } 0 < t < \tau \\ g_2(t) = \frac{1}{\theta_2}\exp\big\{-\frac{1}{\theta_2}(t-\tau) - \frac{1}{\theta_1}\tau\big\} & \text{if } \tau \leq t < \infty \end{cases}. \tag{9.4}$$

Based on the progressively Type-II censored sample, we have n identical units under an initial stress level s_0. The stress level is changed to s_1 at a pre-fixed time τ, and the life-testing experiment is terminated when the r^{th} failure time $T_{r:r:n}$ occurs, where $2 \le r \le n$. Let N_1 be the number of units that fail before time τ at stress level s_0 and N_2 be the number of units that fail after time τ at stress level s_1. With these notations, we will observe the following progressively censored data:

$$\boldsymbol{t} = \left\{ t_{1:r:n} < \cdots < t_{N_1:r:n} \le \tau < t_{N_1+1:r:n} < \cdots < t_{r:r:n} \right\} \tag{9.5}$$

with the corresponding progressive censoring scheme $\boldsymbol{R} = (R_1, \ldots, R_r)$, where $\sum_{j=1}^{r} R_j = n - r$.

From the CED in (9.3) and the corresponding PDF in (9.4), we obtain the likelihood function of θ_1 and θ_2 based on the progressively Type-II censored sample in (9.5) as follows:

1. If $N_1 = r$ and $N_2 = 0$ in (9.5), the likelihood function of θ_1 and θ_2 is

$$\begin{aligned} L(\theta_1, \theta_2 | \boldsymbol{t}) &= C_p \left\{ \prod_{k=1}^{r} g_1\big(t_{k:r:n}\big) \Big[1 - G_1\big(t_{k:r:n}\big)\Big]^{R_k} \right\} \\ &= \frac{C_p}{\theta_1^r} \exp\left\{ -\frac{1}{\theta_1} \sum_{k=1}^{r} \big(R_k + 1\big) t_{k:r:n} \right\}, \quad 0 < t_{1:r:n} < \cdots < t_{r:r:n} < \tau, \end{aligned} \tag{9.6}$$

   where

$$C_p = n(n-1-R_1)(n-2-R_1-R_2)\cdots\left(n-r+1-\sum_{k=1}^{r-1} R_k\right) = \prod_{j=1}^{r} R_j^{\star} \tag{9.7}$$

   and $R_j^{\star} = \sum_{k=j}^{r} (R_k + 1)$.

2. If $N_1 = 0$ and $N_2 = r$ in (9.5), the likelihood function of θ_1 and θ_2 is

$$\begin{aligned} L(\theta_1, \theta_2 | \boldsymbol{t}) &= C_p \left\{ \prod_{k=1}^{r} g_2\big(t_{k:r:n}\big) \Big[1 - G_2\big(t_{k:r:n}\big)\Big]^{R_k} \right\} \\ &= \frac{C_p}{\theta_2^r} \exp\left\{ -\frac{1}{\theta_2} \sum_{k=1}^{r} \big(R_k + 1\big)\big(t_{k:r:n} - \tau\big) - \frac{1}{\theta_1} \sum_{k=1}^{r} \big(R_k + 1\big)\tau \right\}, \\ &\qquad \tau < t_{1:r:n} < \cdots < t_{r:r:n} < \infty. \end{aligned} \tag{9.8}$$

3. In all other cases, the likelihood function of θ_1 and θ_2 is

$$\begin{aligned} L(\theta_1, \theta_2 | \boldsymbol{t}) &= C_p \left\{ \prod_{k=1}^{N_1} g_1\big(t_{k:r:n}\big) \Big[1 - G_1\big(t_{k:r:n}\big)\Big]^{R_k} \right\} \\ &\quad \times \left\{ \prod_{k=N_1+1}^{r} g_2\big(t_{k:r:n}\big) \Big[1 - G_2\big(t_{k:r:n}\big)\Big]^{R_k} \right\} \\ &= \frac{C_p}{\theta_1^{N_1} \theta_2^{N_2}} \exp\left\{ -\frac{1}{\theta_1} D_1 - \frac{1}{\theta_2} D_2 \right\}, \\ &\qquad 0 < t_{1:r:n} < \cdots < t_{N_1:r:n} \le \tau < t_{N_1+1:r:n} < \cdots < t_{r:r:n} < \infty, \end{aligned} \tag{9.9}$$

where $r = N_1 + N_2$ $(2 \le r \le n)$ and

$$D_1 = \sum_{k=1}^{N_1} \big(R_k + 1\big) t_{k:r:n} + \tau \sum_{k=N_1+1}^{r} \big(R_k + 1\big),$$

$$D_2 = \sum_{k=N_1+1}^{r} \big(R_k + 1\big)\big(t_{k:r:n} - \tau\big).$$

From the likelihood functions in (9.6), (9.7) and (9.8), we observe the following:

(1) If $N_1 = r$ and $N_2 = 0$ in (9.5), the MLE of θ_2 does not exist;
(2) If $N_1 = 0$ and $N_2 = r$ in (2.5), the MLE of θ_1 does not exist;
(3) If at least one failure occurs before τ and after τ in (9.5), the MLEs of θ_1 and θ_2 do exist, and $\big(D_1, D_2\big)$ is a joint complete sufficient statistic for (θ_1, θ_2). In this situation, the log-likelihood function of θ_1 and θ_2 is obtained from (9.9) as

$$l(\theta_1, \theta_2|\boldsymbol{t}) = \log C_p - N_1 \log \theta_1 - N_2 \log \theta_2 - \frac{D_1}{\theta_1} - \frac{D_2}{\theta_2}. \tag{9.10}$$

From (9.10), the MLEs of θ_1 and θ_2 are readily obtained as

$$\hat{\theta}_1 = \frac{D_1}{N_1} \qquad \text{and} \qquad \hat{\theta}_2 = \frac{D_2}{N_2}, \tag{9.11}$$

respectively.

Remark 1. In the model considered above, we have not assumed any relationship between the mean failure times under two stress levels.

Remark 2. In some situations, we may know the mean failure time $\theta_2 = \lambda\theta_1$ for a known λ. In this situation, the MLE of θ_1 exists when at least one failure occurs, and its exact distribution can be derived explicitly. One can also use the likelihood ratio test to test the hypothesis $H_0 :\ \theta_2 = \lambda\theta_1$ for a specified λ.

9.3 Conditional Distributions of the MLEs

To find the exact conditional distributions of $\hat{\theta}_1$ and $\hat{\theta}_2$, we first derive the joint conditional moment generating function (CMGF) of $\hat{\theta}_1$ and $\hat{\theta}_2$, conditioned on the event $\big\{1 \le N_1 \le r-1\big\}$, and then obtain from it the CMGFs of $\hat{\theta}_1$ and $\hat{\theta}_2$. For notational convenience, we denote $M_{12}(\nu, \omega|N_1\big)$ for the joint CMGF of $\hat{\theta}_1$ and $\hat{\theta}_2$, and $M_k\big(\omega|N_1\big)$ for the CMGF of $\hat{\theta}_k,\ k = 1, 2$. Evidently, we can write

$$\begin{aligned} M_{12}\big(\nu, \omega|N_1\big) &= \mathrm{E}\Big\{e^{\nu\hat{\theta}_1 + \omega\hat{\theta}_2}\big|1 \le N_1 \le r-1\Big\} \\ &= \sum_{i=1}^{r-1} \mathrm{E}_{\theta_1,\theta_2}\Big\{e^{\nu\hat{\theta}_1 + \omega\hat{\theta}_2}\big|N_1 = i\Big\} \cdot \mathrm{P}_{\theta_1,\theta_2,c}\big\{N_1 = i\big\} \end{aligned} \tag{9.12}$$

and

$$M_k(\omega|N_1) = \mathrm{E}\Big\{e^{\omega\hat{\theta}_k}\big|1 \le N_1 \le r-1\Big\}$$
$$= \sum_{i=1}^{r-1} \mathrm{E}_{\theta_1,\theta_2}\Big\{e^{\omega\hat{\theta}_k}\big|N_1 = i\Big\} \cdot \mathrm{P}_{\theta_1,\theta_2,c}\big\{N_1 = i\big\}, \tag{9.13}$$

where

$$\mathrm{P}_{\theta_1,\theta_2,c}\big\{N_1 = i\big\} = \mathrm{P}\Big\{N_1 = i \;\Big|\; 1 \le N_1 \le r-1\Big\}.$$

In order to obtain $\mathrm{P}\Big\{N_1 = i \;\Big|\; 1 \le N_1 \le r-1\Big\}$, we need the following lemma.

Lemma 1. *Let $T_{1:r:n} < \cdots < T_{r:r:n}$ denote the progressively Type-II censored sample from the cumulative exposure PDF $g(t)$ given in (9.4). Then, the joint density function of $T_{1:r:n}, \ldots, T_{r:r:n}$ is [see Balakrishnan and Aggarwala (2000)]*

$$f\big(t_1,\ldots,t_r\big)$$
$$= C_p\left\{\prod_{k=1}^{N_1} g_1\big(t_k\big)\Big[1-G_1\big(t_k\big)\Big]^{R_k}\right\}\left\{\prod_{k=N_1+1}^{r} g_2\big(t_k\big)\Big[1-G_2\big(t_k\big)\Big]^{R_k}\right\},$$
$$0 < t_1 < \cdots < t_{N_1} \le \tau < t_{N_1+1} < \cdots < t_r \le \infty; \tag{9.14}$$

further, the probability of the event $\big\{N_1 = i,\ i = 1,\ldots,r-1\big\}$ is given by

$$\mathrm{P}\big\{N_1 = i\big\} = C_p \sum_{k=0}^{i}\sum_{l=0}^{r-i-1} \frac{C_{k,i}(\mathbf{S_i})C_{l,r-i-1}(\mathbf{S}_{i+\mathbf{1}})}{B_{l,r-i}(\mathbf{S}_{i+\mathbf{1}})} \cdot \exp\left\{-\frac{\tau}{\theta_1}\sum_{j=i-k+1}^{r} S_j\right\}, \tag{9.15}$$

where

$$S_j = R_j + 1, \qquad \mathbf{S_i} = (S_1,\ldots,S_i), \qquad \mathbf{S}_{i+\mathbf{1}} = (S_{i+1},\ldots,S_{i+l}),$$
$$B_{l,r-i}(\mathbf{S}_{i+\mathbf{1}}) = \sum_{j=r-i-l}^{r-i} S_{i+j} \quad \text{with} \quad \sum_{j=i}^{0} A_j \equiv 0,$$
$$C_{k,i}(\mathbf{S_i}) = \frac{(-1)^k}{\Big\{\prod_{j=1}^{k}\sum_{m=i-k+1}^{i-k+j} S_m\Big\}\Big\{\prod_{j=1}^{i-k}\sum_{m=j}^{i-k} S_m\Big\}},$$
$$C_{l,r-i-1}(\mathbf{S}_{i+\mathbf{1}}) = \frac{(-1)^l}{\Big\{\prod_{j=1}^{l}\sum_{m=r-i-l}^{r-i-l+j-1} S_{i+m}\Big\}\Big\{\prod_{j=1}^{r-i-l-1}\sum_{m=j}^{r-i-l-1} S_{i+m}\Big\}},$$

with $\prod_{j=1}^{0} A_j \equiv 1$ and C_p is as given earlier in (9.7).

Proof. We have

$$\mathrm{P}\big\{N_1 = i\big\} = \int_\tau^\infty\int_\tau^{t_r}\cdots\int_\tau^{t_{i+2}}\int_0^\tau\cdots\int_0^{t_2} f\big(t_1,\ldots,t_r\big)\mathrm{d}t_1\cdots\mathrm{d}t_i\mathrm{d}t_{i+1}\cdots\mathrm{d}t_r$$
$$C_p\left(=\int_0^\tau\cdots\int_0^{t_2}\prod_{k=1}^{i} g_1\big(t_k\big)\Big\{1-G_1\big(t_k\big)\Big\}^{R_k}\mathrm{d}t_1\cdots\mathrm{d}t_i\right)$$
$$\times\left(\int_\tau^\infty\int_\tau^{t_r}\cdots\int_\tau^{t_{i+2}}\prod_{k=i+1}^{r} g_2\big(t_k\big)\Big\{1-G_2\big(t_k\big)\Big\}^{R_k}\mathrm{d}t_{i+1}\cdots\mathrm{d}t_{r-1}\mathrm{d}t_r\right).$$

Upon substituting the expressions for $g_1(\cdot), g_2(\cdot)$, $G_1(\cdot)$ and $G_2(\cdot)$, (9.15) follows from the identity

$$\int_a^{x_{m+1}} \cdots \int_a^{x_3} \int_a^{x_2} \prod_{j=1}^{m} f(x_j)\Big\{1 - F(x_j)\Big\}^{A_j - 1} \mathrm{d}x_1 \mathrm{d}x_2 \cdots \mathrm{d}x_m$$

$$= \sum_{k=0}^{m} C_{k,m}(\boldsymbol{A_m})\Big\{1 - F(x_{m+1})\Big\}^{B_{k,m}(\boldsymbol{A_m})}\big\{1 - F(a)\big\}^{\sum_{j=1}^{m-k} A_j}, \tag{9.16}$$

where $f(x)$ and $F(x)$ denote the PDF and CDF of an absolutely continuous random X. Here, $A_j > 0$ for $j = 1, \ldots, m$, $\boldsymbol{A_m} = (A_1, \ldots, A_m)$,

$$B_{k,m}(\boldsymbol{A_m}) = \sum_{j=m-k+1}^{m} A_j$$

and

$$C_{k,m}(\boldsymbol{A_m}) = \frac{(-1)^k}{\Big\{\prod_{j=1}^{k} \sum_{l=m-k+1}^{m-k+j} A_l\Big\}\Big\{\prod_{j=1}^{m-k} \sum_{l=j}^{m-k} A_l\Big\}}$$

with the usual conventions that $\prod_{j=1}^{0} A_j \equiv 1$ and $\sum_{j=i}^{0} A_j \equiv 0$. ■

From Lemma 1, we have the conditional probability of $N_1 = i$, given $1 \le N_1 \le r-1$, as

$$\mathrm{P}_{\theta_1,\theta_2,c}\big\{N_1 = i\big\} = \frac{\mathrm{P}\big\{N_1 = i\big\}}{\sum_{j=1}^{r-1} \mathrm{P}\big\{N_1 = j\big\}}, \tag{9.17}$$

where $\mathrm{P}\big\{N_1 = i\big\}$ is as presented in (9.15).

Now, for the derivation of the conditional expectation $\mathrm{E}_{\theta_1,\theta_2}\Big\{e^{\nu\hat{\theta}_1 + \omega\hat{\theta}_2}\big|N_1 = i\Big\}$, we need the following lemma.

Lemma 2. *The joint conditional density of $T_{1:r:n}, \ldots, T_{r:r:n}$, given $N_1 = i$, is given by [see Balakrishnan and Aggarwala (2000)]*

$$f(t_1, \ldots, t_r | N_1 = i) = \frac{C_p}{\mathrm{P}\big\{N_1 = i\big\}}\left\{\prod_{k=1}^{i} g_1(t_k)\Big[1 - G_1(t_k)\Big]^{R_k}\right\}$$
$$\times\left\{\prod_{k=i+1}^{r} g_2(t_k)\Big[1 - G_2(t_k)\Big]^{R_k}\right\}, \tag{9.18}$$
$$0 < t_1 < \cdots < t_i \le \tau < t_{i+1} < \cdots < t_r \le \infty,$$

where $\mathrm{P}\big\{N_1 = i\big\}$ is as given in (9.15).

Theorem 1. *The joint CMGF of $\hat{\theta}_1$ and $\hat{\theta}_2$, given $1 \le N_1 \le r-1$, is*

$$M_{12}(\nu, \omega | N_1) = D \sum_{i=1}^{r-1} \sum_{k=0}^{i} \sum_{l=0}^{r-i-1} D_{ikl} \cdot \frac{e^{\frac{\tau}{i}\sum_{j=i-k+1}^{r} S_j \nu}}{\big(1 - \frac{\theta_1}{i}\nu\big)^i \big(1 - \frac{\theta_2}{r-i}\omega\big)^{r-i}}, \nu < \frac{1}{\theta_1}, \omega < \frac{1}{\theta_2}, \tag{9.19}$$

where

$$D = \frac{C_p}{\sum_{j=1}^{r-1} \mathrm{P}\{N_1 = j\}},$$

$$D_{ikl} = \frac{C_{k,i}(\mathbf{S_i}) C_{l,r-i-1}(\mathbf{S_{i+1}})}{B_{l,r-i}(\mathbf{S_{i+1}})} \cdot \exp\left\{ -\frac{\tau}{\theta_1} \sum_{j=i-k+1}^{r} S_j \right\}$$

and C_p is as defined earlier.

Proof. Using (9.16) and the results in Lemmas 1 and 2 into Eq. (9.12), and simplifying the resulting expression, we obtain (9.19). ■

Corollary 1. *The CMGF of $\hat{\theta}_1$, given $1 \le N_1 \le r-1$, is*

$$M_1(\omega|N_1) = D \sum_{i=1}^{r-1} \sum_{k=0}^{i} \sum_{l=0}^{r-i-1} D_{ikl} \cdot \frac{e^{\frac{\tau}{i}\sum_{j=i-k+1}^{r} S_j \omega}}{\left(1 - \frac{\theta_1}{i}\omega\right)^i}, \qquad \omega < \frac{1}{\theta_1}. \tag{9.20}$$

Proof. From Theorem 1, we readily obtain (9.20). ■

Corollary 2. *The CMGF of $\hat{\theta}_2$, given $1 \le N_1 \le r-1$, is*

$$M_2(\omega|N_1) = D \sum_{i=1}^{r-1} \sum_{k=0}^{i} \sum_{l=0}^{r-i-1} D_{ikl} \cdot \frac{1}{\left(1 - \frac{\theta_2}{r-i}\omega\right)^{r-i}}, \qquad \omega < \frac{1}{\theta_2}. \tag{9.21}$$

Proof. From Theorem 1, we readily obtain (9.21). ■

Now, in order to obtain the exact joint conditional density of $\hat{\theta}_1$ and $\hat{\theta}_2$, we need the following lemma.

Lemma 3. *If X is a gamma random variable with shape parameter α and scale parameter β, then the PDF of $Y = X + h$ is of the form*

$$\gamma(x - h; \alpha, \beta) = \begin{cases} \frac{1}{\Gamma(\alpha)\beta^\alpha} \left(x-h\right)^{\alpha-1} \mathrm{e}^{-(x-h)/\beta} & \text{if } x > h \\ 0 & \text{otherwise} \end{cases}, \tag{9.22}$$

and the MGF of $Y = X + h$ is of the form

$$M_Y(\omega) = \frac{e^{\omega h}}{\left(1 - \beta\omega\right)^\alpha}, \qquad |\omega| < 1/\beta. \tag{9.23}$$

Proof. The proof follows from the well-known properties of the gamma distribution; see, for example, Johnson et al. (1994). ■

Theorem 2. *The joint conditional PDF of $\hat{\theta}_1$ and $\hat{\theta}_2$, given $1 \le N_1 \le r-1$, is*

$$f_{\hat{\theta}_1,\hat{\theta}_2}(x,y) = D \sum_{i=1}^{r-1} \sum_{k=0}^{i} \sum_{l=0}^{r-i-1} D_{ikl} \cdot \gamma\left(x - \tau_{ik}; i, \frac{\theta_1}{i}\right) \cdot \gamma\left(y; r-i, \frac{\theta_2}{r-i}\right), \tag{9.24}$$

where $\tau_{ik} = \frac{\tau}{i} \sum_{j=i-k+1}^{r} (R_j + 1)$ and $\gamma(\cdot)$ is as defined in (9.22).

PROOF. The result follows readily from (9.19) upon using Lemma 3. ■

Theorem 3. *The conditional PDF of* $\hat{\theta}_1$*, given* $1 \le N_1 \le r-1$*, is*

$$f_{\hat{\theta}_1}(x) = D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\cdot\gamma\left(x-\tau_{ik}; i, \frac{\theta_1}{i}\right), \tag{9.25}$$

where $\gamma(\cdot)$ *is as defined in (9.22).*

PROOF. The result follows readily from (9.20) upon using Lemma 3. ■

Theorem 4. *The conditional PDF of* $\hat{\theta}_2$*, given* $1 \le N_1 \le r-1$*, is*

$$f_{\hat{\theta}_2}(x) = D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\cdot\gamma\left(x; r-i, \frac{\theta_2}{r-i}\right), \tag{9.26}$$

where $\gamma(\cdot)$ *is as defined in (9.22).*

PROOF. The result follows readily from (9.21) upon using Lemma 3. ■

Remark 3. If $R_1 = \cdots = R_{r-1} = 0$ and $R_r = n-r$, which corresponds to the conventional Type-II right censoring scheme, Eq. (9.24) becomes

$$f_{\hat{\theta}_1,\hat{\theta}_2}(x,y) = D^*\sum_{i=1}^{r-1}\sum_{k=0}^{i} D^*_{ik}\cdot\gamma\left(x-\tau_{ik}; i, \frac{\theta_1}{i}\right)\cdot\gamma\left(y; r-i, \frac{\theta_2}{r-i}\right), \tag{9.27}$$

where $D^* = \left\{\sum_{j=1}^{r-1}\binom{n}{j}p^j(1-p)^{n-j}\right\}^{-1}$ and $D^*_{ik} = (-1)^k\binom{n}{i}\binom{i}{k}(1-p)^{n-i+k}$ with $p = 1-e^{-\tau/\theta_1}$. Furthermore, the marginal conditional densities of $\hat{\theta}_1$ and $\hat{\theta}_2$ in this case become

$$f_{\hat{\theta}_1}(x) = D^*\sum_{i=1}^{r-1}\sum_{k=0}^{i} D^*_{ik}\cdot\gamma\left(x-\tau_{ik}; i, \frac{\theta_1}{i}\right) \tag{9.28}$$

and

$$f_{\hat{\theta}_2}(x) = D^*\sum_{i=1}^{r-1}\binom{n}{i}p^i(1-p)^{n-i}\cdot\gamma\left(x; r-i, \frac{\theta_2}{r-i}\right), \tag{9.29}$$

respectively. The expressions in Eqs. (9.28) and (9.29) are exactly the same expressions as derived by Balakrishnan et al. (2007).

Corollary 3. *The mean and variance of* $\hat{\theta}_1$ *are given by*

$$\mathrm{E}(\hat{\theta}_1) = \theta_1 + D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\ \tau_{ik} \tag{9.30}$$

and

$$\mathrm{Var}(\hat{\theta}_1) = D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\left(\tau_{ik}^2 + \frac{\theta_1^2}{i}\right) - \left(D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\ \tau_{ik}\right)^2, \tag{9.31}$$

respectively.

PROOF. These expressions follow readily from the conditional PDF of $\hat{\theta}_1$ in (9.25). ■

Corollary 4. *The mean and variance of* $\hat{\theta}_2$ *are*

$$\mathrm{E}\big(\hat{\theta}_2\big) = \theta_2 \tag{9.32}$$

and

$$\mathrm{Var}\big(\hat{\theta}_2\big) = D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\cdot\frac{\theta_2^2}{r-i}, \tag{9.33}$$

respectively.

PROOF. These expressions follow readily from the conditional PDF of $\hat{\theta}_2$ in (3.15). ■

Remark 4. From (9.30), we observe that $\hat{\theta}_1$ is a biased estimator of θ_1 while $\hat{\theta}_2$ is observed from (9.32) to be an unbiased estimator of θ_2. Furthermore, from the joint density of $\hat{\theta}_1$ and $\hat{\theta}_2$ in (9.24), we obtain

$$\begin{aligned}\mathrm{E}\big(\hat{\theta}_1\hat{\theta}_2\big) &= D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\left(\tau_{_{ik}} + i\frac{\theta_1}{i}\right)\left[(r-i)\frac{\theta_2}{r-i}\right]\\ &= D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\big(\tau_{_{ik}} + \theta_1\big)\theta_2\\ &= \mathrm{E}\big(\hat{\theta}_1\big)\mathrm{E}\big(\hat{\theta}_2\big)\end{aligned}$$

so that $\mathrm{Cov}\big(\hat{\theta}_1, \hat{\theta}_2\big) = 0$.

Corollary 5. *The tail probabilities of* $\hat{\theta}_1$ *and* $\hat{\theta}_2$*, given* $1 \le N_1 \le r-1$*, are*

$$\mathrm{P}_{\theta_1}\Big\{\hat{\theta}_1 > \xi\Big\} = D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\cdot\Gamma\left(\frac{i}{\theta_1}\big\langle\xi - \tau_{_{ik}}\big\rangle; i\right) \tag{9.34}$$

and

$$\mathrm{P}_{\theta_2}\Big\{\hat{\theta}_2 > \xi\Big\} = D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\cdot\Gamma\left(\frac{r-i}{\theta_2}\big\langle\xi\big\rangle; r-i\right), \tag{9.35}$$

respectively, where $\big\langle w\big\rangle = \max\{0, w\}$ *and*

$$\Gamma(w;\alpha) = \int_w^\infty \gamma\big(x;\alpha,1\big)dx = \int_w^\infty \frac{1}{\Gamma(\alpha)}x^{\alpha-1}e^{-x}dx.$$

PROOF. The expressions in (9.34) and (9.35) follow by integration from (9.25) and (9.26), respectively. ■

9.4 Confidence Intervals

In this section, we present different methods of constructing confidence intervals (CIs) for the unknown parameters θ_1 and θ_2. From Theorems 3 and 4, we can construct the exact CI for θ_1 and θ_2, respectively. Since the exact conditional PDF of $\hat{\theta}_1$ and $\hat{\theta}_2$ are quite complicated, we also present the approximate CIs for θ_1 and θ_2 for larger sample sizes. Finally, we use the parametric bootstrap method to construct CIs for θ_1 and θ_2.

9.4.1 Exact confidence intervals

To guarantee the invertibility for the parameters θ_1 and θ_2, we assume that the tail probabilities of $\hat{\theta}_1$ and $\hat{\theta}_2$ presented in Corollary 5 are increasing functions of θ_1 and θ_2, respectively. Several authors including Chen and Bhattacharyya (1988), Kundu and Basu (2000), and Childs et al. (2003) have used this approach to construct exact CI in different contexts. Like all of them, we are also unable to establish the required monotonicity, but the extensive numerical computations we carried out seem to support this monotonicity assumption; see figure 9.3, for example.

(1) **CI for $\boldsymbol{\theta_1}$**
The exact CI for θ_1 can be constructed by solving the equations

$$\mathrm{P}_{\theta_{1L}}\Big\{\hat{\theta}_1 > \hat{\theta}_{obs}\Big\} = \frac{\alpha}{2} \quad \text{and} \quad \mathrm{P}_{\theta_{1U}}\Big\{\hat{\theta}_1 > \hat{\theta}_{obs}\Big\} = 1 - \frac{\alpha}{2}$$

for θ_{1L} (the lower bound of θ_1) and θ_{1U} (the upper bound of θ_1), respectively.
A two-sided $100(1-\alpha)\%$ CI for θ_1, denoted by $(\theta_{1L}, \theta_{1U})$, can then be obtained by solving the following two non-linear equations (by using the bisection method):

$$\frac{\alpha}{2} = D\big(\theta_{1L}, \hat{\theta}_2\big) \sum_{i=1}^{r-1} \sum_{k=0}^{i} \sum_{l=0}^{r-i-1} D_{ikl}\big(\theta_{1L}, \hat{\theta}_2\big) \cdot \Gamma\bigg(\frac{i}{\theta_{1L}} \big\langle \hat{\theta}_1 - \tau_{_{ik}} \big\rangle; i\bigg)$$

and

$$1 - \frac{\alpha}{2} = D\big(\theta_{1U}, \hat{\theta}_2\big) \sum_{i=1}^{r-1} \sum_{k=0}^{i} \sum_{l=0}^{r-i-1} D_{ikl}\big(\theta_{1U}, \hat{\theta}_2\big) \cdot \Gamma\bigg(\frac{i}{\theta_{1U}} \big\langle \hat{\theta}_1 - \tau_{_{ik}} \big\rangle; i\bigg),$$

where $D,\ D_{ikl},\ \tau_{_{ik}}$ and $\Gamma(w;\alpha)$ are all as defined earlier.

(2) **CI for $\boldsymbol{\theta_2}$**
Similarly, a two-sided $100(1-\alpha)\%$ CI for θ_2, denoted by $(\theta_{2L}, \theta_{2U})$, can be obtained by solving the following two non-linear equations:

$$\frac{\alpha}{2} = D\big(\hat{\theta}_1, \theta_{2L}\big) \sum_{i=1}^{r-1} \sum_{k=0}^{i} \sum_{l=0}^{r-i-1} D_{ikl}\big(\hat{\theta}_1, \theta_{2L}\big) \cdot \Gamma\bigg(\frac{r-i}{\theta_{2L}} \big\langle \hat{\theta}_2 \big\rangle; r-i\bigg)$$

and

$$1 - \frac{\alpha}{2} = D\big(\hat{\theta}_1, \theta_{2U}\big) \sum_{i=1}^{r-1} \sum_{k=0}^{i} \sum_{l=0}^{r-i-1} D_{ikl}\big(\hat{\theta}_1, \theta_{2U}\big) \cdot \Gamma\bigg(\frac{r-i}{\theta_{2U}} \big\langle \hat{\theta}_2 \big\rangle; r-i\bigg),$$

where $D,\ D_{ikl},\ \tau_{_{ijk}}$ and $\Gamma(w;\alpha)$ are all as defined earlier.

9.4.2 Asymptotic confidence intervals

For large N_1 and N_2, the observed Fisher information matrix of θ_1 and θ_2 is

$$\hat{I}(\theta_1,\theta_2) = \begin{bmatrix} \hat{I}_{11} & \hat{I}_{12} \\ \hat{I}_{21} & \hat{I}_{11} \end{bmatrix}_{\theta_1=\hat{\theta}_1,\theta_2=\hat{\theta}_2} = \begin{bmatrix} \frac{N_1}{\hat{\theta}_1^2} & 0 \\ 0 & \frac{N_2}{\hat{\theta}_2^2} \end{bmatrix}, \tag{9.36}$$

where

$$\hat{I}_{ij} = -\mathrm{E}\left\{ \frac{\partial^2 l(\theta_1,\theta_2|\boldsymbol{t})}{\partial\theta_i\partial\theta_j} \right\}\Bigg|_{\theta_1=\hat{\theta}_1,\theta_2=\hat{\theta}_2}, \quad i,j=1,2,$$

and $\hat{\theta}_1$ and $\hat{\theta}_2$ are as in (9.11). The asymptotic variances of $\hat{\theta}_1$ and $\hat{\theta}_2$ can be obtained from (9.36) as

$$V_{11} = \widehat{\mathrm{Var}}(\hat{\theta}_1) = \frac{\hat{\theta}_1^2}{N_1} \quad \text{and} \quad V_{22} = \widehat{\mathrm{Var}}(\hat{\theta}_2) = \frac{\hat{\theta}_2^2}{N_2}.$$

We can then express two-sided $100(1-\alpha)\%$ approximate CIs for θ_1 and θ_2 as

$$(\hat{\theta}_1 - W) \pm z_{1-\alpha/2}\sqrt{V_{11}} \quad \text{and} \quad \hat{\theta}_2 \pm z_{1-\alpha/2}\sqrt{V_{22}},$$

where

$$W = D(\hat{\theta}_1,\hat{\theta}_2)\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}(\hat{\theta}_1,\hat{\theta}_2)\ \tau_{ik},$$

and $z_{1-\alpha/2}$ is the upper $(\alpha/2)$ percentile of the standard normal distribution.

9.4.3 Bootstrap confidence intervals

In this subsection, we present several bootstrap methods to construct CIs for θ_1 and θ_2, viz., Studentized-t interval, Percentile interval, and Adjusted percentile (BCa) interval; see Efron and Tibshirani (1998) and Hall (1988) for details. First, we describe the algorithm to obtain the progressively Type-II censored sample. This algorithm will be utilized in the resampling needed for the bootstrap confidence intervals in the following subsections.

Bootstrap progressively Type-II sample

Step 1. Given τ and the original progressively Type-II censored sample with the censoring scheme $\boldsymbol{R} = (R_1,\ldots,R_r)$, we obtain $\hat{\theta}_1$ and $\hat{\theta}_2$ from (9.11).

Step 2. Based on n, r, $\boldsymbol{R}$, τ, $\hat{\theta}_1$ and $\hat{\theta}_2$, we generate a random sample of size n from Uniform$(0,1)$ distribution, and obtain the progressively Type-II censored uniform sample $(U_{1:r:n},\ldots,U_{r:r:n})$, using the algorithm of Balakrishnan and Sandhu (1995).

Step 3. Find N_1 such that

$$U_{N_1:r:n} < 1 - e^{-\tau/\hat{\theta}_1} \le U_{N_1+1:r:n}\ .$$

Then, for $1 \le k \le N_1$, we set

$$t^*_{k:r:n} = -\hat{\theta}_1 \log\left(1 - U_{k:r:n}\right)$$

and for $N_1 + 1 \le k \le r$, we set

$$t^*_{k:r:n} = \tau - \hat{\theta}_2 \log\left(1 - U_{k:r:n}\right) - \frac{\hat{\theta}_2}{\hat{\theta}_1}\tau.$$

Step 4. Based on $r,\ N_1,\ \tau$ and the progressively Type-II censored sample

$$\left\{t^*_{1:r:n}, \ldots, t^*_{N_1:r:n}, t^*_{N_1+1:r:n}, \ldots, t^*_{r:r:n}\right\},$$

we obtain $\hat{\theta}^*_1$ and $\hat{\theta}^*_2$ from (2.11).

Step 5. Repeat Steps 2-4 M times and arrange all $\hat{\theta}^*_1$'s and $\hat{\theta}^*_2$'s in ascending order to obtain the bootstrap sample

$$\left\{\hat{\theta}^{*[1]}_k, \hat{\theta}^{*[2]}_k, \ldots, \hat{\theta}^{*[M]}_k\right\}, \quad k = 1, 2.$$

Studentized-t interval

1. First, we consider the statistic

$$T^{*[j]}_k = \frac{\hat{\theta}^{*[j]}_k - \hat{\theta}_k}{\sqrt{V\left(\hat{\theta}^*_k\right)}}, \quad j = 1, \ldots, M,\ k = 1, 2.$$

We then obtain the ordered bootstrap sample $T^{*[1]}_k < \cdots < T^{*[M]}_k$.

2. Next, we consider all possible $100(1-\alpha)\%$ CIs of the form

$$\left(T^{*[i]}_k,\ T^{*[(1-\alpha)M+i]}_k\right), \quad i = 1, \ldots, \alpha M,\ k = 1, 2,$$

and choose the interval for which the width is minimum, say $\left(T^*_{kL}, T^*_{kU}\right)$.

3. A two-sided $100(1-\alpha)\%$ Studentized-t bootstrap confidence interval for θ_k is either

$$\left(\hat{\theta}_k - T^*_{kL}\sqrt{V\left(\hat{\theta}_k\right)},\ \hat{\theta}_k - T^*_{kU}\sqrt{V\left(\hat{\theta}_k\right)}\right) \tag{9.37}$$

or

$$\left(\hat{\theta}_k - T^{*[(1-\alpha/2)M]}_k\sqrt{V\left(\hat{\theta}_k\right)},\ \hat{\theta}_k - T^{*[\alpha M/2]}_k\sqrt{V\left(\hat{\theta}_k\right)}\right), \tag{9.38}$$

where $V\left(\hat{\theta}_k\right)$ can be estimated by the asymptotic variance from the original progressively Type-II censored sample.

It is of interest to mention here that we could use the sample variance of the bootstrap sample of $\hat{\theta}_k$ as an estimate of $V\left(\hat{\theta}_k\right)$ instead of the asymptotic variance in Eqs. (9.37) and (9.38). However, we found in our Monte Carlo simulations that the use of the asymptotic variance resulted in better coverage probabilities in general. Furthermore, of the two confidence intervals presented in (9.37) and (9.38), we found the confidence interval in (9.37) to have better coverage probabilities in general than the confidence interval in (9.38). Therefore, all the numerical results we have presented in tables 9.1–9.4 and tables 9.8–9.11 are based on the formula in (9.37).

Percentile interval

1. First, we consider all possible $100(1-\alpha)\%$ CIs of the form

$$\left(\hat{\theta}_k^{*[i]},\ \hat{\theta}_k^{*[(1-\alpha)M+i]}\right), \quad i=1,\ldots,\alpha M,\ k=1,2,$$

and choose the interval with minimum width, say $\left(\hat{\theta}_{kL}^{*},\ \hat{\theta}_{kU}^{*}\right)$.

2. A two-sided $100(1-\alpha)\%$ Percentile bootstrap confidence interval for θ_k is either

$$\left(\hat{\theta}_{kL}^{*},\ \hat{\theta}_{kU}^{*}\right) \quad \text{or} \quad \left(\hat{\theta}_k^{*[\alpha M/2]},\ \hat{\theta}_k^{*[(1-\alpha/2)M]}\right).$$

Adjusted percentile (BCa) interval

A two-sided $100(1-\alpha)\%$ BCa bootstrap confidence interval for θ_k is

$$\left(\hat{\theta}_k^{*[\alpha_{1k}M]},\ \hat{\theta}_k^{*[(1-\alpha_{2k})M]}\right), \quad k=1,2,$$

where

$$\alpha_{1k}=\Phi\left\{\hat{z}_{0k}+\frac{\hat{z}_{0k}+z_{\alpha/2}}{1-\hat{a}_k(\hat{z}_{0k}+z_{\alpha/2})}\right\}$$

and

$$\alpha_{2k}=\Phi\left\{\hat{z}_{0k}+\frac{\hat{z}_{0k}+z_{1-\alpha/2}}{1-\hat{a}_k(\hat{z}_{0k}+z_{1-\alpha/2})}\right\}.$$

Here, $\Phi(\cdot)$ is the CDF of the standard normal distribution, and

$$\hat{z}_{0k}=\Phi^{-1}\left\{\frac{\#\text{ of }\hat{\theta}_k^{*[j]}<\hat{\theta}_k}{M}\right\}, \quad j=1,\ldots,M,\ k=1,2.$$

A good estimate of the acceleration factor a_k is

$$\hat{a}_k=\frac{\sum_{i=1}^{N_k}\left[\hat{\theta}_k^{(\cdot)}-\hat{\theta}_k^{(i)}\right]^3}{6\left\{\sum_{i=1}^{N_k}\left[\hat{\theta}_k^{(\cdot)}-\hat{\theta}_k^{(i)}\right]^2\right\}^{3/2}}, \quad i=1,\ldots,N_k,\ k=1,2,$$

where $\hat{\theta}_k^{(i)}$ is the MLE of θ_k based on the simulated progressively Type-II censored sample with the i^{th} observation removed (i.e., the jackknife estimate), and

$$\hat{\theta}_k^{(\cdot)}=\frac{1}{N_k}\sum_{i=1}^{N_k}\hat{\theta}_k^{(i)}, \quad i=1,\ldots,N_k,\ k=1,2,$$

where $N_1+N_2=r$.

9.5 Simulation Study

In this section, we present the results of a Monte Carlo simulation study carried out in order to compare the performance of all the methods of inference described in Section 9.4. We chose the values of the parameters θ_1 and θ_2 to be $e^{2.5}$ and $e^{1.5}$, respectively; we also chose for n the value of 20, and several different choices for τ. We then determined the true coverage probabilities of the $90\%, 95\%, 99\%$ confidence intervals for θ_1 and θ_2 by all the methods described in Section 9.4. These values, based on 1000 Monte Carlo simulations and $M = 1000$ bootstrap replications, are presented in tables 9.1–9.4 in the Appendix. For convenience notation in progressive censoring, we have used in these tables and elsewhere, for example, $(8, 4\star 0)$ to denote the progressive censoring scheme $(8, 0, 0, 0, 0)$.

From these tables, it is clear that the exact method of constructing confidence intervals (based on the exact conditional densities of $\hat{\theta}_1$ and $\hat{\theta}_2$ derived in Section 9.3) always maintains its coverage probability at the pre-fixed nominal level. The approximate method of constructing confidence intervals (based on the asymptotic normality of $\hat{\theta}_1$ and $\hat{\theta}_2$) has its true coverage probability to be always less than the nominal level. Though the coverage probability improves for large sample size, we still found it to be unsatisfactory even for n as large as 35, particularly when τ is not too large. Therefore, the approximate CIs should not be used unless n is considerably large.

Among the three bootstrap methods of constructing confidence intervals described in Section 9.4, the Studentized-t interval seems to have considerably low coverage probabilities compared to the nominal level. The percentile interval and the adjusted percentile interval seem to have their coverage probabilities better and somewhat closer to the nominal level. Even though the percentile method seems to be sensitive, the method does improve a bit for larger sample size. Overall, the adjusted percentile method seems to be the one (among the three bootstrap methods) with somewhat satisfactory coverage probabilities and hence may be used in case of large sample sizes when the computation of the exact CIs becomes difficult.

9.6 Optimal Censoring Scheme

With $(R_1, \ldots, R_r)$ as the progressive censoring scheme in a simple step-stress test, we may consider the determination of the optimal choice of $\boldsymbol{R} = (R_1, \ldots, R_r)$, denoted by $\boldsymbol{R}^* = (R_1^*, \ldots, R_r^*)$. For determining such an optimal censoring scheme among all possible progressive censoring schemes, we could use *variance optimality*, for example, which minimizes the total variance of the MLEs. The objective function is then given by

$$\begin{aligned} \psi(\boldsymbol{R}) &= \mathrm{Var}\big(\hat{\theta}_1 + \hat{\theta}_2\big) \\ &= \mathrm{Var}\big(\hat{\theta}_1\big) + \mathrm{Var}\big(\hat{\theta}_2\big) + 2\mathrm{Cov}\big(\hat{\theta}_1, \hat{\theta}_2\big), \end{aligned} \tag{9.39}$$

where $\mathrm{Var}\big(\hat{\theta}_1\big)$ and $\mathrm{Var}\big(\hat{\theta}_2\big)$ are as given in (9.31) and (9.33), respectively. Since $\mathrm{Cov}\big(\hat{\theta}_1, \hat{\theta}_2\big) = 0$ (see Remark 4), Eq. (9.39) becomes

$$\psi(\boldsymbol{R}) = D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\left(\tau_{ik}^2 + \frac{\theta_1^2}{i} + \frac{\theta_2^2}{r-i}\right) - \left(D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\ \tau_{ik}\right)^2. \quad (9.40)$$

Hence, the optimal censoring scheme can be found by minimizing $\psi(\boldsymbol{R})$, with fixed time τ, so that

$$\psi(\boldsymbol{R}^*) \le \psi(\boldsymbol{R}).$$

However, since $\hat{\theta}_1$ is a biased estimator of θ_1 while $\hat{\theta}_2$ is an unbiased estimator of θ_2 (see Corollaries 3 and 4), it is more reasonable to consider the objective function as

$$\begin{aligned}\varphi(\boldsymbol{R}) &= \mathrm{MSE}(\hat{\theta}_1) + \mathrm{Var}(\hat{\theta}_2)\\ &= D\sum_{i=1}^{r-1}\sum_{k=0}^{i}\sum_{l=0}^{r-i-1} D_{ikl}\left(\tau_{ik}^2 + \frac{\theta_1^2}{i} + \frac{\theta_2^2}{r-i}\right) \end{aligned} \quad (9.41)$$

and determine the optimal censoring scheme $\boldsymbol{R}^*$ that minimizes the function $\varphi(\boldsymbol{R})$ in (9.41). This is referred to as *mean square error optimality*.

For $\theta_1 = e^{1.5}$ and $\theta_2 = e^{0.5}$, we have presented in tables 9.5 and 9.6 the best and worst censoring schemes with variance optimality and mean square error optimality, respectively, for different choices of $n,\ r$ and τ. The relative efficiency values of worst to best censoring schemes presented in these two tables reveal the distinct advantage of adopting an optimal censoring scheme in the simple step-stress life-test.

Furthermore, the objective function $\varphi(\boldsymbol{R})$ in (9.41) can be utilized to determine an optimal time τ for changing the stress level with a specified choice of $n,\ r,\ \boldsymbol{R},\ \theta_1$ and θ_2. Table 9.7 presents these results for different choices of $n,\ r$ and $\boldsymbol{R}$ in the cases of (1) $\theta_1 = e^{1.5}$ and $\theta_2 = e^{0.5}$, and (2) $\theta_1 = e^{2.5}$ and $\theta_2 = e^{1.5}$. These results will be quite useful in designing an optimal simple step-stress life-test with prior information on θ_1 and θ_2. For example, given $n = 12,\ r = 8,\ \theta_1 = e^{2.5}$ and $\theta_2 = e^{1.5}$, if we had planned to adopt $\boldsymbol{R} = (4,\ 7 \star 0)$ as the progressive Type-II censoring scheme in the step-stress test, then we find from table 9.7 the optimal time $\tau^* = 23.347150$. Figure 9.1 displays the relationship between time τ and $\varphi(\boldsymbol{R})$ in (9.41) for different choices of $n,\ r,\ \boldsymbol{R},\ \theta_1$ and θ_2.

Moreover, the objective function $\varphi(\boldsymbol{R})$ in (9.41) can also be utilized to determine simultaneously an optimal time τ for changing the stress level and the optimal censoring scheme $\boldsymbol{R}^*$ for a specified choice of $n,\ r,\ \theta_1$ and θ_2. In this case, we find an optimal time τ^* and the corresponding optimal progressive censoring scheme $\boldsymbol{R}^*$ when the MSE is minimum among all possible progressive Type-II censoring schemes. Figure 9.2 displays the relationship between time τ and $\varphi(\boldsymbol{R})$ in (9.41) when (i) $n = 12,\ r = 6,\ \theta_1 = e^{1.5}$ and $\theta_2 = e^{0.5}$, and (ii) $n = 16,\ r = 8,\ \theta_1 = e^{2.5}$ and $\theta_2 = e^{1.5}$ are fixed in advance.

From figure 9.2, we find that, in the case of (i), the optimal time is $\tau^* = 5.429890$, the corresponding optimal censoring scheme is $\boldsymbol{R}^* = (3\star 0,\ 6,\ 2\star 0)$, and the minimum MSE is 7.866258; in the case of (ii), the optimal time is $\tau^* = 13.10505$, the corresponding optimal censoring scheme is $\boldsymbol{R}^* = (4\star 0,\ 8,\ 3\star 0)$, and the minimum MSE is 40.95032; see figure 9.3 which, in addition to showing the optimal censoring scheme and the near optimal censoring schemes, also shows some censoring schemes which are worst from MSE point of view.

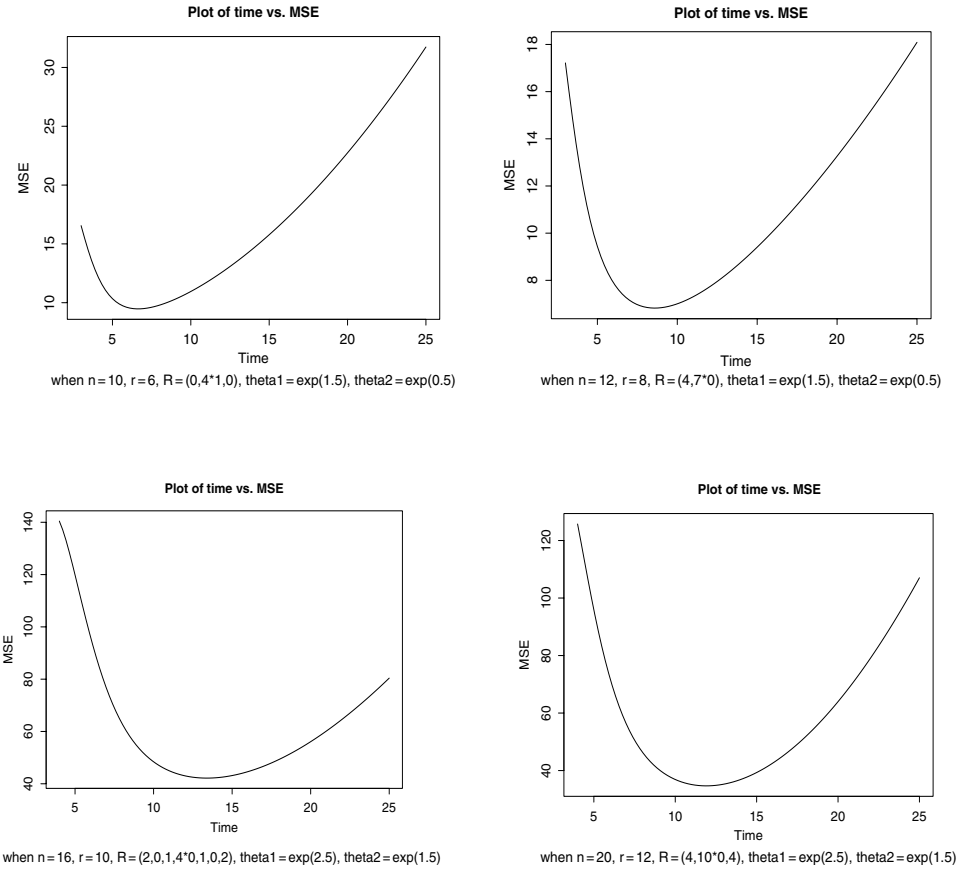

Figure 9.1. Plots of time τ vs. $\varphi(\boldsymbol{R})$ for different choices of $n,\ r,\ \theta_1$ and θ_2

9.7 Illustrative Examples

In this section, we consider two examples. Example 1 presents some plots to show the monotonicity of the tail probabilities of $\hat{\theta}_1$ and $\hat{\theta}_2$ presented in Corollary 5. Example 2 presents a data using which the estimation of θ_1 and θ_2 are illustrated for different progressive censoring schemes.

Example 1 Although we can not prove the monotonic increasing property of the tail probability functions given in Corollary 5, we present some plots of $P\{\hat{\theta}_k > \xi\}$ for different choices of $n,\ \mathbf{R}$ and τ in figure 9.4 when (1) $n = 10,\ \boldsymbol{R} = (7\star 0,\ 4)$ with $\tau = 1$, (2) $n = 20,\ \boldsymbol{R} = (4,\ 15\star 0)$ with $\tau = 3$, and (3) $n = 35,\ \boldsymbol{R} = (8\star 0, 4\star 1,\ 2, 4\star 1, 8\star 0)$ with $\tau = 5$. These plots all display the monotonicity of the probabilities of interest.

Example 2 Let us consider the following data when $n = 20$ with $\tau = 5,\ \theta_1 = e^{2.5}$ and $\theta_2 = e^{1.5}$:

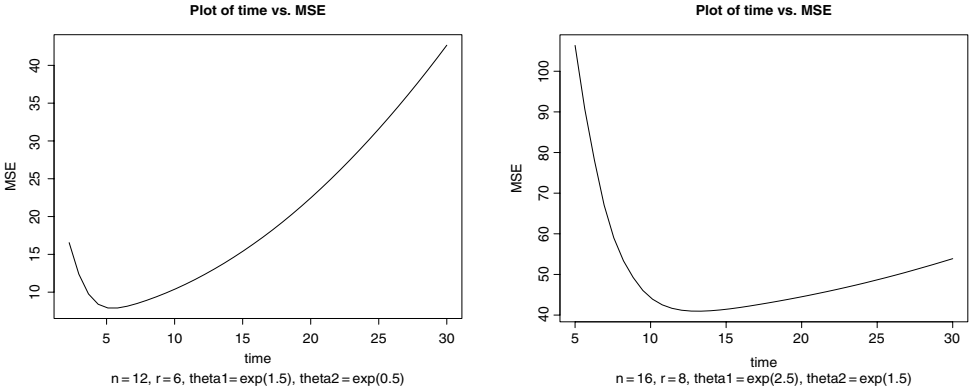

Figure 9.2. Plots of time τ vs. $\varphi(\boldsymbol{R})$ with $n,\ r,\ \theta_1$ and θ_2 fixed

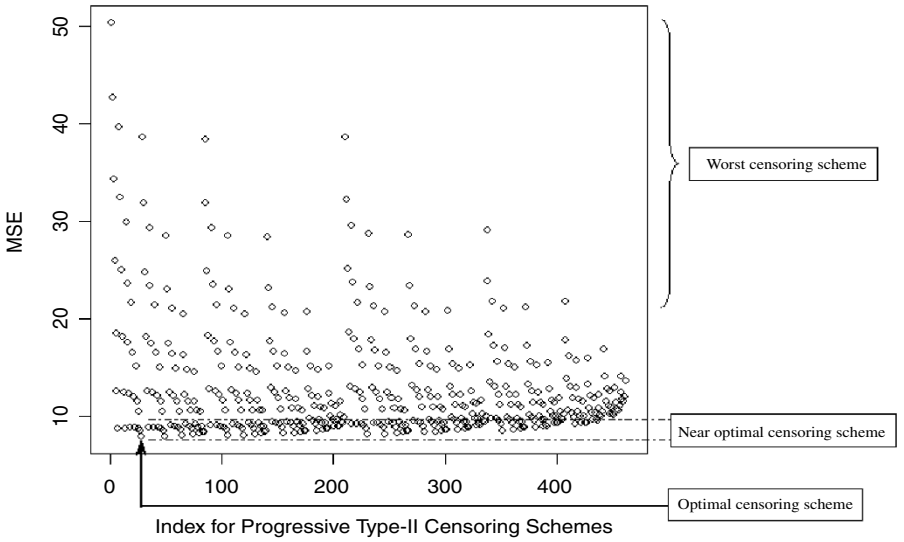

Figure 9.3. Plot of censoring schemes vs. MSE when $n = 12,\ r = 6,\ \theta_1 = e^{1.5},\ \theta_2 = e^{0.5}$

Stress Level	**Times-to-Failure**						
$e^{2.5}$	0.21	0.60	1.53	1.75	2.10	3.21	
$e^{1.5}$	5.38	5.62	6.42	7.30	7.34	9.17	9.92
	10.15	10.20	10.21	11.09	12.00	12.61	15.79

In this case, we obtain the MLEs of θ_1 and θ_2 for different choices of progressive censoring schemes as follows:
The MSEs of the best and worst optimal progressive censoring schemes when $r = 12$ are 72.58156 and 125.5496, respectively, and so the relative efficiency of worst to best censoring schemes is 57.81%. The MSEs of the best and worst optimal progressive censoring schemes when $r = 16$ are 71.39777 and 94.34234, respectively, and so the relative efficiency of worst to best censoring schemes is 75.68%. The confidence intervals for θ_1

r	**Censoring Scheme**	$\hat{\theta}_1$	$\hat{\theta}_2$
12	(11⋆0, 8)	13.233333	7.431667
	(8, 11⋆0)‡	6.846667	1.871667
	(10⋆0, 4, 4)	13.233333	6.211667
	(4, 4, 10⋆0)	7.106667	1.871667
	(4⋆0, 4⋆2, 4⋆0)	11.670000	2.205000
	(2, 0, 2, 6⋆0, 2, 0, 2)	10.480000	4.028333
	(3⋆0, 8, 8⋆0)†	8.900000	1.871667
16	(15⋆0, 4)	13.233330	5.255000
	(4, 15⋆0)‡	10.040000	3.171000
	(14⋆0, 2, 2)	13.233330	5.253000
	(2, 2, 14⋆0)	10.170000	3.171000
	(6⋆0, 4⋆1, 6⋆0)	13.233330	3.643000
	(1, 2⋆0, 1, 8⋆0, 1, 2⋆0, 1)	11.893330	4.184000
	(3⋆0, 4, 12⋆0)†	11.066670	3.171000

† and ‡ correspond to the best and worst optimal progressive censoring scheme, respectively

and θ_2 obtained by all five methods are presented in tables 9.8–9.11. Note that the approximate confidence interval and the Studentized-t interval are both unsatisfactory as mentioned earlier. We also observe that all three bootstrap methods yield confidence intervals for θ_2 to be close to the exact confidence interval for θ_2, but not so for θ_1.

9.8 Conclusions

In this paper, we have considered a simple step-stress model with two stress levels from the exponential distribution when the data are progressively Type-II censored. We have derived the conditional MLEs of the unknown parameters θ_1 and θ_2 and their exact joint and marginal conditional distributions. We have discussed the optimal censoring scheme and the optimal time for change of stress which are applicable with some preliminary estimates of θ_1 and θ_2. We have also proposed several different procedures for constructing confidence intervals for θ_1 and θ_2. We have carried out a simulation study to compare the performance of all these procedures. We have observed that the approximate method of constructing confidence intervals (based on the asymptotic normality of the MLEs $\hat{\theta}_1$ and $\hat{\theta}_2$) and the Studentized-t bootstrap confidence interval are both unsatisfactory in terms of coverage probabilities. Even though the percentile bootstrap method seems to be sensitive for small values of τ, the method does improve for large sample sizes. Overall, the adjusted percentile method seems to be the one (among all three bootstrap methods) with somewhat satisfactory coverage probabilities (not so for θ_1 when τ is small). Hence, our recommendation is to use the exact method

whenever possible, and the adjusted percentile method in case of large sample sizes when the computation of the exact confidence interval becomes difficult. We have also presented some examples to illustrate all the methods of inference discussed here as well as to support the conclusions drawn.

Appendix: Tables and Figures

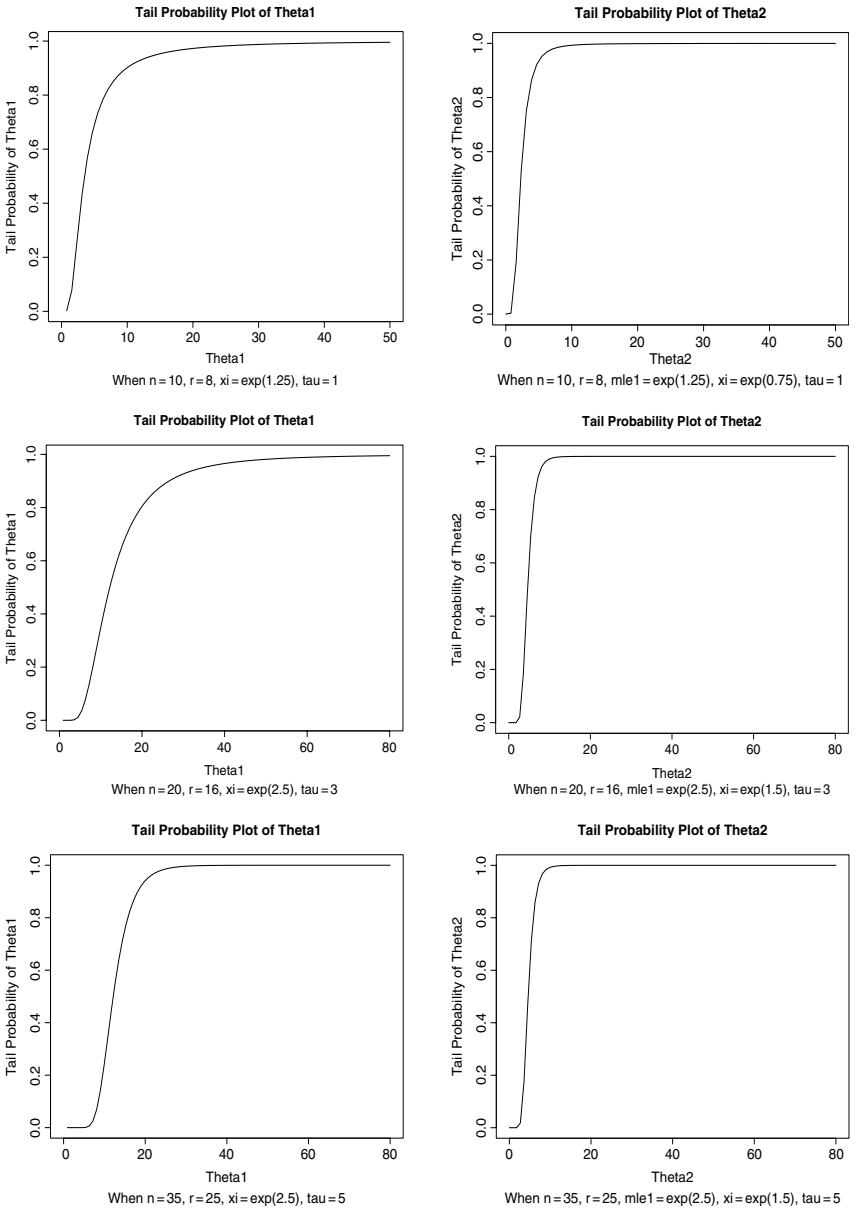

Figure 9.4. Tail probability plots of $\hat{\theta}_1$ and $\hat{\theta}_2$

Table 9.1. Estimated coverage probabilities (in %) of confidence intervals for θ_1 based on 1000 simulations and $M = 1000$ replications with $n = 20,\ r = 8,\ \theta_1 = e^{2.5}$ and $\theta_2 = e^{1.5}$

		90% C.I.					95% C.I.					99% C.I.				
Censoring Scheme	τ	Bootstrap			App.	Exact	Bootstrap			App.	Exact	Bootstrap			App.	Exact
		P	St	BCa			P	St	BCa			P	St	BCa		
(7⋆0,12)	1	96.9	51.0	82.0	75.4	89.9	97.5	52.4	85.9	73.5	96.7	100.0	50.1	93.2	93.9	99.0
	2	96.7	61.6	79.3	83.6	88.9	100.0	62.8	85.3	81.7	94.4	100.0	65.8	92.0	90.9	98.4
	3	89.7	63.3	75.8	78.8	90.9	95.6	65.1	81.4	83.6	94.8	97.3	66.5	88.5	93.4	99.4
	4	94.2	66.2	76.5	83.1	88.5	93.2	65.2	80.0	90.5	94.6	98.8	64.4	88.5	94.5	99.0
	5	83.2	65.8	73.0	79.1	92.1	91.5	67.0	80.2	87.0	96.0	97.6	68.2	89.9	92.1	98.8
	6	88.9	71.8	70.7	82.3	90.8	93.9	74.8	85.6	89.4	96.0	97.0	76.2	93.7	93.8	98.5
	7	92.3	69.0	74.9	79.9	90.1	96.0	71.3	89.0	85.7	94.3	98.7	73.7	96.9	91.0	98.7
	8	89.1	70.1	78.3	79.1	91.2	94.7	72.7	87.5	86.9	95.5	97.9	75.9	95.9	90.9	98.5
	9	87.9	65.0	76.7	84.0	89.8	92.6	78.7	86.3	88.4	94.2	98.0	73.4	97.1	90.3	98.9
	10	88.9	72.2	70.0	82.5	90.6	94.2	73.6	89.9	87.7	95.9	99.0	73.8	94.0	90.8	98.5
(12, 7⋆0)	1	88.8	69.0	80.7	75.7	89.2	96.4	76.3	87.6	79.4	94.8	99.1	82.3	94.5	80.9	98.9
	2	96.1	69.9	83.5	79.6	89.0	97.6	76.1	89.6	84.8	95.4	99.2	77.5	91.3	86.2	99.2
	3	94.2	74.7	86.8	79.5	90.0	97.4	77.7	92.8	86.1	96.0	99.2	81.8	96.1	90.7	98.9
	4	90.5	75.3	87.9	82.4	90.6	96.3	80.7	94.1	83.7	93.8	99.2	83.9	97.0	91.9	99.3
	5	91.5	80.2	91.8	80.5	89.0	94.3	81.2	94.4	86.6	95.0	99.0	85.4	98.0	90.8	99.2
	6	88.6	78.6	86.9	84.3	91.0	94.1	84.2	93.3	84.5	95.8	99.4	86.8	97.4	92.1	99.2
	7	91.5	80.1	88.0	79.3	88.8	93.5	81.1	90.8	88.0	95.2	99.4	88.5	98.4	93.6	99.2
	8	89.3	77.9	86.7	81.5	90.2	95.0	82.5	91.3	87.5	95.5	98.2	86.8	96.0	91.8	99.0
	9	88.4	75.8	84.1	82.0	91.7	94.1	80.1	89.4	86.8	95.9	98.9	87.1	95.5	91.2	98.7
	10	89.8	75.7	85.6	82.5	90.0	94.5	81.4	90.4	86.0	95.0	99.0	87.1	95.9	92.4	99.4
(6⋆0,	1	97.0	50.3	79.8	75.9	89.8	99.4	53.6	86.5	74.5	94.6	99.8	57.6	92.2	92.2	98.8
6, 6)	2	96.3	70.7	83.0	81.4	89.8	99.5	72.1	87.8	83.3	95.3	100.0	72.3	92.2	91.9	98.6
	3	87.8	67.3	77.4	76.4	88.5	95.0	74.4	84.1	86.3	94.8	97.8	73.1	90.6	92.9	98.7
	4	92.4	63.6	76.0	82.7	90.3	94.5	67.2	83.8	88.9	95.6	98.8	76.2	92.7	92.7	98.9
	5	90.5	65.4	72.7	80.1	88.1	92.6	71.1	83.3	87.3	95.2	97.9	75.2	89.9	93.4	98.2
	6	88.9	69.2	69.3	82.0	89.4	93.0	75.6	79.5	88.8	94.1	96.3	76.8	88.6	93.6	98.7
	7	92.8	69.8	74.5	81.9	89.2	91.1	76.1	86.9	87.4	94.5	96.8	79.4	89.5	92.9	99.1
	8	87.8	67.9	79.2	83.9	89.9	93.9	73.5	86.6	88.7	95.1	99.0	73.1	91.1	91.0	98.5
	9	90.8	63.2	73.1	80.5	90.0	95.9	75.2	86.9	88.8	95.3	97.8	74.4	93.5	92.0	98.8
	10	92.3	63.1	73.5	81.8	89.7	96.0	74.6	85.8	88.9	95.9	99.1	76.4	93.2	92.3	99.3
(6, 6,	1	94.1	59.5	77.5	69.8	89.6	97.7	61.2	81.7	78.4	94.4	99.4	70.6	90.3	85.5	99.0
6⋆0)	2	92.1	69.5	85.3	79.8	91.0	95.3	73.6	89.8	83.6	94.7	99.3	74.4	94.8	89.2	99.0
	3	92.3	81.1	89.3	80.2	91.3	96.7	81.3	93.5	87.3	94.8	99.6	84.9	96.6	89.5	99.2
	4	89.9	79.8	85.1	83.4	91.5	94.2	81.8	92.4	84.9	95.9	99.4	86.6	98.1	90.2	99.4
	5	91.3	80.8	87.5	83.7	91.4	93.9	83.5	91.5	86.9	94.8	98.6	85.9	96.4	91.4	98.9
	6	88.8	78.3	86.2	83.2	90.4	95.9	83.5	90.7	87.8	95.6	98.6	87.3	97.2	92.7	99.3
	7	89.7	78.9	85.9	82.3	89.2	94.9	82.9	91.9	86.7	95.9	99.1	87.5	96.8	89.6	99.3
	8	88.8	78.8	85.4	84.6	90.7	94.3	82.8	90.7	88.1	94.8	99.4	89.4	97.2	92.9	99.2
	9	90.4	79.0	86.4	83.2	90.9	96.1	83.7	91.5	88.5	95.5	99.0	88.9	96.3	93.2	98.8
	10	92.0	81.1	86.3	85.7	90.3	96.1	80.5	89.1	88.7	94.6	99.5	89.4	96.0	92.7	99.3
(3, 0, 3, 2⋆0,	1	95.8	44.9	78.7	79.8	90.5	98.2	48.1	84.0	79.7	95.9	99.8	49.7	90.5	83.2	98.7
3, 0, 3)	2	95.5	75.1	85.0	77.7	89.8	97.5	73.3	88.1	83.4	95.0	99.1	78.5	93.3	90.8	99.6
	3	90.5	70.2	84.8	81.8	91.4	92.2	71.2	88.7	86.6	94.0	99.5	73.2	94.3	91.2	98.8
	4	88.6	69.5	82.0	83.7	89.7	96.1	75.1	89.1	86.6	94.8	98.5	79.8	94.2	91.9	98.8
	5	93.9	67.5	80.3	85.6	90.4	96.0	72.3	87.0	87.6	94.8	99.7	76.3	93.1	92.9	98.5
	6	92.4	70.1	78.0	86.8	90.1	98.2	74.0	86.2	90.7	93.6	99.2	79.0	92.9	95.3	99.3
	7	94.7	71.6	79.3	88.5	89.1	96.3	76.3	85.3	92.3	95.1	99.5	83.9	93.8	97.5	99.8
	8	92.3	73.2	76.4	91.2	90.5	96.6	79.4	84.9	94.1	95.2	99.7	86.0	93.1	98.1	98.9
	9	89.4	76.1	77.1	92.1	89.4	95.1	80.5	83.8	97.7	95.6	99.2	86.3	92.5	98.2	98.1
	10	82.7	76.9	69.1	95.2	90.9	91.1	81.3	80.0	98.2	95.0	98.6	83.6	90.5	99.4	99.0
(2⋆0,3,3,	1	93.4	52.1	82.4	74.5	89.3	96.9	54.2	85.0	75.3	95.8	99.3	58.9	92.0	89.1	98.3
3, 3, 2⋆0)	2	94.8	72.9	86.3	79.2	89.0	95.8	76.7	91.0	86.4	94.2	98.0	78.7	94.0	90.6	99.1
	3	87.9	77.1	83.8	82.6	91.3	92.2	80.3	90.0	86.6	94.7	98.5	84.4	95.7	92.2	98.5
	4	86.6	73.4	84.9	82.3	89.5	92.7	77.4	90.8	85.0	95.3	97.4	82.0	95.5	93.2	98.8
	5	87.3	78.1	86.0	83.9	89.7	93.7	82.1	91.7	88.1	95.8	98.0	87.2	96.0	92.3	98.9
	6	90.3	83.0	88.7	85.0	90.9	93.5	83.3	91.1	89.9	94.3	98.1	89.3	97.3	93.3	99.2
	7	89.9	81.1	86.8	87.2	91.3	95.6	87.6	92.8	88.4	94.5	98.3	88.4	96.5	94.4	98.9
	8	91.3	82.0	87.3	85.7	90.0	95.2	86.9	91.8	87.1	95.5	98.3	88.7	96.3	92.4	99.2
	9	92.3	83.5	86.7	85.2	90.8	96.2	87.6	91.6	88.6	94.8	99.1	91.7	98.0	95.4	98.9
	10	93.5	83.7	85.8	87.2	89.9	97.4	89.6	92.8	90.4	94.6	99.1	91.8	97.5	94.5	99.0

Table 9.2. Estimated coverage probabilities (in %) of confidence intervals for θ_2 based on 1000 simulations and $M = 1000$ replications with $n = 20,\ r = 8,\ \theta_1 = e^{2.5}$ and $\theta_2 = e^{1.5}$

		90% C.I.					95% C.I.					99% C.I.				
Censoring Scheme	τ	Bootstrap			App.	Exact	Bootstrap			App.	Exact	Bootstrap			App.	Exact
		P	St	BCa			P	St	BCa			P	St	BCa		
(7⋆0, 12)	1	83.6	88.8	89.7	84.1	91.3	91.1	96.1	96.7	88.4	96.1	96.1	98.6	97.6	93.2	98.6
	2	84.2	89.6	90.6	83.9	91.3	88.1	94.9	95.0	87.7	95.5	94.2	99.2	97.3	90.2	99.3
	3	81.4	90.5	88.9	80.7	90.7	86.1	95.5	93.5	81.2	95.4	93.2	99.6	96.3	88.4	99.1
	4	80.1	90.3	86.7	77.0	88.8	83.1	95.8	91.8	81.1	95.6	91.8	99.5	94.5	85.8	99.1
	5	79.3	90.1	83.5	75.6	87.5	79.6	95.3	88.5	79.7	95.4	89.0	99.6	93.6	83.8	98.6
	6	78.3	90.9	83.4	74.7	90.5	79.2	94.9	88.4	79.7	93.7	87.1	99.3	91.0	82.0	99.2
	7	78.4	91.5	83.1	73.1	89.6	79.1	94.6	87.1	78.4	94.9	86.5	99.4	91.4	82.9	99.3
	8	77.6	89.7	80.7	73.6	89.8	78.6	95.3	86.7	78.7	95.3	85.5	98.6	89.2	81.3	99.5
	9	76.3	88.8	79.8	73.6	90.0	78.3	94.3	86.1	76.2	94.9	85.9	98.9	89.5	79.4	98.6
	10	76.0	89.9	79.5	72.7	91.6	77.2	95.4	85.7	75.8	94.1	84.8	98.6	88.2	78.8	98.8
(12, 7⋆0)	1	86.8	90.6	90.9	86.2	89.4	92.5	95.5	95.2	88.7	95.0	96.0	98.0	97.1	93.1	98.9
	2	87.4	89.4	89.7	83.6	89.2	92.3	95.5	95.9	85.9	94.3	96.1	99.0	97.7	91.8	99.1
	3	86.0	88.7	89.6	83.1	89.7	89.8	95.8	95.6	86.0	94.4	95.1	99.0	97.5	92.1	98.8
	4	87.3	90.4	91.3	84.9	90.0	92.1	95.4	95.7	87.6	94.3	95.4	99.4	97.9	90.3	99.5
	5	84.5	90.7	90.7	83.5	91.1	90.8	96.2	96.4	85.6	96.5	94.3	98.5	97.2	91.6	99.6
	6	83.8	89.3	90.2	82.6	89.5	90.6	95.9	96.8	86.4	95.3	94.4	99.8	98.0	91.1	99.2
	7	83.1	89.4	89.7	82.2	90.0	89.1	94.7	94.9	85.4	96.0	93.8	99.2	96.6	91.6	98.7
	8	81.9	89.8	89.2	80.2	91.1	89.4	95.4	95.2	81.7	95.8	94.8	99.3	96.5	87.9	99.1
	9	83.7	91.9	91.9	78.4	88.9	88.6	94.8	94.2	84.5	94.6	92.6	99.2	96.0	87.9	98.3
	10	82.3	91.2	90.7	77.0	90.4	86.9	95.4	93.2	84.2	95.0	92.6	99.1	95.1	86.7	99.4
(6⋆0, 6, 6)	1	86.8	89.2	90.1	84.9	90.8	91.1	95.0	96.1	87.4	94.8	96.3	98.5	97.8	92.1	98.9
	2	85.7	89.7	91.4	80.3	88.6	91.2	95.4	95.2	86.4	95.1	95.6	99.1	97.4	90.4	98.9
	3	81.2	88.7	88.6	79.4	91.1	88.9	96.2	95.4	83.7	95.0	92.7	98.9	95.0	87.6	98.4
	4	79.4	90.1	87.3	79.4	91.4	85.0	96.7	93.1	80.7	95.7	89.5	99.3	93.3	85.9	98.9
	5	77.5	90.3	83.9	73.3	89.1	81.0	96.2	89.4	78.9	94.2	90.4	99.7	94.1	81.5	98.7
	6	73.9	91.6	82.7	74.0	89.6	80.1	96.5	88.5	76.3	94.8	86.4	99.6	89.8	81.6	99.6
	7	72.2	91.0	79.3	72.2	89.9	80.5	95.7	86.8	75.2	94.5	84.8	99.3	88.9	78.4	99.1
	8	73.3	91.8	80.1	74.4	91.0	77.7	97.2	86.0	74.3	95.3	83.7	99.3	87.5	79.6	99.3
	9	71.3	90.2	78.3	71.4	89.3	76.7	95.8	83.2	73.8	94.5	81.5	98.6	86.6	77.9	99.0
	10	67.1	88.7	75.5	70.3	89.1	75.4	95.7	82.7	76.3	93.2	81.4	99.2	86.0	77.6	99.6
(6, 6, 6⋆0)	1	85.9	90.6	90.1	82.9	88.3	91.2	95.0	94.5	88.0	95.5	95.0	98.8	97.0	93.5	99.0
	2	86.8	90.1	90.8	84.5	91.4	91.8	94.8	95.4	89.4	94.7	96.8	99.6	98.4	91.2	99.0
	3	87.6	91.0	91.6	82.3	89.2	91.5	94.9	94.7	86.6	96.3	94.5	98.4	96.9	91.3	99.2
	4	85.2	89.0	89.4	84.3	90.2	90.0	95.5	95.4	85.9	95.6	94.4	99.4	97.6	91.5	99.2
	5	84.5	90.2	90.7	83.5	88.4	91.6	95.7	96.1	85.4	94.2	95.5	99.0	97.0	90.0	98.8
	6	84.6	90.3	91.7	82.1	90.9	88.3	93.9	94.8	84.7	95.1	94.3	99.3	97.2	89.3	99.5
	7	83.5	90.5	91.6	78.1	88.4	89.9	95.1	95.0	82.7	94.8	95.5	99.1	97.0	87.7	98.8
	8	82.9	90.7	90.0	80.9	90.0	86.8	95.8	95.1	83.5	95.3	94.6	99.4	96.7	87.1	99.1
	9	83.7	92.0	90.8	78.9	88.1	87.9	95.8	94.5	82.6	95.4	92.6	99.0	95.5	89.2	99.1
	10	81.3	90.5	89.4	78.0	90.4	87.1	95.6	94.0	82.0	94.7	92.2	99.6	95.3	86.8	99.1
(3, 0, 3, 2⋆0, 3, 0, 3)	1	89.3	91.7	92.5	82.1	88.6	91.0	94.7	95.1	89.1	94.6	96.5	98.9	98.3	90.9	99.0
	2	84.7	90.5	91.2	84.9	90.0	90.9	94.7	94.6	87.3	95.1	96.6	99.5	98.2	89.3	98.7
	3	85.0	90.6	91.1	81.1	89.8	88.5	94.5	95.0	86.5	95.2	94.4	99.1	97.0	89.7	99.1
	4	84.6	91.8	91.6	80.2	90.5	88.3	95.9	95.4	83.7	95.4	93.1	99.1	95.7	88.7	99.0
	5	79.4	90.2	88.6	79.3	90.0	86.2	95.3	92.3	79.2	94.3	93.5	99.9	96.0	84.1	99.2
	6	80.4	90.1	87.0	76.0	91.1	82.8	96.1	90.7	76.7	94.1	90.7	99.5	93.5	83.7	99.3
	7	80.7	91.3	86.9	71.7	90.8	81.4	95.8	90.2	77.9	94.5	87.7	99.5	92.8	83.6	98.8
	8	78.7	89.9	84.5	76.5	90.2	82.5	95.3	89.4	77.7	95.1	86.4	99.3	90.7	82.4	99.5
	9	76.4	89.5	82.8	74.6	89.1	79.9	94.6	87.0	75.1	95.9	87.2	99.4	90.5	79.3	99.2
	10	76.2	91.6	85.0	74.1	88.9	81.6	97.0	89.9	76.0	96.3	88.7	99.0	92.2	79.7	98.6
(2⋆0, 3, 3, 3, 3, 2⋆0)	1	86.6	89.1	90.4	85.7	90.7	91.4	95.2	95.2	87.9	94.8	96.4	98.9	97.9	92.0	98.7
	2	86.5	90.8	91.5	83.3	90.3	89.7	94.6	95.2	85.7	95.2	95.0	98.7	97.4	89.9	99.4
	3	85.2	91.5	91.3	80.6	92.7	86.4	94.9	93.7	84.9	94.7	94.1	99.0	97.6	88.6	99.4
	4	83.1	88.7	88.7	79.4	90.7	84.8	95.1	92.4	85.1	94.2	93.1	99.6	96.0	86.9	99.5
	5	81.6	90.1	89.5	81.3	91.1	86.8	94.7	93.3	80.2	95.2	92.8	99.3	96.0	84.3	98.3
	6	81.0	88.9	88.0	77.9	89.5	83.0	95.2	92.5	83.1	94.5	90.5	98.9	93.1	84.1	99.3
	7	79.5	92.0	88.9	75.5	89.4	84.2	96.8	92.7	78.5	94.6	89.9	99.4	93.9	86.5	99.2
	8	76.5	89.8	86.1	74.4	90.8	84.0	96.7	92.1	78.9	94.6	89.1	99.9	92.3	82.0	98.5
	9	76.4	88.4	84.5	75.1	92.1	82.7	95.5	89.9	76.1	95.2	89.0	99.1	91.9	83.2	99.1
	10	78.1	91.5	85.9	71.1	90.1	80.4	94.8	88.3	76.9	95.2	87.4	99.0	91.9	79.8	99.4

Table 9.3. Estimated coverage probabilities (in %) of confidence intervals for θ_1 based on 1000 simulations and $M = 1000$ replications with $n = 20,\ r = 12,\ \theta_1 = e^{2.5}$ and $\theta_2 = e^{1.5}$

		90% C.I.					95% C.I.					99% C.I.				
Censoring Scheme	τ	Bootstrap			App.	Exact	Bootstrap			App.	Exact	Bootstrap			App.	Exact
		P	St	BCa			P	St	BCa			P	St	BCa		
(11⋆0, 8)	1	96.6	49.5	82.9	72.7	90.2	97.6	54.0	84.7	74.5	95.0	99.8	58.5	93.1	90.9	98.5
	2	95.9	73.0	85.3	84.6	91.1	98.4	73.5	88.0	81.0	95.3	99.8	77.7	93.2	92.9	99.1
	3	86.8	79.0	84.4	81.2	89.2	95.5	81.9	88.9	88.0	95.8	97.5	80.7	91.9	91.6	98.5
	4	90.9	75.1	84.7	83.1	91.4	95.1	77.8	90.3	87.0	95.0	98.3	76.5	92.4	92.5	98.8
	5	92.8	73.0	83.3	83.4	90.1	94.9	71.8	88.1	88.6	95.7	98.5	74.6	94.5	93.1	99.2
	6	94.2	68.8	80.4	84.1	90.2	95.0	73.8	87.1	88.4	94.7	97.9	75.5	92.0	93.2	98.6
	7	92.8	70.2	77.6	86.1	90.5	96.3	72.8	85.4	91.0	96.0	99.0	78.0	92.1	92.8	98.9
	8	90.6	72.7	76.4	92.0	90.7	94.5	74.2	82.2	90.9	95.3	99.1	79.7	92.5	94.8	99.0
	9	89.8	74.5	76.0	97.0	90.3	94.2	79.1	81.6	89.3	95.0	98.1	83.9	91.3	92.2	99.6
	10	89.4	79.6	75.6	99.4	89.8	92.2	81.9	79.0	90.0	94.7	95.8	85.3	89.5	91.9	99.3
(8, 11⋆0)	1	97.2	65.5	80.2	74.5	89.3	98.8	70.6	86.5	80.6	94.9	99.8	74.3	90.1	88.0	98.6
	2	96.6	62.9	85.9	76.0	90.0	98.0	66.8	88.9	85.0	95.9	99.7	67.9	92.8	88.4	99.4
	3	91.4	75.8	88.9	80.2	90.2	97.7	81.4	93.5	85.7	94.2	99.7	80.8	95.8	92.1	98.9
	4	89.7	77.3	85.3	83.3	90.1	92.1	81.0	90.0	88.5	94.7	98.9	83.8	96.0	91.6	99.1
	5	90.3	79.6	87.8	82.9	90.4	94.6	80.6	91.3	86.5	95.0	98.6	85.6	96.1	94.2	99.1
	6	88.3	81.3	87.2	83.7	89.9	93.1	82.1	90.6	88.6	95.1	98.1	87.8	96.8	93.4	99.5
	7	90.2	80.7	89.3	85.8	90.9	93.1	80.8	90.6	87.2	94.5	98.5	87.4	95.9	93.3	99.4
	8	87.4	81.5	86.2	85.9	90.8	94.7	86.0	93.3	90.1	94.2	98.5	91.0	97.0	94.7	99.2
	9	87.5	78.3	86.9	83.7	88.8	94.5	86.8	93.4	88.7	95.0	98.3	90.5	97.3	93.5	98.8
	10	86.7	80.4	86.1	84.6	90.7	93.3	86.4	92.0	88.8	96.1	99.0	89.8	96.4	94.7	99.4
(10⋆0, 4, 4)	1	96.8	49.2	81.0	75.5	91.7	97.9	52.6	86.1	71.5	94.1	99.8	57.4	90.7	91.1	99.0
	2	95.9	72.8	84.5	84.3	91.7	99.4	73.2	88.7	81.0	94.3	99.5	77.8	92.9	92.7	99.4
	3	86.8	78.2	83.9	84.7	90.2	94.8	81.2	88.0	86.3	94.7	97.6	83.5	92.3	93.4	98.9
	4	91.2	77.5	86.1	83.7	89.0	93.0	77.7	89.9	85.1	95.2	99.0	80.2	94.5	93.9	99.1
	5	90.7	72.2	83.7	84.6	90.1	94.3	76.1	89.7	89.6	95.2	97.8	78.7	95.1	92.0	98.4
	6	92.4	73.4	83.0	83.8	90.0	96.7	75.0	89.3	89.9	95.3	98.9	80.7	94.3	94.0	98.7
	7	93.5	77.0	82.8	87.6	91.6	95.7	76.7	87.3	90.5	94.1	99.2	83.0	95.1	95.1	98.8
	8	92.0	74.2	79.2	87.4	89.2	96.6	78.3	86.8	92.4	94.4	98.9	83.4	93.1	98.0	99.2
	9	90.7	76.8	77.4	92.1	90.1	95.8	81.7	84.9	95.4	95.7	98.6	85.8	93.6	98.7	99.1
	10	86.7	78.1	74.3	94.6	89.2	94.3	84.1	84.3	97.3	95.8	98.7	88.0	92.8	99.1	98.7
(4, 4, 10⋆0)	1	95.7	45.3	76.1	79.6	89.5	98.4	51.9	85.4	82.9	94.2	99.4	56.5	90.5	87.2	98.7
	2	95.4	72.1	85.5	79.6	89.1	98.3	77.3	90.6	86.3	94.9	99.9	77.5	93.3	90.3	98.7
	3	88.8	76.7	86.3	81.7	91.3	95.7	80.1	93.0	84.1	95.8	99.1	84.0	96.4	90.0	98.8
	4	91.9	79.1	87.5	81.4	89.0	94.8	81.3	91.0	85.4	95.2	98.3	84.7	94.7	93.0	98.9
	5	86.0	79.5	86.4	82.9	89.3	93.2	81.9	92.0	87.5	94.8	98.5	86.3	95.8	94.1	99.0
	6	88.0	80.8	86.1	85.7	91.2	94.2	86.3	93.5	89.2	94.6	98.9	90.1	96.9	94.4	98.7
	7	89.0	81.5	89.2	84.9	90.4	95.3	87.6	94.4	90.7	94.8	98.1	88.8	97.1	93.1	99.2
	8	89.0	83.9	88.1	86.5	90.2	94.0	87.4	93.1	89.4	95.0	97.9	90.0	97.4	93.4	98.5
	9	88.0	82.3	86.9	87.6	90.1	94.2	86.2	92.9	89.0	95.4	99.0	91.4	96.3	94.0	98.9
	10	86.9	80.6	85.5	85.8	90.5	93.9	86.6	92.5	88.3	94.4	98.2	90.5	96.7	93.3	99.0
(2, 0, 2, 6⋆0, 2, 0, 2)	1	95.3	49.1	81.2	80.1	90.6	99.0	50.5	85.5	77.8	94.8	99.9	52.9	90.8	84.4	99.1
	2	94.4	72.6	84.2	74.3	91.0	97.4	79.0	89.3	86.0	95.7	99.3	80.6	94.0	91.6	98.9
	3	90.1	76.0	85.4	85.9	89.9	92.4	76.4	90.3	86.8	94.9	99.8	78.9	96.1	92.2	99.0
	4	86.2	73.1	84.1	85.4	90.1	94.2	80.6	91.5	85.9	94.6	98.1	81.6	95.2	94.0	98.9
	5	90.0	78.9	87.2	84.0	91.0	95.4	81.5	91.3	88.6	94.7	98.5	84.0	94.7	93.3	98.8
	6	88.8	77.1	84.9	85.0	89.6	93.5	82.3	90.9	88.8	95.2	98.6	84.6	95.4	93.3	98.8
	7	89.2	80.0	85.8	84.5	89.9	95.3	83.2	91.9	88.2	93.9	99.0	87.4	95.4	94.1	99.2
	8	91.9	77.8	85.4	84.2	89.1	96.1	82.3	90.4	89.5	94.7	99.1	87.5	96.1	95.3	99.2
	9	93.2	79.2	84.5	86.7	90.1	95.9	81.7	88.4	88.6	95.3	99.6	85.9	94.0	95.1	99.3
	10	95.4	81.3	86.4	87.1	89.9	96.9	81.3	87.6	90.5	95.5	99.3	87.7	95.0	95.7	99.4
(4⋆0, 2, 2, 2, 2, 4⋆0)	1	96.8	50.9	82.5	76.7	90.2	97.9	54.5	86.6	77.3	94.7	99.4	58.4	91.8	90.7	99.1
	2	95.6	73.9	84.1	83.9	90.4	98.1	77.3	90.5	81.0	94.8	99.5	77.8	92.2	92.0	98.7
	3	85.8	80.7	85.2	79.0	90.8	93.5	81.8	87.6	88.1	94.6	98.1	84.4	91.8	91.3	98.8
	4	88.8	79.4	86.3	82.6	90.2	92.2	85.2	91.6	87.6	94.8	97.6	85.6	96.0	93.4	99.3
	5	86.6	78.7	87.2	86.2	91.3	91.6	82.5	92.4	90.1	95.3	96.1	83.6	95.3	94.6	99.0
	6	85.3	82.0	87.3	83.7	88.9	91.6	86.0	93.6	89.2	95.6	98.8	87.8	97.7	94.7	99.3
	7	87.4	82.8	86.1	86.3	91.5	94.2	89.1	93.4	89.6	94.4	98.0	91.0	97.4	94.2	99.3
	8	88.2	85.0	88.3	88.2	90.3	94.0	88.5	92.3	90.4	95.4	97.7	91.6	97.6	95.1	99.4
	9	88.1	85.3	87.6	83.7	88.3	93.1	88.1	91.4	91.3	95.0	98.4	92.3	97.6	95.0	99.1
	10	89.8	85.6	88.8	84.4	91.1	95.0	89.5	93.2	90.3	95.4	98.6	92.3	97.6	93.8	98.7

Table 9.4. Estimated coverage probabilities (in %) of confidence intervals for θ_2 based on 1000 simulations and $M = 1000$ replications with $n = 20,\ r = 12,\ \theta_1 = e^{2.5}$ and $\theta_2 = e^{1.5}$

		90% C.I.					95% C.I.					99% C.I.				
Censoring Scheme	τ	Bootstrap			App.	Exact	Bootstrap			App.	Exact	Bootstrap			App.	Exact
		P	St	BCa			P	St	BCa			P	St	BCa		
(11⋆0, 8)	1	88.1	89.7	90.6	86.3	89.9	92.6	95.3	95.7	90.7	95.2	97.6	98.6	97.9	95.2	99.1
	2	88.3	90.4	91.6	86.5	92.1	93.1	95.5	95.5	90.1	94.7	97.0	99.1	98.5	92.6	99.5
	3	88.0	89.1	90.3	85.6	90.6	93.2	96.5	96.1	89.3	94.7	96.4	99.3	98.0	93.6	99.3
	4	84.7	90.8	91.5	85.2	90.7	89.7	95.0	95.6	86.8	94.7	96.2	99.3	98.6	91.9	98.6
	5	83.9	89.3	91.6	83.2	89.4	89.9	95.4	95.8	87.7	96.1	96.6	99.6	98.4	91.6	99.0
	6	83.2	88.8	88.2	82.4	88.8	86.9	94.5	93.0	84.6	94.4	93.9	99.2	97.2	88.9	98.8
	7	82.2	89.3	87.7	81.3	90.3	86.6	95.6	94.2	85.5	96.5	92.4	99.5	98.7	87.3	99.1
	8	82.3	91.3	87.7	79.2	90.6	85.7	95.7	92.3	85.1	93.7	91.1	99.0	97.2	86.6	98.8
	9	80.3	90.3	86.3	78.4	90.7	84.9	95.2	90.3	84.6	94.7	91.0	99.3	96.8	86.6	99.1
	10	80.1	89.9	86.6	78.4	91.4	84.0	95.9	91.2	84.9	95.0	90.5	99.0	96.9	81.2	98.5
(8, 11⋆0)	1	86.5	88.7	89.3	88.1	91.1	90.9	95.3	95.0	90.6	95.1	97.9	98.9	99.0	95.2	99.1
	2	88.1	90.4	90.6	86.9	91.5	93.7	95.8	95.9	90.4	95.3	96.2	98.8	97.8	94.6	99.4
	3	87.4	90.8	91.0	86.1	90.0	91.3	94.1	94.8	88.6	94.6	97.6	99.1	98.7	95.3	99.2
	4	88.1	90.1	91.5	86.0	90.1	92.7	94.5	94.4	89.1	94.5	96.2	99.3	98.1	94.2	98.9
	5	87.4	89.0	90.2	85.0	88.5	92.6	95.5	96.2	91.7	95.9	96.6	98.7	98.4	94.6	98.9
	6	88.7	90.3	92.0	86.4	90.8	93.4	95.3	95.0	88.1	95.2	95.1	99.4	97.6	92.9	99.2
	7	87.1	91.7	92.0	85.9	90.9	90.9	95.7	96.0	88.2	94.2	96.7	98.8	98.4	91.2	99.0
	8	87.9	90.7	90.8	82.4	89.1	90.8	94.5	95.0	88.5	95.1	96.8	99.1	98.6	90.9	99.1
	9	86.7	89.1	89.3	83.1	90.1	89.5	94.0	94.3	87.5	95.0	95.3	98.9	97.5	90.8	98.4
	10	85.9	89.9	91.4	82.9	88.8	90.9	95.0	96.0	84.9	94.4	95.7	99.1	97.7	91.2	99.6
(10⋆0, 4, 4)	1	88.1	89.3	89.4	87.3	89.5	92.4	94.9	95.4	90.5	95.5	96.4	99.2	97.9	94.1	98.9
	2	87.7	91.9	92.8	86.0	91.3	91.3	95.5	95.6	88.8	94.4	97.0	98.5	97.6	93.4	98.6
	3	87.3	88.6	89.7	85.8	90.8	92.4	95.9	96.4	87.8	95.4	97.0	99.0	98.1	92.7	99.2
	4	86.7	89.3	90.2	85.0	91.3	90.7	95.1	95.8	89.7	94.7	96.7	98.6	98.4	92.8	98.6
	5	86.4	90.5	90.6	80.7	90.6	90.7	95.4	96.3	85.8	95.3	96.0	99.4	98.2	91.5	98.7
	6	85.0	90.8	90.2	83.0	89.1	89.1	96.5	95.2	82.9	95.7	95.7	99.6	97.8	88.7	99.1
	7	83.3	91.2	90.2	79.4	89.5	86.7	96.8	95.0	82.8	94.7	93.3	99.6	96.7	87.6	99.1
	8	78.3	91.3	87.1	76.7	88.2	85.7	95.0	91.5	80.6	94.8	90.9	99.2	94.7	85.7	99.1
	9	78.6	89.7	84.6	77.0	90.7	83.5	96.8	90.9	79.6	94.0	90.2	99.7	93.6	86.0	99.6
	10	77.0	90.6	82.2	76.9	90.2	79.2	95.0	86.3	78.9	94.8	87.5	99.7	92.7	81.4	99.6
(4, 4, 10⋆0)	1	89.3	92.0	91.6	89.4	90.9	92.3	94.6	94.3	88.8	95.3	96.6	98.7	97.4	94.1	98.6
	2	88.3	89.6	89.7	87.6	90.6	92.6	95.6	96.2	90.9	96.1	97.5	99.0	98.8	92.5	99.1
	3	88.2	89.5	89.9	85.9	89.1	92.8	95.9	95.7	89.9	94.4	96.2	99.4	98.5	93.9	98.7
	4	86.8	88.7	89.7	87.1	90.8	92.0	96.5	95.4	89.1	94.3	97.0	99.1	98.1	94.5	99.1
	5	88.2	92.0	92.2	84.7	90.9	93.4	95.2	96.1	89.4	94.8	96.7	99.4	98.4	92.1	99.6
	6	85.7	87.8	88.9	85.6	90.6	91.9	95.2	95.8	89.8	94.5	97.1	99.5	98.6	93.5	99.0
	7	86.9	91.6	91.8	83.6	91.2	92.0	95.0	95.2	87.5	95.0	96.0	98.9	97.9	91.7	99.3
	8	86.4	91.0	91.4	84.9	89.9	91.0	95.9	96.2	86.5	94.7	95.5	99.0	97.6	91.7	98.2
	9	85.2	89.3	89.8	83.6	89.9	90.2	94.6	94.8	87.8	95.0	94.6	99.0	97.0	90.9	98.9
	10	86.4	91.8	92.5	80.5	91.1	90.1	95.2	94.7	86.8	94.6	95.3	99.3	97.5	91.6	99.2
(2, 0, 2, 6⋆0, 2, 0, 2)	1	88.9	89.7	90.6	85.4	88.5	93.8	96.0	96.0	90.8	95.9	96.8	99.2	98.1	94.0	99.1
	2	86.7	89.4	90.5	87.4	90.4	92.2	94.1	94.6	91.1	95.7	97.0	99.1	98.8	92.8	99.4
	3	89.4	90.7	91.9	86.7	88.9	91.9	95.5	95.8	89.5	94.4	96.9	99.6	98.4	93.4	99.3
	4	85.4	90.1	91.3	85.9	90.0	92.4	94.5	95.4	88.1	95.4	97.1	99.4	98.1	92.7	99.2
	5	87.2	90.4	91.4	85.3	89.1	92.4	94.9	96.2	87.0	95.3	97.1	99.5	98.1	92.2	99.4
	6	86.2	93.4	93.3	83.8	89.3	90.4	95.5	96.2	86.2	95.7	95.7	99.6	98.4	90.9	99.5
	7	84.7	91.5	92.0	83.4	87.4	91.1	96.5	96.9	85.7	95.3	94.8	99.1	97.2	89.8	99.6
	8	82.9	90.3	90.1	79.6	89.1	88.0	96.3	95.0	85.1	95.1	93.4	99.4	96.7	87.9	99.0
	9	81.2	89.5	88.9	79.1	91.4	88.5	97.6	94.5	83.2	95.9	94.0	99.2	96.1	87.4	99.2
	10	80.9	91.1	89.2	80.3	89.8	84.1	97.0	93.4	83.5	95.6	92.9	99.3	96.1	86.8	99.6
(4⋆0, 2, 2, 2, 2, 4⋆0)	1	90.1	89.6	90.1	87.7	89.9	93.2	95.7	95.4	90.4	95.6	96.8	99.0	98.3	94.7	98.9
	2	87.0	91.9	91.9	84.8	90.0	93.5	95.1	95.6	90.5	94.1	96.4	98.9	98.0	94.5	98.7
	3	88.0	91.2	92.2	86.7	91.3	91.2	95.2	95.3	88.7	94.9	96.1	98.9	98.0	94.5	98.9
	4	84.6	87.9	88.7	83.0	88.0	92.4	95.7	96.0	88.4	94.6	95.4	99.1	97.6	91.6	99.2
	5	86.5	88.1	89.5	85.1	89.7	91.4	96.5	95.9	88.4	95.7	96.4	99.0	98.6	92.2	99.1
	6	83.8	90.2	90.1	82.3	90.2	89.0	96.1	95.6	86.5	94.6	96.2	99.0	98.4	91.9	99.2
	7	83.1	91.2	90.7	81.1	87.2	90.2	94.9	94.4	85.7	95.5	94.6	99.4	97.5	89.1	99.0
	8	82.3	90.2	89.8	82.3	90.2	88.8	95.6	94.9	84.6	95.6	94.8	98.6	96.7	88.9	98.9
	9	82.9	89.3	88.8	81.2	88.9	86.6	93.0	92.4	82.1	94.6	92.0	99.4	96.3	90.3	99.8
	10	85.0	89.8	89.2	79.1	90.4	88.9	95.9	94.8	81.8	94.4	91.1	99.3	95.6	88.1	98.9

Table 9.5. The optimal censoring scheme under variance optimality when $\theta_1 = e^{1.5}$ and $\theta_2 = e^{0.5}$ are fixed

n	r	τ	Best Censoring Scheme	Variance	Worst Censoring Scheme (%)	Variance	Relative Efficiency (%)
10	4	1	(6, 3⋆0)	6.6727	(0, 6, 2⋆0)	11.4759	58.1454
		3	(0, 6, 2⋆0)	16.1995	(3⋆0, 6)	27.3317	59.2700
		5	(2⋆0, 6, 0)	11.1018	(3⋆0, 6)	28.7591	38.6028
		7	(2⋆0, 6, 0)	9.5829	(3⋆0, 6)	25.9970	36.8617
		9	(2⋆0, 6, 0)	9.4267	(3⋆0, 6)	22.8246	41.3007
	6	1	(4, 5⋆0)	6.9724	(0, 4, 4⋆0)	10.1330	68.8085
		3	(0, 4, 4⋆0)	14.8958	(4, 5⋆0)	19.7418	75.4531
		5	(3⋆0, 4, 2⋆0)	8.4993	(4, 5⋆0)	13.9872	60.7647
		7	(3⋆0, 4, 2⋆0)	6.9918	(4, 5⋆0)	10.1147	69.1257
		9	(3⋆0, 3, 0, 1)	6.7351	(4, 5⋆0)	8.4086	80.0981
	8	1	(2, 7⋆0)	7.8990	(0, 2, 6⋆0)	9.3971	84.0574
		3	(2⋆0, 2, 5⋆0)	14.1761	(2, 7⋆0)	16.8237	84.2629
		5	(3⋆0, 2, 4⋆0)	7.3983	(2, 7⋆0)	9.4502	78.2870
		7	(4⋆0, 1, 2⋆0, 1)	5.7126	(2, 7⋆0)	6.7263	84.9295
		9	(7⋆0, 2)	5.2843	(1, 5⋆0, 1, 0)	5.9111	89.3970
12	6	1	(6, 5⋆0)	8.8650	(0, 6, 4⋆0)	13.2089	67.1138
		3	(2⋆0, 6, 3⋆0)	11.7538	(6, 5⋆0)	19.3985	60.5913
		5	(3⋆0, 6, 2⋆0)	7.2209	(6, 5⋆0)	13.3790	53.9722
		7	(3⋆0, 5, 0, 1)	6.6979	(6, 5⋆0)	9.8590	67.9368
		9	(3⋆0, 4, 0, 2)	6.6551	(6, 5⋆0)	8.3026	80.1562
	8	1	(4, 7⋆0)	9.7988	(0, 4, 6⋆0)	12.4552	78.6724
		3	(2⋆0, 4, 5⋆0)	11.0070	(4, 7⋆0)	16.1089	68.3286
		5	(4⋆0, 3, 2⋆0, 1)	6.0520	(4, 7⋆0)	8.9574	67.5640
		7	(4⋆0, 2, 2⋆0, 2)	5.2297	(4, 7⋆0)	6.5859	79.4070
		9	(4⋆0, 1, 2⋆0, 3)	5.0820	(3, 5⋆0, 1, 0)	5.8779	86.4595
	10	1	(2, 9⋆0)	10.8169	(2⋆0, 2, 7⋆0)	12.0106	90.0607
		3	(3⋆0, 2, 6⋆0)	10.6109	(2, 9⋆0)	12.9132	82.1712
		5	(9⋆0, 2)	5.4010	(2, 9⋆0)	6.4747	83.4170
		7	(9⋆0, 2)	4.4593	(8⋆0, 2, 0)	5.0836	87.7205
		9	(9⋆0, 2)	4.2934	(8⋆0, 2, 0)	4.9774	86.2583
16	8	2	(2⋆0, 8, 5⋆0)	12.4683	(8, 7⋆0)	19.2231	64.8613
		4	(4⋆0, 6, 2⋆0, 2)	5.5620	(8, 7⋆0)	10.8427	51.2971
		6	(4⋆0, 3, 2⋆0, 5)	5.0132	(8, 7⋆0)	7.1757	69.8644
		8	(3⋆0, 1, 1, 2⋆0, 6)	5.0050	(8, 7⋆0)	6.0342	82.9431
		10	(2, 6⋆0, 6)	5.0485	(7, 5⋆0, 1, 0)	5.7532	87.7510
	10	2	(2⋆0, 5, 6⋆0, 1)	12.1242	(6, 9⋆0)	17.5246	69.1836
		4	(5⋆0, 6, 4⋆0)	4.8650	(6, 9⋆0)	7.8610	61.8872
		6	(5⋆0, 1, 3⋆0, 5)	4.1519	(6, 9⋆0)	5.3362	77.8071
		8	(9⋆0, 6)	4.0965	(3, 7⋆0, 3, 0)	5.0449	81.2004
		10	(9⋆0, 6)	4.1734	(3, 7⋆0, 3, 0)	4.9841	83.7334
	12	2	(11⋆0, 4)	11.8977	(4, 11⋆0)	15.4878	76.8197
		4	(5⋆0, 4, 6⋆0)	4.4038	(4, 11⋆0)	5.9742	73.7133
		6	(11⋆0, 4)	3.6505	(10⋆0, 4, 0)	4.5211	80.7428
		8	(11⋆0, 4)	3.6233	(10⋆0, 4, 0)	4.5502	79.6290
		10	(11⋆0, 4)	3.7310	(10⋆0, 4, 0)	4.5498	82.0030
20	10	2	(3⋆0, 8, 5⋆0, 2)	8.4432	(10, 9⋆0)	16.7017	50.5527
		4	(5⋆0, 4, 3⋆0, 6)	4.2271	(10, 9⋆0)	7.5217	56.1985
		6	(5⋆0, 1, 3⋆0, 9)	4.0393	(10, 9⋆0)	5.2656	76.7106
		8	(1, 8⋆0, 9)	4.0891	(7, 7⋆0, 3, 0)	5.0372	81.1779
		10	(3, 8⋆0, 7)	4.1885	(7, 7⋆0, 3, 0)	4.9817	84.0786
	12	2	(3⋆0, 4, 7⋆0, 4)	8.1759	(8, 11⋆0)	14.4642	56.5255
		4	(6⋆0, 1, 4⋆0, 7)	3.7239	(8, 11⋆0)	5.7208	65.0935
		6	(11⋆0, 8)	3.4959	(1, 9⋆0, 7, 0)	4.6220	75.6359
		8	(11⋆0, 8)	3.5874	(3, 9⋆0, 5, 0)	4.5676	78.5407
		10	(11⋆0, 8)	3.7234	(3, 9⋆0, 5, 0)	4.5500	81.8334
	16	2	(15⋆0, 4)	7.8617	(4, 15⋆0)	10.5172	74.7509
		4	(7⋆0, 4, 8⋆0)	3.0856	(4, 15⋆0)	3.7742	81.7557
		6	(8⋆0, 4, 7⋆0)	2.8102	(14⋆0, 4, 0)	3.5043	80.1930
		8	(3, 6⋆0, 1, 8⋆0)	2.9742	(14⋆0, 4, 0)	3.8680	76.8932
		10	(4, 15⋆0)	3.1557	(14⋆0, 4, 0)	4.0119	78.6583

Table 9.6. The optimal censoring scheme under MSE optimality when $\theta_1 = e^{1.5}$ and $\theta_2 = e^{0.5}$ are fixed

n	r	τ	Best Censoring Scheme	MSE	Worst Censoring Scheme	MSE	Relative Efficiency (%)
10	4	1	(6, 3⋆0)	6.6861	(0, 6, 2⋆0)	11.6232	57.5239
		3	(0, 6, 2⋆0)	17.4733	(3⋆0, 6)	68.4492	25.5274
		5	(2⋆0, 6, 0)	14.0161	(3⋆0, 6)	150.7494	9.2976
		7	(2⋆0, 6, 0)	15.0415	(3⋆0, 6)	274.8084	5.4734
		9	(2⋆0, 6, 0)	18.4278	(3⋆0, 6)	444.7415	4.1435
	6	1	(4, 5⋆0)	7.0630	(0, 4, 4⋆0)	10.4003	67.9115
		3	(2⋆0, 4, 3⋆0)	15.6672	(5⋆0, 4)	21.8711	71.6346
		5	(3⋆0, 4, 2⋆0)	9.2602	(5⋆0, 4)	26.6702	34.7212
		7	(3⋆0, 4, 2⋆0)	8.5444	(5⋆0, 4)	45.3267	18.8507
		9	(3⋆0, 4, 2⋆0)	9.6248	(5⋆0, 4)	75.6365	12.7250
	8	1	(2, 7⋆0)	8.2403	(0, 2, 6⋆0)	9.8242	83.8780
		3	(2⋆0, 2, 5⋆0)	14.9405	(2, 7⋆0)	18.0579	82.7366
		5	(3⋆0, 2, 4⋆0)	7.7356	(2, 7⋆0)	9.9645	77.6312
		7	(4⋆0, 2, 3⋆0)	6.3094	(7⋆0, 2)	10.4581	60.3299
		9	(4⋆0, 2, 3⋆0)	6.5303	(7⋆0, 2)	15.2085	42.9385
12	6	1	(6, 5⋆0)	9.2057	(2⋆0, 6, 3⋆0)	13.9979	65.7646
		3	(2⋆0, 6, 3⋆0)	12.1921	(5⋆0, 6)	24.6396	49.4816
		5	(3⋆0, 6, 2⋆0)	7.9370	(5⋆0, 6)	43.2473	18.3527
		7	(3⋆0, 6, 2⋆0)	8.3719	(5⋆0, 6)	84.8345	9.8685
		9	(2, 2⋆0, 4, 2⋆0)	9.6266	(5⋆0, 6)	146.2384	6.5828
	8	1	(4, 7⋆0)	10.5137	(2⋆0, 4, 5⋆0)	13.4514	78.1603
		3	(2⋆0, 4, 5⋆0)	11.4579	(4, 7⋆0)	17.2163	66.5526
		5	(4⋆0, 4, 3⋆0)	6.3131	(7⋆0, 4)	11.9590	52.7895
		7	(4⋆0, 4, 3⋆0)	5.9694	(7⋆0, 4)	20.7164	28.8149
		9	(1, 2⋆0, 1, 2, 3⋆0)	6.5141	(7⋆0, 4)	36.0754	18.0569
	10	1	(2, 9⋆0)	11.8325	(2⋆0, 2, 7⋆0)	13.1238	90.1602
		3	(3⋆0, 2, 6⋆0)	11.0928	(2, 9⋆0)	13.6951	80.9980
		5	(4⋆0, 2, 5⋆0)	5.5700	(2, 9⋆0)	6.7247	82.8295
		7	(5⋆0, 2, 4⋆0)	4.8283	(9⋆0, 2)	6.5828	73.3470
		9	(5⋆0, 2, 4⋆0)	5.0255	(9⋆0, 2)	9.3537	53.7279
16	8	2	(2⋆0, 8, 5⋆0)	12.9156	(8, 7⋆0)	21.0105	61.4718
		4	(4⋆0, 8, 3⋆0)	5.7315	(7⋆0, 8)	18.4851	31.0061
		6	(4⋆0, 8, 3⋆0)	5.6963	(7⋆0, 8)	44.8061	12.7131
		8	(4, 2⋆0, 1, 3, 3⋆0)	6.2036	(7⋆0, 8)	88.9667	6.9729
		10	(6, 2⋆0, 1, 1, 3⋆0)	6.8775	(7⋆0, 8)	149.0573	4.6140
	10	2	(2⋆0, 6, 7⋆0)	12.6996	(6, 9⋆0)	19.0171	66.7800
		4	(5⋆0, 6, 4⋆0)	4.9477	(6, 9⋆0)	8.1961	60.3670
		6	(5⋆0, 6, 4⋆0)	4.5543	(9⋆0, 6)	14.8544	30.6594
		8	(3, 4⋆0, 3, 4⋆0)	4.8472	(9⋆0, 6)	30.0448	16.1334
		10	(5, 3⋆0, 1, 5⋆0)	5.2338	(9⋆0, 6)	51.9260	10.0793
	12	2	(2⋆0, 4, 9⋆0)	12.6024	(4, 11⋆0)	16.6980	75.4726
		4	(5⋆0, 4, 6⋆0)	4.4919	(4, 11⋆0)	6.1988	72.4641
		6	(6⋆0, 4, 5⋆0)	3.8446	(11⋆0, 4)	5.8876	65.3005
		8	(1, 3⋆0, 1, 0, 2, 5⋆0)	4.0288	(11⋆0, 4)	10.3097	39.0774
		10	(4, 11⋆0)	4.2959	(11⋆0, 4)	17.5642	24.4585
20	10	2	(3⋆0, 17⋆0)	8.6806	(10, 9⋆0)	18.0305	48.1437
		4	(5⋆0, 15⋆0)	4.3825	(9⋆0, 10)	13.5660	32.3051
		6	(2, 3⋆0, 1, 7, 4⋆0)	4.5426	(9⋆0, 10)	37.2891	12.1822
		8	(7, 4⋆0, 3, 4⋆0)	4.8494	(9⋆0, 10)	77.1804	6.2832
		10	(9, 3⋆0, 1, 5⋆0)	5.2376	(9⋆0, 10)	131.6731	3.9778
	12	2	(3⋆0, 8, 8⋆0)	8.4912	(8, 11⋆0)	15.5191	54.7146
		4	(6⋆0, 8, 5⋆0)	3.7665	(11⋆0, 8)	6.1571	61.1732
		6	(1, 5⋆0, 7, 5⋆0)	3.7939	(11⋆0, 8)	14.8794	25.4979
		8	(6, 5⋆0, 2, 5⋆0)	4.0302	(11⋆0, 8)	31.9149	12.6280
		10	(8, 11⋆0)	4.2998	(11⋆0, 8)	56.2560	7.6433
	16	2	(4⋆0, 4, 11⋆0)	8.2964	(4, 15⋆0)	11.1870	74.1609
		4	(7⋆0, 4, 8⋆0)	3.1363	(4, 15⋆0)	3.8880	80.6654
		6	(8⋆0, 4, 7⋆0)	2.8388	(14⋆0, 4, 0)	3.6107	78.6215
		8	(3, 6⋆0, 1, 8⋆0)	3.0273	(15⋆0, 4)	5.5949	54.1078
		10	(4, 15⋆0)	3.2745	(15⋆0, 4)	9.3924	34.8628

Table 9.7. The optimal-time with minimum MSE when n, r, $\boldsymbol{R}$, θ_1 and θ_2 are fixed

			$\theta_1 = e^{1.5}$ and $\theta_2 = e^{0.5}$		$\theta_1 = e^{2.5}$ and $\theta_2 = e^{1.5}$	
n	**r**	**Censoring Scheme**	**Optimal-time**	**min. MSE**	**Optimal-time**	**min. MSE**
10	4	(3⋆0, 6)	0.497247	3.774531	1.351752	27.890224
		(6, 3⋆0)	6.917718	24.93450	18.804600	184.242430
		(2, 1, 1, 2)	0.536917	4.090915	1.459510	30.228000
		(3, 2⋆0, 3)	0.572172	3.985142	1.555255	29.446441
		(0, 3, 3, 0)	5.661822	14.922759	15.390590	110.265100
	6	(5⋆0, 4)	3.286667	21.790941	8.934054	161.014485
		(4, 5⋆0)	8.787287	11.016664	23.886290	81.402750
		(1, 0, 1, 1, 0, 1)	5.563263	12.115872	15.122720	89.524860
		(2, 4⋆0, 2)	4.939339	17.089034	13.426430	126.271830
		(2⋆0, 2, 2, 2⋆0)	6.461862	8.619150	17.565470	63.687380
	8	(7⋆0, 2)	5.535736	9.186648	15.048050	67.880650
		(2, 7⋆0)	8.744945	6.873914	23.771070	50.791740
		(0, 1, 4⋆0, 1, 0)	7.613914	7.108081	20.696700	52.522010
		(1, 6⋆0, 1)	6.629429	8.022364	18.020720	59.277700
		(3⋆0, 1, 1, 3⋆0)	7.485085	6.320418	20.346550	46.701920
12	6	(5⋆0, 6)	0.407177	3.387775	1.106907	25.032460
		(6, 5⋆0)	8.629530	10.896890	23.457460	80.517720
		(2, 0, 1, 1, 0, 2)	4.410210	14.159480	11.988590	104.625200
		(3, 4⋆0, 3)	3.977177	18.621750	10.811110	137.597160
		(2⋆0, 3, 3, 2⋆0)	5.602603	8.055846	15.229430	59.525100
	8	(7⋆0, 4)	4.125926	10.873441	11.215420	80.344460
		(4, 7⋆0)	8.588989	6.823374	23.347150	50.418290
		(1, 0, 1, 2⋆0, 1, 0, 1)	5.766066	7.419517	15.673870	54.823230
		(2, 6⋆0, 2)	5.348949	8.879327	14.539540	65.609850
		(3⋆0, 2, 2, 3⋆0)	6.417017	5.970594	17.443040	44.117050
	10	(9⋆0, 2)	5.631031	5.928696	15.306910	43.807470
		(2, 9⋆0)	8.406206	5.094936	22.850350	37.646770
		(0, 1, 6⋆0, 1, 0)	7.201301	5.353277	19.574970	39.555670
		(1, 8⋆0, 1)	6.638238	5.495566	18.044140	40.607040
		(4⋆0, 1, 1, 4⋆0)	7.249650	4.844249	19.706610	35.794430
16	8	(7⋆0, 8)	2.754655	13.103435	7.488088	96.822019
		(8, 7⋆0)	8.416617	6.769414	22.878680	50.019580
		(2, 0, 2, 2⋆0, 2, 0, 2)	4.259059	7.663110	11.577480	56.623150
		(4, 6⋆0, 4)	3.909109	10.150602	10.625930	75.003370
		(3⋆0, 4, 4, 3⋆0)	5.021862	5.610600	13.650850	41.457040
	10	(9⋆0, 6)	3.559850	7.230336	9.676677	53.425358
		(6, 9⋆0)	8.226907	5.065642	22.363060	37.430320
		(2, 0, 1, 4⋆0, 1, 0, 2)	4.925676	5.706721	13.389370	42.167280
		(3, 8⋆0, 3)	4.741041	6.151359	12.887440	45.452730
		(4⋆0, 3, 3, 4⋆0)	5.535666	4.557247	15.047520	33.673760
	12	(11⋆0, 4)	4.493343	4.769220	12.214110	35.240040
		(4, 11⋆0)	7.869169	4.111233	21.390640	30.378130
		(1, 0, 1, 6⋆0, 1, 0, 1)	5.909970	4.302062	16.064980	31.788180
		(2, 10⋆0, 2)	5.624875	4.416294	15.289940	32.632250
		(5⋆0, 2, 2, 5⋆0)	6.010544	3.861178	16.338340	28.530460
20	10	(9⋆0, 10)	2.639540	8.117453	7.174925	59.980313
		(10, 9⋆0)	8.128679	5.050435	22.096030	37.317950
		(3, 0, 2, 4⋆0, 2, 0, 3)	3.918498	5.840517	10.651550	43.155910
		(5, 8⋆0, 5)	3.737177	6.657241	10.158710	49.190730
		(4⋆0, 5, 5, 4⋆0)	4.477177	4.404244	12.170290	32.543210
	12	(11⋆0, 8)	3.215065	5.302418	8.739480	39.179860
		(8, 11⋆0)	7.762102	4.100461	21.099500	30.298540
		(2, 0, 1, 0, 1, 2⋆0, 1, 0, 1, 0, 2)	4.654535	4.271674	12.652350	31.563640
		(4, 10⋆0, 4)	4.380831	4.693092	11.908370	34.677520
		(5⋆0, 4, 4, 5⋆0)	4.803153	3.712437	13.056220	27.431410
	16	(15⋆0, 4)	4.728859	3.149274	12.854350	23.270160
		(4, 15⋆0)	6.894444	2.979400	18.741080	22.014950
		(1, 2⋆0, 1, 8⋆0, 1, 2⋆0, 1)	5.724124	3.048205	15.559860	22.523360
		(2, 14⋆0, 2)	5.658468	3.059654	15.381320	22.607960
		(7⋆0, 2, 2, 7⋆0)	5.560621	2.831259	15.115370	20.920330

Table 9.8. Interval estimation for θ_1 based on the data in Example 2 when $n = 20,\ r = 12$ and $\tau = 5$ for different progressive censoring schemes

Censoring Scheme	Method	90%	95%	99%
(11⋆0, 8)	Bootstrap (P)	(7.6192, 30.6300)	(7.0170, 31.2968)	(6.1664, 49.1116)
	(ST)	(7.9323, 25.5874)	(7.8356, 28.3682)	(7.7060, 33.7679)
	(BCa)	(7.7022, 31.0159)	(7.4645, 47.4902)	(6.7018, 99.3545)
	Approximation	(1.8022, 19.5748)	(0.0998, 21.2771)	(0.0000, 24.6043)
	Exact	(6.7551, 26.4410)	(5.9857, 31.0852)	(4.7131, 43.8428)
(8, 11⋆0)‡	Bootstrap (P)	(3.5444, 14.2814)	(3.3792, 16.3905)	(2.5526, 27.1662)
	(ST)	(3.9892, 14.8601)	(3.8481, 15.8082)	(3.7015, 22.4038)
	(BCa)	(3.9624, 18.0095)	(3.7556, 21.9938)	(3.1813, 61.6967)
	Approximation	(1.3653, 10.5605)	(0.4846, 11.4413)	(0.0000, 13.1627)
	Exact	(3.7957, 14.1406)	(3.4280, 16.6016)	(2.8302, 23.3008)
(10⋆0, 4, 4)	Bootstrap (P)	(7.6641, 31.0573)	(6.8046, 45.9254)	(5.8634, 96.3478)
	(ST)	(7.9039, 25.2230)	(7.7977, 29.7070)	(7.6935, 35.7553)
	(BCa)	(7.8097, 31.2686)	(7.0459, 47.6600)	(6.2765, 99.7112)
	Approximation	(1.8336, 19.6062)	(0.1312, 21.3086)	(0.0000, 24.6358)
	Exact	(6.8890, 26.4432)	(6.1505, 31.0852)	(4.9405, 43.8428)
(4, 4, 10⋆0)	Bootstrap (P)	(3.7920, 13.9467)	(3.5969, 18.4519)	(2.3967, 26.1617)
	(ST)	(4.2487, 14.7487)	(3.9500, 15.5997)	(3.7317, 26.0164)
	(BCa)	(4.2737, 18.7861)	(3.8351, 20.1726)	(3.3187, 36.6394)
	Approximation	(1.4857, 11.0300)	(0.5714, 11.9443)	(0.0000, 13.7311)
	Exact	(3.9483, 14.7708)	(3.5657, 17.3578)	(2.9439, 24.4287)
(4⋆0, 2, 2, 2, 2, 4⋆0)	Bootstrap (P)	(5.8335, 23.4714)	(5.2811, 30.7903)	(4.4210, 49.6410)
	(ST)	(6.9205, 25.8092)	(6.5870, 28.7427)	(6.4750, 34.6064)
	(BCa)	(6.4304, 31.0234)	(6.3702, 48.4823)	(5.0651, 99.7232)
	Approximation	(2.2362, 17.9092)	(0.7349, 19.4105)	(0.0000, 22.3446)
	Exact	(6.5358, 24.2108)	(5.9136, 28.4491)	(4.9084, 40.0830)
(2, 0, 2, 6⋆0, 2, 0, 2)	Bootstrap (P)	(5.7044, 25.0609)	(5.1417, 26.9826)	(4.3019, 41.7131)
	(ST)	(6.1685, 21.6505)	(5.9779, 24.5269)	(5.7198, 30.5802)
	(BCa)	(5.9333, 26.9192)	(6.0312, 42.7513)	(5.0517, 48.0536)
	Approximation	(1.8669, 15.9418)	(0.5188, 17.2899)	(0.0000, 19.9249)
	Exact	(5.6962, 21.5512)	(5.1228, 25.3516)	(4.1867, 35.8105)
(3⋆0, 8, 8⋆0)†	Bootstrap (P)	(4.7232, 18.1680)	(4.2184, 20.3091)	(3.4659, 31.1892)
	(ST)	(5.1448, 18.1312)	(4.8177, 20.9644)	(4.4267, 25.9902)
	(BCa)	(5.2925, 31.1765)	(4.8851, 46.8117)	(4.6630, 99.5848)
	Approximation	(2.0845, 14.0373)	(0.9396, 15.1823)	(0.0000, 17.4200)
	Exact	(4.9359, 18.9557)	(4.4518, 22.3907)	(3.6679, 31.9482)

† and ‡ correspond to the best and worst optimal progressive censoring scheme, respectively

Table 9.9. Interval estimation for θ_2 based on the data in Example 2 when $n = 20,\ r = 12$ and $\tau = 5$ for different progressive censoring schemes

Censoring Scheme	Method	90%	95%	99%
(11⋆0, 8)	Bootstrap (P)	(2.9197, 13.9012)	(2.2737, 15.4757)	(1.2029, 19.1343)
	(ST)	(4.3684, 17.8598)	(3.7036, 21.8055)	(3.2409, 30.6980)
	(BCa)	(4.1206, 22.4190)	(3.5766, 23.1080)	(2.9650, 25.3142)
	Approximation	(2.4412, 12.4221)	(1.4852, 13.3781)	(0.0000, 15.2466)
	Exact	(4.0903, 19.3707)	(3.6078, 24.9707)	(2.7612, 51.8994)
(8, 11⋆0)‡	Bootstrap (P)	(0.7069, 3.4105)	(0.5734, 3.8266)	(0.3063, 4.9397)
	(ST)	(1.1011, 4.6370)	(1.0141, 5.4108)	(0.7822, 9.9626)
	(BCa)	(1.0573, 4.8731)	(0.8153, 6.0384)	(0.6392, 8.6880)
	Approximation	(0.6148, 3.1285)	(0.3740, 3.3693)	(0.0000, 3.8399)
	Exact	(1.0308, 4.7848)	(0.9140, 6.0010)	(0.7178, 10.6030)
(10⋆0, 4, 4)	Bootstrap (P)	(2.3507, 11.5815)	(1.9436, 12.8934)	(0.8473, 15.5043)
	(ST)	(3.6280, 15.0959)	(3.2017, 17.4813)	(2.5272, 29.7463)
	(BCa)	(3.4104, 15.4120)	(2.9497, 20.0069)	(2.0473, 27.1174)
	Approximation	(2.0405, 10.3829)	(1.2414, 11.1819)	(0.0000, 12.7437)
	Exact	(3.4146, 16.2793)	(3.0090, 21.0889)	(2.2949, 45.1611)
(4, 4, 10⋆0)	Bootstrap (P)	(0.7597, 3.3935)	(0.6315, 3.8579)	(0.2945, 4.6152)
	(ST)	(1.0753, 4.2903)	(0.9770, 5.1445)	(0.7936, 9.5134)
	(BCa)	(0.9690, 4.5006)	(0.8847, 5.3209)	(0.6593, 7.2495)
	Approximation	(0.6148, 3.1285)	(0.3740, 3.3693)	(0.0000, 3.8399)
	Exact	(1.0318, 4.7673)	(0.9154, 5.9628)	(0.7202, 10.4199)
(4⋆0, 2, 2, 2, 2, 4⋆0)	Bootstrap (P)	(0.8970, 4.0304)	(0.7043, 4.5353)	(0.4326, 5.1445)
	(ST)	(1.2614, 5.1032)	(1.1344, 6.4068)	(1.0015, 9.9530)
	(BCa)	(1.0772, 4.8804)	(1.0049, 6.1737)	(0.7415, 6.3388)
	Approximation	(0.7243, 3.6857)	(0.4407, 3.9693)	(0.0000, 4.5237)
	Exact	(1.2224, 5.5020)	(1.0879, 6.7883)	(0.8670, 11.0791)
(2, 0, 2, 6⋆0, 2, 0, 2)	Bootstrap (P)	(1.7490, 7.2193)	(1.2287, 8.2428)	(0.5398, 11.9232)
	(ST)	(2.3513, 9.0882)	(2.1360, 11.7481)	(1.7936, 23.0902)
	(BCa)	(2.1919, 9.1754)	(1.9217, 15.4783)	(1.4421, 17.3095)
	Approximation	(1.3233, 6.7334)	(0.8051, 7.2516)	(0.0000, 8.2644)
	Exact	(2.2157, 10.4214)	(1.9589, 13.2550)	(1.5185, 25.2881)
(3⋆0, 8, 8⋆0)†	Bootstrap (P)	(0.7405, 3.3836)	(0.5818, 3.7401)	(0.4078, 4.8563)
	(ST)	(1.1026, 4.4840)	(0.9732, 5.8714)	(0.7799, 7.0224)
	(BCa)	(1.0459, 4.6043)	(0.9624, 6.0527)	(0.7540, 6.3487)
	Approximation	(0.6148, 3.1285)	(0.3740, 3.3693)	(0.0000, 3.8399)
	Exact	(1.0422, 4.6208)	(0.9286, 5.6882)	(0.7403, 9.3213)

† and ‡ correspond to the best and worst optimal progressive censoring scheme, respectively

Table 9.10. Interval estimation for θ_1 based on the data in Example 2 when $n = 20,\ r = 16$ and $\tau = 5$ for different progressive censoring schemes

Censoring Scheme	Method	90%	95%	99%
(15⋆0, 4)	Bootstrap (P)	(7.7205, 31.0638)	(7.2833, 46.5117)	(6.1618, 48.7250)
	(ST)	(7.8785, 24.9563)	(7.7689, 27.8029)	(7.6913, 34.7115)
	(BCa)	(8.2103, 32.1004)	(7.4564, 47.3957)	(6.4107, 96.5373)
	Approximation	(1.8831, 19.6557)	(0.1807, 21.3581)	(0.0000, 24.6853)
	Exact	(7.1480, 26.4453)	(6.4679, 31.0852)	(5.3601, 43.8428)
(4, 15⋆0)‡	Bootstrap (P)	(5.3282, 24.0386)	(4.8693, 26.9841)	(4.2137, 40.9931)
	(ST)	(5.8845, 21.5367)	(5.7643, 23.8038)	(5.6449, 28.8365)
	(BCa)	(5.5550, 24.6928)	(5.3355, 39.4726)	(4.7075, 82.4953)
	Approximation	(1.7027, 15.1866)	(0.4112, 16.4782)	(0.0000, 19.0025)
	Exact	(5.5236, 20.3805)	(5.0008, 23.9203)	(4.1562, 33.5889)
(14⋆0, 2, 2)	Bootstrap (P)	(7.4699, 30.5301)	(6.9216, 31.9434)	(5.5611, 48.7172)
	(ST)	(7.9447, 26.5075)	(7.7987, 28.8120)	(7.6864, 38.5929)
	(BCa)	(7.6898, 30.9446)	(7.2449, 47.1811)	(6.0841, 99.8929)
	Approximation	(1.8832, 19.6558)	(0.1808, 21.3581)	(0.0000, 24.6853)
	Exact	(7.1507, 26.4453)	(6.4717, 31.0852)	(5.3693, 43.8428)
(2, 2, 14⋆0)	Bootstrap (P)	(5.7763, 23.6235)	(4.9931, 25.4672)	(4.1218, 42.2223)
	(ST)	(5.9695, 19.9079)	(5.8391, 23.8068)	(5.5879, 30.3764)
	(BCa)	(6.0477, 25.3383)	(5.2593, 39.3973)	(4.6981, 45.0710)
	Approximation	(1.8002, 15.4587)	(0.4919, 16.7670)	(0.0000, 19.3240)
	Exact	(5.6082, 20.7202)	(5.0770, 24.3304)	(4.2187, 34.2041)
(6⋆0, 1, 1, 1, 1, 6⋆0)	Bootstrap (P)	(7.3080, 31.2168)	(6.2011, 31.9030)	(5.1995, 48.1872)
	(ST)	(7.8832, 26.4767)	(7.7799, 32.9499)	(7.7191, 40.9189)
	(BCa)	(7.5467, 31.4499)	(6.4568, 47.2244)	(5.8610, 97.5159)
	Approximation	(1.9275, 19.7001)	(0.2251, 21.4025)	(0.0000, 24.7297)
	Exact	(7.1553, 26.4453)	(6.4801, 31.0852)	(5.3906, 43.8428)
(1, 2⋆0, 1, 8⋆0, 1, 2⋆0, 1)	Bootstrap (P)	(6.5878, 27.7176)	(6.1081, 29.8341)	(5.2458, 49.4007)
	(ST)	(7.0962, 24.1443)	(6.8439, 26.7152)	(6.7381, 32.2997)
	(BCa)	(6.6201, 28.4727)	(6.5875, 44.4735)	(5.4979, 97.5127)
	Approximation	(1.9282, 17.9011)	(0.3982, 19.4311)	(0.0000, 22.4214)
	Exact	(6.5247, 24.1702)	(5.9064, 28.4064)	(4.9054, 40.0488)
(3⋆0, 4, 12⋆0)†	Bootstrap (P)	(6.0557, 22.3669)	(5.2670, 30.0157)	(4.3681, 48.1113)
	(ST)	(6.5452, 22.6138)	(6.1842, 27.1483)	(5.9840, 34.8190)
	(BCa)	(6.8388, 30.7426)	(6.1729, 45.9260)	(5.6860, 99.2218)
	Approximation	(2.1269, 16.9896)	(0.7032, 18.4132)	(0.0000, 21.1957)
	Exact	(6.1448, 22.9205)	(5.5604, 26.9751)	(4.6170, 38.1689)

† and ‡ correspond to the best and worst optimal progressive censoring scheme, respectively

Table 9.11. Interval estimation for θ_2 based on the data in Example 2 when $n = 20,\ r = 16$ and $\tau = 5$ for different progressive censoring schemes

Censoring Scheme	Method	90%	95%	99%
(15⋆0, 4)	Bootstrap (P)	(2.7866, 7.9334)	(2.4479, 8.8422)	(1.8304, 10.4831)
	(ST)	(3.5748, 9.8201)	(3.2255, 11.2764)	(2.8688, 15.1626)
	(BCa)	(3.4420, 10.0787)	(3.1213, 12.5051)	(2.6220, 11.9991)
	Approximation	(2.5216, 7.9884)	(1.9980, 8.5120)	(0.9745, 9.5355)
	Exact	(3.2999, 9.9950)	(3.0145, 11.4789)	(2.5281, 15.5835)
(4, 15⋆0)‡	Bootstrap (P)	(1.7472, 4.8536)	(1.4680, 5.5189)	(0.9051, 6.3976)
	(ST)	(2.1087, 5.7230)	(1.8459, 6.5634)	(1.6037, 10.8823)
	(BCa)	(2.0115, 5.7987)	(1.7200, 6.4434)	(1.5072, 8.1269)
	Approximation	(1.5216, 4.8204)	(1.2056, 5.1364)	(0.5881, 5.7539)
	Exact	(1.9889, 6.0384)	(1.8176, 6.9272)	(1.5277, 9.3396)
(14⋆0, 2, 2)	Bootstrap (P)	(2.7246, 8.1049)	(2.3914, 8.9676)	(1.3873, 10.6279)
	(ST)	(3.3663, 9.9867)	(3.1185, 11.1234)	(2.7329, 16.9733)
	(BCa)	(3.1730, 9.7300)	(3.0033, 10.7044)	(2.2676, 16.3365)
	Approximation	(2.5207, 7.9853)	(1.9972, 8.5088)	(0.9742, 9.5318)
	Exact	(3.2986, 9.9911)	(3.0133, 11.4758)	(2.5268, 15.5835)
(2, 2, 14⋆0)	Bootstrap (P)	(1.7215, 5.0009)	(1.3441, 5.5100)	(0.9355, 6.7688)
	(ST)	(2.0506, 5.8740)	(1.9056, 7.0181)	(1.6112, 9.9742)
	(BCa)	(1.9822, 5.9733)	(1.6555, 6.9376)	(1.4157, 7.3832)
	Approximation	(1.5216, 4.8204)	(1.2056, 5.1364)	(0.5881, 5.7539)
	Exact	(1.9884, 6.0406)	(1.8172, 6.9295)	(1.5277, 9.3396)
(6⋆0, 1, 1, 1, 1, 6⋆0)	Bootstrap (P)	(2.0153, 5.7452)	(1.6665, 6.2160)	(1.4218, 7.8402)
	(ST)	(2.3377, 6.5351)	(2.1432, 7.6423)	(1.8363, 8.6357)
	(BCa)	(2.2275, 6.1985)	(2.1258, 7.5606)	(1.7220, 9.7381)
	Approximation	(1.7481, 5.5379)	(1.3851, 5.9009)	(0.6756, 6.6104)
	Exact	(2.2935, 6.8867)	(2.0978, 7.8854)	(1.7663, 10.5664)
(1, 2⋆0, 1, 8⋆0, 1, 2⋆0, 1)	Bootstrap (P)	(2.1555, 6.5910)	(2.0295, 7.6299)	(1.3209, 8.2178)
	(ST)	(2.7670, 8.1150)	(2.4158, 8.5607)	(2.1197, 11.3166)
	(BCa)	(2.5255, 7.7236)	(2.3689, 8.6886)	(1.9080, 11.1337)
	Approximation	(2.0077, 6.3603)	(1.5908, 6.7772)	(0.7759, 7.5921)
	Exact	(2.6247, 7.9682)	(2.3982, 9.1458)	(2.0142, 12.3669)
(3⋆0, 4, 12⋆0)†	Bootstrap (P)	(1.5736, 5.1370)	(1.4143, 5.3534)	(1.2943, 6.2831)
	(ST)	(2.0191, 6.1451)	(1.8971, 6.8944)	(1.6676, 7.1841)
	(BCa)	(1.8129, 5.7948)	(1.8495, 6.7222)	(1.4934, 8.6884)
	Approximation	(1.5216, 4.8204)	(1.2056, 5.1364)	(0.5881, 5.7539)
	Exact	(1.9893, 6.0326)	(1.8188, 6.9119)	(1.5314, 9.2786)

† and ‡ correspond to the best and worst optimal progressive censoring scheme, respectively

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Part IV

Engineering Modeling

10

Non-Gaussian State Estimation in Power Systems

Roberto Mínguez[1], Antonio J. Conejo[2], and Ali S. Hadi[3]

[1] Department of Mathematics, University of Castilla-La Mancha, Spain
[2] Department of Electrical Engineering, University of Castilla-La Mancha, Spain
[3] Department of Mathematics, American University in Cairo

Abstract: Most power system state estimators consider measurements as independent Gaussian random variables and use a weighted least squares approach to estimate the most likely system state. More often than not, in practice the Gaussian and independent measurements assumptions do not hold. In this paper we relax these questionable assumptions and develop techniques to accurately estimate the system state through appropriate transformations of correlated non-Gaussian measurements. An example illustrates the proposed estimation technique. In addition to its generality to include more complex statistical models, the results show that the proposed estimation technique is more accurate and more robust with respect to outliers than the weighted least squares approach.

Keywords and phrases: Cholesky decomposition, maximum likelihood, non-gaussian random variables, Nataf transformation, orthogonal transformation, Rosenblatt transformation, weighted least squares estimation

10.1 Introduction

Owing to the complexities of operating large, interconnected networks, more and more electric utilities replace their traditional dispatch offices with modern Energy Management System (EMS). The purpose of an EMS is to monitor, control, and optimize the transmission and generation facilities with advanced computer technologies. The aim of the state estimation is to get the best estimate of the current system states processing a set of real-time redundant measures and network parameters available in the EMS database. The performance of state estimation, therefore, depends on the accuracy of the measured data as well as the parameters of the network model. The measured data are subject to noise or errors in the metering system and the communication process. Large errors in the analog measurements, the so-called bad data, may happen in practice. Network parameters such as impedence of transmission lines may be incorrect as a result of inaccurate data provided by the manufacturer, error in calibration, etc. In addition, due to the lack of field information and possible errors in calculations, transformer tap positions may be erroneous.

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The purpose of a state estimator is to filter all these errors to achieve the best possible estimate of the state of the system. Background on state estimation can be found, for instance, in Larson et al. (1970), Schweppe and Wildes (1970), Schweppe and Rom (1970), Schweppe (1970), García et al. (1979), Holten et al. (1988), Monticelli and García (1990), Monticelli (2000), and Abur and Expósito (2004).

This paper is related to and partly motivated by state estimation in distribution networks where the number of available real time measurements is generally low and load predictions are used as pseudomeasurements. Past work on statistical modeling of the states of distribution networks has shown that loads are not normally distributed, Borkowska (1974), Allan and Al-Shakarchi (1976), Dopazo et al. (1975), EPRI Report EA-3467 (1984), Anders (1990), and Herman and Kritzinger (1993), i.e., loads are not generally Gaussian random variables. It is also recognized that certain measurements, such as voltage and active and reactive power injections at a given bus, are correlated in both transmission and distribution networks. Due to these reasons variables in state estimation cannot be modeled as independent Gaussian random variables.

A general weighted-least-squares (WLS) state estimator that does not require the measurements to be either Gaussian or statistically independent is proposed. It is based on the maximum likelihood estimation using appropriate statistical transformations.

This paper is organized as follows. In Section 10.2 the maximum likelihood estimation method and associated statistical assumptions are presented. In Section 10.4 the likelihood estimation using different transformations (Transformed Likelihood Estimation, TLE) is explained. In Section 10.5 the TLE method is applied to the power system state estimation problem (General State Estimation, GSE). In Section 10.6 a method for bad data detection is provided. Section 10.7 gives results from an illustrative example to demonstrate the functioning of the method. And finally, Section 10.8 provides some conclusions.

10.2 Maximum Likelihood Estimation

The objective of the state estimation is to determine the most likely state of a system based on the quantities that are measured, i.e., measurements. One way to accomplish this is by the maximum likelihood estimation (MLE), a method widely used in statistics.

Suppose we have a vector $\boldsymbol{z} = (z_1, z_2, \ldots, z_m)^T$ of m measurements. These measurements are assumed to have a known probability distribution with unknown parameters, that is, the joint probability density function of $\boldsymbol{z}$ is given by

$$f_Z(\boldsymbol{z}; \boldsymbol{\theta}) = f_Z(z_1, z_2, \ldots, z_m; \boldsymbol{\theta}), \tag{10.1}$$

where $\boldsymbol{\theta}$ is a vector containing the parameters of the probability density function. Viewed as a function of $\boldsymbol{\theta}$ given the measurements $\boldsymbol{z}$, (10.1) can be written as

$$f_Z(\boldsymbol{z}; \boldsymbol{\theta}) = L(\boldsymbol{\theta}; \boldsymbol{z}). \tag{10.2}$$

The function $L(\boldsymbol{\theta}; \boldsymbol{z})$ is referred to as the likelihood function and will attain its peak value if the unknown parameters are selected to be closest to their actual values. Hence, an optimization problem can be set up in order to maximize the likelihood function

as a function of the unknown parameters. The solution gives the maximum likelihood estimates for the parameters of interest.

The objective of the maximum likelihood estimation is to maximize the likelihood function (10.1) by varying the assumed parameters $\boldsymbol{\theta}$. In determining the maximum likelihhod estimate of $\boldsymbol{\theta}$, the likelihood function is commonly replaced by its logarithm in order to simplify the optimization procedure. The modified function

$$\ell(\boldsymbol{\theta}; \boldsymbol{z}) = \log L(\boldsymbol{\theta}; \boldsymbol{z}) \tag{10.3}$$

is called log-likelihood function. Thus, the likelihood estimation problem can be stated as:

$$\underset{\boldsymbol{\theta}}{\text{maximize}}\ \ell(\boldsymbol{\theta}; \boldsymbol{z}). \tag{10.4}$$

The solution of (10.4) gives the maximum likelihood estimates for the parameters of interest.

The complexity of the log-likelihood function depends on the assumed joint probability density and on whether the independents are independent. Its expression can be very simple when the variables are assumed independent. In this case, the log-likelihood function in (10.3) becomes

$$\ell(\boldsymbol{\theta}; \boldsymbol{z}) = \sum_{i=1}^{m} \log f_{Z_i}(z_i; \boldsymbol{\theta}), \tag{10.5}$$

where $f_{Z_i}(z_i; \boldsymbol{\theta})$ is the marginal probability density function of the ith measurement Z_i.

In addition to the assumption of independence, the measurements are also customarily assumed to have a Gaussian distribution. These two assumptions are made only to simplify the form of the log-likelihood. In practical state estimation problems, these two assumptions do not hold, and the general form of the log-likelihood function in (10.3) is much more complex than in its special case in (10.5) because the joint probability density function (10.1) must be completely described.

In this paper we relax both the independence and normality assumptions and show that it is possible, through appropriate transformation, to obtain a set of independent normal random variables which may then be used with regression methods, hence reducing substantially the complexity of the general state estimation problem.

10.3 Transformation of Random Variables

Consider the general vector $\boldsymbol{z}$ of random variables with known joint probability density function (10.1) which is related to another vector of random variables $\boldsymbol{y}$ (Freeman (1963)) by a known function:

$$\boldsymbol{y} = \boldsymbol{y}(\boldsymbol{z})$$

having unique (i.e., one to one) inverse

$$\boldsymbol{z} = \boldsymbol{z}(\boldsymbol{y}).$$

Then

$$f_Y(\boldsymbol{y};\boldsymbol{\theta}) = f_Z(\boldsymbol{z};\boldsymbol{\theta})|\boldsymbol{J}|, \tag{10.6}$$

where $\boldsymbol{J}$ is the Jacobian of the transformation whose elements are $J_{ij} = \partial z_j/\partial y_i$. Transformation (10.6) is valid provided its uniqueness.

In this context the next subsections present several methods for transforming arbitrary random variables into independent standard normal variables.

10.3.1 Rosenblatt transformation

Consider a vector of uniformly distributed random variables denoted by $\boldsymbol{U}$. Let these be the intermediaries between the random variables in the original space $\boldsymbol{Z}$, and the standardized normal variables $\boldsymbol{Y}$. Provided that the joint probability distribution function $F_Z(\boldsymbol{z})$ it is known, its conditional distributions $F_i(z_i|z_1, z_2, \ldots, z_{i-1})$ are available. The Rosenblatt (1952) transformation in the m-dimensional space becomes:

$$\begin{aligned} \Phi(y_1) = u_1 &= F_1(z_1), \\ \Phi(y_2) = u_2 &= F_2(z_2|z_1), \\ &\vdots \\ \Phi(y_m) = u_m &= F_m(z_m|z_1, z_2, \ldots, z_{m-1}), \end{aligned} \tag{10.7}$$

where $\Phi(\cdot)$ is the standard normal cumulative distribution function and $u_1, \ldots, u_m$ are the uniformly distributed variables $U(0,1)$. The component of the vector $\boldsymbol{Y}$ can be obtained by successive inversion:

$$\begin{aligned} y_1 &= \Phi^{-1}[F_1(z_1)], \\ y_2 &= \Phi^{-1}[F_2(z_2|z_1)], \\ &\vdots \\ y_m &= \Phi^{-1}[F_m(z_m|z_1, z_2, \ldots, z_{m-1})]. \end{aligned} \tag{10.8}$$

We also need to obtain the jacobian of the transformation. For simplicity, the inverse of the Jacobian is obtained first:

$$J_{ij}^{-1} = \frac{\partial y_i}{\partial z_j} = \begin{cases} 0, & \text{if } i < j, \\ \dfrac{f_i(z_i|z_1, \ldots, z_{i-1})}{\phi(y_i)}, & \text{if } i = j, \\ \dfrac{1}{\phi(y_i)} \dfrac{\partial F_i(z_i|z_1, \ldots, z_{i-1})}{\partial z_i}, & \text{if } i > j, \end{cases} \tag{10.9}$$

where the Jacobian is given in terms of $\boldsymbol{z}$. Note that $\boldsymbol{J}^{-1}$ and $\boldsymbol{J}$ are lower triangular matrices, where $\boldsymbol{J}$ can be obtained from $\boldsymbol{J}^{-1}$ by back substitution.

10.3.2 Nataf transformation

If only marginal probability distributions and correlation data are available, even for non-normal random variables, the Nataf transformation may be applied to give a set of independent normal random variables. Note that because there is no information about the conditional distributions, the Rosenblatt transformation cannot be applied. This transformation creates an approximation based on a joint normal distribution.

Considering the marginal cumulative distribution functions $F_{Z_i}(z_i)$ the transformation in (10.8) becomes:

$$\begin{aligned} y_1 &= \Phi^{-1}[F_1(z_1)], \\ y_2 &= \Phi^{-1}[F_2(z_2)], \\ &\vdots \\ y_m &= \Phi^{-1}[F_m(z_m)]. \end{aligned} \tag{10.10}$$

It is now assumed that $\boldsymbol{Y}$ is jointly normal, with m-dimensional standard normal probability density function $\phi_m(\boldsymbol{y}, \boldsymbol{\rho})$ having zero means, unit standard deviations and correlation matriz $\boldsymbol{\rho} = \{\rho_{ij}\}$. The Nataf (1962) approximation for the joint probability density function is given by:

$$f_Z(\boldsymbol{z}; \boldsymbol{\theta}) = \phi_m(\boldsymbol{y}, \boldsymbol{\rho}; \boldsymbol{\theta})|\boldsymbol{J}|, \tag{10.11}$$

where the Jacobian determinant $|\boldsymbol{J}|$ is obtained, taking into account (10.9), by:

$$|J| = \frac{\phi(y_1)\phi(y_2)\cdots\phi(y_m)}{f_{Z_1}(z_1)f_{Z_2}(z_2)\cdots f_{Z_m}(z_m)}. \tag{10.12}$$

Methods for obtaining $\boldsymbol{\rho}$ are shown in Liu and Der Kiureghian (1986).

Note that the resulting distribution may be transformed to an independent standarized distribution $\phi_m(\boldsymbol{t}, \boldsymbol{I})$ through the orthogonal transformation shown below.

10.3.3 Orthogonal transformation of normal random variables

Let $\boldsymbol{Z}$ be a correlated vector of random variables, with mean $\boldsymbol{\mu}_Z$ and covariance matrix $\boldsymbol{C}_Z$. This matrix is diagonal if the variables are uncorrelated. This is a sufficient measurement of dependence for normal distributions. An uncorrelated vector $\boldsymbol{U}$, and a linear transformation matrix $\boldsymbol{A}$, is now sought, such that

$$\boldsymbol{U} = \boldsymbol{A}\boldsymbol{Z}. \tag{10.13}$$

It is desirable that the transformation in (10.13) is also orthogonal so that the Euclidean distances remain unchanged. From matrix theory (Golub (1996)), this implies that $\boldsymbol{A}^T = \boldsymbol{A}^{-1}$.

Under the linear transformation (10.13) the covariance matrix of $\boldsymbol{U}$ becomes

$$\boldsymbol{C}_U = \boldsymbol{A}\boldsymbol{C}_Z\boldsymbol{A}^T. \tag{10.14}$$

To obtain an uncorrelated vector $\boldsymbol{U}$, the matrix $\boldsymbol{C}_U$ has to be strictly diagonal. This can be achieved by finding the characteristic values (eigenvalues) of $\boldsymbol{C}_Z$, which can be transformed into:

$$\boldsymbol{C}_Z = \boldsymbol{A}_Z\boldsymbol{C}_U\boldsymbol{A}_Z^T, \tag{10.15}$$

where matrix $\boldsymbol{C}_U$ contains the characteristic values λ_{ii} and the columns of matrix $\boldsymbol{A}_Z$ are the characteristic vectors. Proceeding in this way matrix $\boldsymbol{A}$ in (10.14) is equal to $\boldsymbol{A}_Z$.

Note that under the transformation in (10.13) the inverse of the Jacobian becomes matrix $\boldsymbol{A}$, which is orthogonal. It follows readily that in this case $|\boldsymbol{J}^{-1}| = \pm 1$.

There is another alternative manner to get an orthogonal transformation. Note that the standard deviations of $\boldsymbol{C}_U$ $(\lambda_{ii}^{1/2})$ must all be positive, since they have no

physical meaning otherwise. This means that $\boldsymbol{C}_Z$ must be a positive definite matrix, thus Cholesky decomposition can be applied

$$\boldsymbol{C}_Z = \boldsymbol{L}\boldsymbol{L}^T.$$

Substituting this expression in (10.14) and considering that our aim is to get $\boldsymbol{C}_U = \boldsymbol{I}$ we have:

$$\begin{aligned} \boldsymbol{C}_U &= \boldsymbol{A}\boldsymbol{C}_Z\boldsymbol{A}^T \\ &= (\boldsymbol{A}\boldsymbol{L})\left(\boldsymbol{L}^T\boldsymbol{A}^T\right) = \boldsymbol{I}. \end{aligned} \tag{10.16}$$

For expression (10.16) to hold $\boldsymbol{A}$ must be equal to $\boldsymbol{L}^{-1}$. This way matrix $\boldsymbol{A}$ will be lower-triangular. The last step is to transform the variables $\boldsymbol{U} \sim N(\boldsymbol{\mu}_Z, \boldsymbol{I})$ into the standardized normal random variables $\boldsymbol{Y} \sim N(\boldsymbol{0}, \boldsymbol{I})$ by means of:

$$\boldsymbol{Y} = \boldsymbol{A}(\boldsymbol{Z} - \boldsymbol{\mu}_Z). \tag{10.17}$$

Using transformation (10.17) equation (10.6) becomes:

$$\prod_{i=1}^{m} f_{Y_i}(y_i; \boldsymbol{\theta}) = f_Z(\boldsymbol{z}; \boldsymbol{\theta})|\boldsymbol{A}|, \tag{10.18}$$

where the Jacobian $\boldsymbol{J}$ corresponds to matrix $\boldsymbol{A}$.

10.4 The Transformed Likelihood Estimation Problem

An alternative formulation of the Maximum Likelihood Estimation problem (10.4) consists of transforming a vector $\boldsymbol{Z}$ of random variables into an independent standardized normal random vector $\boldsymbol{Y}$ using the transformations stated in Section 10.2.

Thus using expression (10.6) problem (10.4) becomes:

$$\underset{\boldsymbol{\theta}}{\text{maximize}} \log(f_Y(\boldsymbol{y}; \boldsymbol{\theta})/|\boldsymbol{J}|) \tag{10.19}$$

subject to

$$\boldsymbol{y} = T(\boldsymbol{z}; \boldsymbol{\theta}), \tag{10.20}$$

$$\boldsymbol{\theta}^{\min} \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^{\max}, \tag{10.21}$$

where (10.20) is the transformation, i.e., Rosenblatt (10.8), Nataf (10.10) or the orthogonal transformation (10.17), $\boldsymbol{J}$ is the Jacobian of the corresponding transformation, and (10.21) is the constraint fixing limits for the parameters involved.

As in the transformations above, $\boldsymbol{Y}$ is a vector of standardized normal random variables, the objective function (10.19) is equivalent to:

$$\underset{\boldsymbol{\theta}}{\text{minimize}} \sum_{i=1}^{m} y_i^2 \,. \tag{10.22}$$

10.5 General State Estimation (GSE) Formulation

Most state estimation models in practical use are formulated as overdetermined systems of nonlinear equations. Consider the nonlinear measurement model

$$\boldsymbol{z} = \boldsymbol{h}(\boldsymbol{x}^{\text{true}}) + \boldsymbol{e}, \tag{10.23}$$

where $\boldsymbol{z}$ is the vector of measurements, $\boldsymbol{x}^{\text{true}}$ is the true state vector, i.e. the parameters in the above statistical model ($\boldsymbol{\theta}$), $\boldsymbol{h}$ is a nonlinear function vector relating measurements to states, and $\boldsymbol{e}$ is the measurement error. There are m measurements and n state variables, $n < m$.

In general, the state estimation problem can be formulated mathematically as an optimization problem including equality and inequality constraints as:

$$\underset{\boldsymbol{x}}{\text{minimize}} \sum_{i=1}^{m} y_i^2 \text{ subject to } \begin{cases} \boldsymbol{y} = T(\boldsymbol{z}; \boldsymbol{h}(\boldsymbol{x})), \\ \boldsymbol{c}(\boldsymbol{x}) = \boldsymbol{0}, \\ \boldsymbol{g}(\boldsymbol{x}) \leq \boldsymbol{0}, \end{cases} \tag{10.24}$$

where $\boldsymbol{x}$ is the vector of state variables (parameters to be obtained), $\boldsymbol{h}(\boldsymbol{x})$ are the nonlinear functions relating measurements to states, i.e., power flow quantities (dependent variables), $\boldsymbol{c}(\boldsymbol{x})$ are the equality constraints representing very accurate measurements (zero injections), and $\boldsymbol{g}(\boldsymbol{x})$ are inequality constraints normally used to represent physical operating limits. Note that constraint (10.21) is included in the last constraint in (10.24).

Note that in this paper we consider as state variables nodal voltages and angles. Power flows in branches that follow Kirchoff's laws are dependent variables and can be determined from the state variables. However, in branches where the application of Kirchoff's law is not fruitful, such as branches with unknown impedances, flows can be introduced as additional state variables.

10.5.1 Independent gaussian probability density function

Traditionally, measurement errors in state estimation are assumed to be independent and to have a Gaussian (Normal) distribution. Under these assumptions, and considering (10.17), problem (10.24) becomes:

$$\underset{\boldsymbol{x}}{\text{minimize}} \sum_{i=1}^{m} y_i^2 \text{ subject to } \begin{cases} y_i = \dfrac{z_i - h_i(\boldsymbol{x})}{\sigma_i}, \\ \boldsymbol{c}(\boldsymbol{x}) = \boldsymbol{0}, \\ \boldsymbol{g}(\boldsymbol{x}) \leq \boldsymbol{0}, \end{cases} \tag{10.25}$$

where the first constraint corresponds to the Rosenblatt transformation for this particular statistical assumption.

Considering the residual as $\boldsymbol{r} = \boldsymbol{z} - \boldsymbol{h}(\boldsymbol{x})$ and the weights $w_i = \sigma_i^{-2}$, the above problem can be expressed as:

$$\underset{\boldsymbol{x}}{\text{minimize}} \sum_{i=1}^{m} w_i r_i^2 \text{ subject to } \begin{cases} r_i = z_i - h_i(\boldsymbol{x}), \\ \boldsymbol{c}(\boldsymbol{x}) = \boldsymbol{0}, \\ \boldsymbol{g}(\boldsymbol{x}) \leq \boldsymbol{0}, \end{cases} \tag{10.26}$$

which is the constrained weighted least squares formulation.

10.5.2 Dependent gaussian probability density function

If measurement errors are assumed to be dependent and have a Gaussian (Normal) distribution with correlation matrix $\boldsymbol{\rho}$ and known standard deviation vectors $\boldsymbol{\sigma}$, the problem in (10.24) becomes:

$$\underset{\boldsymbol{x}}{\text{minimize}} \sum_{i=1}^{m} y_i^2 \text{ subject to } \begin{cases} \boldsymbol{y} = \boldsymbol{A}(\boldsymbol{z} - \boldsymbol{h}(\boldsymbol{x})), \\ \boldsymbol{c}(\boldsymbol{x}) = \boldsymbol{0}, \\ \boldsymbol{g}(\boldsymbol{x}) \leq \boldsymbol{0}, \end{cases} \tag{10.27}$$

where matrix $\boldsymbol{A}$ is the inverse of the Cholesky transformation matrix of the covariance matrix whose elements are $\sigma_i \sigma_j \rho_{ij}$.

10.5.3 Dependent non-gaussian probability density function

The most general case corresponds to the case where measurement errors are assumed to be dependent and to have a non-Gaussian distribution. This case corresponds to problem (10.24).

10.6 Bad Data Detection

One advantage of the proposed method is that the Chi-square test can be applied in a simple manner. Note that the transformation (10.20) allows us to obtain a set of independent standard normal random variables $Y_i \sim N(0, 1)$, and considering that the objective function (10.22) of the transformed likelihood estimation problem is the sum of squares of the Y_i variables, therefore, the objective function has a χ^2 distribution with at most $(m - n)$ degrees of freedom, since in power systems, at least n measurements will have to satisfy the power balance equations. Thus, χ^2 test for detecting bad data can be used as follows:

1. Solve the estimation problem and obtain the objective function optimal value $\sum_{i=1}^{m} y_i^2$.
2. Get the value of the Chi-square distribution function corresponding to a detection confidence with probability α, $\chi^2_{m-n,\alpha}$.
3. Check if $\sum_{i=1}^{m} y_i^2 \geq \chi^2_{m-n,\alpha}$; if yes, bad data is suspected; else, data are assumed to be free of error.

10.7 Illustrative Example

The 6-bus electric energy system depicted in figure 10.1 is considered in this example (Sheblé (1999)). The data of a power flow for this system is provided in Conejo et al. (2005). Note that a power flow provides all variables to define a state of the system.

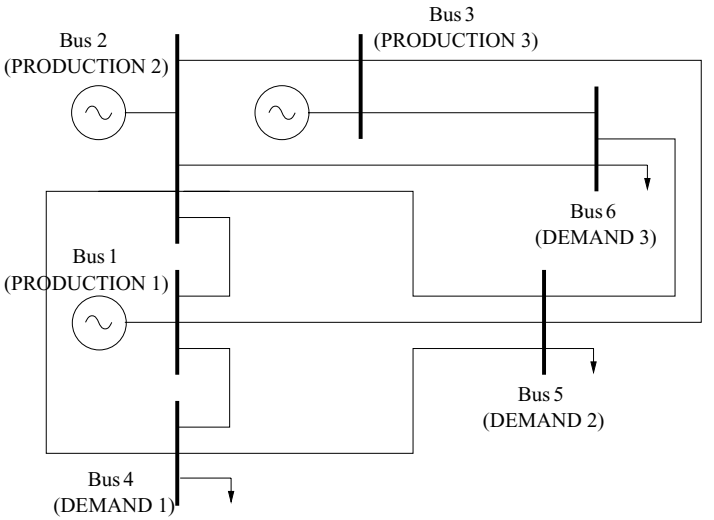

Figure 10.1. Six-bus system

The measurements considered are the following:

1. Voltage magnitude for every node
2. Active and Reactive power injection at every node
3. Active and Reactive power flow at both ends of every line or transformer

Hence the total number of measurements and the number of degrees of freedom for this 6-bus system are: $6 + 2 \times 6 + 2 \times 2 \times 11 = 62$, and $62 - 2 \times 6 + 1 = 51$, respectively.

10.7.1 Statistical assumptions

To show the importance of the dependency between measurements in the estimation process the following statistical model has been used and the results are compared with those obtained using a model that uses the traditional independent normal random variable assumption. Note that the proposed model has been selected for illustration purposes, as additional research is needed on the right estimation of the best measurements probability distribution.

The formula used by the American Electric Company for determining variance values for measurements in its state estimator is (Allemong et al. (1982)):

$$\sigma_i = 0.0067 S_i + 0.0016 F_{S_i} \tag{10.28}$$

where

$$S_i = \begin{cases} \sqrt{P_{F_{km}}^2 + Q_{F_{km}}^2}, & \text{for flow } k-m, \\ \sqrt{P_k^2 + Q_k^2}, & \text{for bus } k, \\ v_k, & \text{for voltage } k, \end{cases} \tag{10.29}$$

and $P_{F_{km}}$, $Q_{F_{km}}$ are the active and reactive power flow magnitudes, respectively, P_k, Q_k are the active and reactive power injection magnitudes, respectively; and v_k and δ_k

are the voltage magnitude and voltage angle in bus k, respectively; and F_{S_i} is the scale factor, which in this paper will be taken as $\max(P_{F_{km}}, Q_{F_{km}})$ for flow measurements, $\max(P_k, Q_k)$ for power injection measurements, and $\max(v_k)$ for voltage measurements, respectively.

Additionally, measurement systems generally establish a correlation between voltage measurements and the remainder measurements (active and reactive power injections, active and reactive power flows) in the same bus. Therefore, dependency between voltage measurements and the remainder measurements is considered. To model this complex mechanism, a correlation coefficient ρ is used, so that, $\rho = \pm 1$ implies the maximum correlation possible (positive or negative), whereas $\rho = 0$ implies independence. Figure 10.2 shows the pattern of the covariance matrix using this model.

Additionally, as the voltage measurements are positive variables they are modeled using random variables with a log-normal distribution $\ln(V_i) \sim N(\mu_{\ln V_i}, \sigma^2_{\ln V_i})$ whose parameters can be obtained form those corresponding to the normal variable as follows:

$$\mu_{\ln V_i} = \ln \frac{v_i}{\sqrt{(1 + \left(\sigma_i^V / v_i\right)^2)}} \quad \text{and} \quad \sigma^2_{\ln V_i} = \ln(1 + \left(\sigma_i^V / v_i\right)^2). \tag{10.30}$$

where σ_i^V is the standard deviation for bus i obtained using (10.28).

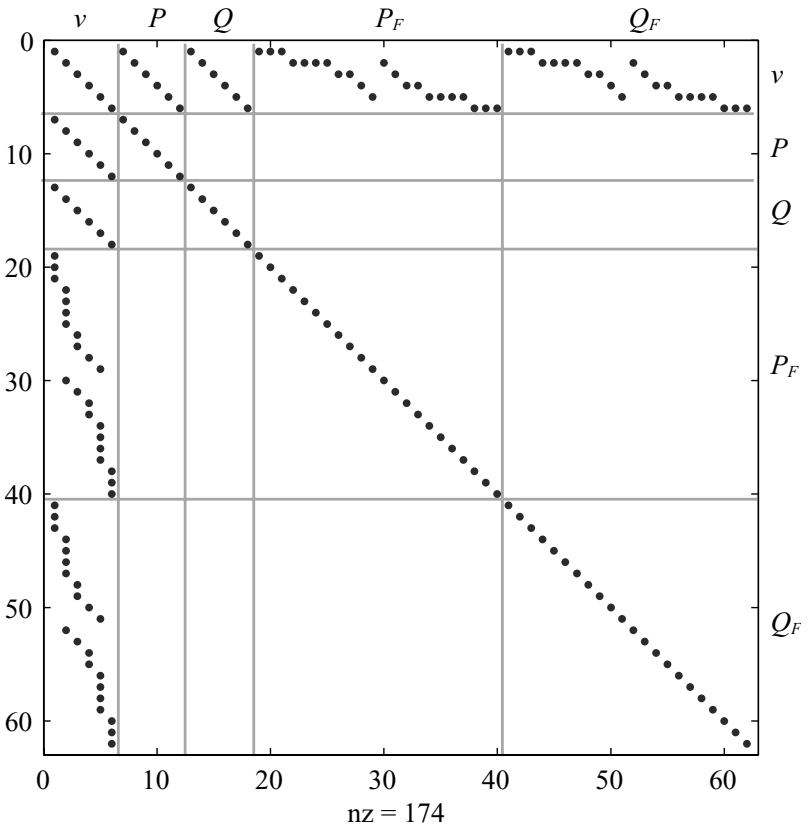

Figure 10.2. Covariance matrix pattern for the six-bus system example

The General State Estimation (GSE) problem in (10.24) for this particular example, and considering the following sets definition:

Ω_i Set of buses adjacent to bus i
Ω^0 Set of transit nodes associated with zero injections
Ω^V Set of available voltage magnitude measurements
Ω^{P_i} Sets of available active power injection measurements, where subindex $i = g, d, b$ refers to only generation, only demand and both
Ω^{Q_i} Sets of available reactive power injection measurements, where subindex $i = g, d, b$ refers to only generation, only demand and both
Ω^{P_F} Set of available active power flow measurements
Ω^{Q_F} Set of available reactive power flow measurements

Is stated below:

$$\underset{v_i, \delta_i, P_i, Q_i; i=1,\ldots,6;\ P_{F_{ij}}, Q_{F_{ij}};\ (i,j)\in\Omega^{P_F}}{\text{Minimize}} \quad J(\boldsymbol{x}), \tag{10.31}$$

where

$$J(\boldsymbol{x}) = \sum_{i\in\Omega^V} (y_i^V)^2 + \sum_{i\in\Omega^P} (y_i^P)^2 + \sum_{i\in\Omega^Q} (y_i^Q)^2 + \sum_{(i,j)\in\Omega^{P_F}} (y_{ij}^{P_F})^2 + \sum_{(i,j)\in\Omega^{Q_F}} (y_{ij}^{Q_F})^2,$$

subject to

$$y_i^V = \frac{\ln(v_i^m) - \ln\left(\frac{v_i}{\sqrt{1+(\sigma_i^V/v_j)^2}}\right)}{\sqrt{\ln(1+(\sigma_i^V/v_i))^2}};\ i\in\Omega^V, \tag{10.32}$$

$$y_i^P = \frac{P_i^m - P_i - \rho\sigma_i^{PQ} y_i^V}{\sigma_i^{PQ}\sqrt{1-\rho^2}};\ i\in\Omega^P, \tag{10.33}$$

$$y_i^Q = \frac{Q_i^m - Q_i - \rho\sigma_i^{PQ} y_i^V}{\sigma_i^{PQ}\sqrt{1-\rho^2}};\ i\in\Omega^Q, \tag{10.34}$$

$$y_{ij}^{P_F} = \frac{P_{F_{ij}}^m - P_{F_{ij}} - \rho\sigma_{ij}^{PQ_F} y_i^V}{\sigma_{ij}^{PQ_F}\sqrt{1-\rho^2}};\ (i,j)\in\Omega^{P_F}, \tag{10.35}$$

$$y_{ij}^{Q_F} = \frac{Q_{F_{ij}}^m - Q_{F_{ij}} - \rho\sigma_{ij}^{PQ_F} y_i^V}{\sigma_{ij}^{PQ_F}\sqrt{1-\rho^2}};\ (i,j)\in\Omega^{Q_F}, \tag{10.36}$$

$$P_i = v_i \sum_j v_j \left(G_{ij}\cos(\delta_i - \delta_j) + B_{ij}\sin(\delta_i - \delta_j)\right);$$
$$i = j;\ (i,j)\in\Omega_i;\ i = 1,\ldots,6, \tag{10.37}$$

$$Q_i = v_i \sum_j v_j \left(G_{ij}\sin(\delta_i - \delta_j) - B_{ij}\cos(\delta_i - \delta_j)\right);$$
$$i = j;\ (i,j)\in\Omega_i;\ i = 1,\ldots,6, \tag{10.38}$$

$$P_{F_{ij}} = v_i v_j (G_{ij} \cos(\delta_i - \delta_j) + B_{ij} \sin(\delta_i - \delta_j)) - G_{ij} v_i^2;\ (i,j) \in \Omega^{P_F}, \tag{10.39}$$

$$Q_{F_{ij}} = v_i v_j (G_{ij} \sin(\delta_i - \delta_j) - B_{ij} \cos(\delta_i - \delta_j)) + v_i^2 (B_{ij} - b_{ij}^s/2);\ (i,j) \in \Omega^{Q_F}, \tag{10.40}$$

$$P_i^{\min} \leq P_i \leq P_i^{\max};\qquad i = 1, \cdots, 3, \tag{10.41}$$

$$Q_i^{\min} \leq Q_i \leq Q_i^{\max};\qquad i = 1, \cdots, 3, \tag{10.42}$$

$$-\pi \leq \delta_i \leq \pi;\qquad i = 2, \cdots, 6, \tag{10.43}$$

$$\delta_1 = 0, \tag{10.44}$$

where (10.31) is the objective function including the sums of the squares of the normalized errors corresponding to voltage, active and reactive power injection, and active and reactive power flow measurements, respectively. The constraints in (10.32)–(10.36) are the equations corresponding to the Rosenblatt transformation, where σ_i^V, σ_i^{PQ}, and $\sigma_{ij}^{PQ_F}$ are the standard deviation values associated with voltage, active and reactive power injection, and active and reactive power flow measurements, respectively, which are obtained using (10.28). The constraints in (10.37)–(10.40) are the active and reactive power injections and flows equations, and the last constraints are physical limits, such as minimum and maximum reactive power generation and angle extreme values ($-\pi$,π). Note also that G_{ij}, B_{ij}, and b_{ij}^S are the ijth element of the real part of the admittance matrix, the ijth element of the imaginary part of the admittance matrix, and the charging susceptance of the ijth line, respectively. Note that the admittance matrix is a constant matrix dependent of the geometry and physical components of the network, it relates nodal current injections and nodal voltages.

The measurements $\mathbf{v}^m$, $\mathbf{P}^m$, $\mathbf{Q}^m$, $\mathbf{P_F}^m$ and $\mathbf{Q_F}^m$ are synthetically generated by adding randomly generated errors to the true values $\mathbf{v}^{\text{true}}$, $\mathbf{P}^{\text{true}}$, $\mathbf{Q}^{\text{true}}$, $\mathbf{P_F}^{\text{true}}$ and $\mathbf{Q_F}^{\text{true}}$. Note that this process is done by generating independent standard normal random numbers and using the inverse of the Rosenblatt transformation to obtain the measurements.

Several synthetically generated measurements using different values of the correlation factor ρ have been performed. Next, the general state estimation problem (10.31)–(10.44) and the usual weighted least squares estimation problem (WLS), considering independent normal random variables, are solved. The corresponding objective functions $J(\boldsymbol{x})$ and the regression curves for both approaches are shown in figure 10.3 (a). In figure 10.3 (b) the true quadratic errors defined as $e^{\text{true}} = \sum_{i=1}^{m} (x_i^{\text{est}} - x_i^{\text{true}})^2$, i.e., the sum of squares over the total number of measurements of the difference between the true and the estimated values. The following observations can be made:

1. For $\rho = 0$ the objective function and the true quadratic error are almost the same, the small difference being due to the use of the log-normal distribution for the voltage measurements in the GSE model.
2. The WLS objective function decreases if the absolute value of the correlation factor increases, whereas the GSE objective function increases slightly. Note that the maximum differences in the WLS and GSE objective functions occur for $\rho = -1$ and $\rho = 1$, the optimal values are 51.39 and 25.31 for $\rho = -1$, and 51.29 and 31.49

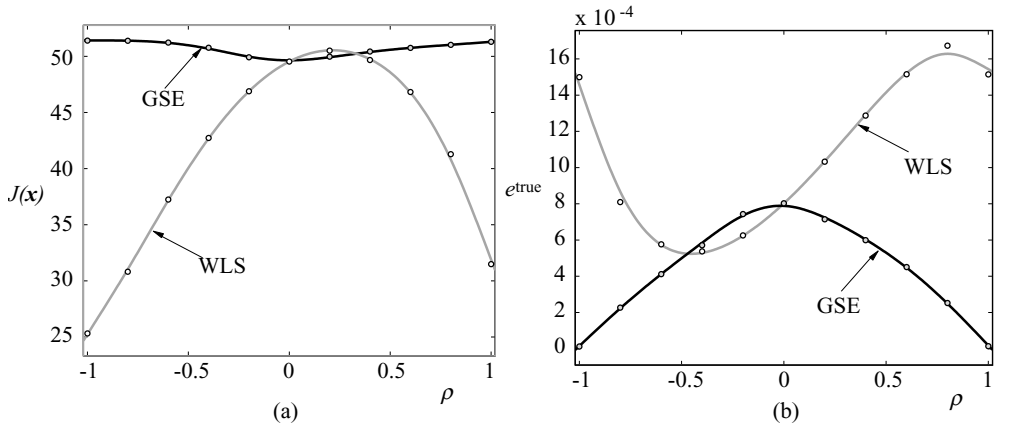

Figure 10.3. Graphical illustration of the the estimation state performance considering WLS and GSE: (a) Objective function, (b) true quadratic error

for $\rho = 1$. These results could suggest that the WLS is a better approach because the chi-square value (objective function) is smaller for all the ρ-values, but the true errors (e^{true}) are clearly smaller for the GSE estimation, as shown in figure 10.3 (b).
3. True errors decrease if the correlation absolute value increases, and the maximum difference between errors using both approaches occurs for $\rho \pm 1$.

Additionally, to check the behavior of both models if outliers (bad measurements) exist, a bias over the measurement in the voltage for bus 1 (a typical bus) equal to 6 standard deviations (a clear outlier) is introduced. The corresponding objective functions $J(\boldsymbol{x})$ and the regression curves for both the WLS and GSE models are shown in figure 10.4 (a), whereas in figure 10.4 (b) the true quadratic errors are shown. The following observations can be made:

1. The behavior of the objective function for both models is analogous to the previous case (see figure 10.3 (a)) but with a larger objective function value due to the outlier.
2. Figure 10.4 (a) also shows horizontal lines corresponding to the $\chi^2_{(m-n),\alpha}$ distribution function corresponding to a detection confidence with probability α. Note that the WLS estimation fails to detect suspicious data if the correlation coefficient absolute value increases. For instance, if the confidence probability is 96%, WLS estimation fails to detect bad data if $\rho \leq -0.5$ and $\rho \geq 0.525$ because in both intervals holds that $\sum_{i=1}^{m} y_i^2 \geq \chi^2_{m-n,\alpha}$. The range where the WLS estimation fails to detect bad data increases with the confidence probability. On the other hand GSE model detects bad data for all values of ρ and α considered.
3. The WLS true error is always greater than the GSE true error. The difference increases as the correlation factor deviates from 0, attaining the maximum value (0.0091) when $\rho = -1$.
4. The GSE is more robust because the maximum difference between the true error with and without outlier is $\approx 13.1\%$ whereas in the WLS model the difference is $\approx 83.6\%$.

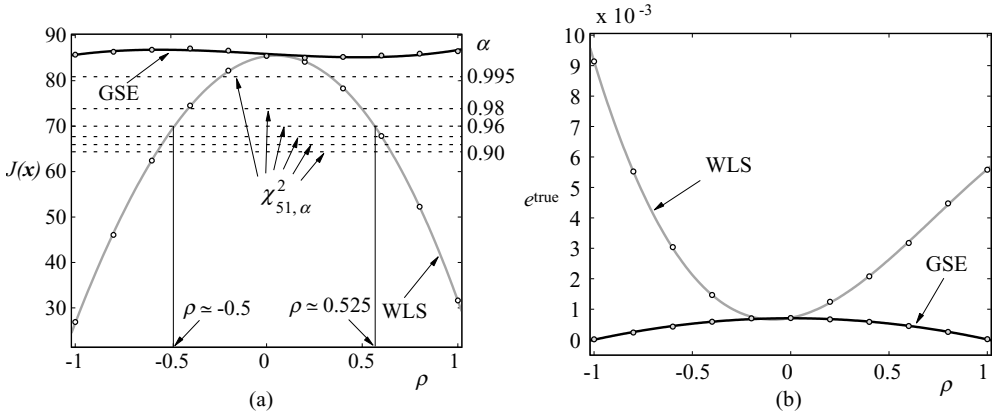

Figure 10.4. Graphical illustration of the state estimation performance considering WLS and GSE when an outlier exists: (a) Objective function and horizontal lines representing the χ^2 distribution function values for different confidence probabilities and 51 degrees of freedom $\chi^2(51, \alpha)$, (b) true quadratic error

Unlike common practice in state estimation, the proposed method is directly based on solving an optimization problem. We advocate this approach due to the versatility, efficiency and robustness of currently available software. We emphasize that the available optimization codes efficiently account for sparsity and possible numerical ill-conditioning.

10.8 Conclusions

This paper provides a procedure for solving the state estimation problem considering that the measurements are non-Gaussian and can be statistically correlated. The method is useful to increase the confidence level of the model and its predictions. It has the following advantages with respect the standard WLS model:

1. It is more robust with respect to outliers.
2. It increases accuracy in identifying bad data.
3. It is flexible allowing the use of complex statistical models.

An example is used to illustrate the performance of the method.

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11

Statistics Applied to Wave Climate on a Beach Profile

Carmen Castillo[1] and Cristina Solares[2]

[1] Civil Engineering Department, University of Castilla-La Mancha, Ciudad Real, Spain
[2] Department of Mathematics, University of Castilla-La Mancha, Ciudad Real, Spain

Abstract: One of the most important subjects in coastal engineering is the forecasting of wave climate evolution along a beach profile and its associated probability.

Many authors have dealt with this problem proposing different CDFs (Cumulative Distribution Functions) and statistical descriptors evolution. One of these works suggests that, for a given sea state, the parameters of the local (at a given point of the profile) wave height CDF depend on the local value of kh and offshore wave parameters. Therefore, it is possible to describe the evolution of the probability distribution of wave heights on a beach profile provided its geometry is known as well as the statistical descriptors of wave oscillation approaching the beach profile (offshore the depth of closure). This model has been validated for waves approaching the beach with normal incidence.

This paper intends to step forward on this work by describing the statistical properties of other local wave parameters such as the maximum wave height. Conditional distributions are also described for two consecutive local wave heights, for consecutive offshore wave parameters (wave height or wave period) and for the most relevant offshore wave parameters (wave height and wave period).

All the information provided in this model will be useful for estimating sediment transport and, therefore, how a beach profile and planform will evolve in time.

Keywords and phrases: Wave climate, maximum wave height, statistics, beach profile distributions

11.1 Introduction

Propagating wave climate along a beach profile is a very interesting subject in coastal engineering since it can be applied to breakwater design, sediment transport or prediction of shoreline evolution.

Castillo (2004) stated that, for a given sea state, local distributions of water column components depend only on local value of kh and offshore wave climate. Castillo et al. (2004) applied the model to wave height and Castillo and Losada (2005) to wave energy dissipation.

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The input for the model consists of the beach profile at the beginning of the sea state and offshore wave climate characteristics. The output are the probabilities associated with different values of variables such as wave height, short wave oscillation and long wave oscillation or probabilities of breaking events (see Castillo and Losada (2000)) at any point of the profile for the given sea state. This means that the probabilities are conditional probabilities to the input conditions.

This paper intends to advance into a more complete model including probabilities for offshore wave climate, in order to transform conditional probabilities to absolute probabilities, and the analysis of other local variables as the maximum wave height.

The paper is organized as follows. Section 11.2 deals with offshore wave climate probabilities. In Section 11.3, local wave height analysis is done. Section 11.4 is devoted to correlation between consecutive waves, and Section 11.5 defines local maximum wave height. Finally, some conclusions are stated.

11.2 Offshore Wave Climate

Offshore wave climate is part of the input of the model together with the beach profile at the beginning of the sea state. Wave climate on a sea state will be defined by three variables (statistical descriptors of the sea state):

- Significant wave height H_S: mean of the $N/3$ highest waves
- Zero up-crossing mean period $\overline{T_z}$: waves are defined by the zero up-crossing method so time between two consecutive zero up-crossing defines a wave period
- Peak period T_p: most energetic period

The model should include another variable, which is the sea level, but since data used for validation keep the level constant, it will not be taken into account for the moment.

All three variables are defined positive. After analyzing all the available information from the Spanish coast, some conclusions about these variables were driven:

- All of them were found to be lognormal (see some examples in figure 11.1).
- All of them are correlated

Therefore, their PDFs (Probability Density Functions) and CDFs are:

- Significant wave height:

$$f_{H_S}(x) = \frac{1}{\sqrt{2\pi}\sigma_s x} \exp\left\{-\frac{(\ln x - \mu_s)^2}{2\sigma_s^2}\right\} \tag{11.1}$$

$$F_{H_S}(x) = \Phi\left(\frac{\ln x - \mu_s}{\sigma_s}\right) \tag{11.2}$$

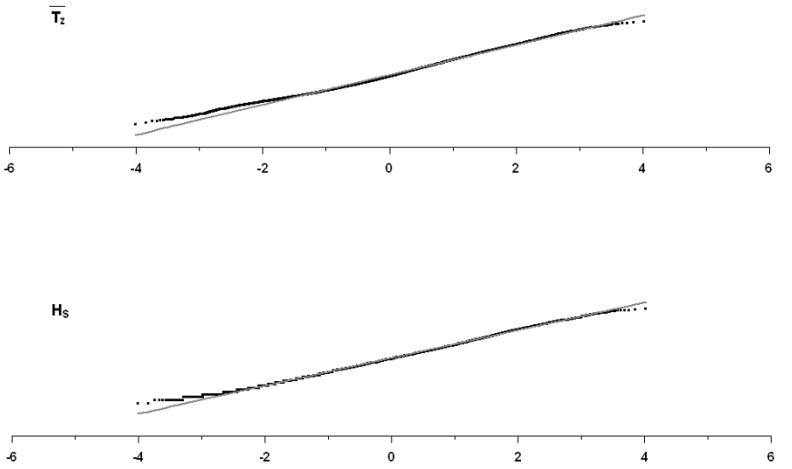

Figure 11.1. Mean zero up-crossing wave period and significant wave height on lognormal scales

- Zero up-crossing mean period:

$$f_{\overline{T_z}}(x) = \frac{1}{\sqrt{2\pi}\sigma_z x} \exp\left\{-\frac{(\ln x - \mu_z)^2}{2\sigma_z^2}\right\} \tag{11.3}$$

$$F_{\overline{T_z}}(x) = \Phi\left(\frac{\ln x - \mu_z}{\sigma_z}\right) \tag{11.4}$$

- Peak period

$$f_{T_p}(x) = \frac{1}{\sqrt{2\pi}\sigma_p x} \exp\left\{-\frac{(\ln x - \mu_p)^2}{2\sigma_p^2}\right\} \tag{11.5}$$

$$F_{T_p}(x) = \Phi\left(\frac{\ln x - \mu_p}{\sigma_p}\right) \tag{11.6}$$

For correlation analysis, some properties of normal variables will be used. A variable X is lognormal if the variable $Y = \ln X$ is normal. Conditional distributions for a normal variable $X\left(\mu_x, \sigma_x^2\right)$ given the normal variable $Y\left(\mu_y, \sigma_y^2\right) = y$, $X|Y = y$, is also a normal variable with mean and variance:

$$\mu = \mu_x + \frac{\sigma_{xy}}{\sigma_y^2}(y - \mu_y) \tag{11.7}$$

$$\sigma^2 = \frac{\sigma_y^2\sigma_x^2 - \sigma_{xy}^2}{\sigma_y^2} \tag{11.8}$$

Conditional distribution for a normal variable $Z\left(\mu_z, \sigma_z^2\right)$ given the normal variables $Y\left(\mu_y, \sigma_y^2\right) = y$ and $X\left(\mu_x, \sigma_x^2\right) = x$, $Z|\left(X = x, Y = y\right)$, is also a normal variable with mean and variance:

$$\mu = \mu_z + \frac{\sigma_{xz}\sigma_y^2 - \sigma_{xy}\sigma_{yz}}{\sigma_x^2\sigma_y^2 - \sigma_{xy}^2}(x - \mu_x) + \frac{\sigma_{yz}\sigma_x^2 - \sigma_{xy}\sigma_{xz}}{\sigma_x^2\sigma_y^2 - \sigma_{xy}^2}(y - \mu_y) \tag{11.9}$$

$$\sigma^2 = \frac{\sigma_x^2\sigma_y^2\sigma_z^2 + 2\sigma_{xy}\sigma_{xz}\sigma_{yz} - \sigma_x^2\sigma_{yz}^2 - \sigma_y^2\sigma_{xz}^2 - \sigma_z^2\sigma_{xy}^2}{\sigma_x^2\sigma_y^2 - \sigma_{xy}^2} \tag{11.10}$$

For lognormal variables, the results are similar, that is, conditional variables are also lognormal with values for μ and σ shown in Eq. (11.7) to Eq. (11.10).

Therefore, the resulting CDFs are:

- Significant wave height:

$$F_{H_S}(x) = \Phi\left(\frac{\ln x - \mu_s}{\sigma_s}\right) \tag{11.11}$$

- Peak period given significant wave height:

$$F_{T_p|H_s=y}(x) = \Phi\left(\frac{\ln x - \mu}{\sigma}\right) \tag{11.12}$$

with

$$\mu = \mu_p + \frac{\sigma_{sp}}{\sigma_s^2}(y - \mu_s)$$
$$\sigma^2 = \frac{\sigma_s^2\sigma_p^2 - \sigma_{sp}^2}{\sigma_s^2}$$

- Zero up-crossing period given significant wave height and peak period:

$$F_{\overline{T_z}|(H_S=y,T_p=x)}(z) = \Phi\left(\frac{\ln z - \mu}{\sigma}\right) \tag{11.13}$$

with

$$\mu = \mu_z + \frac{\sigma_{pz}\sigma_s^2 - \sigma_{sp}\sigma_{sz}}{\sigma_p^2\sigma_s^2 - \sigma_{sp}^2}(x - \mu_p) + \frac{\sigma_{sz}\sigma_p^2 - \sigma_{sp}\sigma_{pz}}{\sigma_p^2\sigma_s^2 - \sigma_{sp}^2}(y - \mu_s)$$
$$\sigma^2 = \frac{\sigma_p^2\sigma_s^2\sigma_z^2 + 2\sigma_{sp}\sigma_{pz}\sigma_{sz} - \sigma_p^2\sigma_{sz}^2 - \sigma_s^2\sigma_{pz}^2 - \sigma_z^2\sigma_{sp}^2}{\sigma_p^2\sigma_s^2 - \sigma_{sp}^2}$$

The number of waves in the sea state is defined as $N = d/\overline{T_z}$ (rounded to the closest integer) where d is the sea state duration.

$$Prob[N = n] = Prob\left[n - 0.5 \leq \frac{d}{\overline{T_z}} < n + 0.5\right] \tag{11.14}$$

$$Prob[N = n] = F_{d/\overline{T_z}}(n + 0.5) - F_{d/\overline{T_z}}(n - 0.5) \tag{11.15}$$

with

$$F_{d/\overline{T_z}}(x) = Prob\left[\frac{d}{\overline{T_z}} \leq x\right] = Prob\left[\overline{T_z} \geq \frac{d}{x}\right] = 1 - F_{\overline{T_z}}\left(\frac{d}{x}\right) \tag{11.16}$$

Therefore:

$$Prob\left[N = n\right] = F_{\overline{T_z}}\left(\frac{d}{n - 0.5}\right) - F_{\overline{T_z}}\left(\frac{d}{n + 0.5}\right) \tag{11.17}$$

11.3 Local Wave Height Description

11.3.1 Conditional probabilities

This section provides local wave height description for a given sea state, that is, for a given set of wave climate values $\left(H_s, T_p, \overline{T_z}\right)$. Therefore, all the probabilities defined are conditional probabilities to a given sea state's characteristics.

Castillo et al. (2004) showed that local wave height at any fixed point of a beach profile is a Weibull for minima variable with location parameter $\lambda = 0$, and scale and shape parameters δ, β depend on local value of kh and an offshore wave height parameter as shown in figure 11.2. Figure 11.3 shows the validation of the model for some of the SUPERTANK data from Kraus and Smith (1994).

Local CDFs and PDFs are given by:

$$F_H(x) = 1 - \exp\left\{-\left(\frac{x}{\delta}\right)^{\beta}\right\} \tag{11.18}$$

for $x > 0$

$$f_H(x) = \frac{\beta x^{\beta-1}}{\delta^{\beta}} \exp\left\{-\left(\frac{x}{\delta}\right)^{\beta}\right\} \tag{11.19}$$

for $x > 0$

These equations allow us for the evaluation of local wave height parameters:

- Mean wave height: $\overline{H}$

$$\overline{H} = \int_0^{\infty} x f_H(x)\, dx = \delta \Gamma\left(1 + \frac{1}{\beta}\right) \tag{11.20}$$

- Root mean squared wave height: H_{rms}

$$H_{rms}^2 = \int_0^{\infty} x^2 f_H(x)\, dx = \delta^2 \Gamma\left(1 + \frac{2}{\beta}\right) \tag{11.21}$$

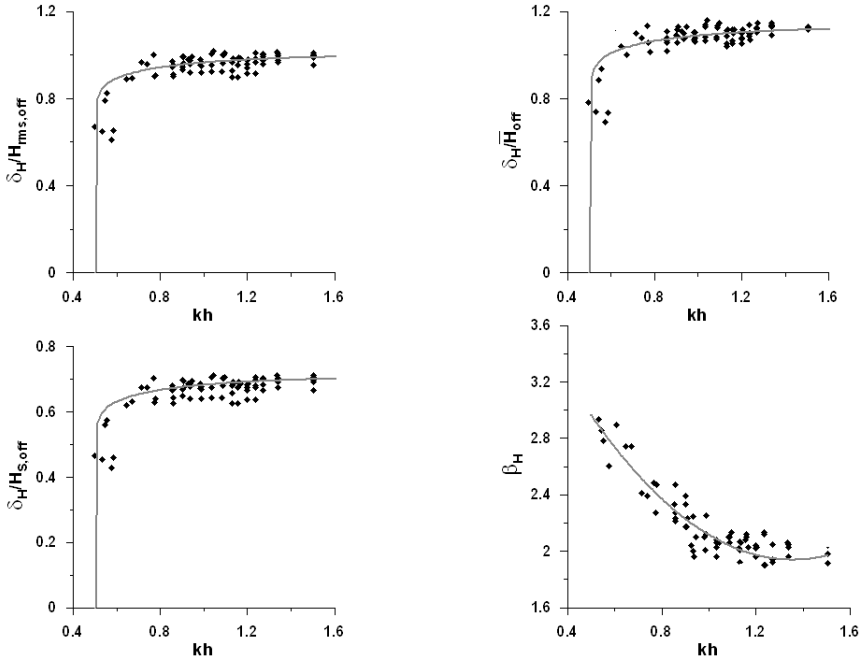

Figure 11.2. Local wave height parameters

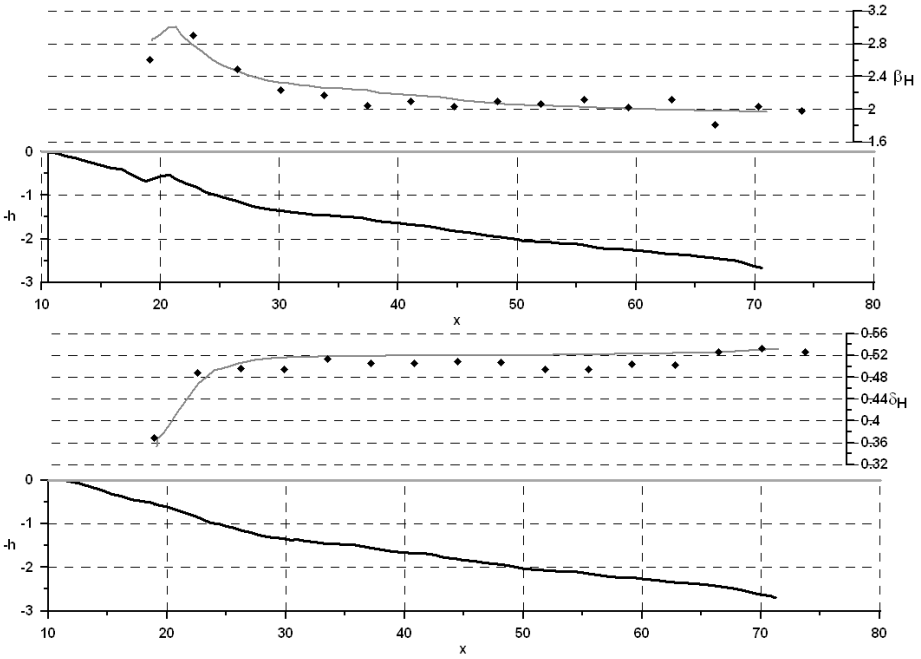

Figure 11.3. Wave height parameters along a beach profile

- Significant wave height: H_S. It is a particular case of the parameter $H_{1/n}$ (mean of the N/n highest waves) for $n = 3$ with N the number of waves in the sea state.

$$H_{1/n} = \frac{\int_{H_u}^{\infty} x f_H(x)\, dx}{\int_{H_u}^{\infty} f_H(x)\, dx} \tag{11.22}$$

where $Prob[H > H_u] = \frac{N/n}{N} = 1/n$, which for Weibull for minima becomes:

$$\exp\left\{-\left(\frac{H_u}{\delta}\right)^{\beta}\right\} = \frac{1}{n} \tag{11.23}$$

Therefore, $H_u = \delta (\ln n)^{1/\beta}$. Operating,

$$H_{1/n} = \delta \left[(\ln n)^{1/\beta} + \frac{n}{\beta} \Gamma\left(\frac{1}{\beta}, \ln n\right)\right] \tag{11.24}$$

So, significant wave height $H_S = H_{1/3}$ will result in:

$$H_S = \delta \left[(\ln 3)^{1/\beta} + \frac{3}{\beta} \Gamma\left(\frac{1}{\beta}, \ln 3\right)\right] \tag{11.25}$$

When $kh > \pi/3$, $\beta = 2$ which means the Weibull for minima is transformed into a Rayleigh distribution. In this case:

- Mean wave height: $\overline{H}$

$$\overline{H} = 0.886\delta \tag{11.26}$$

- Root mean squared wave height: H_{rms}

$$H_{rms} = \delta \tag{11.27}$$

- Significant wave height: H_S.

$$H_S = 1.41\delta \tag{11.28}$$

Offshore wave height must satisfy $\beta = 2$. Therefore, $H_{rms,off}/\delta_{off} = 1$ as stated on Eq. (11.27). Figure 11.2 shows how $\delta/H_{rms,off}$ tends asymptotically to 1 as it should be for $kh > \pi$, that is deep water depth, where waves do not feel the bottom so, if there are no other boundaries affecting wave propagation, CDF should not change. Eq. (11.26) and (11.28) are also related to the asymptotic values of $\delta/\overline{H}_{off}$ and $\delta/H_{S,off}$, respectively. They are the inverse of the numerical values shown in the equations.

11.3.2 Absolute probabilities

This section is devoted to analyzing absolute probabilities associated with local wave height. Applying the total probability theorem:

$$F_H(x) = Prob[H \le x] = \sum Prob[H \le x | (N = n, H_S = h, T_p = t)] \times Prob[N = n, H_S = h, T_p = t] \quad (11.29)$$

where $Prob[H \le x | (N = n, H_S = h, T_p = t)] = F_{H,c}(x)$ is the CDF in Eq. (11.18).

$$\begin{aligned} & F_H(x) = \sum F_{H,c}(x) \, Prob[H_S = h] \, Prob[(N = n, T_p = t) | H_S = h] \\ & = \sum F_{H,c}(x) \, Prob[H_S = h] \, Prob[T_p = t | H_S = h] \\ & Prob[N = n | (T_p = t, H_S = h)] \\ & = \sum F_{H,c}(x) \, f_{H_S}(h) \, f_{T_p | H_S = h}(t) \\ & Prob\left[n - 0.5 \le \frac{d}{\overline{T_z}} < n + 0.5 | (T_p = t, H_S = h)\right] \\ & = \sum F_{H,c}(x) \, f_{H_S}(h) \, f_{T_p | H_S = h}(t) \\ & \times \left[F_{\overline{T_z}|(T_p = t, H_S = h)}\left(\frac{d}{n - 0.5}\right) - F_{\overline{T_z}|(T_p = t, H_S = h)}\left(\frac{d}{n + 0.5}\right)\right] \end{aligned} \quad (11.30)$$

$$\begin{aligned} & F_H(x) = \sum_n \int_0^\infty \int_0^\infty F_{H_{max,n}} f_{H_S}(h) \, f_{T_p | H_S = h}(t) \\ & \left[F_{\overline{T_z}|(T_p = t, H_S = h)}\left(\frac{d}{n - 0.5}\right) - F_{\overline{T_z}|(T_p = t, H_S = h)}\left(\frac{d}{n + 0.5}\right)\right] dhdt \end{aligned} \quad (11.31)$$

11.4 Consecutive Wave Heights

Usually, waves propagate in groups of higher and lower heights. Therefore, correlation between consecutive waves has been analyzed by an independence test. The results are shown in figure 11.4.

Correlation between waves decreases as they are more separated in time. It is clear that correlation between a wave and the previous one is very strong but it is not that clear when related to the two previous waves or the three previous ones. The model will only consider correlation between a wave and the previous one.

Castillo (2004) used the conditional probability of two correlated Weibull for minima variables based on the joint survival function $G_{X,Y}(x, y)$ described by Arnold et al. (1999).

$$G_{X,Y}(x, y) = Prob[X > x, Y > y] \quad (11.32)$$

$$F_{X,Y}(x, y) = Pr[X \le x, Y \le y] = G_{X,Y}(x, y) + F_X(x) + F_Y(x) - 1 \quad (11.33)$$

This distribution is applied to a wave height given the previous one is known as both of them are Weibull for minima. The conditional CDF is defined as:

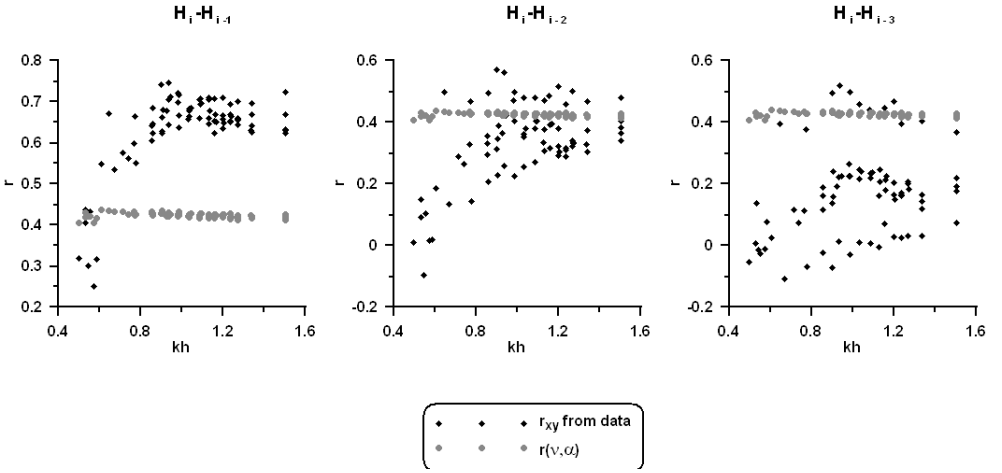

Figure 11.4. Independence test results for consecutive wave heights

$$F_{H_i|H_{i-1}=x}(y) = 1 - \exp\left\{-\left[1+\theta\left(\frac{x}{\delta}\right)^{\beta}\right]\left(\frac{y}{\delta}\right)^{\beta}\right\}\left[1+\theta\left(\frac{y}{\delta}\right)^{\beta}\right] \qquad (11.34)$$

with $x, y > 0$

Estimating the value of θ, it was found that it depends on local value of kh as it happened with the rest of the parameters of local wave height. Figure 11.5 shows the dependence of θ on kh.

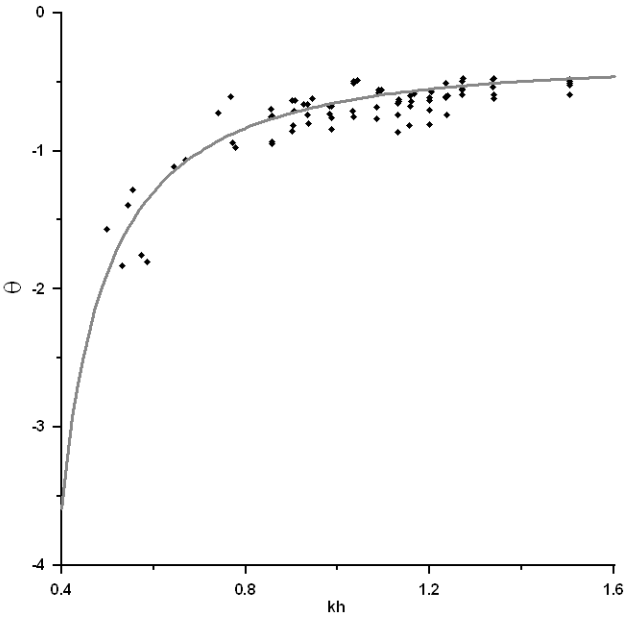

Figure 11.5. Correlation parameter

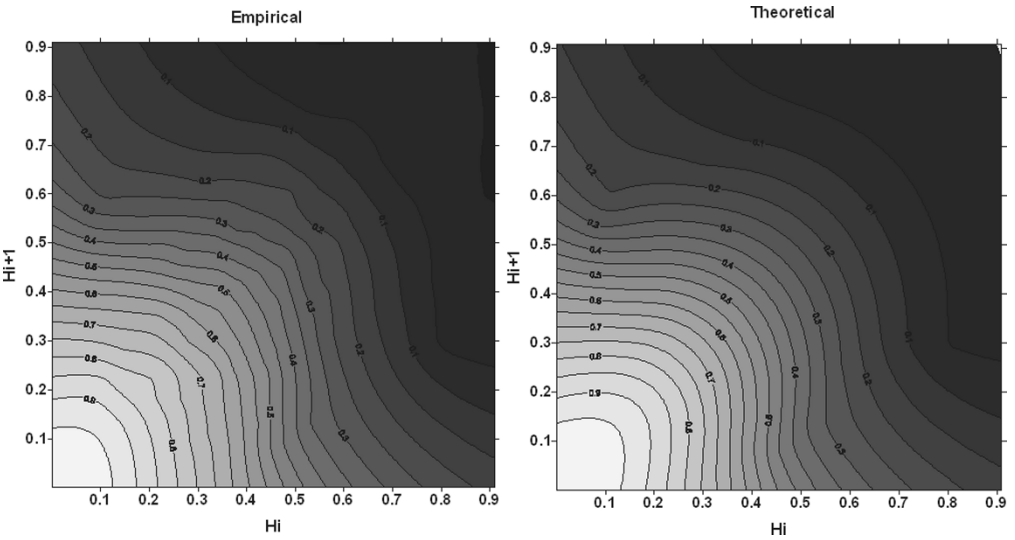

Figure 11.6. Survival function for consecutive wave heights. Comparison between data and the model

Figure 11.6 shows the comparison between the survival function attained from the data and the one resulting from the model for one of the cases that were analyzed. It shows good agreement between data and the model.

11.5 Maximum Wave Height

Maximum wave height is a very important parameter for designing in coastal engineering. There will be two case studies: the first one under the hypothesis that waves in a sea state are uncorrelated and the second one using the results in Section 11.4.

11.5.1 Conditional probabilities

This section is dedicated to analyzing probabilities associated to maximum wave height provided the number of waves in the sea state N and the offshore wave parameters H_s and T_p are known.

Uncorrelated waves

If waves in a sea state are independent, the CDF for the maximum wave height out of N (number of waves in the sea state) is defined by:

$$F_{H_{max,N}}(x) = Prob\left[H_{max,N} \leq x\right] = Prob\left[H_1 \leq x, H_2 \leq x, \ldots, H_N \leq x\right] = Prob\left[H_1 \leq x\right] \cdot Prob\left[H_2 \leq x\right] \cdot \ldots \cdot Prob\left[H_N \leq x\right] = \left[F_H(x)\right]^N \quad (11.35)$$

Correlated waves

If consecutive wave heights and only them are correlated:

$$F_{H_{max,N}}(x) = Prob[H_{max,N} \leq x] = Prob[H_1 \leq x, H_2 \leq x, \ldots, H_N \leq x] = Prob[H_1 \leq x]\, Prob[(H_2 \leq x, \ldots H_N \leq x)\,|H_1 \leq x] = Prob[H_1 \leq x]\, Prob[H_2 \leq x|H_1 \leq x] \ldots Prob[H_N \leq x|H_{N-1} \leq x] \quad (11.36)$$

Applying conditional probability:

$$F_{H_{max,N}}(x) = F_{H_1}(x)\frac{F_{H_1,H_2}(x,x)}{F_{H_1}(x)} \ldots \frac{F_{H_{N-1},H_N}(x,x)}{F_{H_{N-1}}(x)} = F_H(x)\left[\frac{F_{H,H}(x,x)}{F_H(x)}\right]^{N-1} \quad (11.37)$$

which finally gives:

$$F_{H_{max,N}}(x) = \frac{[F_{H,H}(x,x)]^{N-1}}{[F_H(x)]^{N-2}} \quad (11.38)$$

where $F_H(x)$ is defined in equation (11.18) and $F_{H,H}(x,x)$ can be derived from equation (11.34).

11.5.2 Absolute probabilities

This section is dedicated to analyzing absolute probabilities associated to maximum wave height. Applying the total probability theorem:

$$F_{H_{max}}(x) = Prob[H_{max} \leq x] = \sum Prob[H_{max,n} \leq x]\, Prob[N = n, H_S = h, T_p = t] \quad (11.39)$$

where $Prob[H_{max,n} \leq x]$ is the CDF in Section 11.5.1.

$$F_{H_{max}}(x) = \sum F_{H_{max,n}} Prob[H_S = h]\, Prob[(N = n, T_p = t)\,|H_S = h] =$$
$$\sum F_{H_{max,n}} Prob[H_S = h]\, Prob[T_p = t|H_S = h]$$
$$Prob[N = n|\,(T_p = t, H_S = h)] = \sum F_{H_{max,n}} f_{H_S}(h)\, f_{T_p|H_S=h}(t)$$
$$Pr\left[n - 0.5 \leq \frac{d}{\overline{T_z}} < n + 0.5|\,(T_p = t, H_S = h)\right] =$$
$$\sum F_{H_{max,n}} f_{H_S}(h)\, f_{T_p|H_S=h}(t) \times$$
$$\left[F_{\overline{T_z}|(T_p=t,H_S=h)}\left(\frac{d}{n-0.5}\right) - F_{\overline{T_z}|(T_p=t,H_S=h)}\left(\frac{d}{n+0.5}\right)\right] \quad (11.40)$$

$$F_{H_{max}}(x) = \sum_n \int_0^\infty \int_0^\infty F_{H_{max,n}} f_{H_S}(h)\, f_{T_p|H_S=h}(t) \left[F_{\overline{T_z}|(T_p=t,H_S=h)}\left(\frac{d}{n-0.5}\right) - F_{\overline{T_z}|(T_p=t,H_S=h)}\left(\frac{d}{n+0.5}\right)\right] dhdt \quad (11.41)$$

11.6 Conclusions

A model is proposed for establishing wave climate at any point of a beach profile for a given sea state. Therefore, probabilities of local wave height and local maximum wave height assuming both correlated or uncorrelated consecutive waves are derived.

A model is also defined for offshore wave climate that is defined by significant wave height, peak period and zero up-crossing mean period (related to the number of waves of a sea state).

Both models have been combined in order to derive absolute probabilities of wave climate at any point of the beach profile.

The model can be applied to design of breakwaters or to the estimation of how a beach profile and planform will evolve in time.

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Part V

Extreme Value Theory

12

On Some Dependence Measures for Multivariate Extreme Value Distributions

Ishay Weissman

Faculty of Industrial Engineering and Management, Technion-Israel Institute of Technology, Israel

Abstract: This paper deals with the dependence structure of multivariate extremes. Two particular measures of dependence among the components are proposed. They are suitable for any (finite) dimension, and are invariant under increasing transformations of the marginal distributions. It is shown that both have a desired property that other coefficients of dependence lack. That is, for the mixture model, mixture between complete dependence and total independence, both measures are equal to the weight of the complete dependence model. Other properties are discussed and illustrated through examples.

Keywords and phrases: Coefficient of dependence, extremal coefficient, extremal index, Pickands dependence function

12.1 Introduction

Let $\mathbf{X} = (X_1, X_2, \cdots, X_d) \in \mathbf{R}^d$ be a random vector G-distributed, where G is a multivariate extreme value distribution (MEVD). The purpose of this paper is to propose two coefficients of dependence τ_1 and τ_2, which will measure the degree of dependence among the components X_j of $\mathbf{X}$. We are interested in coefficients that are invariant under increasing transformations, that is, independent of the marginal distributions of the X_j.

Background. It is well known (see Tiago de Oliveira (1962), Marshall and Olkin (1983)) that

$$\prod_{j=1}^{d} G_j(x_j) \le G(\mathbf{x}) \le \min_{1\le j\le d} G_j(x_j), \tag{12.1}$$

where G_j is the marginal distribution function of X_j. The inequality on the right holds true for every multivariate distribution. The inequality on the left is a property of MEVD, called *positive quadrant dependence* (when d=2) and it implies *positive*

B.C. Arnold et al. (eds.), *Advances in Mathematical and Statistical Modeling*,
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association. The two bounds of (12.1) are both special cases of MEVD — complete dependence on the right and total independence on the left.

Let $\lambda = -\log G$, $\lambda_j = -\log G_j$ be the respective exponent functions, $y_j = 1/\lambda_j(x_j)$ and

$$\lambda_*(\mathbf{y}) = \lambda(\lambda_1^{-1}(1/y_1), \cdots, \lambda_d^{-1}(1/y_d)).$$

Then, Equation (12.1) becomes

$$\max_{1\le j\le d} y_j^{-1} \le \lambda_*(\mathbf{y}) \le \Sigma_{j=1}^d y_j^{-1}. \tag{12.2}$$

The proximity of G to one of its bounds (or λ_* to its bounds) can serve as a measure of dependence. Indeed, Pickands (1981) defined a *dependence function* on the simplex

$$\Omega = \Omega_d = \{\mathbf{v} \in \mathbf{R}^{d-1} \,:\, v_j \ge 0,\ \Sigma_{j=1}^{d-1} v_j \le 1\,\}$$

by

$$A(\mathbf{v}) = \lambda_*(v_1^{-1}, v_2^{-1}, \cdots, v_d^{-1}) \quad (\mathbf{v} \in \Omega),$$

where here and in the sequel, $v_d = 1 - \Sigma_{j=1}^{d-1} v_j$. It follows that for $\mathbf{y} \in \mathbf{R}_+^d$,

$$\lambda_*(\mathbf{y}) = A(\mathbf{v}) \sum_{j=1}^d y_j^{-1} \qquad (v_j = \frac{y_j^{-1}}{\Sigma_{i=1}^d y_i^{-1}},\ j = 1, 2, \cdots, d).$$

The function A is convex and invariant under increasing transformations of the X_j. The transformation from λ to λ_* is for convenience and is equivalent to transforming X_j to $Y_j = 1/\lambda_j(X_j)$ which are unit-Fréchet distributed, namely, $P\{Y_j \le y\} = \exp(-1/y)$ $(y > 0)$.

Looking back at Equation (12.2), this is equivalent to

$$\frac{1}{d} \le A_0(\mathbf{v}) := \max_{1\le j\le d} v_j \le A(\mathbf{v}) \le 1 \qquad (\mathbf{v} \in \Omega), \tag{12.3}$$

$A \equiv 1$ corresponds to total independence and $A \equiv A_0$ to complete dependence. We note in passing that if $\mathbf{e}_j \in \Omega$ is the unit vector with 1 at its jth position and 0 elsewhere $(j = 1, 2, \cdots, d-1)$ and $\mathbf{e}_d = \mathbf{0}$, then $A(\mathbf{e}_j) = 1$ for all j.

A famous example of MEVD is the *logistic model*, for which

$$A(\mathbf{v}) = (\Sigma_1^d v_j^{1/\alpha})^\alpha \qquad (0 < \alpha \le 1).$$

When $\alpha = 1$ we have independence and as $\alpha \downarrow 0$, $A \to A_0$ (complete dependence). Figure 12.1 shows graphically the function A for several values of α for the case $d = 2$.

12.2 Dependence Coefficients

The function A depicts the dependence structure among the X_j (or the Y_j). Let $\mathbf{v}_* = (d^{-1}, \cdots, d^{-1}) \in \Omega$, then $\eta = A(\mathbf{v}_*)$ has an interesting interpretation:

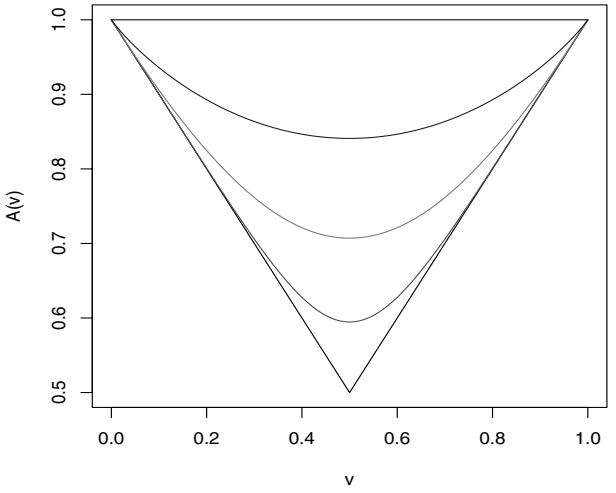

Figure 12.1. Pickands dependence function for the Logistic Model, $A(v) = (v^{1/\alpha} + (1 - v)^{1/\alpha})^{\alpha}$ with $\alpha = 0,\ .25,\ .50,\ .75,\ 1$

$$P\{\max Y_j \le y\} = \exp(-\lambda_*(y\mathbf{v}_*) = \exp(-d\eta/y) \qquad (12.4)$$
$$= (P\{Y_1 \le y\})^{d\eta} \quad (y > 0).$$

Namely, the maximum of d random variables Y_j behaves as the maximum of $\theta = d\eta = dA(\mathbf{v}_*)$ independent ones. Clearly, $1 \le \theta \le d$, $\theta = 1$ corresponds to complete dependence and $\theta = d$ to total independence. Smith (1990) and later Schlather and Tawn (2002, 2003) use the term *extremal coefficient* for θ and use it as a measure of dependence.

Remark. Suppose $\mathbf{X}$ is a sequence (i.e., $d = \infty$) and Pickands dependence function for the first n components of $\mathbf{X}$ is A_n. Then, the so called *extremal index* of $\mathbf{X}$ (if exists) is $\lim_{n\to\infty} A_n(n^{-1}, n^{-1}, \cdots, n^{-1})$ (see Leadbetter et al (1983)).

Other coefficients of dependence often used (for bivariate extremes) are Kendall's τ (here τ_K), Spearman's ρ,

$$\rho_S = \mathrm{corr}(G_1(X_1), G_2(X_2)) = \mathrm{corr}(e^{-1/Y_1}, e^{-1/Y_2})$$

and

$$\rho = \mathrm{corr}(\lambda_1(X_1), \lambda_2(X_2)) = \mathrm{corr}(1/Y_1, 1/Y_2)$$

(see Beirlant et al. (2004), pp. 274–275). One obvious advantage of θ is that it can be used for any model with $d \ge 2$. To be on the same scale as the other coefficients of dependence, we define

$$\tau_1 = \frac{d - \theta}{d - 1} = \frac{d(1 - \eta)}{d - 1}, \qquad (12.5)$$

for which $\tau_1 = 0$ or 1 according as the X_j are totally independent or completely dependent. Another coefficient of a similar nature is

$$\tau_2 = \frac{\int_{\Omega_d}(1 - A(\mathbf{v}))d\mathbf{v}}{\int_{\Omega_d}(1 - A_0(\mathbf{v}))d\mathbf{v}} =: \frac{S_d(A)}{S_d(A_0)}, \qquad (12.6)$$

which is the ratio between the volume enclosed between the function A and its upper bound 1 and the largest possible volume. This ratio is equal to 0 when $A \equiv 1$ (total independence) and to 1 when $A \equiv A_0$ (complete dependence). The coefficient τ_2 is briefly mentioned by Tiago de Oliveira:97, p. 319, in the context of bivariate extremes. We advocate its use for any $d \geq 2$.

Since the denominator in τ_2 depends on d only, while the numerator is case-specific, it would be useful to have a formula for $S_d(A_0)$:

$$S_d(A_0) = \int_{\Omega_d} (1 - A_0(\mathbf{v}))d\mathbf{v} = \frac{1}{(d-1)!} - \frac{1}{d!}\left\{1 + \frac{1}{2} + \cdots + \frac{1}{d}\right\}. \tag{12.7}$$

The proof appears in Onn and Weissman (2006).

The question which one is preferred has no definite answer. It is clear that one coefficient cannot preserve all the information about the function A. A similar question might be raised in the context of *mode vs mean* as representatives of a whole distribution. However, we might require that a coefficient of dependence of MEVD will satisfy a simple condition. Let $V_0, V_1, V_2, \cdots$ be a sequence of independent unit-Fréchet random variables and consider the *mixture model* for some $\alpha \in [0, 1]$:

$$X_j = \max\{\alpha V_0, (1-\alpha)V_j\} \quad (j = 1, 2, \cdots, d).$$

Then $\mathbf{X} = (X_1, X_2, \cdots, X_d)$ has unit-Fréchet margins and its A function is given by

$$A(\mathbf{v}) = \alpha A_0(\mathbf{v}) + (1-\alpha) \cdot 1,$$

a mixture between complete dependence and total independence. A reasonable requirement is that a coefficient of dependence equals α in this case. Indeed, $\tau_1 = \tau_2 = \alpha$ for all $d \geq 2$. For comparison, when $d = 2$, one can show that

$$\tau_K = \rho = \frac{\alpha}{2-\alpha} \leq \rho_S = \frac{3\alpha}{4-\alpha} \leq \alpha = \tau_1 = \tau_2.$$

Hence, in this respect of fulfilling the intuitive condition, τ_1 and τ_2 are preferred. To be fair, if (X_1, X_2) has a mixture distribution (not a mixture exponent), that is, for some independent and identically distributed random variables U, V, the pair $(X_1, X_2) = (U, V)$ with probability $1 - \alpha$ and $= (U, U)$ with probability α, then $\rho_S = \rho = \alpha$ (the distribution of (X_1, X_2) cannot be MEVD if $0 < \alpha < 1$). This example shows that in the context of multivariate extremes, τ_1 and τ_2 are more intuitive coefficients of dependence.

12.3 Examples

1. *Mixed model.* For $\alpha \in [0, 1]$, the exponent function is given by

$$\lambda(x, y) = \frac{1}{x} + \frac{1}{y} - \frac{\alpha}{x+y},$$

from which we get

$$A(v) = 1 - \alpha(1-v)v \quad (0 \le v \le 1)$$

$$\tau_1 = \frac{1}{2}\alpha, \quad \tau_2 = \frac{2}{3}\alpha$$

$$\tau_K = \frac{8tan^{-1}(\alpha/(4-\alpha))^{1/2}}{\alpha^{1/2}(4-\alpha)^{1/2}} - 2$$

$$\rho = \frac{8tan^{-1}(\alpha/(4-\alpha))^{1/2}}{\alpha^{1/2}(4-\alpha)^{3/2}} - \frac{2-\alpha}{4-\alpha}$$

$$\rho_S = 12\left\{\frac{8tan^{-1}(\alpha/(8-\alpha))^{1/2}}{\alpha^{1/2}(8-\alpha)^{3/2}} + \frac{1}{8-\alpha}\right\} - 3.$$

Table 12.1 gives the coefficients of dependence in increasing order. We notice that in this model, complete dependence is impossible.

2. *de Haan-Resnick model.* The exponent function is given by

$$\lambda(x,y,z) = \frac{1}{2}\{\max(x^{-1},y^{-1}) + \max(x^{-1},z^{-1}) + \max(y^{-1},z^{-1})\}.$$

This means

$$X_1 = \max(V_1,V_2)/2, \quad X_2 = \max(V_1,V_3)/2, \quad X_3 = \max(V_2,V_3)/2,$$

$$A(\mathbf{v}) = \frac{1}{2}\{\max(v_1,v_2) + \max(v_1,v_3) + \max(v_2,v_3)\}.$$

Thus we conclude that

$$\eta = A(1/3,1/3,1/3) = 1/2, \quad \tau_1 = (3/2)(1-\eta) = 3/4$$

$$\tau_2 = \frac{36}{7}\cdot\frac{1}{8} = \frac{9}{14} = .642857$$

$$\tau_1(1,2) = \tau_2(1,2) = 1/2$$

(Introducing X_3 to the system increases the dependence).

Table 12.1. Coefficients of dependence for the mixed model

α	τ_K	ρ	τ_1	ρ_S	τ_2
0	0	0	0	0	0
.25	.0877	.0901	.1250	.1299	.1667
.50	.1853	.1958	.2500	.2702	.3333
.75	.2947	.3215	.3750	.4222	.5000
1	.4184	.4728	.5000	.5874	.6667

Table 12.2. Coefficient of dependence for the Cross-Over Model, $d = 3$

h	$\int_\Omega (1-A)$	τ_2	τ_1
0	0	0	0
.1	99/2000	.25457	.15
.2	12/125	.49371	.30
.3	273/2000	.70200	.45
.4	21/125	.86400	.60
.5	3/16	.96429	.75
.6	97/500	.99771	.90
2/3	7/36	1	1

3. *Cross-over model*. The exponent function is given by

$$\lambda(x,y) = \max(hx^{-1}, (1-h)y^{-1}) + \max((1-h)x^{-1}, hy^{-1}).$$

This means

$$X_1 = \max(hV_1, (1-h)V_2), \quad X_2 = \max((1-h)V_1, hV_2),$$

$$A(v) = \max(A_0(v), 1-h) \quad (0 \le v \le 1,\ 0 \le h \le 1/2).$$

Thus we conclude that

$$\eta = A(1/2) = 2h, \quad \tau_2 = 4h(1-h) = 1 - (1-\tau_1)^2.$$

This model can be defined for $d \ge 2$ as follows:

$$A(\mathbf{v}) = \max(A_0(\mathbf{v}), 1-h) \quad (\mathbf{v} \in \Omega_d,\ 0 \le h \le d/(d-1).$$

The X_j can be defined as

$$X_j = \max\{(1-h)V_j, h(d-1)^{-1} \max_{1 \le i \le d,\ i \ne j} V_i\} \quad (j = 1, 2, \cdots, d).$$

Here $\tau_1 = dh/(d-1)$ and τ_2 is computed via Equations (12.6) and (12.7). Table 12.2 gives the coefficient of dependence for some values of h and $d = 3$.

12.4 Relation between τ_1 and τ_2

Theorem 1. *For $d = 2$, $\tau_1 \le \tau_2$.*

Proof. Given an MEVD, let A be its Pickands dependence function (the red graph in figure 12.2) and let $h = 1 - A(1/2)$, so that $\tau_1 = 2h$. Define the mixture model whose Pickands dependence function (the green graph) is $A^*(\mathbf{v}) = 2hA_0(\mathbf{v}) + 1 - 2h$, for which $\tau_1^* = \tau_1 = \tau_2^*$. Since A is convex, $A \le A^*$ (equality at $v = 1/2$),

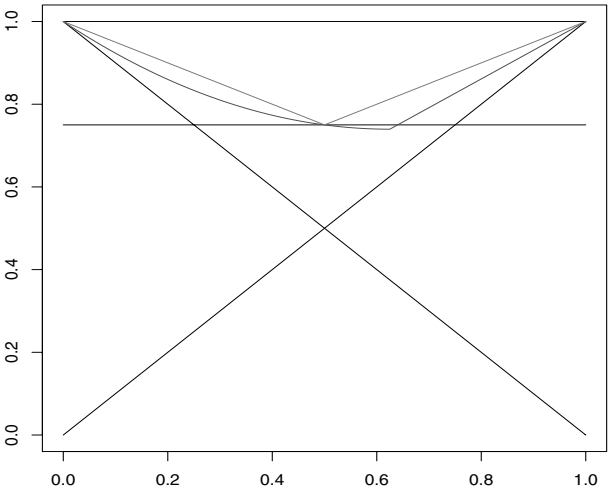

Figure 12.2. Pickands dependence functions A (red) and A^* (green)

$$\int_\Omega (1 - A(\mathbf{v}))d\mathbf{v} \geq \int_\Omega (1 - A^*(\mathbf{v}))d\mathbf{v} = \tau_1 \int_\Omega (1 - A_0(\mathbf{v}))d\mathbf{v},$$

hence,

$$\tau_2 = \frac{\int_\Omega (1 - A(\mathbf{v}))d\mathbf{v}}{\int_\Omega (1 - A_0(\mathbf{v}))d\mathbf{v}} \geq \tau_1.$$

This completes the proof. ■

This is a proper proof for $d = 2$. For $d \geq 3$, figure 12.2 is misleading, namely, $A \leq A^*$ is not necessarily true. The de Haan-Resnick model ($d = 3$) is a counter example. For $v_1 \geq v_2 \geq v_3,\ v_1 + v_2 + v_3 = 1$,

$$A(\mathbf{v}) = v_1 + \frac{1}{2}v_2, \quad A^*(\mathbf{v}) = \frac{3}{4}v_1 + \frac{1}{4}.$$

Since $v_2 > v_3$ if and only if $v_1 + 2v_2 - 1 > 0$, it follows that

$$A(\mathbf{v}) - A^*(\mathbf{v}) = \frac{1}{4}v_1 + \frac{1}{2}v_2 - \frac{1}{4} = \frac{1}{4}(v_1 + 2v_2 - 1) > 0.$$

Indeed, in this case, $\tau_1 = 3/4 > \tau_2 = 9/14$. On the other hand, the logistic model ($d = 3$) is a model for which $\tau_1 \leq \tau_2$, as is demonstrated by the table 12.3.
Here $\tau_1 = (3 - 3^\alpha)/2$ and $\tau_2 = \int_\Omega (1 - A)36/7$.

Going back to the case $d = 2$, we ask how big can the difference $\tau_2 - \tau_1$ be?

Consider all the (symmetric) models for which $A(1/2) = 1 - h$.
Clearly, the one with the largest area enclosed between A and 1 is the one pertains to the cross-over model (the red graph in figure 3) $A_{co}(\mathbf{v}) = \max(A_0(\mathbf{v}), 1 - h)$. The one with the smallest area pertains to the mixture model $A^*(\mathbf{v}) = 2hA_0(\mathbf{v}) + 1 - 2h$ (the green graph). For both models $\tau_1 = 2h$, while $\tau_2 = \tau_1 = 2h$ for the mixture model and

$$\tau_2 = 4h(1 - h) = 1 - (1 - \tau_1)^2$$

Table 12.3. Coefficients of dependence for the Logistic Model, $d = 3$

α	τ_1	τ_2
0	1	1
1/4	.8420	.9457
1/2	.6340	.7670
3/4	.3602	.4559
1	0	0

for the cross-over model. Hence for every A between these cases,

$$\tau_1 = 2h \leq \tau_2 \leq 4h(1-h) = 1 - (1-\tau_1)^2.$$

It follows that

$$\max_{0 \leq h \leq 1/2} (\tau_2 - \tau_1) = \frac{1}{4},$$

and this max is attained at $h = 1/4,\ \tau_1 = 1/2,\ \tau_2 = 3/4$. It turns out that this is also the largest possible difference for all A (including asymmetric ones), but we skip the details.

One could hold τ_2 constant (i.e. the area) and let τ_1 vary. For instance, for all triangles with height h ($h \in [0, 1/2]$), $\tau_2 = 2h$ while

$$\frac{h}{1-h} \leq \tau_1 \leq 2h.$$

This has maximum range of $3 - 2^{3/2} = .17157$ at $h = 1 - 2^{-1/2} = .29289$.

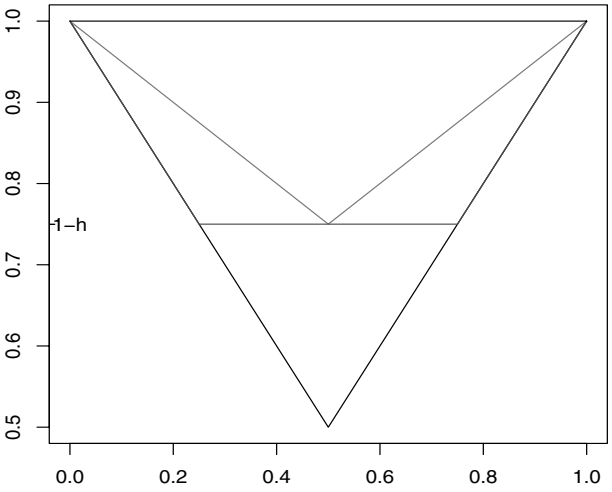

Figure 12.3. Pickands dependence functions A^* (green) and A_{co} (red)

12.5 Combining Two Independent Models

Let $\mathbf{X} = (x_1, \cdots, X_k)$, $\mathbf{Y} = (Y_1, \cdots, Y_m)$ be two independent MEVD random vectors, with unit-Fréchet margins. We combine them into

$$\mathbf{Z} = (X_1, \cdots, X_k, Y_1, \cdots, Y_m) \quad (k + m = d)$$

and want to compute τ_{1Z}, τ_{2Z} on the basis of τ_{1X}, τ_{2X}, τ_{1Y}, τ_{2Y}. For convenience we denote

$$B_k = 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{k}.$$

Theorem 2. *If $\mathbf{X} \in \mathbf{R}^k$, $\mathbf{Y} \in \mathbf{R}^m$ are independent, MEVD , then*

$$\tau_{1Z} = \frac{k-1}{d-1}\tau_{1X} + \frac{m-1}{d-1}\tau_{1Y} \tag{12.8}$$

and

$$\tau_{2Z} = \frac{k - B_k}{d - B_d}\tau_{2X} + \frac{m - B_m}{d - B_d}\tau_{2Y}. \tag{12.9}$$

Proof. The proof of (12.8) is straightforward. The independence assumption implies that

$$\theta_Z = \theta_X + \theta_Y. \tag{12.10}$$

Using Equation (12.5) to substitute $\theta_Z = d - (d-1)\tau_{1Z}$ etc. in Equation (12.10) leads to Equation (12.8).

To prove the second assertion, we write the Pickands dependence function for $\mathbf{Z}$ as

$$A_Z(\mathbf{v}) = tA_X(\mathbf{u}) + (1-t)A_Y(\mathbf{w}) \quad (\mathbf{v} \in \Omega_d,\ \mathbf{u} \in \Omega_k,\ \mathbf{w} \in \Omega_m), \tag{12.11}$$

where

$$t = v_1 + v_2 + \cdots + v_k;\ \ u_i = \frac{v_i}{t},\ i = 1, 2, \cdots, k;\ \ w_i = \frac{v_{i+k}}{1-t},\ i = 1, 2, \cdots, m.$$

The Jacobian of the transformation

$$(v_1, v_2, \cdots, v_{d-1}) \mapsto (t, u_1, \cdots, u_{k-1}, w_1, \cdots, w_{m-1})$$

is

$$J = t^{k-1}(1-t)^{m-1} \quad (t \in [0, 1])$$

and

$$1 - A_Z(\mathbf{v}) = t(1 - A_X(\mathbf{u})) + (1-t)(1 - A_Y(\mathbf{w})).$$

Hence,

$$\begin{aligned} S_d(A_Z) &= \int_{\Omega_d} (1 - A_Z(\mathbf{v}))d\mathbf{v} = \\ &= \int_0^1 \int_{\Omega_k} \int_{\Omega_m} (1 - A_Z(\mathbf{v}))d\mathbf{u}d\mathbf{w}t^{k-1}(1-t)^{m-1}dt \end{aligned}$$

$$= \frac{1}{(m-1)!}\int_0^1 t^k(1-t)^{m-1}dt \int_{\Omega_k}(1-A_X(\mathbf{u}))d\mathbf{u}$$
$$+\frac{1}{(k-1)!}\int_0^1 t^{k-1}(1-t)^m dt \int_{\Omega_m}(1-A_Y(\mathbf{w}))d\mathbf{w}$$
$$= \frac{k!}{d!}S_k(A_0)\tau_{2X} + \frac{m!}{d!}S_m(A_0)\tau_{2Y}.$$

Division by $S_d(A_0)$ completes the proof. ■

We note that τ_{1Z} and τ_{2Z} are "almost" weighted averages; "almost" because the sums of the respective weights are less than 1. However, for k and m large, these sums tend to 1. Two special cases of interest are $k \geq 2$, $m = 1$ and $k = m = 2$. For the first case we have

$$\tau_{1Z} = \frac{k-1}{k}\tau_{1X}, \quad \tau_{2Z} = \frac{k-B_k}{k+1-B_{k+1}}\tau_{2X}.$$

For $k = m = 2$ we have

$$\tau_{1Z} = \frac{1}{3}(\tau_{1X}+\tau_{1Y}), \quad \tau_{2Z} = \frac{6}{23}(\tau_{2X}+\tau_{2Y}).$$

Expressions (12.8) and (12.9) are exact for independent $\mathbf{X}$, $\mathbf{Y}$, but they can serve as lower bounds for dependent pairs $\mathbf{X}$, $\mathbf{Y}$. Inequalities of this kind concerning the extremal coefficients are dealt with by Schlather and Tawn (2002, 2003). Given 2^d numbers $\{\theta_B\}$, corresponding to all subsets $B \subseteq \{1, 2, \cdots, d\}$, Schlather and Tawn (2002, 2003) give necessary and sufficient conditions on $\{\theta_B\}$ so that they can be self-consistent as extremal coefficients of all sub-vectors of the MEVD $\mathbf{X} \in \mathbf{R}^d$. These conditions imply analog conditions on τ_{1B}.

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13

Ratio of Maximum to the Sum for Testing Super Heavy Tails

Cláudia Neves and Isabel Fraga Alves[2]

[1] UIMA, Department of Mathematics, University of Aveiro, Portugal
[2] CEAUL, DEIO, Faculty of Sciences, University of Lisbon, Portugal

Abstract: An extreme value approach to the modeling of rare and damaging events quite frequently involves heavy tailed distributions associated with power decaying tails. The positive counterpart of this power, which determines the tail heaviness of the distribution function pertaining to the sample observations, is consensually known as the tail index. In this paper, we allow the tail index α to be zero so as to embrace the class of super-heavy tailed distributions. We then present a test statistic consisting of the ratio of maximum to the sum of log-excesses in order to discern between distributions with heavy and super-heavy tails. Under suitable yet reasonable assumptions, we cast an account of consistency of the Hill estimator for α equal to zero from the asymptotic features of the referred testing procedure.

Keywords and phrases: Extreme value theory, Hill estimator, max-domains of attraction, regular variation theory, test of hypothesis

13.1 Introduction

The potential of Extreme Value theory in assessing statistical models for tail-related values has gained widespread recognition in fields ranging from hydrology to insurance, finance and, more recently, in telecommunications and teletraffic engineering. In extreme value analysis the main concern is not towards the accumulation of many events, none of these being dominant (in which case the Central Limit Theorem would serve our purposes), but the interest goes instead to a single event capable of compromising the integrity of a certain system, making therefore the normal distribution inadequate to describe the small set of data arising with such individual large and thus dominant contributors. The Fisher-Tippett Theorem of extreme values (Fisher and Tippett, 1928) states that all possible non-degenerate weak limit distributions of maxima of independent and identically distributed (i.i.d.) random variables $X_1, X_2, \ldots, X_n$ with the same parent distribution function F are Extreme Value distributions. It can be considered the fundamental result in Extreme Value theory, detaining the same prominent status in the study of partial maxima of i.i.d. sequences of random variables

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as the Central Limit Theorem holds in the study of partial sums. Assuming there are normalizing constants $a_n > 0$ and $b_n \in \mathbb{R}$ such that

$$\lim_{n\to\infty} P\Big\{a_n^{-1}\Big(\max(X_1,\ldots,X_n) - b_n\Big) \le x\Big\} = \lim_{n\to\infty} F^n(a_n\, x + b_n) = G(x), \quad (13.1)$$

for all $x \in \mathbb{R}$ with G a non-degenerate distribution function, then the Fisher and Tippett theorem asserts that we can redefine the constants in such a way that the distribution function F is in the domain of attraction of the Generalized Extreme Value distribution $G_\gamma = G$ (notation: $F \in \mathcal{D}(G_\gamma)$), i.e.,

$$\lim_{n\to\infty} F^n(a_n\, x + b_n) = G_\gamma(x) := \exp(-(1+\gamma x)^{-1/\gamma}), \quad (13.2)$$

for $1+\gamma x > 0$, where $\gamma \in \mathbb{R}$ is the extreme value index. The Generalized Extreme Value distribution G_γ comprises three classes of distributions discriminated by the extreme value index sign: Weibull ($\gamma < 0$), Gumbel ($\gamma = 0$) and Fréchet ($\gamma > 0$).

The particularly interesting case of Fréchet domain of attraction contains distributions with polynomially decaying tails. These are heavy-tailed distributions with infinite endpoint, for which there exists a tail index $\alpha = 1/\gamma$, such that the tail distribution function $\overline{F} := 1 - F$ satisfies $\lim_{t\to\infty} \overline{F}(tx)/\overline{F}(t) = x^{-\alpha}$, for every $x > 0$. Then, we say that $\overline{F}$ is of regular variation near infinity with index $-\alpha$ (notation: $\overline{F} \in RV_{-\alpha}$), meaning that $\overline{F}$ can be decomposed as $\overline{F}(x) = x^{-\alpha}L(x)$ where L is of slow variation, i.e., $\lim_{t\to\infty} L(tx)/L(t) = 1$, for any $x > 0$, which entails $L \in RV_0$ (see, e.g., 5. in Section 13.3).

Although most classical distribution functions admit sequences $a_n > 0$ and $b_n \in \mathbb{R}$ such that a non-degenerate limit is attained in (13.1), the existence of such sequences is not guaranteed. In fact, it can be shown that if $\overline{F}$ is of slow variation, there is no possibility of normalizing the sequence of partial maxima in order to make (13.1) to hold mainly because there is too much weight on the tail. Therefore, the term *super-heavy* can be fairly assigned to the tail distribution function $\overline{F}$. A common example is the log-Pareto distribution function (its expression gives an explanation for the term log-Pareto)

$$F(x) = 1 - (\log x)^{-1},\ x \ge e.$$

It is also worthwhile to mention that super-heavy tailed distributions do not possess finite moments of any order and, as a consequence, any statistical inference based on empirical moments is meaningless for these kinds of models. Altogether, with any distribution function F such that $\overline{F} \in RV_{-\alpha}$, the tail index $\alpha \ge 0$ gives the order of finite moments.

The theory of Regular Variation has been a prolific contributor to Extreme Value theory as it provides a formal framework for a more systematic study of relevant properties of distribution functions belonging to extreme domains of attraction. With this respect, we refer to de Haan and Ferreira (2006). In particular, a necessary and sufficient condition for $F \in \mathcal{D}(G_\gamma)$ is the extended regular variation property:

$$\lim_{t\to\infty} \frac{U(tx) - U(t)}{a(t)} = \frac{x^\gamma - 1}{\gamma}, \quad (13.3)$$

for every $x > 0$ and some positive measurable function a, where U stands for a quantile type function pertaining to F defined by the generalized inverse

$$U(t) := \Big(\frac{1}{1-F}\Big)^{\leftarrow}(t) = \inf\Big\{x : F(x) \geq 1 - \frac{1}{t}\Big\}.$$

Moreover, $\gamma = 1/\alpha > 0$ and $a(t) = tU(t)/q(t)$ yield the equivalence of (13.3) to the following regular variation property

$$\lim_{t\to\infty} \frac{U\big(t + x\,q(t)\big)}{U(t)} = (1 + \alpha\,x)^{\frac{1}{\alpha}} \tag{13.4}$$

for all $1 + \alpha x > 0$, $\alpha \geq 0$, with a positive measurable function q such that

$$\lim_{t\to\infty} \frac{q\big(t + x\,q(t)\big)}{q(t)} = 1 + \alpha x$$

(cf. Lemma 1 below). This function q is called auxiliary function for U. If $\alpha = 0$, the right hand side of (13.4) should be understood in the limiting sense as e^x while q becomes a self-neglecting function. According to de Haan (1970), Definition 1.5.1, we then say that the tail quantile function U belongs to the class Γ of functions of rapid variation (notation: $U \in \Gamma$). We emphasize that super-heavy tailed distributions are here addressed by this relation. Owing to condition (13.4), we find appropriate to use a suitably normalized version of the test statistic

$$T_n(k) = \frac{\log(X_{n,n}) - \log(X_{n-k,n})}{\sum_{i=0}^{k-1} \big(\log(X_{n-i,n}) - \log(X_{n-k,n})\big)}, \tag{13.5}$$

where $X_{1,n} \leq X_{2,n} \leq \ldots \leq X_{n,n}$ are the order statistics corresponding to the random sample $X_1, X_2, \ldots, X_n$, with the ultimate aim of distinguishing between heavy and super-heavy tails. In Section 13.2, we present some results concerning the asymptotic behavior of $T_n(k)$ for large n, which allows us to establish eventually a critical region for the test at a certain nominal level $\overline{\alpha}$. The remainder of this paper unfolds as follows. In Section 13.3 we display some simulation results concerning not only estimated power but also type I error of the test. A brief application to two published data sets in teletraffic and seismology fields is also given. Section 13.4 comprises results on regular variation required to obtain the asymptotic statements involving the testing procedure. Finally, Section 13.5 contains the proofs of the main results formulated in Section 13.2. There is also a proof for consistency of the Hill estimator in the super-heavy tailed case that hinges on the proof given for the main theorem.

13.2 Main Results

The present section concentrates on the asymptotic behavior of the test statistic introduced in (13.5). While the main theorem below encloses a general result for distributions with heavy or super-heavy tails, thus suggesting a possible normalization for the test statistic to attain a non-degenerate limit, on the other hand, results (i) and (ii) of its corollary expound eventual differences in stochastic behavior between the two classes of distributions, accounting for power and consistency of the test, respectively.

Theorem 1. *Suppose the function U is such that condition (13.4) holds for some $\alpha \geq 0$. Let $k = k_n$ be an intermediate sequence, i.e., a sequence of positive integers such that $k_n \to \infty$ and $k_n = o(n)$ as $n \to \infty$. Then*

$$T_n(k) = O_p\Big(\frac{1}{\log k}\Big),$$

with $T_n(k)$ as defined in (13.5).

Corollary 1. *Under the conditions of Theorem 1,*

(i) if $\alpha = 0$,

$$\log k\, T_n(k) \xrightarrow[n\to\infty]{d} T^*, \tag{13.6}$$

where the limiting random variable T^* has a Fréchet distribution function $\Phi(x) = \exp\big(-x^{-1}\big)$, $x \geq 0$;

(ii) if $\alpha > 0$,

$$\log k\, T_n(k) \xrightarrow[n\to\infty]{P} 0. \tag{13.7}$$

Therefore, taking only the k most extreme observations from a sample of size n such that k/n amounts to a small top sample fraction, the critical region for the one-sided test $H_0 : \alpha = 0$ *versus* $H_1 : \alpha > 0$ of nominal size $\overline{\alpha}$ is given by $\mathcal{R} : \log k\, T_n(k) < \Phi^{-1}(\overline{\alpha})$, where Φ^{-1} denotes the inverse of the Fréchet distribution function.

13.3 Simulation Results and Real Data Analysis

It should be noticed at this point that we are dealing with a test of asymptotic size $\overline{\alpha}$, where in fact the closeness of the true actual size of the test to the nominal one is determined by how precise the approximation to the Fréchet law is. Under these circumstances, simulations are generally needed to gain insight. In this section, we present small sample Monte Carlo simulations in order to study more thoroughly the behavior of the testing procedure, taking the following distributions as key examples:

1. Consider a random variable Y with standard Pareto distribution function $F(y) = 1-y^{-1}$, all $y \geq 1$. We say that a random variable W follows a log-Pareto distribution with parameter $\beta > 0$ if and only if $W = e^{\beta Y}$. The tail quantile function pertaining to W is simply $U_W(t) = e^{\beta t}$. Thus, condition (13.4) holds with $\alpha = 0$ and $q(t) = 1/\beta$.
2. A random variable X has a log-Fréchet distribution with parameter $\beta > 0$ if and only if $Y = \log X/\beta$ has a Fréchet distribution function

$$\Phi(x) = \exp\{-x^{-1}\},\ x > 0.$$

Since $U(t) = \exp\big\{-\beta/\log(1-1/t)\big\}$, for $t \geq 1$, then condition (13.4) holds with $\alpha = 0$ and auxiliary function $q(t) = 1/\beta$.

3. Let X be a random variable with log-Weibull distribution function

$$F(x) = 1 - \exp\{-(\log x)^{\beta}\},\ x \geq 1,\ 0 < \beta < 1.$$

Then $U \in \Gamma$ with auxiliary function $q(t) = \beta t(\log t)^{1-1/\beta}$.

4. A random variable X is said to have a log-Cauchy distribution if and only if $Y = \log X$ is a Cauchy random variable for which $U_Y(t) = \tan(\pi/2 - \pi/t)$ admits the expansion $U_Y(t) = t/\pi + \pi/3t^{-1} + o(t^{-1})$, $t \to \infty$. Hence, U_Y satisfies (13.4) with $\alpha = 1$ and $q(t) = t$ whereas (13.4) holds immediately for U_X with $\alpha = 0$ and $q(t) = \pi$ once we notice that $U_X = \exp U_Y$.

5. A random variable X has a log-Gamma distribution with parameters $\beta > 0$ and $\alpha > 0$ if it has probability density function

$$f_{\beta,\alpha}(x) = \frac{\alpha^{\beta}}{\Gamma(\beta)}(\log x)^{\beta-1}x^{-\alpha+1},\ x > 1.$$

In other words, X is log-Gamma distributed for $X > 1$ if and only if $Z = \log X$ is Gamma distributed for $Z > 0$. Then L'Hopital ascertains that $1 - F(x) \sim x^{-\alpha}(\log x)^{\beta-1}$ $(x \to \infty)$. The case $\beta = 1$ reduces to the Pareto distribution function $F(x) = 1 - x^{-\alpha}$, for all $x \geq 1$, while for other values of β we have essentially a Pareto distribution contaminated by the slowly varying function $L(x) = (\log x)^{\beta-1}$.

Furthermore, we shall draw comparisons of the now proposed test with the test introduced in Fraga Alves et al. (2006), liable to the test statistic

$$S_n(k) := \sqrt{24}\Big(\sum_{i=0}^{k-1}\frac{X_{n-k,n}}{X_{n-i,n}}\Big)^{1/2}\left(\frac{\sum_{i=0}^{k-1}\big(X_{n-k,n}/X_{n-i,n}\big)^2}{\sum_{i=0}^{k-1}X_{n-k,n}/X_{n-i,n}} - \frac{1}{2}\right). \tag{13.8}$$

Under suitable and reasonable restrictions upon the growth of the intermediate sequence $k = k_n$, the statistic $S_n(k)$ is asymptotically standard normal. The corresponding rejection region of the test at a significance level $\overline{\alpha}$ is thus given by $\mathcal{R} : S_n(k) > z_{1-\overline{\alpha}}$, where z_{ε} denotes the standard normal ε-quantile. Figures 13.1 and 13.2 display the relative frequency of rejections for each one of the models specified above as a function of the number k of the most extreme observations in samples of size $n = 1000$, obtained by generating 5000 samples from each one of the parent distributions specified above. Concerning empirical power, it seems that any trajectory determined by the test based on $T_n(k)$ will tend to agree with the ones displayed in figure 13.1 (a). This is particularly true for Fréchet and Pareto distributions, where the parameter β can be disregarded. On the contrary, the statistic $S_n(k)$ yields a great variety of patterns for the empirical power as the true value of α changes and only surpasses the now proposed test for α greater than, say, 0.5. Regarding simulated Type I error in figure 13.2, the test based on $T_n(k)$ is somewhat conservative. However this may not be all disadvantageous, specially if we look at the less heavy distributions lying in the class of super-heavy tails, since, under these distributions, the number of wrong rejections is likely to raise high above the nominal level of the test just as happens with the log-Cauchy. Moreover, for log-Pareto and log-Fréchet models, the statistic $T_n(k)$ is *parameter-free*, i.e., its distribution does not depend on the particular parameter β in 1. or 2.

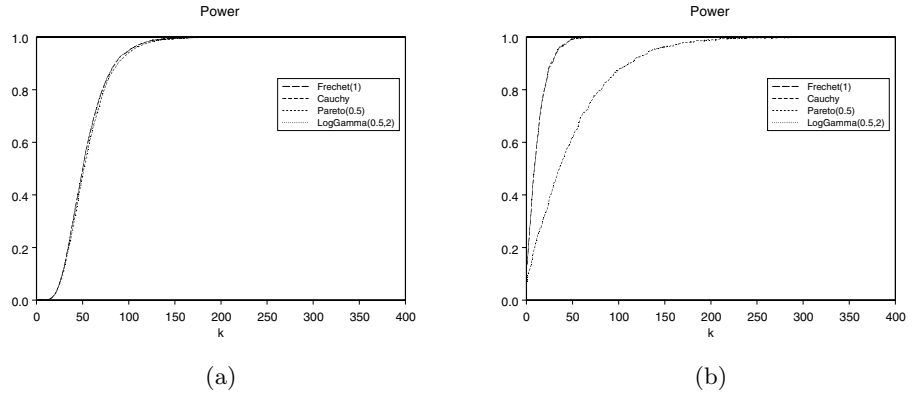


Figure 13.1. (a) Empirical power of $\log k\, T_n(k)$ and (b) empirical power of $S_n(k)$, at a nominal level $\overline{\alpha} = 0.05$ and built on 5000 samples of size $n = 1000$, all plotted against $k = 1, 2, \ldots, 200$

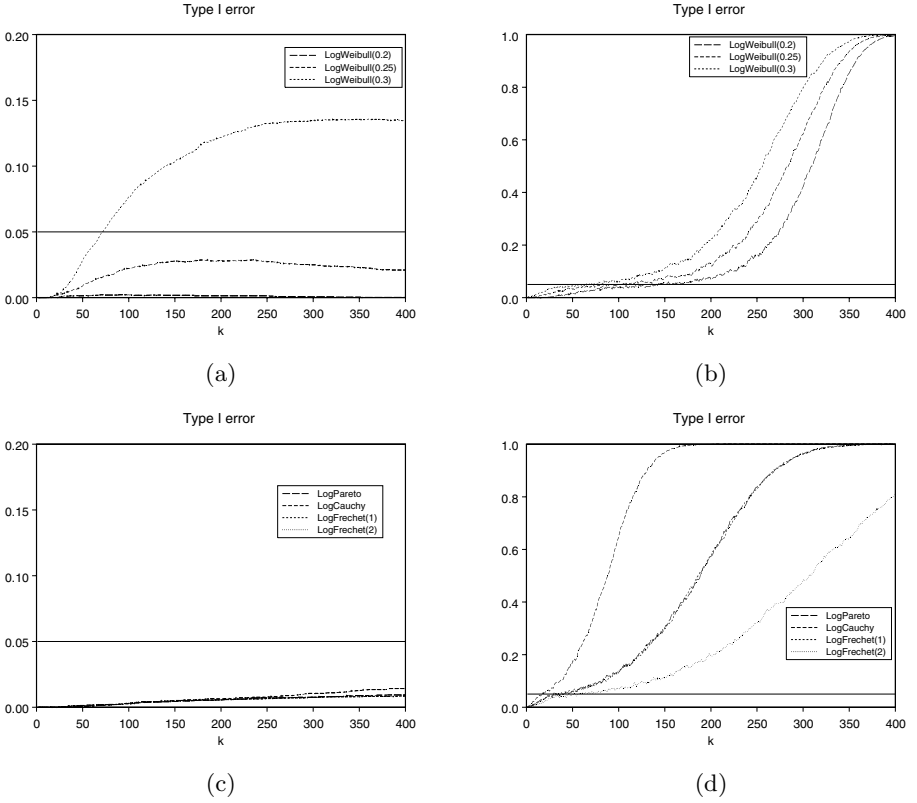


Figure 13.2. (a) and (c) Estimated Type I error of $\log k\, T_n(k)$, (b) and (d) Estimated Type I error of $S_n(k)$ at a nominal level $\overline{\alpha} = 0.05$, built on 5000 samples of size $n = 1000$, all plotted against $k = 1, 2, \ldots, 200$

As illustrative examples, consider the 36 699 file lengths in bytes included in the Internet Traffic Archive (`http://ita.ee.lbl.gov/index.html`) along with seismic data consisting of seismic moment for California seismicity, for magnitude $m \geq 5.5$, during the last two centuries (1800-1999). The seismic data set was extracted from Toppozada et al. (2000) earthquake catalog, available at `http://www.consrv.ca.gov/CGS/rghm/quakes/ms49epicenters.txt`. These referred magnitudes were then converted into seismic moments (for further details, see Zaliapin et al. (2005)).

In figure 13.3 we depict the trajectories resulting from the application of both test statistics to the data together with the corresponding critical values for $\overline{\alpha} = 0.05$. In what concerns the teletrafic data, we distinctly reject a distribution with super-heavy tail as underlying the data. The decision on whether we should reject the super-heavy tailed case is not so clear anymore when we consider the seismic data. The test statistic $S_n(k)$ exhibits a very erratic behaviour around the critical line, contrasting with the smooth sample path for the new test statistic $\log k\, T_n(k)$, which for a wide range of values of k, returns values below the critical line; therefore it is reasonable to reject a super-heavy tailed distribution to model underlying the seismic data. The proposed T-test reveals to be a valuable complement to the S-test. Attending to the relatively

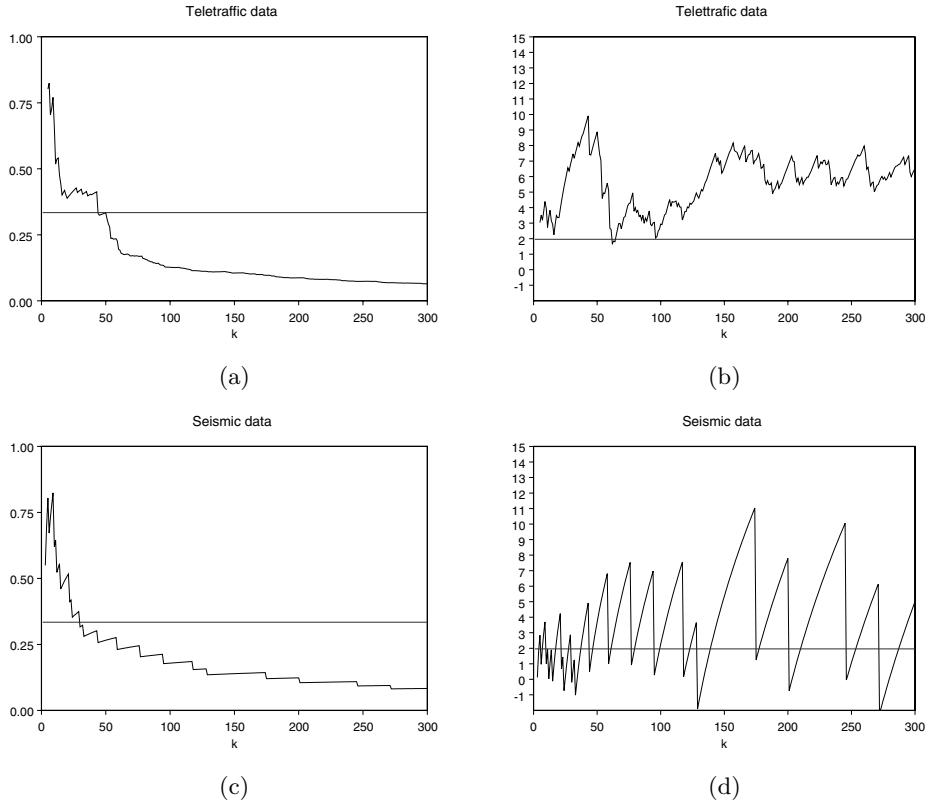
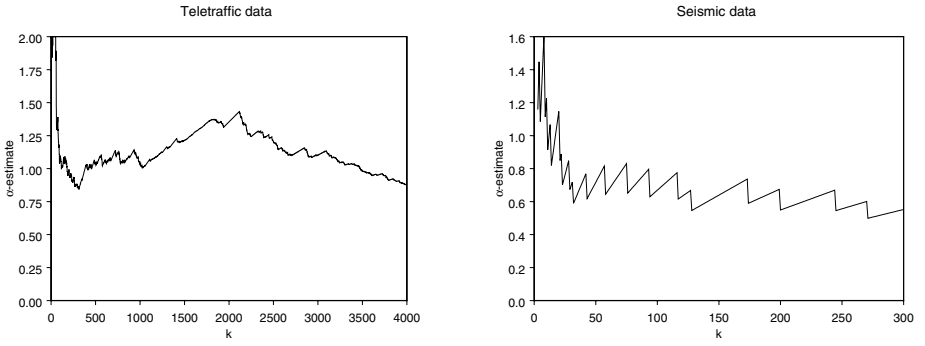


Figure 13.3. Sample paths and straight lines corresponding respectively to: $\log k\, T_n(k)$ and $\Phi^{-1}(0.05) \simeq 0.334$ in (a) and (c); $S_n(k)$ and $q_{0.95} \simeq 1.96$ in (b) and (d), against k



(a) (b)

Figure 13.4. α-Hill plot of: (a) file lengths (in bytes) and (b) seismic data

stable regions of the Hill-plots in figure 13.4 subject to small values of k, we can pinpoint $\hat{\alpha} = 1.0$ and $\hat{\alpha} = 0.6$ as valid estimates for the tail index with respect to the teletraffic data and seismic data, respectively. To sum up, the models underlying these two data sets reveal a considerable tail weight, and for that reason the use of empirical moments for statistical inference, as means and variances for instance, should be avoided.

13.4 Auxiliary Results

In this section, we gather some results on the theory of Regular Variation, necessary for the proof of the main theorem.

Lemma 1. *Suppose the function U is such that relation (13.4) holds with some $\alpha \geq 0$. Then, the auxiliary function q satisfies*

$$\lim_{t\to\infty} \frac{q(t)}{t} = \alpha \tag{13.9}$$

and

- *if $\alpha > 0$, then $U(\infty) := \lim_{t\to\infty} U(t) = \infty$ and U is of regular variation near infinity with index $1/\alpha$, i.e., $U \in RV_{1/\alpha}$;*
- *if $\alpha = 0$, then $U(\infty) = \infty$ and U is ∞-varying at infinity.*

Furthermore, for $\alpha = 0$,

$$\lim_{t\to\infty} \Big(\log U\big(t + x\, q(t)\big) - \log U(t) \Big) = x, \quad \textit{for every } x \in \mathbb{R}. \tag{13.10}$$

Proof. In case $\alpha > 0$, the first part of the Lemma follows directly from (13.4) whereas in case $\alpha = 0$ it is ensured by Lemma 1.5.1 and Theorem 1.5.1 of de Haan (1970). Relation (13.10) follows immediately from (13.4) with respect to $\alpha = 0$. ■

Proposition 1. *Suppose condition* (13.4) *holds for some* $\alpha \geq 0$.

(i) If $\alpha > 0$, *then for any* $\varepsilon > 0$ *there exists* $t_0 = t_0(\varepsilon)$ *such that for* $t \geq t_0$, $x \geq 0$,

$$(1-\varepsilon)\,(1+\alpha\,x)^{\frac{1}{\alpha}-\varepsilon} \leq \frac{U\big(t+x\,q(t)\big)}{U(t)} \leq (1+\varepsilon)\,(1+\alpha\,x)^{\frac{1}{\alpha}+\varepsilon}. \tag{13.11}$$

(ii) If (13.4) holds with $\alpha = 0$ *then, for any* $\varepsilon > 0$, *there exists* $t_0 = t_0(\varepsilon)$ *such that for* $t \geq t_0$, *for all* $x \in \mathbb{R}$,

$$\frac{U(t+x\,q(t))}{U(t)} \leq (1+\varepsilon)\,\exp\big(x(1+\varepsilon)\big). \tag{13.12}$$

Proof. Inequalities in (13.11) follow immediately from Proposition 1.7 in Geluk and de Haan (1987) when we settle $q(t) = \alpha t$ (see also (13.9) in Lemma 1) while (13.12) was extracted from Beirlant and Teugels (1989), p. 153. ■

Lemma 2.

(i) If $U \in RV_{1/\alpha}$, $\alpha > 0$, *then for any* $\varepsilon > 0$ *there exists* $t_0 = t_0(\varepsilon)$ *such that for* $t \geq t_0$, $x \geq 1$,

$$(1-\varepsilon)\frac{1}{\alpha}\log x \leq \log U(tx) - \log U(t) \leq (1+\varepsilon)\frac{1}{\alpha}\log x. \tag{13.13}$$

(ii) If $U \in \Gamma$ *then, for any* $\varepsilon > 0$, *there exists* $t_0 = t_0(\varepsilon)$ *such that for* $t \geq t_0$, *for all* $x \in \mathbb{R}$,

$$\log U\big(t+x\,q(t)\big) - \log U(t) \leq \varepsilon + x(1+\varepsilon). \tag{13.14}$$

Proof. Notice that once we apply the logarithmic transformation to relation (13.11) for large enough t, it becomes

$$(1-\varepsilon)\log(1+\alpha\,x)^{\frac{1}{\alpha}} \leq \log U\big(t+x\,q(t)\big) - \log U(t) \leq (1+\varepsilon)\log(1+\alpha\,x)^{\frac{1}{\alpha}}.$$

As before, the precise result is obtained by taking $q(t) = \alpha\,t$ with the concomitant translation of (13.4) for $\alpha > 0$ into the regularly varying property of U (cf. Lemma 1 again). The proof for (13.14) is similar and therefore obviated. ■

13.5 Proofs

Proof of Theorem 1. Let $\big\{Y_{i,n}\big\}_{i=1}^{n}$ be the order statistics corresponding to the independent and identically distributed random variables $\big\{Y_i\big\}_{i=1}^{n}$ with standard Pareto distribution function $1 - y^{-1}$, for all $y \geq 1$. Taking into account the equality in distribution

$$\big\{X_{i,n}\big\}_{i=1}^{n} \stackrel{d}{=} \big\{U(Y_{i,n})\big\}_{i=1}^{n}, \tag{13.15}$$

and defining

$$Q_n^{(i)} := \frac{Y_{n-i,n} - Y_{n-k,n}}{q(Y_{n-k,n})}, \quad i = 0, 1, \ldots, k-1 \tag{13.16}$$

and

$$M_n^{(1)} := \frac{1}{k} \sum_{i=0}^{k-1} \log U(Y_{n-i,n}) - \log U(Y_{n-k,n}), \tag{13.17}$$

we get in turn

$$T_n(k) \stackrel{d}{=} \frac{\log U(Y_{n,n}) - \log U(Y_{n-k,n})}{k\, M_n^{(1)}} \tag{13.18}$$

$$= \frac{\log U(Y_{n,n}) - \log U(Y_{n-k,n})}{\sum_{i=0}^{k-1} \big(\log U(Y_{n-i,n}) - \log U(Y_{n-k,n})\big)}$$

$$= \frac{\log U\big(Y_{n-k,n} + Q_{k,n}^{(0)}\, q(Y_{n-k,n})\big) - \log U(Y_{n-k,n})}{\sum_{i=0}^{k-1} \Big(\log U\big(Y_{n-k,n} + Q_{k,n}^{(i)}\, q(Y_{n-k,n})\big) - \log U(Y_{n-k,n})\Big)}. \tag{13.19}$$

Bearing on the fact that the almost sure convergence $Y_{n-k,n} \xrightarrow[n\to\infty]{as} \infty$ holds with an intermediate sequence $k = k_n$ (cf. Embrechts et al. (1997), Proposition 4.1.14), we can henceforth make use of condition (13.4). For ease of exposition, we shall consider the cases $\alpha > 0$ and $\alpha = 0$ separately.

• *Case* $\alpha > 0$*:* As announced, the core of this part of the proof lies at relation (13.4). Added (13.13) from Lemma 2, we obtain the following inequality for any $\varepsilon > 0$ and sufficiently large n:

$$M_n^{(1)} = \frac{1}{k} \sum_{i=0}^{k-1} \log U\Big(\frac{Y_{n-i,n}}{Y_{n-k,n}}\, Y_{n-k,n}\Big) - \log U(Y_{n-k,n})$$

$$\leq (1+\varepsilon) \frac{1}{k} \sum_{i=0}^{k-1} \frac{1}{\alpha} \big(\log Y_{n-i,n} - \log Y_{n-k,n}\big).$$

Owing to Rényi's important representation for exponential spacings,

$$E_{k-i,k} \stackrel{d}{=} E_{n-i,n} - E_{n-k,n} \;=\; \log(Y_{n-i,n}) - \log(Y_{n-k,n}), \tag{13.20}$$

where $E_{n-i,n}$, $i = 0, 1, \ldots, k-1$, are the order statistics pertaining to independent standard exponential random variables $E_i = \log Y_i$, we thus obtain

$$M_n^{(1)} = \frac{1}{k} \sum_{i=0}^{k-1} \log U(Y_{n-i,n}) - \log U(Y_{n-k,n}) \leq \frac{1}{\alpha}\,(1+\varepsilon) \frac{1}{k} \sum_{i=0}^{k-1} \log Y_{k-i,k}. \tag{13.21}$$

We can also establish a similar lower bound. Now, the Law of Large Numbers ensures the convergence in probability of the term on the right hand side of (13.21) since, for an intermediate sequence $k = k_n$,

$$\frac{1}{k}\sum_{i=0}^{k-1}\log Y_i \xrightarrow[k\to\infty]{P} \int_1^\infty \log y\,\frac{dy}{y^2} \;=\; 1.$$

In conjunction with with (13.9), the latter entails

$$L_n(k) := \frac{q(Y_{n-k,n})}{Y_{n-k,n}}\,M_n^{(1)} = 1 + o_p(1). \quad (n\to\infty) \tag{13.22}$$

Hence, using (13.13) followed by (13.20) upon (13.18), we obtain as $n\to\infty$

$$\begin{aligned} T_n(k) &\stackrel{d}{=} \frac{1}{k}\,\frac{q(Y_{n-k,n})}{Y_{n-k,n}}\,\frac{\log U(Y_{n,n}) - \log U(Y_{n-k,n})}{L_n(k)} \\ &= \frac{1}{k}\,(E_{k,k} - \log k)\big(1+o_p(1)\big) + \frac{\log k}{k}\big(1+o_p(1)\big). \end{aligned} \tag{13.23}$$

Finally, noticing that $E_{k,k} - \log k \xrightarrow[k\to\infty]{d} \Lambda$, where Λ is denoting a Gumbel random variable, we obtain a slightly stronger result than the one stated in the theorem. More specifically, we get from (13.23) that $T_n(k) = o_p(k^{-1/2})$, for any intermediate sequence $k = k_n$.

• *Case* $\alpha = 0$*:* The proof concerning this case of super-heavy tailed distributions, virtually mimics the steps followed in the heavy tailed case ($\alpha > 0$). We get from (13.19) that $M_n^{(1)}$ as defined in (13.17) can be written as

$$M_n^{(1)} = \frac{1}{k}\sum_{i=0}^{k-1}\log U\big(Y_{n-k,n} + Q_{k,n}^{(i)}\,q(Y_{n-k,n})\big) - \log U(Y_{n-k,n}).$$

Giving heed to the fact that, for each $i = 0, 1, \ldots, k-1$,

$$Q_{k,n}^{(i)} = \frac{Y_{n-k,n}}{q(Y_{n-k,n})}\Big(\frac{Y_{n-i,n}}{Y_{n-k,n}} - 1\Big)$$

is stochastically bounded away from zero (see Lemma 1), we can thus apply relation (13.14) from Lemma 2 in order to obtain, for any intermediate sequence $k = k_n$,

$$\frac{1}{k}\sum_{i=0}^{k-1}\log U\big(Y_{n-k,n} + Q_{k,n}^{(i)}\,q(Y_{n-k,n})\big) - \log U(Y_{n-k,n}) \le (1+\varepsilon)\,\frac{1}{k}\sum_{i=0}^{k-1} Q_{k,n}^{(i)},$$

as $n\to\infty$. Using Rényi's representation (13.20), we get

$$\frac{q(Y_{n-k,n})}{Y_{n-k,n}}\,M_n^{(1)} \le (1+\varepsilon)\,\frac{1}{k}\sum_{i=0}^{k-1}\big(Y_{k-i,k} - 1\big). \tag{13.24}$$

It is worth noticing at this point that with constants $a_k^* > 0$, $b_k^* \in \mathbb{R}$ such that $a_k^* \sim k\pi/2$ and $b_k^* a_k^*/k \sim \log k$ as $k\to\infty$, this new random variable S_k^*

$$S_k^* := \frac{1}{a_k^*}\sum_{i=0}^{k-1}\big(Y_i - 1\big) - b_k^*, \tag{13.25}$$

converges in distribution to a sum-stable law (cf. Geluk and de Haan (2000)). Embedding S_k^* defined above in the right hand side of (13.24), we ensure that $L_n(k)$ as introduced in (13.22) satisfies $L_n(k) = O_p(\log k)$. Therefore, in view of (13.19), the proof is concluded by showing that is possible to normalize the maximum of the log-spacings in a way to exhibit a non-degenerate behavior eventually. Since $U \in \Gamma$ we get in a similar way as before, for large enough n,

$$\begin{aligned}
&\frac{q(Y_{n-k,n})}{k\,Y_{n-k,n}}\Big(\log U\big(Y_{n-k,n} + Q_{k,n}^{(0)}\, q(Y_{n-k,n})\big) - \log U(Y_{n-k,n})\Big) \\
&= k^{-1}\Big(\frac{Y_{n,n}}{Y_{n-k,n}} - 1\Big)\big(1 + o_p(1)\big) \\
&= k^{-1}\big(Y_{k,k} - 1\big)\big(1 + o_p(1)\big) \;= O_p(1).
\end{aligned}$$

■

Remark 1. Notice that if $\alpha > 0$, then the consistency property of the well-know Hill estimator for $\gamma = \alpha^{-1}$,

$$\hat{\gamma}_n^H(k) := \frac{1}{k}\sum_{i=0}^{k-1} \log X_{n-i,n} - \log X_{n-k,n}$$

holds for an intermediate sequence $k = k_n$, i.e., $\big(\hat{\gamma}_n^H(k)\big)^{-1} \xrightarrow[n\to\infty]{P} \alpha$ and with a further restriction upon the growth of k, the Hill estimator is asymptotically normal (see, e.g., de Haan and Ferreira (2006)). Because the Hill estimator is always positive, we must inevitably consider a normalization in location if we want to attain the normal limit for $\alpha = 0$. However, Examples 1 and 2 below serve to show that even so the Hill estimator is sometimes asymptotically normal and sometimes not. Despite the asymptotic normality is not always achieved, the Hill estimator enjoys the consistency property even for super-heavy tails. The latter is sustained on the proof of Theorem 1. Notice that, since we have the identity in distribution $\hat{\gamma}_n^H(k) \stackrel{d}{=} M_n^{(1)}$ with $M_n^{(1)}$ defined in (13.17), we get from (13.24) and subsequent text, for any $\varepsilon > 0$ and large enough n,

$$\frac{q(Y_{n-k,n})}{Y_{n-k,n}}\,\frac{1}{\log k}\,\hat{\gamma}_n^H(k) < (1+\varepsilon)\Big(\frac{S_k^*}{\log k} + \frac{2}{\pi} + o(1)\Big),$$

meaning that the left hand-side of the above inequality is with high probability contained in the interval $(0, 2/\pi+\varepsilon)$, eventually. Lemma 1 ascertains that $q(Y_{n-k,n})/Y_{n-k,n} = o_p(1)$ for any intermediate sequence $k = k_n$. Hence $1/\hat{\gamma}_n^H(k)$ is also $o_p(1)$.

The following examples arise in the sequence of Remark 1.

Example 1. Consider a random sample taken from a standard log-Pareto population $X = e^Y$, with Y denoting a standard Pareto random variable. Then, the Hill estimator acquires the simple form

$$\hat{\gamma}_n^H(k) = \frac{1}{k}\sum_{i=0}^{k-1} Y_{n-i,n} - Y_{n-k,n}$$

Since $(k/n)Y_{n-k,n} \xrightarrow[n\to\infty]{P} 1$, with $k = k_n$ an intermediate sequence (see, e.g., Wellner, 1978), we get that

$$\hat{\gamma}_n^H(k) \stackrel{d}{=} Y_{n-k,n}\Big(\frac{1}{k}\sum_{i=0}^{k-1} Y_i^* - 1\Big) = \frac{n}{k}\left(S_k^* + b_k\right)\big(1 + o_p(1)\big),$$

with $\{Y_i^*\}_{i=0}^{k-1}$ denoting i.i.d. standard Pareto random variables independent of the random threshold $Y_{n-k,n}$, $b_k = O(\log k)$ and where S_k^* is the random variable (13.25) with limiting sum-stable distribution.

Example 2. Considering the log-Weibull distribution with $0 < \beta < 1$, the Hill estimator may be written as

$$H_n(k) = \frac{1}{k}\sum_{i=0}^{k-1}\big(\log Y_{n-i,n}\big)^{1/\beta} - \big(\log Y_{n-k,n}\big)^{1/\beta}$$

Similarly as in Example 1, we can replace the random threshold $Y_{n-k,n}$ by the fraction n/k and ultimately obtain that

$$\begin{aligned} H_n(k) &\stackrel{d}{=} \big(\log Y_{n-k,n}\big)^{1/\beta-1}\frac{1}{\beta}\left(\frac{1}{k}\sum_{i=1}^{k}\log Y_i^* + o_p(1)\right) \\ &= k^{-1/2}\big(\log\frac{n}{k}\big)^{1/\beta-1}\frac{1}{\beta}\left(S_k + \sqrt{k}\right)\big(1 + o_p(1)\big), \end{aligned}$$

where S_k converges to a standard normal random variable.

Proof of Corollary 1.
(i) For $\alpha = 0$, the last part of the proof of Theorem 1 emphasizes that, as $n \to \infty$,

$$\begin{aligned} \log k\, T_n(k) &\stackrel{d}{=} \frac{k^{-1}\big(\log U(Y_{n,n}) - \log U(Y_{n-k,n})\big)}{L_n(k)/\log k}\,\frac{q(Y_{n-k,n})}{Y_{n-k,n}} \\ &= \big(T^* + o_p(1)\big)/\big(1 + o_p(1)\big) \\ &= T^*\big(1 + o_p(1)\big) \end{aligned}$$

because, after suitably normalization by $a_k = k^{-1}$, the maximum of a sample of size k with standard Pareto parent distribution is attracted to a Fréchet law.
(ii) The precise result follows from (13.23) by straightforward calculations. ■

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14

Tail Behaviour: An Empirical Study

M. Ivette Gomes[1], Dinis Pestana[1], Lígia Rodrigues[2], and Clara Viseu[3]

[1] UIMA, Universidade de Lisboa, DEIO, FCUL, and CEAUL, Portugal
[2] Instituto Politécnico de Tomar, and CEAUL, Universidade de Lisboa, Portugal
[3] Instituto Politécnico de Coimbra, ISCA, and CEAUL, Universidade de Lisboa, Portugal

Abstract: In many areas of application, like for instance *statistical quality control*, *insurance* and *finance*, a typical requirement is to estimate a *high quantile*, i.e., the *Value at Risk* at a level p, high enough, so that the chance of an exceedance of that value is equal to p, small. In this paper we provide an empirical data analysis of log-returns associated to a set of financial data, through the use of reduced-bias tail index and associated high quantile estimators. These tail index estimators depend on two second order parameters, and in order to achieve a reduction in bias without any inflation of the asymptotic variance, the second order parameters in the bias are both estimated at a level of a higher order than the one used for the estimation of the tail index. A percentile method for quantile estimation and a heuristic adaptive choice of the threshold for reduced-bias estimators are considered, and their finite sample properties are studied via small-scale Monte Carlo simulations.

Keywords and phrases: Heavy tails, high quantiles, value at risk, semi-parametric estimation, percentile estimation, statistics of extremes

14.1 Introduction

In risk management it is crucial to evaluate adequately the risk of a big loss that occurs very rarely. The risk is generally expressed as the *Value at Risk* (VaR_p), i.e., a *high quantile* $\chi_{1-p} := F^{\leftarrow}(1-p)$ of a probability distribution function (d.f.) F, with $F^{\leftarrow}(y) := \inf\{x : F(x) \geq y\}$, the generalized inverse function of F. Let us denote $U(t)$ the inverse function of $1/(1-F)$. Then, for small p, we want to estimate the parameter

$$VaR_p = U\left(1/p\right), \quad p = p_n \to 0, \quad n\, p_n \leq 1.$$

Usually, we have in fact $n\, p_n < 1$, i.e., we want to extrapolate beyond the sample. Since we are dealing with a small probability, we may confine ourselves to modeling the tail. Moreover, since in financial applications we find generally heavy tails, we shall assume that the d.f. underlying the data satisfies, for some positive constant C,

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$$1 - F(x) \ \sim \ (x/C)^{-1/\gamma}, \quad \text{as } x \to \infty, \quad \text{with } \gamma > 0. \tag{14.1}$$

Weissman et al. (1978) proposed the following semi-parametric estimator of a high quantile (i.e., the Value-at-Risk):

$$Q_{\hat{\gamma}}^{(p)}(k) := X_{n-k+1:n} \left(k/(np)\right)^{\hat{\gamma}}, \tag{14.2}$$

where $X_{n-k+1:n}$ is the k-th top order statistic (o.s.), $\hat{\gamma}$ any consistent estimator for γ and Q stands for the quantile function. Further details on semi-parametric estimation of extremely high quantiles for a general tail index $\gamma \in \Re$ may be found in de Haan and Rootzén (1993) and, more recently, in Ferreira et al. (2003) and Matthys and Beirlant (2003). Matthys et al. (2004), Gomes and Pestana (2007a), Gomes and Figueiredo (2006) and Beirlant et al. (2006), among others, dealt with reduced-bias quantile estimation. Interesting references on parametric quantile estimation, also used in this paper, are Castillo and Hadi (1994, 1995). As usual in semi-parametric estimation of parameters of extreme events, we need to work with an *intermediate* sequence of integers, i.e., with

$$k \in [1, n): \ k = k_n \to \infty \quad \text{and} \quad k = o(n) \quad \text{as } n \to \infty. \tag{14.3}$$

For heavy tails, the classical semi-parametric tail index estimator, usually the one which is used in (14.2) for a semi-parametric quantile estimation, is the Hill estimator $\hat{\gamma} = \hat{\gamma}(k) =: H(k)$ (Hill, 1975), with the functional expression,

$$H(k) := \frac{1}{k} \sum_{i=1}^{k} U_i, \quad U_i := i \left(\ln X_{n-i+1:n} - \ln X_{n-i:n}\right), \ 1 \le i \le k. \tag{14.4}$$

If we insert in (14.2) the Hill estimator, $H(k)$, we get the so-called classical quantile estimator, $Q_{H}^{(p)}(k)$. In order to be able to study the asymptotic non-degenerate behavior of $Q_{H}^{(p)}(k)$, as well as of alternative VaR_p-estimators, it is useful to impose a second order expansion on the tail function $1 - F$ or on the quantile function U. We shall assume that we are working in Hall-Welsh class of models (Hall and Welsh, 1985), where, with $C, \ \gamma > 0$, $\rho < 0$ and β non-zero,

$$U(t) = C t^{\gamma} \left(1 + \gamma \ \beta \ t^{\rho}/\rho + o\left(t^{\rho}\right)\right), \quad \text{as } t \to \infty. \tag{14.5}$$

We shall further use the notation

$$A(t) := \gamma \ \beta \ t^{\rho}, \quad \gamma > 0, \ \beta \neq 0, \ \rho < 0. \tag{14.6}$$

The class in (14.5) is a wide class of models that contains heavy-tailed parents like the Fréchet, the Generalized Pareto and the Student's t.

From the results of de de Haan and Peng (1998), we may say that in Hall-Welsh class of models in (14.5) and for *intermediate* k,

$$H(k) - \gamma \ \stackrel{d}{=} \ \gamma \ P_k/\sqrt{k} + A(n/k)(1 + o_p(1))/(1 - \rho), \tag{14.7}$$

with $A(\cdot)$ the function in (14.6) and P_k an asymptotically standard normal r.v.

Regarding semi-parametric quantile estimation: under condition (14.5), the asymptotic behavior of $Q_{H}^{(p)}(k)$ is also well-known:

$$\sqrt{k}\left(Q_{_H}^{(p)}(k)/\,VaR_p - 1\right)/\ln(k/(np)) \xrightarrow[n\to\infty]{d} Normal\left(\lambda/(1-\rho),\ \gamma^2\right),$$

provided the sequence $k = k_n$ is intermediate, $\ln(k/(np)) = o(\sqrt{k})$ and $\lim_{n\to\infty}\sqrt{k}\ A(n/k) = \lambda \in \Re$, finite, with $A(\cdot)$ the function in (14.6).

On the basis of the results in Gomes and Figueiredo (2006), Gomes and Pestana (2007a) and Beirlant et al. (2006), we here proceed to the use in (14.2) of specific reduced-bias tail index estimators. Those tail index estimators and associated quantile estimators are described in Section 14.3, after a brief review, in Section 14.2, of a possible methodology to build asymptotic confidence intervals (CI's) for the tail index and the VaR on the basis of classical semi-parametric estimators. Section 14.4 is dedicated to the description, in an algorithmic way, of procedures dedicated to the semi-parametric estimation of the second order parameters (β, ρ), of the tail index γ and of an extreme quantile or VaR. In Section 14.5, we perform a small-scale Monte Carlo simulation to illustrate the performance of the percentile method, devised in a parametric set-up, and to present some simulated properties of the heuristic adaptive choice considered for the tail estimation through reduced-bias estimators. Finally, in Section 14.6, we provide an empirical data analysis of log-returns associated to the Euro-Great Britain Pound (EGBP) daily exchange rates, collected from January 4, 1999, until November 17, 2005, representative of other log-returns data analysed in Gomes and Pestana (2007a).

14.2 Asymptotic CI's for the Tail Index and the VaR

Let $a_k := 1.96/\sqrt{k} + \beta(n/k)^\rho/(1-\rho)$ and $b_k := 1.96/\sqrt{k} - \beta(n/k)^\rho/(1-\rho)$. Since from (14.7), together with the definition of $A(t)$ in (14.6), we may guarantee that $\sqrt{k}\,\{H(k)/\gamma - 1 - \beta(n/k)^\rho/(1-\rho)\} \approx Normal(0,1)$, provided that $\sqrt{k}\ (n/k)^\rho \to \lambda$, finite, we may get approximate 95% CI's for γ, given by

$$\left(H(k)/(1+a_k),\ H(k)/(1-b_k)\right) =: \left(LCL_{_H}(k),\ UCL_{_H}(k)\right). \tag{14.8}$$

If $\lambda = 0$, we may replace in (14.8) the bias summand $\beta(n/k)^\rho/(1-\rho)$ by 0. Moreover, for models in (14.5) the optimal k-value for the tail index estimation through the Hill estimator, in (14.4), is well approximated by

$$k_0^H \equiv k_0^H(n;\beta,\rho) := \arg\min_k \left\{\frac{1}{k} + \frac{\beta^2(n/k)^{2\rho}}{(1-\rho)^2}\right\} = \left(\frac{(1-\rho)n^{-\rho}}{\beta\ \sqrt{-2\rho}}\right)^{2/(1-2\rho)}, \tag{14.9}$$

and $\sqrt{k_0^H}\left(n/k_0^H\right)^\rho \to (1-\rho)/\left(\beta\sqrt{-2\rho}\right)$. If we use $H(k_0^H)$ to build a CI for γ, we may thus replace in (14.8) the bias summand $\beta(n/k)^\rho/(1-\rho)$ by $1/\sqrt{-2\rho k}$.

Similarly to what has been done for the Hill estimator, we may estimate, now numerically, the "optimal" threshold for the VaR estimation through $Q_{_H}$,

$$k_0^{Q_H} \equiv k_0^{Q_H}(n,p;\beta,\rho) := \arg\min_k \left\{\ln^2\left(\frac{k}{np}\right)\left(\frac{1}{k} + \frac{\beta^2(n/k)^{2\rho}}{(1-\rho)^2}\right)\right\}. \tag{14.10}$$

We may also find approximate CI's for VaR_p on the basis of $Q_{_H}^{(p)}(k)$ and for any level k such that $\sqrt{k}\ A(n/k) \to \lambda$, finite. A 95% CI, dependent on γ, is given by $\left(Q_{_H}(k)\,(k/(np))^{-\gamma a_k}\,,\ Q_{_H}(k)\,(k/(np))^{\gamma b_k}\,\right)$. In order to have a guarantee of a coverage probability at least equal to 95%, and with $LCL_{_H}(k)$ and $UCL_{_H}(k)$ given in (14.8), we shall work with

$$LCL_{Q_{_H}}(k) = Q_{_H}(k)\ \min\left((k/(np))^{-a_k LCL_{_H}(k)}\,,(k/(np))^{-a_k UCL_{_H}(k)}\right), \tag{14.11}$$

$$UCL_{Q_{_H}}(k) = Q_{_H}(k)\ \max\left((k/(np))^{b_k LCL_{_H}(k)}\,,(k/(np))^{b_k UCL_{_H}(k)}\right). \tag{14.12}$$

14.3 Reduced Bias Tail Index and Quantile Estimators

14.3.1 Tail index estimation

We shall work here with the reduced-bias tail index estimators in Caeiro et al. (2004) and Gomes et al. (2005). The estimator in Caeiro et al. (2004), also used in Gomes and Pestana (2007a) for quantile estimation, is given by

$$\overline{H}_{\hat\beta,\hat\rho}(k) := H(k)\left(1-\hat\beta\,(n/k)^{\hat\rho}\,/(1-\hat\rho)\right), \tag{14.13}$$

where $(\hat\beta,\hat\rho)$ is an adequate consistent estimator of (β,ρ), with both $\hat\beta$ and $\hat\rho$ based on a number of top o.s. k_1 of an order larger than k, the number of top o.s. used for the tail index estimation. Note that the estimator in (14.13) is a bias-corrected Hill estimator: the dominant component of the bias of Hill's estimator, provided in (14.7) and given by $\gamma\ \beta(n/k)^{\rho}/(1-\rho)$, is estimated through $H(k)\ \hat\beta\ (n/k)^{\hat\rho}/(1-\hat\rho)$ and directly removed from the Hill estimator in (14.4).

Apart from the class of estimators in (14.13), we shall also consider the reduced-bias class of estimators in Gomes et al. (2005). Such a class is of the same type as the one in (14.13), but it has been inspired in the tail index estimator provided in Gomes and Martins (2002), i.e., it is based on an approximate maximum likelihood approach associated to the scaled log-spacings U_i in (14.4). With the same notation as before, we shall work with the tail index estimator

$$ML_{\hat\beta,\hat\rho}(k) := H(k) - \hat\beta\,(n/k)^{\hat\rho}\,D_k\,(\hat\rho)\,,\ D_k(\alpha) := \frac{1}{k}\sum_{i=1}^{k}(i/k)^{-\alpha}\,U_i. \tag{14.14}$$

This is another example of a bias-corrected Hill estimator, where we are using $D_k(\hat\rho)$ as an estimator of $\gamma/(1-\rho)$. We may state the following:

Proposition 1 (Caeiro et al. (2004); Gomes et al. (2005)). *For models in* (14.5), *let us assume that* (14.3) *holds and that, with* $A(t)$ *given in* (14.6), $\sqrt{k}\ A(n/k) \to \lambda$, *finite and non necessarily null, as* $n \to \infty$. *Then, with* T *denoting either* $\overline{H}$ *in* (14.13) *or* ML *in* (14.14),

$$\sqrt{k}\,(T_{\beta,\rho}(k)-\gamma) \xrightarrow[n\to\infty]{d} Normal\left(0,\ \gamma^2\right).$$

This same limiting behaviour holds if we replace $T_{\beta,\rho}$ by $T_{\hat{\beta},\hat{\rho}}$, provided that we consider a ρ-estimator $\hat{\rho}$, such that $\hat{\rho}-\rho = o_p(1/\ln n)$, and we choose $\hat{\beta}$ consistent for the estimation of β. More specifically, and with V_k^T an asymptotically standard normal r.v., we may write

$$T_{\hat{\beta},\hat{\rho}}(k) \stackrel{d}{=} \gamma + \gamma\ V_k^T/\sqrt{k} + o_p(A(n/k)).$$

Remark 1. Contrarily to what happens in Drees' class of functionals (Drees, 1998), where the minimal asymptotic variance of a reduced-bias tail index estimator is given by $(\gamma(1-\rho)/\rho)^2$, here we have been able to obtain a reduced-bias tail index estimator with an asymptotic variance equal to γ^2, the asymptotic variance of Hill's estimator, which is indeed the maximum likelihood estimator of γ for the strict Pareto model $F(x;\gamma,C) = 1-(x/C)^{-1/\gamma}$, $x \geq C$, $\gamma > 0$.

14.3.2 Asymptotic CI's for γ based on second order reduced-bias tail index estimation

On the basis of the statistics $\overline{H}$ and ML in (14.13) and (14.14), respectively, with $a_k^* = 1+1.96/\sqrt{k}$, $b_k^* = 1-1.96/\sqrt{k}$, for levels k such that $\sqrt{k}\ (n/k)^\rho \to \lambda$, finite, and again with T denoting any of the estimators in either (14.13) or (14.14), Proposition 1 enables us to get the following 95% approximate CI for γ,

$$(LCL_{_T}(k), UCL_{_T}(k)) = (T(k)/a_k^*,\ T(k)/b_k^*)\,. \tag{14.15}$$

14.3.3 Adaptive choice of the level for reduced-bias estimators

Here, we have decided to use the heuristic adaptive choice of k suggested in Gomes and Pestana (2007a). Up to now, we do not have simple techniques to estimate the optimal threshold of second order reduced-bias estimators. If we plot the 95% approximate confidence region in (14.8) as a function of k, the Hill estimate is sooner or later going to cross this region. We have thus decided to use such a k-value for the tail index estimation through the second order reduced-bias tail index estimator $\overline{H}(k)$ and $ML(k)$ in (14.13) and (14.14), respectively, as well as for the associated *VaR* estimation. Such a crossing level is solution of the equation $|\beta|\ (n/k)^\rho/(1-\rho) = 1.96/\sqrt{k}$, i.e., we get

$$k_{01} \equiv k_{01}(n;\beta,\rho) = \left(1.96(1-\rho)n^{-\rho}/|\beta|\right)^{2/(1-2\rho)}. \tag{14.16}$$

For levels of this type, $\sqrt{k}\ A(n/k) \to \lambda$, finite, i.e., they are not yet optimal for the tail index estimation through second order reduced-bias tail index estimators. However, with a tail index estimator of the type of the ones in (14.13) and (14.14) we are safe for all k, and the level in (14.16) has revealed to provide an interesting adaptive choice of the threshold.

14.3.4 Extreme quantile or *VaR* estimation

We shall now consider the alternative VaR_p estimators $Q_{\overline{H}}^{(p)}$ and $Q_{ML}^{(p)}$, with $Q_{\hat{\gamma}}^{(p)}$, $\overline{H}$ and ML given in (14.2), (14.13) and (14.14), respectively. Under the same conditions as before, i.e., under conditions (14.3), (14.5) and provided that $\ln(k/(np)) = o(\sqrt{k})$ and $\lim_{n\to\infty} \sqrt{k}\ A(n/k) = \lambda$, finite, if we work with any of the reduced-bias tail index estimators $\overline{H}$ or ML, generally denoted T, we get

$$\sqrt{k}\left(Q_{T}^{(p)}(k)/\,VaR_p - 1\right)/\ln(k/(np)) \xrightarrow[n\to\infty]{d} Normal\left(0,\ \gamma^2\right),$$

even when $\lambda \neq 0$. Note that with a "classical" reduced-bias tail index estimator, i.e., a tail index estimator of the type of the ones used for quantile estimation in Gomes and Figueiredo (2006), we were able to also get a null bias, but at expenses of a higher asymptotic variance.

14.3.5 Asymptotic CI's for VaR_p on the basis of reduced-bias estimators

Whenever working with Q_{T}, with T denoting either $\overline{H}$ in (14.13) or ML in (14.14), levels k such that $\sqrt{k}\ A(n/k) \to \lambda$, finite, and with UCL_{T} given in (14.15), we shall use the CI,

$$\left(LCL_{Q_{T}}, UCL_{Q_{T}}\right) = Q_{T} \times \left((k/(np))^{-\frac{1.96\ UCL_{T}}{\sqrt{k}}},\ (k/(np))^{\frac{1.96\ UCL_{T}}{\sqrt{k}}}\right). \qquad (14.17)$$

14.4 An Algorithm for Semi-Parametric Tail Estimation

We propose the following algorithm:

1. Given a sample $(X_1, X_2, \cdots, X_n)$, and for $k = 1, 2, \cdots, n_0$, with n_0 the number of positive values in the sample, plot, for $\tau = 0$ and $\tau = 1$, the estimates

$$\hat{\rho}_\tau(k) := \min\left\{0,\ \left(3(T_n^{(\tau)}(k) - 1\right)\right) / \left(T_n^{(\tau)}(k) - 3\right)\right\}, \qquad (14.18)$$

where, with $M_n^{(j)}(k) := \frac{1}{k}\sum_{i=1}^{k}\left\{\ln X_{n-i+1:n} - \ln X_{n-k:n}\right\}^j, \quad j = 1, 2, 3$, and the notation $a^{b\tau} = b \ln a$ whenever $\tau = 0$,

$$T_n^{(\tau)}(k) := \frac{\left(M_n^{(1)}(k)\right)^{\tau} - \left(M_n^{(2)}(k)/2\right)^{\tau/2}}{\left(M_n^{(2)}(k)/2\right)^{\tau/2} - \left(M_n^{(3)}(k)/6\right)^{\tau/3}}, \quad \tau \in \Re.$$

2. Consider $\{\hat{\rho}_\tau(k)\}_{k\in\mathcal{K}}$, for large k, say $k \in \mathcal{K} = \left(\left[n_0^{0.995}\right], \left[n_0^{0.999}\right]\right)$, and compute their median, denoted χ_τ. Next choose the *tuning parameter*

$$\tau^* := \arg\min_{\tau} \sum_{k\in\mathcal{K}} \left(\hat{\rho}_\tau(k) - \chi_\tau\right)^2.$$

3. Work then with $(\hat{\rho}_{\tau^*}, \hat{\beta}_{\tau^*}) := (\hat{\rho}_{\tau^*}(k_1), \hat{\beta}_{\hat{\rho}_{\tau^*}}(k_1))$, where,
$$k_1 = \left[n_0^{0.995}\right], \tag{14.19}$$
and
$$\hat{\beta}_{\hat{\rho}}(k) := \left(\frac{k}{n}\right)^{\hat{\rho}} \frac{d_k(\hat{\rho})\ D_k(0) - D_k(\hat{\rho})}{d_k(\hat{\rho})\ D_k(\hat{\rho}) - D_k(2\hat{\rho})}, \quad d_k(\alpha) := \frac{1}{k}\sum_{i=1}^{k}(i/k)^{-\alpha}, \tag{14.20}$$
being $D_k(\alpha)$ and $\hat{\rho}_\tau(k)$ given in (14.14) and (14.18), respectively.
4. Plot the classical Hill estimates $H(k)$, given in (14.4), and adaptively consider $H(\hat{k}_0^H)$, $\hat{k}_0^H = k_0^H(n; \hat{\beta}_{\tau^*}, \hat{\rho}_{\tau^*})$, $k_0^H(n; \beta, \rho)$ given in (14.9), together with the 95% approximate CI, $(LCL_{_H}(\hat{k}_0^H),\ UCL_{_H}(\hat{k}_0^H))$, given in (14.8) for a general k.
5. Plot also the reduced-bias tail index estimates $\overline{H} \equiv \overline{H}_{\tau^*}(k)$ and $ML \equiv ML_{\tau^*}(k)$, associated to the estimates $(\hat{\rho}_{\tau^*},\ \hat{\beta}_{\tau^*})$ obtained in step 3. Adaptively consider $\overline{H}(\hat{k}_{01})$, $ML(\hat{k}_{01})$, $\hat{k}_{01} = k_{01}(n; \hat{\beta}_{\tau^*}, \hat{\rho}_{\tau^*})$, $k_{01}(n; \beta, \rho)$ given in (14.16), and with T standing either for $\overline{H}_{\tau^*}$ or ML_{τ^*}, obtain the 95% CI $(LCL_{_T}(\hat{k}_{01}),\ UCL_{_T}(\hat{k}_{01}))$, provided in (14.15) for a general k.
6. Choose the tail index estimate providing the smallest 95% confidence size. Let us denote Γ the associated estimator (either H, $\overline{H}$ or ML).
7. Plot the classical VaR estimates $Q_{_H}(k)$, with $Q_{\hat{\gamma}}(k)$ and H given in (14.2) and (14.4), respectively, and adaptively consider $Q_{_H}(\hat{k}_0^{Q_{_H}})$, where $\hat{k}_0^{Q_{_H}} = k_0^{Q_{_H}}(n, p; \hat{\beta}_{\tau^*}, \hat{\rho}_{\tau^*})$, with $k_0^{Q_{_H}}(n, p; \beta, \rho)$ given in (14.10). Consider also the approximate CI, $(LCL_{Q_{_H}}(\hat{k}_0^{Q_{_H}}), UCL_{Q_{_H}}(\hat{k}_0^{Q_{_H}}))$, given in (14.11) and in (14.12) for a general k;
8. If the estimator Γ chosen in step 6. is one of the reduced-bias estimators, plot $Q_\Gamma^{(p)}(k)$ and adaptively consider $Q_\Gamma^{(p)}(\hat{k}_{01})$, $\hat{k}_{01} = k_{01}(n; \hat{\beta}_{\tau^*}, \hat{\rho}_{\tau^*})$, with $k_{01}(n; \beta, \rho)$ given in (14.16), together with the CI in (14.17) at $k = \hat{k}_{01}$.

Remark 2. For asymptotic and finite sample details on the estimators of ρ in (14.18), see Fraga Alves et al. (2003). The estimator of β in (14.20) has been introduced in Gomes and Martins (2002), where conditions that enable its asymptotic normality have been set, whenever ρ is estimated at a level k_1 of a larger order than the level k used for the estimation of β. Details on the asymptotic distribution of $\hat{\beta}_{\hat{\rho}(k)}(k)$ may be found in Gomes et al. (2004).

Remark 3. Steps 1 and 2 of the algorithm lead in almost all situations to the *tuning parameter* $\tau^* = 0$ whenever $|\rho| \le 1$ and $\tau^* = 1$, otherwise. Such an educated guess usually provides better results than a possibly "noisy" estimation of τ, and it is highly recommended in practice. For details on this and similar algorithms for the ρ-estimation, see Gomes and Pestana (2007b).

14.5 The Use of a Parametric Quantile Method in Tail Index and Quantile Estimation

Castillo and Hadi (1994, 1995) introduced a percentile (P) method for the estimation of parameters and quantiles of the Extreme-Value (EV) d.f., given by $EV_\gamma(x) :=$

$\exp(-(1+\gamma x)^{-1/\gamma})$, $1+\gamma x > 0$, $\gamma \in \Re$. Whenever $\gamma > 0$, i.e., whenever we are dealing with heavy-tailed models, the EV_γ parent is usually called Fréchet. Here, we shall work with a standard Fréchet$_\gamma$ d.f., $F(x) = \exp\big(-x^{-1/\gamma}\big)$, $x \geq 0$. Apart from the Fréchet, we shall work with Generalized Pareto GP parents, with d.f. $F(x) = 1-(1+\gamma x)^{-1/\gamma}$, $x \geq 0$.

The estimation procedure considered by Castillo and Hadi consists of a two-stage P-method. In a first stage we obtain initial estimates $\hat{\gamma}_{ijr}$ of γ, applying the P-method, through the use of the o.s., $x_{i:n}, x_{j:n}$ and $x_{r:n}$, the quotient $(x_{j:n}-x_{r:n})/(x_{i:n}-x_{j:n})$ and the bisection method. We fix the levels $i=1$ and $r=n$ and, in a second stage, compute the median of the $(n-2)$-vector of estimates $\hat{\gamma}_{1jn}$, $j=2,\cdots,n-1$. The final estimate is denoted $\hat{\gamma}_{_P}$. The estimate of the quantile of probability $1-p$ is then $\hat{\chi}_P^{(p)} := (-\ln(1-p))^{-\hat{\gamma}_P}$ for Fréchet models and $\hat{\chi}_P^{(p)} := (p^{-\hat{\gamma}_P}-1)/\hat{\gamma}_{_P}$ for GP_γ models.

We shall proceed here to a small-scale Monte Carlo comparison of the tail index P-estimators with Hill's estimator computed at the estimated value of k_0^H in (14.9), as well as with the reduced-bias estimators $\overline{H}$ and ML, in (14.13) and (14.14), respectively, both computed at the estimated value of k_{01} in (14.16). The simulation results were obtained on the basis of 1000 runs, from the above mentioned parents with $\gamma = \{0.2, 0.5, 1 \text{ and } 2\}$ and samples of size $n = 1000$. The estimates obtained are summarized in table 14.1. The values in brackets are the simulated mean squared errors (MSE) for each estimator and each value of γ. The underlined values are the ones providing minimum squared bias, that correspond in all cases to minimum MSE.

The ln-VaR_p-estimates presented in table 14.2 have been obtained again on the basis of 1000 runs, for the same parents as before, for sample size $n = 1000$ and $p = 0.001$. Once again the values in brackets are the simulated MSE's for each estimator and each value of γ and the underlined values are the ones leading to minimum bias, again correspondent to minimum MSE.

Tables 14.1 and 14.2 clearly show, overall, that the P-estimators of tail index and high quantiles are, for Fréchet parents, better than any of the adaptive semi-parametric estimators. Indeed, apart from quantile estimation for $\gamma = 2$, they exhibit simultaneously minimum bias and minimum MSE. For other parents, things may work

Table 14.1. Simulated mean values (mean squared errors) of the γ-estimators under comparison

γ	0.2	0.5	1.0	2.0
Fréchet$_\gamma$ parent: ($\rho = -1$)				
$\hat{\gamma}_{_P}$	<u>0.2003</u> (1.3E-7)	<u>0.5000</u> (7.2E-8)	<u>0.9987</u> (1.8E-6)	<u>1.9934</u> (4.3E-5)
$H(\hat{k}_0^H)$	0.2228 (5.2E-4)	0.6282 (0.0164)	1.1420 (0.0203)	2.2210 (0.0488)
$\overline{H}(\hat{k}_{01})$	0.2103 (1.1E-4)	0.5779 (0.0061)	1.0048 (2.3E-5)	2.0689 (0.0047)
$ML(\hat{k}_{01})$	0.2101 (1.0E-4)	0.5763 (0.0058)	1.0077 (6.0E-5)	2.0528 (0.0028)
GP$_\gamma$ parent: ($\rho = -\gamma$)				
$\hat{\gamma}_{_P}$	<u>0.3748</u> (0.0313)	0.6120 (0.0129)	1.0418 (0.0018)	1.9488 (0.0027)
$H(\hat{k}_0^H)$	0.4391 (0.0572)	0.5638 (0.0041	1.0773 (0.0060)	2.3532 (0.1247)
$\overline{H}(\hat{k}_{01})$	0.4031 (0.0413)	0.5531 (0.0028)	<u>1.0021</u> (4.5E-6)	1.9496 (0.0025)
$ML(\hat{k}_{01})$	0.3987 (0.0395)	<u>0.5484</u> (0.0023)	0.9932 (5.6E-5)	<u>1.9600</u> (0.0016)

Table 14.2. Simulated mean values (mean squared errors) for the different estimators of $\ln VaR_p$ under comparison, $p = 0.001$

γ	0.2	0.5	1.0	2.0
Fréchet$_\gamma$ parent: ($\rho = -1$)				
ln-VaR_p	1.3815	3.4536	6.9073	13.8145
$\ln \hat{\chi}_P^{(p)}$	1.3835 (6.4E-6)	3.4539 (3.5E-6)	6.8986 (8.6E-5)	13.7691 (0.0021)
$\ln Q_H(\hat{k}_0^{Q_H})$	1.5364 (0.0240)	4.0833 (0.3965)	7.5201 (0.3756)	14.8708 (1.1157)
$\ln Q_{\overline{H}}(\hat{k}_{01})$	1.4247 (0.0019)	3.7841 (0.1092)	6.7719 (0.0183)	13.8907 (0.0058)
$\ln Q_{ML}(\hat{k}_{01})$	1.4237 (0.0018)	3.7744 (0.1029)	6.7888 (0.0140)	13.8004 (2.0E-4)
GP$_\gamma$ parent: ($\rho = -\gamma$)				
ln-VaR_p	2.7017	4.1149	6.9068	13.1224
$\ln \hat{\chi}_P^{(p)}$	3.4934 (0.6449)	4.7045 (0.3581)	7.1547 (0.0636)	12.7949 (0.1097)
$\ln Q_H(\hat{k}_0^{Q_H})$	2.8574 (0.0242)	4.7683 (0.4270)	7.1303 (0.0500)	14.6295 (2.2713)
$\ln Q_{\overline{H}}(\hat{k}_{01})$	2.7728 (0.0050)	4.0123 (0.0105)	6.7724 (0.0180)	12.8383 (0.0807)
$\ln Q_{ML}(\hat{k}_{01})$	2.7503 (0.0024)	4.0156 (0.0099)	6.7264 (0.0325)	12.8971 (0.0507)

differently. For instance, for GP parents, the reduced-bias estimators have an overall better performance. Also, we cannot forget that we are comparing two different approaches on quantile and tail index estimation, and we are not being totally fair to the semi-parametric approach. Indeed in a parametric context, like the one in this simulation study, we would expect to observe a even higher performance of the P-estimators, specifically devised for a specific model. Note further that, both in terms of minimum squared bias and minimum MSE, the choice of either $\overline{H}(\hat{k}_{01})$ or $ML(\hat{k}_{01})$ has always led to a better performance than the one achieved by $H(\hat{k}_0^H)$. This is thus a point in favor of the reduced-bias estimators here proposed.

14.6 Financial Data Analysis

14.6.1 Second order parameter estimation

The number of positive log-returns of the $EGBP$ data is $n_0 = 835$. The sample paths of the ρ-estimates associated to $\tau = 0$ and $\tau = 1$ lead us to choose the estimate associated to $\tau = 0$, on the basis of any stability criterion for large k, like the one in step 2 of the algorithm. The estimates obtained are $\left(\hat{\rho}_0, \hat{\beta}_0\right) = (-0.686, 1.047)$. In figure 14.1, for the $EGBP$ data, we picture the sample paths of the estimators of the second order parameters.

14.6.2 Tail index and VaR_p estimation

The sample paths of the classical Hill estimator H in (14.4), the second order reduced-bias tail index estimators $\overline{H}_0 = \overline{H}_{\hat{\beta}_0,\hat{\rho}_0}$ and $ML_0 = ML_{\hat{\beta}_0,\hat{\rho}_0}$, provided in (14.13) and (14.14), respectively, as well as the associated Var_p estimators, for $p = 0.001$, are pictured in figure 14.2.

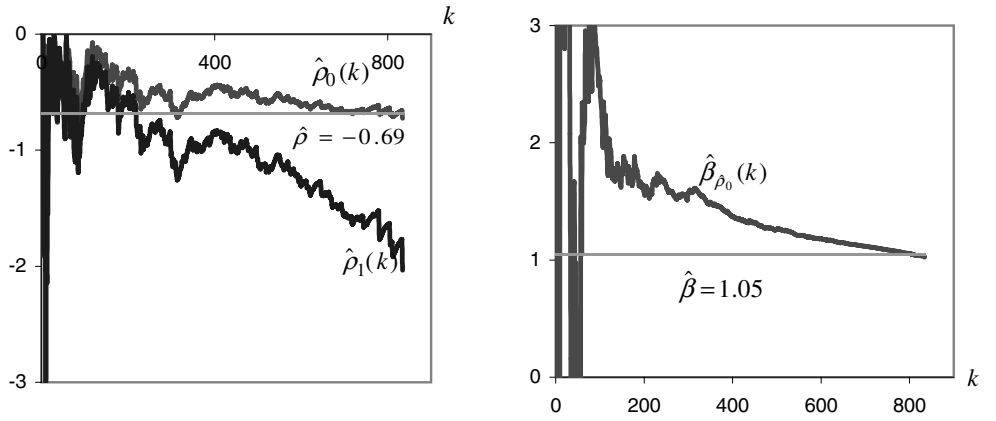

Figure 14.1. Estimates of ρ, through $\hat{\rho}_\tau(k)$ in (14.18), $\tau = 0$ and 1 (*left*) and of β, through $\hat{\beta}_{\hat{\rho}_0}(k)$ in (14.20) (*right*), for the positive log-returns on EGBP data

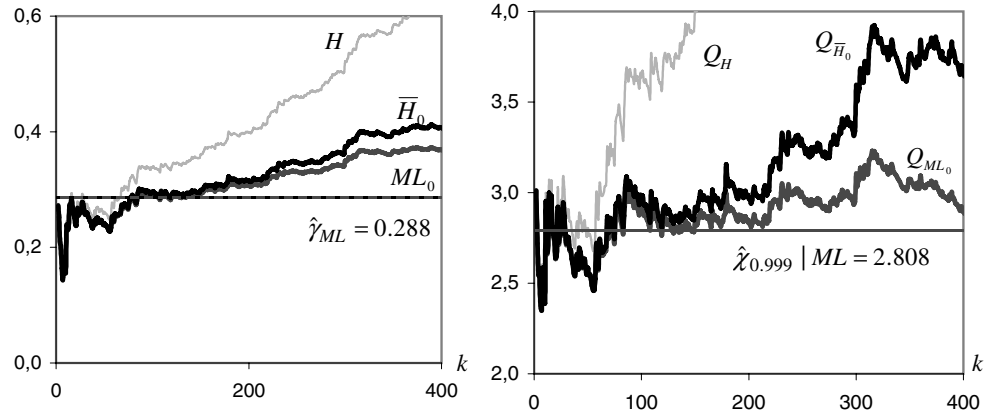

Figure 14.2. Estimates provided through H, $\overline{H}_0$ and ML_0 in (14.4), (14.13) and (14.14) (*left*) and the associated ln-VaR_p estimates, for the positive log-returns on EGBP data and $p = 0.001$

From a theoretical point a view the chosen estimate in step 6 of the algorithm should be $\overline{H}_0(\hat{k}_{01})$ or $ML_0(\hat{k}_{01})$. Indeed, for this data set, we have been led to the choice $ML_0(\hat{k}_{01})$. Relevant characteristics, related to both tail index and quantile estimates are presented in table 14.3.

14.6.3 Graphical illustration of the adaptive threshold choice for tail index and VaR estimation

In figure 14.3 (*left*) we illustrate graphically steps 4-6 in the algorithm, for the data set under analysis. Figure 14.3 (*right*) exhibits steps 7-8, in the algorithm. Again, the $VaR_{0.001}$ estimate is denoted $\hat{\chi}_{0.999}$ and is associated to ML_0.

Table 14.3. Estimates of the different parameters characterising the tail behaviour of the data set

$(\hat{k}_0^H, \hat{k}_{01}) = (65, 130)$	$H(\hat{k}_0^H)) = 0.286$	$\overline{H}_0(\hat{k}_{01}) = 0.291$	$ML_0(\hat{k}_{01}) = \underline{0.288}$
$(LCL_\bullet,\ UCL_\bullet)$	(0.211,0.332)	(0.249, 0.352)	(0.246, 0.346)
$\hat{k}_0^{Q_H} = 47$	$Q_H(\hat{k}_0^{Q_H}) = 2.803$		$Q_{ML}(\hat{k}_{01}) = 2.808$
$(LCL_{Q_\bullet}, UCL_{Q_\bullet})$	(1.726, 3.729)		(2.077, 3.796)

14.6.4 The use of a percentile method in quantile estimation

The direct application of the P-method in Section 14.5 to the data set has not been successful, in the sense that we could not adequately fit to the data a model with a closed form for the quantile function. The better fit has been provided by Student-t models, and for such models the P-method is computationally expensive and not at all promising.

We have here used a mixed technique based upon the percentile P-method in Castillo and Hadi, but estimating γ only on the basis of high quantiles of probability $1 - p = 0.9, 0.95, 0.975, 0.990$ and 0.995. On the basis of the approximation in (14.1), or equivalently the approximation $U(t) = Ct^\gamma$, the use of any pair of p-values, (p_1, p_2), in the above mentioned set, enables us to get γ-estimates, $\hat{\gamma}_P^\bullet := -\ln\left(X_{[n(1-p_1)]+1:n}/X_{[n(1-p_2)]+1:n}\right)/\ln\left(p_1/p_2\right)$. The median of these estimates, denoted $\hat{\gamma}_P^*$, was then considered as the overall estimate of γ provided by this technique. The estimation of C through the percentile method led us to very large estimates of C, based upon estimates $\hat{C}_P := X_{[n(1-p_1)]+1:n}(p_1)^{\hat{\gamma}_P^*}$, very large high quantile estimates, and was consequently discarded. We have then used a least squares technique based on the points $\left(q_i = -\ln(1 - i/(n+1)), (\ln X_{n-i+1:n} - \ln C)/\hat{\gamma}_P^*\right)$, for large i, getting an estimate $\hat{C}_{LS}$. A high quantile of probability $1 - p$ is then estimated through $\hat{\chi}_P^* = \hat{C}_{LS}\ p^{-\hat{\gamma}_P^*}$. The estimates of γ, C and $\chi_{0.999}$ provided by this method are now summarised, together with the estimates obtained through the Hill estimator H and the ML_0 estimator, $\left(\hat{\gamma}_H, \hat{\gamma}_{ML_0}, \hat{\gamma}_P^*, \hat{C}_{LS}, \hat{\chi}_H, \hat{\chi}_{ML_0}, \hat{\chi}_P^*\right) =$

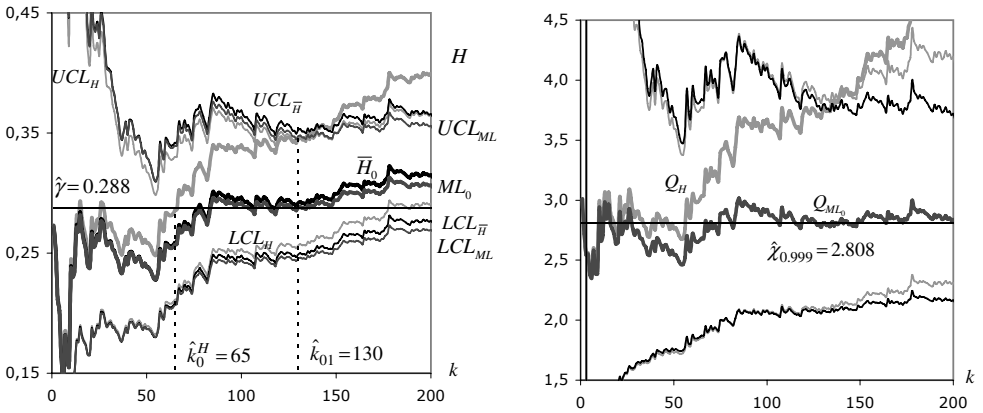

Figure 14.3. Confidence intervals for γ (*left*) and VaR_p, $p = 0.001$ (*right*) (EGBP data)

$(0.30, 0.29, 0.32, 0.283, 2.80, 2.83, 2.60)$. From these results we see that, in this case, the percentile method seems to provide a slight overestimation of the tail index and underestimation of high quantiles. When we compare the methodologies in what regards the size of associated $CI's$, the method based on reduced-bias tail index estimation seems indeed to be, among the techniques considered in this paper, the one providing the best results.

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15

An Example of Real–Life Data Where the Hill Estimator is Correct

Rolf–Dieter Reiss and Ulf Cormann

Department of Mathematics, University of Siegen, Germany

Abstract: We assume that the normalized excesses over a fixed threshold are distributed according to a Pareto distribution with unknown shape and scale parameters. If the scale parameter is equal to one, then the famous Hill estimator is the maximum likelihood estimator and, therefore, the asymptotically optimal estimator for the shape parameter. Otherwise, the performance of the Hill estimator can be very bad. We present a real-life data set where is evidence that the 1–parameter modeling can be justified. Within the 2–parameter model, we apply the maximum likelihood estimator and modifications of an estimator proposed in Castillo and Hadi (1997).

Keywords and phrases: Exceedances, Hill estimator, modified Pickands estimators, Pareto models, plankton species data, heavy tails

15.1 Introduction

If the original data are distributed according to a random variable X with distribution function (df) F, then the exceedances over a threshold u are distributed according to the exceedance df

$$\begin{aligned} F^{[u]}(x) &= P(X \le x | X > u) \\ &= \frac{F(x) - F(u)}{1 - F(u)}, \quad x \ge u. \end{aligned}$$

Notice that $F^{[u]}$ is the truncation of F left of the threshold u.

The possible continuous, limiting dfs of the exceedance dfs $F^{[u]}$, as u goes to the right endpoint of the support of F, are the generalized Pareto dfs (GPDs) with real-valued shape parameter γ which is called the tail index. This is the mathematical justification for the replacement of the actual df $F^{[u]}$ by some GPD, where, in addition, location and/or scale parameters μ and σ must be added.

Despite the nice mathematical theory, one has to justify the use of GPDs in statistical analysis either by applying a goodness–of–fit test or by finding some empirical

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evidence for this choice of parametric dfs. In the next step, statistical inference for the actual dfs may be carried out within a parametric model of GPDs. The present article is focused on those GPDs that possess a heavy upper tail and, therefore, we merely deal with Pareto dfs with tail indices $\gamma > 0$. We refer to the books by Reiss and Thomas (1997) and Falk et al. (1994) for a practical and theoretically oriented introduction to exceedances and GPDs.

For estimating the heavy tailed Pareto dfs, theoretically oriented probabilitists and statisticians prefer the Hill estimator because of its simple structure, which facilitates the verification of mathematical results. In addition, this is the maximum likelihood estimator with respect to a restricted Pareto model, cf. (15.1) and (15.3). This makes the Hill estimator also attractive for practitioners. However, this can have serious consequences if the choice of the restricted Pareto model is unsuitable.

The article is organized as follows: in Section 15.2 we introduce the restricted and the full Pareto model for normalized excesses, and explain in Section 15.3 why the Hill estimator has such poor performance within the full Pareto model. In Section 15.4 we introduce certain scale–invariant estimators for the tail index $\gamma > 0$ and estimators of the scale parameter which are related to those in Pickands (1975) and Castillo and Hadi (1997). In Section 15.5 we analyze a data set that is exceptional in two directions: Firstly, the use of the Hill estimator can be justified and, secondly, an estimate $\hat{\gamma} > 0.5$ of the tail index is obtained which yields that the underlying df possesses very heavy tails. The article is concluded in Section 15.6 with some remarks about the performance of different modified Pickands estimators and computational aspects.

15.2 The Pareto Modeling

If the statistical inference for the upper tail of a distribution is based on the exceedances $x_i,\ i = 1, \ldots, k$, over a threshold $u > 0$, then one basic statistical model is that of Pareto dfs

$$H_\gamma(x/u) = 1 - (x/u)^{-1/\gamma}, \quad x \geq u, \tag{15.1}$$

where $\gamma > 0$ is called the tail index. By taking x_i/u in place of x_i one gets the statistical model of dfs

$$H_\gamma(x) = 1 - x^{-1/\gamma}, \quad x \geq 1.$$

Alternatively, one may consider the normalized excesses

$$y_i = (x_i - u)/u \tag{15.2}$$

which correspond to the dfs

$$F_\gamma(x) = 1 - (1 + x)^{-1/\gamma}, \quad x \geq 0. \tag{15.3}$$

One gets the full Pareto model for the normalized excesses y_i by adding a scale parameter $\sigma > 0$. This model consists of the dfs

$$F_{\gamma,\sigma}(x) = 1 - (1 + x/\sigma)^{-1/\gamma}, \quad x \geq 0. \tag{15.4}$$

We also note the pertaining quantile function

$$F^{-1}_{\gamma,\sigma}(q) = \sigma\left((1-q)^{-\gamma} - 1\right), \quad 0 < q < 1, \tag{15.5}$$

which will be used in Section 15.4 for the construction of modified Pickands estimators.

We remark that a continuous parametrization of the unified GPD family with real tail index γ is achieved by dfs of the form

$$W_\gamma(x) = 1 - (1+\gamma x)^{-1/\gamma} \quad \text{for} \quad \begin{cases} 0 < x, & \gamma > 0; \\ & \text{if} \\ 0 < x < 1/|\gamma|, & \gamma < 0. \end{cases} \tag{15.6}$$

where, in addition, $W_0(x) = \lim_{\gamma\to 0} W_\gamma(x)$ is the exponential df. For $\gamma > 0$ one again gets Pareto dfs, and for $\gamma < 0$ one has to deal with certain beta dfs.

The use of Pareto dfs in the form (15.4) can facilitate the construction of estimators as, e.g., in Castillo and Hadi (1997) and in the subsequent Section 15.4, or in Reiss and Thomas (1999) in conjunction with certain Bayesian estimators.

15.3 The Hill Estimator

An estimator for the tail index $\gamma > 0$ of Pareto dfs proposed by Hill (1975)—based on the exceedances x_i over a threshold u—plays an important role within the statistical extreme value theory. This estimator has the simple form

$$\gamma_H = \frac{1}{k}\sum_{i=1}^{k} \log\frac{x_i}{u}. \tag{15.7}$$

We will shortly explain the behavior of the Hill estimator within the enlarged model (15.4). The Hill estimator, expressed by the normalized excesses y_i in (15.2), is given by

$$\gamma_H = \frac{1}{k}\sum_{i=1}^{k} \log\frac{x_i}{u} = \frac{1}{k}\sum_{i=1}^{k} \log(1+y_i)$$

which is closely centered around the unknown tail index γ according to the excellent performance of the Hill estimator with respect to the models (15.1) and (15.3), respectively.

If a scale parameter $\sigma > 0$ is included as in (15.4), then one observes the data

$$z_i = \sigma y_i, \tag{15.8}$$

and the Hill estimator based on the z_i is of the form

$$\gamma_H = \frac{1}{k}\sum_{i=1}^{k} \log(1+z_i) = \frac{1}{k}\sum_{i=1}^{k} \log(1+\sigma y_i).$$

One realizes that the Hill estimator is not invariant under the scale parameter σ which entails that the performance can be poor if $\sigma \neq 1$. If $\sigma > 1$ ($\sigma < 1$) then one overestimates (underestimates) the tail index γ.

Thus, the Hill estimator is "correct" if the restricted Pareto model (15.3) is correct. If this is not the case, there is the possibility of carrying out the statistical inference with estimators tailored for the enlarged model (15.4) of Pareto dfs where a scale parameter is added.

For a further discussion of the poor performance of the Hill estimator we refer to Reiss and Thomas (1997), pages 117 and 149 in the 1st edition, pages 143–144 in the 2nd edition (the latter reference includes an illustration of simulated densities of the Hill estimator as presented by the first author at the Gothenburg meeting about Extremes—Risk and Safety in the year 1998), and to Fraga Alves (2001).

15.4 Modified Pickands Estimators

In view of the discussion in Section 15.3 we define estimators of the tail index γ that are invariant under the scale parameter σ. We make use of estimators which can be represented in a closed form based on certain order statistics.

For the Pareto quantile function $F^{-1}_{\gamma,\sigma}$ in (15.5) the following two equations hold:

$$\log\left(\frac{F^{-1}_{\gamma,\sigma}(q_2) - F^{-1}_{\gamma,\sigma}(q_1)}{F^{-1}_{\gamma,\sigma}(q_1)}\right) \Big/ \log(1/a) = \gamma \tag{15.9}$$

and

$$\frac{\left(F^{-1}_{\gamma,\sigma}(q_1)\right)^2}{F^{-1}_{\gamma,\sigma}(q_2) - 2F^{-1}_{\gamma,\sigma}(q_1)} = \sigma \tag{15.10}$$

for $q_1 = 1 - a$, $q_2 = 1 - a^2$ and $0 < a < 1$ (cf. also Reiss and Thomas (1997), pp. 118, for this choice of values q_i).

Therefore, one may deduce closed–form estimators of γ and σ for each $0 < a < 1$ by plugging in appropriate order statistics. Let

$$\hat{\gamma}_a = \log\left(\frac{z_{j(a,k):k} - z_{i(a,k):k}}{z_{i(a,k):k}}\right) \Big/ \log(1/a) \tag{15.11}$$

and

$$\hat{\sigma}_a = \frac{z^2_{i(a,k):k}}{z_{j(a,k):k} - 2z_{i(a,k):k}} \tag{15.12}$$

where $i(a,k) = [k(1-a)]$ and $j(a,k) = [k(1-a^2)]$.

For $a = 1/2$ one gets the Pickands (1975) estimators. Convex combinations of several Pickands estimators were studied by Falk (1994) and Drees (1995). Likewise one may take the median of such estimators as it was done by Castillo and Hadi (1997). In the latter article, the estimators are established as numerical solutions of certain equations, cf. (15.16), with the Pickands estimators mentioned as special cases.

We make use of the medians

$$\gamma_{MP} = \text{median}\{\hat{\gamma}_{a(i)} : i = [k/4], \ldots, [3k/4]\} \tag{15.13}$$

and

$$\sigma_{MP} = \text{median}\{\hat{\sigma}_{a(i)} : i = [k/4], \ldots, [3k/4]\} \tag{15.14}$$

where the $a(i)$ are given by $i = k(1 - a(i))$ for $i = 1, \ldots, k$. Thus, we have $i(a(i), k) = i$ in (15.11) and (15.12). We refer to Section 15.6 for a discussion about this choice of initial estimators $\hat{\gamma}_{a(i)}$ and $\hat{\sigma}_{a(i)}$.

It is apparent that the estimators $\hat{\gamma}_a$ and γ_{MP} of γ are invariant under the scale parameter σ.

15.5 Analyzing the Long Term Copepod Data

We continue the analysis in the article by Schmitt et al. (2006) of certain copecod data where the Hill estimate of the tail index γ is applied, giving the value $\tilde{\gamma}_H = 0.8$. This indicates an extraordinary case in so far that for tail indices $\gamma > 0.5$ the pertaining Pareto distribution does not possess a finite variance.

15.5.1 The data set

The data are deduced from weekly measurements of the abundance of a plankton species (a copepod called Centropages typicus) from January 1967 to December 1997 in the Villefranche Bay near Nice, France. The samples were collected by Serge Dallot using a Juday-Bogorov net and the countings were done by Juan Carlos Molinero. Countings were separately made for females and males. The data set mentioned above concerns the product of the countings for females and males. This product is an index for the mating encounter rate, which is regarded as a critical issue in plankton ecology.

The data set is of size $n = 1353$. The data range from 0 to 908,782. According to the visual insight gained from Q–Q–plots, sample excess functions and diagrams of estimates we choose a threshold $u = 34,000$ which entails a number of $k = 100$ exceedances $x_1, \ldots, x_{100}$. The data set, which has to be analyzed, therefore consists of the normalized excesses $y_i = x_i/34,000 - 1$.

15.5.2 Parametric estimates for the copepod data

Based on the y_i one gets the Hill estimate $\gamma_H = 0.84$ (it is understood that $\sigma = 1$) and the modified Pickands estimates $\gamma_{MP} = 0.78$ and $\sigma_{MP} = 1.08$. The latter estimate indicates that the underlying df is sufficiently close to the restricted Pareto model (15.3) so that the Hill estimate of γ can be correct. The estimates γ_H and γ_{MP} are sufficiently close together and confirm the estimate $\tilde{\gamma}_H = 0.8$ in Schmitt et al. (2006). The maximum likelihood estimates in the 2-parameter model are $\gamma_{ML} = 0.68$ and $\sigma_{ML} = 1.43$, which is within a reasonable agreement with the previous estimates.

It is remarkable that there is a strong evidence of a df with a tail index $\gamma > 0.5$. This incident occurs for the first time to the 1st author after having analyzed a greater number of data sets from finance, hydrology, insurance, telecommunication, ecology, etc. There are rumours that there are real–life data (business interruption and, as recently mentioned in a talk by Paul Embrechts, operational risk data in an Italian bank) having such very heavy tails, yet these data are not available to the public.

15.5.3 Median excess functions

This above mentioned evidence is supported by empirical investigations. In the following lines we compare parametric excess functions pertaining to the Hill estimate and the modified Pickands estimates to a sample excess function. The excess df above the threshold u, pertaining to a df F, is

$$F^{(u)}(x) = F^{[u]}(u+x),\ x \geq 0.$$

The mean and median excess functions are given by the means and, respectively, medians of excess dfs as functions in u. Because the present data set is related to a very heavy–tailed df we merely deal with the median excess function

$$m_F(u) = \left(F^{(u)}\right)^{-1}(1/2), \quad u > 0. \tag{15.15}$$

Excess functions of GPDs are straight lines. For the df $F_{\gamma,\sigma}$ in (15.4) one gets the median excess function

$$m_{F_{\gamma;\sigma}}(u) = \sigma(2^\gamma - 1)(1 + x/\sigma), \quad u > 0.$$

A sample version of the median excess function is obtained by plugging in the sample df.

In figure 15.1, one realizes that there is a good correspondence between the estimated parametric and the sample median excess functions.

When looking at the plots in figure 15.1 one should keep in mind that 56 (respectively, 80) excesses out of total number of $n = 100$ excesses are smaller than 1 (respectively, smaller than 3). One cannot expect that sample excess functions are smooth in the upper range because they are neither monotone nor close to a constant (like sample dfs or sample densities).

We remark that Q–Q–plots, in conjunction with estimated tail indizes and unknown location and scale parameters, support the previous conclusions.

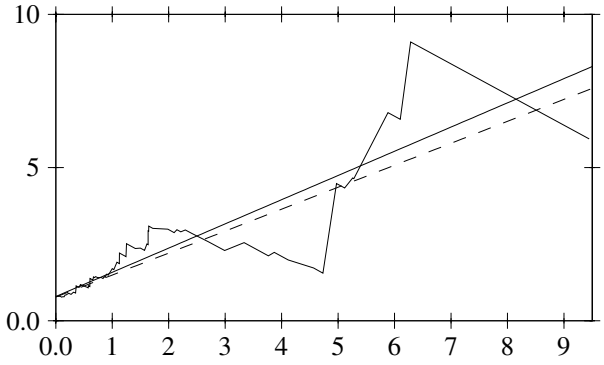

Figure 15.1. Median excess functions: sample version, Hill (solid) and modified Pickands (dashed) based on 100 normalized excesses

15.6 Computational Aspects

As mentioned above, the modified Pickands estimates in (15.13) and (15.14) applied to the normalized excesses of the copepod data are 0.78 for γ and 1.07 for σ. These estimates are based on pairs $(y_{i:k}, y_{j:k})$ with i between $[k/4]$ and $[3k/4]$ and j satisfying a certain condition.

The choice $[k/4] \le i \le [3k/4]$ was made because simulations show that the initial estimators in (15.11) and (15.12) are inaccurate if i is too close to 1 or k. The plot of simulated medians of $\hat{\gamma}_{a(i)}$ against i is downward U–shaped, below γ and near to γ for $\lfloor 1/4\,k \rfloor \le i \le \lfloor 3/4\,k \rfloor$. As a consequence the estimator γ_{MP} in (15.13) has a tendency to underestimate γ. Because our estimator is given in a closed form it should be possible to construct an improved version of this estimator. The estimator σ_{MP} in (15.14) of σ is amazingly accurate.

Castillo and Hadi (1997) study in detail the case of negative tail indices γ. We briefly mention the required modifications to get estimators for positive γ. From $F_{\gamma,\sigma}(F^{-1}_{\gamma,\sigma}(q)) = q$, $0 < q < 1$, one gets the equations

$$\log(1 + F^{-1}_{\gamma,\sigma}(q)/\sigma) = -\gamma \log(1 - q) \tag{15.16}$$

which yield the equations (15.9) and (15.10) for the specific choice of values q_1 and q_2.

To get the estimator in Castillo and Hadi (1997),

- plug in the order statistics $y_{i:k}$ and $y_{j:k}$ in place of $F^{-1}_{\gamma,\sigma}(q_i)$ and $F^{-1}_{\gamma,\sigma}(q_j)$, with $q_i = i/(k+1)$ and $q_j = j/(k+1)$, for each pair $i < j$;
- compute numerical solutions of each pair of equations in order to get initial estimates of γ and σ,
- establish the final estimator by taking again the median of the initial estimates.

For the copepod data, the Castillo–Hadi estimates are 0.85 for γ and 1.04 for σ.

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Part VI

Business and Economics Applications

16

Deriving Credibility Premiums Under Different Bayesian Methodology

Emilio Gómez Déniz

UIMA, Department of Quantitative Methods, University of Las Palmas de Gran Canaria, Spain

Abstract: Credibility theory is a set of quantitative methods that allows an insurer to adjust future premiums based on past experience. Generally, the credibility expression obtained is written as a weighted sum of the sample mean and the collective premium, the premium to be charged to a collective of policyholders in a portfolio. The weighted factor is referred to as the credibility factor. In this paper, a review of credibility theory is presented and new credibility formulae are obtained in a simple and extensive Bayesian methodology.

Keywords and phrases: Credibility, Bayes, loss function, premium, regret

16.1 Introduction

Credibility theory is an experience rating technique in actuarial science used usually in automobile insurance, worker's compensation premium, loss reserving and IBNR (Incurred But Not Reported) claims to the insurer–where credibility theory can be used to estimate the claim size amount. Experience rating is the process whereby the experience of an individual risk is used to calculate the premium rate for that individual. Under this theory, the premium for an individual risk is computed by combining the experience of the individual (contract or policyholder) with the experience of a collective (portfolio).

In this sense, credibility theory is used to determine the expected claims experience of an individual risk when those risks are not homogeneous, given that the individual risk belongs to a heterogeneous collective. The main objective of the credibility theory is to calculate the weight that should be assigned to the individual risk data to determine a fair premium to be charged.

In credibility theory, it is assumed that the risk $X \in \mathcal{X}$ follows a probability density function $f(x|\theta)$ depending on an unknown risk parameter $\theta \in \Theta$. Now the unknown premium $P \equiv P(\theta)$, called the risk premium, can be obtained by minimizing the expected loss $E_f\left[L_1(\theta, P)\right]$, with $P \in \mathcal{P}$, the action space. L_1 is taken usually as the weighted squared–error loss function (WLF henceforth), i.e. $L_1(a, x) = h(x)(x-a)^2$.

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Using different functional forms for $h(x)$ we have different premium principles. For example for $h(x) = 1$ and $h(x) = \exp\{cx\}, c > 0$, we have the net and Esscher premium principles respectively (Heilmann, 1989), (Gómez Déniz et al., 2006), among others.

If experience is not available, the actuary computes the collective premium, PC, which is given by minimizing the risk function, i.e., minimizing $E_\pi\left[L_1(P(\theta), PC)\right]$. Finally, if experience is available, the actuary takes a sample $\mathbf{x}$ from the random variables $X_i,\ \ i = 1, 2, \ldots, t$, assuming X_i i.i.d., and uses this information to estimate the unknown risk premium $P(\theta)$, through the Bayes premium PB, obtained by minimizing the Bayes risk, i.e., minimizing $E_{\pi^{\mathbf{x}}}\left[L_1(P(\theta), PB)\right]$. Here, $\pi^{\mathbf{x}}$ is the posterior distribution of the risk parameter, $\theta \in \Theta$, given the sample information $\mathbf{x}$.

If the practitioner uses the quadratic loss function the risk, collective and Bayes net premiums are given by (see Eichenauer et al. (1988), Heilmann (1989) and Gómez Déniz et al. (2006)).

$$P(\theta) = \int_{\mathcal{X}} x f(x|\theta) dx, \tag{16.1}$$

$$P(\pi) = \int_{\Theta} P(\theta)\pi(\theta) d\theta, \tag{16.2}$$

$$P(\pi^{\mathbf{x}}) = \int_{\Theta} P(\theta)\pi^{\mathbf{x}}(\theta) d\theta, \tag{16.3}$$

respectively.

Suppose now we have a portfolio of k policyholders. The problem of credibility theory is how to compute a fair premium to the policyholder in class $j,\ \ j = 1, \ldots, k$, by using his own information and the information of the whole portfolio. The following solution was suggested by Whitney (1918).

$$M_j^c = \text{Premium}_j = (1 - Z)m + ZM_j, \tag{16.4}$$

where

- Premium_j is the credibility adjusted premium.
- m is the overall mean.
- M_j is the mean for individual risk j.
- Z is the credibility factor, a number between 0 and 1.

Under this approach, a compromise M_j^c is computed by (16.4) and graphically (see figure 16.1) we see that M_j^c is somewhere on the line segment between m and M_j.

The main problem now is how to choose the credibility factor Z. In order to do this, some useful results, which we do not present here, have been proposed: limited fluctuation credibility, Hachemeister random coefficient regression model, multi–dimensional credibility, Hilbert spaces methods, etc. The most important contribution in this matter was proposed by Bühlmann (1967) in a simple and elegant form. This result is known

Figure 16.1. Credibility premium

as the classical model of Bühlmann. Firstly, Bailey (1950) and later some approaches to the credibility problem were obtained under the Bayesian methodology.

The paper is organized as follows. In Section 16.2, the classical model of Bühlmann is presented. Credibility premiums under standard Bayesian methodology and based on robust Bayesian analysis are showed in Section 6.3 and 16.4 respectively. New credibility premiums are obtained under a more general loss function than the squared–error loss in Section 16.5. Finally, some concluding remarks are made in Section 6.6.

16.2 Classical Model of Bühlmann

The idea of the Bühlmann model is to derive a premium

$$E\left(P(\theta)|X_1, X_2, \ldots, X_t\right),$$

based on the observations $X_1, X_2, \ldots, X_t$ by minimizing the squared–error loss function

$$E\left[P(\theta) - c_0 - \sum_{r=1}^{t} X_r\right]^2,$$

i.e., the premium is a linear function of the observed data.

Defining:

- $P(\theta) = E\left(X|\theta\right)$, the risk net premium
- $m = E_{\text{Total}}\left(X\right) = E\left[P(\theta)\right]$, the collective net premium
- $a = \text{Var}\left[E\left(X|\theta\right)\right] = \text{Var}\left[P(\theta)\right]$, the variance of the hypothetical means. It measures the heterogeneity of the portfolio.
- $s^2 = E\left[\text{Var}\left(X|\theta\right)\right]$, expected values of the process of variance

He found that

$$c_r = \frac{a}{s^2 + at} = \frac{Z}{t},$$

where

$$Z \equiv Z(t) = \frac{at}{s^2 + at} = \frac{t\text{Var}\left[E\left(X|\theta\right)\right]}{t\text{Var}\left[E\left(X|\theta\right)\right] + E\left[\text{Var}(X|\theta)\right]}, \tag{16.5}$$

and $c_0 = \left[1 - Z(t)\right] m$. Hence

$$E\left[P(\theta)|X_1, \ldots X_t\right] = Z(t)\bar{X} + \left[1 - Z(t)\right] m.$$

The main advantage of this approach is that this relation does not make any assumption about the type of distributions governing the individual risks or the prior distribution function of the parameters. In actuarial science, it is said that exact credibility exists when the credibility premium has the same credibility factor as in (16.5). Observe that $Z(t)$ is a function of t with $Z(t) \to 1$ when $t \to \infty$, and $Z(t) \to 0$ when $t \to 0$. Furthermore, $Z(t)$ is a decreasing function of s^2 and an increasing function of

a. Thus, the larger the variation associated with the individual combinations of risk characteristics is, the less weight is given to the current observations and the more weight is given to the prior mean.

A generalization of the Bühlmann model is the Bühlmann–Straub model (see Bühlmann (1967)), in which natural weights are assigned to the data and are allowed to vary with time. Again, credibility premium in a distribution free approach is obtained.

16.3 Standard Bayesian Credibility

Expression (16.4) can also be thought as a compromise between the mean of the current observations, the data, and the prior mean, an estimate based on the actuary's prior opinion. In this sense, that expression includes the concept of prior data, in the spirit of the Bayesian paradigm. Bailey (1950) showed that if the likelihood is the binomial distribution and the prior is the beta distribution, exact credibility occurs. In the same paper, Bailey also demonstrated credibility expression in the Poisson–Gamma case. Similar results were obtained by Mayerson (1964). Finally, Jewell (1974) generalized these results showing that for the exponential family of distributions and its conjugate priors, exact credibility premiums were derived. In this case, by using the single exponential family with parametrization,

$$f(x|\theta) = \frac{p(x)e^{-\theta x}}{q(\theta)}, \tag{16.6}$$

where $q(\theta)$ and $p(x)$ are arbitrary functions such that $f(x|\theta)$ is a proper density and the conjugate prior distribution

$$\pi(\theta) = \frac{q(\theta)^{-t_0}e^{-\theta x_0}}{c(t_0, x_0)}, \tag{16.7}$$

Jewell (1974) proved that the Bayesian net premium is given by,

$$P(\pi^{\mathbf{x}}) = \frac{x_0 + \sum_{i=1}^{t} x_i}{t_0 + t} = [1 - Z(t)]\, m + Z(t)\bar{\mathbf{x}}.$$

Here, $Z(t) = t/(t_0 + t)$, while $m = \int_\Theta P(\theta)\pi(\theta)d\theta = x_0/t_0$. It is easy to show that this credibility factor admits the same formulation as the Bühlmann credibility factor in (16.5).

Example 1. In table 16.1 some natural conjugate prior distributions are showed. Now, using (16.1), (16.2) and 16.3) it is straightforward to show that Bayesian premiums for the conjugate distributions in table 16.1 are given by expressions which appear in table 16.2.

Table 16.1. Conjugate distributions

Likelihood Prior	Posterior
$X\|\theta \sim \mathcal{P}o(\theta)$ $\theta \sim \mathcal{G}(a,b)$	$\mathcal{G}(a+t, b+t\bar{\mathbf{x}})$
$X\|\theta \sim \mathcal{NB}(r,\theta)$ $\theta \sim \mathcal{B}(a,b)$	$\mathcal{B}(a+tr, b+t\bar{\mathbf{x}})$
$X\|\theta \sim \mathcal{B}i(m,\theta)$ $\theta \sim \mathcal{B}(a,b)$	$\mathcal{B}(a+t\bar{\mathbf{x}}, b+mt-t\bar{\mathbf{x}})$
$X\|\theta \sim \mathcal{G}(\theta,\nu)$ $\theta \sim \mathcal{G}(a,b)$	$\mathcal{G}(a+t\bar{\mathbf{x}}, b+t\nu)$
$X\|\theta \sim \mathcal{N}(\theta,\sigma^2)$ $\theta \sim \mathcal{N}(a,\tau^2)$	$\mathcal{N}\left(\frac{a\sigma^2+t\bar{\mathbf{x}}\tau^2}{\sigma^2+t\tau^2}, \frac{\sigma^2\tau^2}{\sigma^2+t\tau^2}\right)$

$\mathcal{P}o$: Poisson, $\mathcal{G}$: Gamma, $\mathcal{NB}$: Negative binomial, $\mathcal{B}i$: Binomial, $\mathcal{B}$: Beta, $\mathcal{N}$: Normal

Table 16.2. Credibility premiums under net premium principle

Likelihood Prior	$P(\pi)$	$P(\pi^{\mathbf{x}})$	$Z(t)$
$X\|\theta \sim Po(\theta)$ $\theta \sim \mathcal{G}(a,b)$	$\frac{a}{b}$	$\frac{a+t\bar{\mathbf{x}}}{b+t}$	$\frac{t}{b+t}$
$X\|\theta \sim \mathcal{NB}(r,\theta)$ $\theta \sim \mathcal{B}(a,b)$	$r\frac{b}{a-1}$	$r\frac{b+n\bar{\mathbf{x}}}{a+nr-1}$	$\frac{rt}{b+tr-1}$
$X\|\theta \sim \mathcal{B}i(m,\theta)$ $\theta \sim \mathcal{B}(a,b)$	$m\frac{a}{a+b}$	$m\frac{a+n\bar{\mathbf{x}}}{a+b+mn}$	$\frac{mt}{a+b+mt}$
$X\|\theta \sim \mathcal{G}(\theta,\nu)$ $\theta \sim \mathcal{G}(a,b)$	$\nu\frac{a}{b-1}$	$\nu\frac{a+t\bar{\mathbf{x}}}{b+t\nu-1}$	$\frac{t\tau^2}{a+t\nu-1}$
$X\|\theta \sim \mathcal{N}(\theta,\sigma^2)$ $\theta \sim \mathcal{N}(a,\tau^2)$	a	$\frac{a\sigma^2+t\bar{\mathbf{x}}\tau^2}{\sigma^2+t\tau^2}$	$\frac{t\tau^2}{\sigma^2+t\tau^2}$

16.4 Credibility Based on Robust Bayesian Analysis

Another approach to the Bayes setup analyzed above occurs when practitioners suppose that a correct prior π exists, but they are unable to apply the pure Bayesian assumption, perhaps because they are not sure or are unable to specify it totally. Thus, they assign a prior π to the risk parameter θ, which represents a well approximation of the true prior. This situation can also be considered when the question must be solved by two or more decision–makers and they do not agree about the prior distribution to be used. A common approach to prior uncertainty in Bayesian analysis is to choose a class Γ of prior distributions and to compute the range of Bayes actions as the prior ranges over $\mathcal{Q}$.

This is known as robust Bayesian methodology. A new alternative consists of choosing a procedure that lies between the Bayes action and the Bayes robust methodology. This hybrid approach is known as the Γ–minimax regret principle, or the posterior regret Γ–minimax principle (PRGM, henceforth).

If $\rho(\pi^{\mathbf{x}}, P)$ is the posterior expected loss of an action P under $\pi^{\mathbf{x}}$, the posterior regret of P is defined as (Ríos et al. (1995) and Zen and DasGupta (1993))

$$r(\pi^{\mathbf{x}}, P) = \rho(\pi^{\mathbf{x}}, P) - \rho(\pi^{\mathbf{x}}, P(\pi^{\mathbf{x}})),$$

which measures the loss of optimality by choosing P instead of the optimal action $P(\pi^{\mathbf{x}})$.

Now $RP(\pi^{\mathbf{x}}) \in \mathcal{P}$ is the PRGM action if

$$\inf_{P\in\mathcal{P}} \sup_{\pi\in\mathcal{Q}} r(\pi^{\mathbf{x}}, P) = \sup_{\pi\in\mathcal{Q}} r(\pi^{\mathbf{x}}, RP(\pi^{\mathbf{x}})).$$

It is easy to show (see Ríos et al. (1995) and Zen and DasGupta (1993)) that if we choose $h(x) = 1$, i.e., the premium to be considered is the net premium principle, the PRGM action is the midpoint of the interval $\left[\inf_{\pi\in\mathcal{Q}} P(\pi^{\mathbf{x}}), \sup_{\pi\in\mathcal{Q}} P(\pi^{\mathbf{x}})\right]$.

The PRGM procedure is based on the line that the optimal action minimizes the supremum of the function over distributions in class Γ. Therefore, the actuary would be wise to ensure that the largest possible increase in risk resulting from making the wrong choice of prior distribution should be kept as small as possible.

Suppose that (16.6) is the likelihood function and θ is a single unknown parameter, with prior distribution (16.7), but the investigator is unable to specify completely the parameter of this prior distribution; or perhaps two or more decision–makers may not be agreed with the prior distribution to be used. Thus, we use the following classes of prior distributions:

$$\mathcal{Q}_1 = \left\{\pi(\theta) : x_0^{(1)} \le x_0 \le x_0^{(2)},\ t_0 \ \text{ fixed}\right\}, \tag{16.8}$$

$$\mathcal{Q}_2 = \left\{\pi(\theta) : \gamma_1 \le m \le \gamma_2,\ t_0 \ \text{ fixed}\right\}, \tag{16.9}$$

$$\mathcal{Q}_3 = \left\{\pi(\theta) : t^{(1)} \le t_0 \le t^{(2)}\right\}. \tag{16.10}$$

Now the PRGM premiums under the classes $\mathcal{Q}_j,\ j = 1, 2, 3$ are given in the following result.

Theorem 1. *Consider the single–parameter exponential family (16.6) and the conjugate prior distribution (16.7), then the posterior regret $\Gamma-$minimax net premium under $\mathcal{Q}_j,\ j = 1, 2, 3$, classes are given by:*

$$RP(\pi; \mathcal{Q}_j) = \frac{X_j + \sum_{i=1}^{t} x_i}{T_j + t}, \quad j = 1, 2, 3 \tag{16.11}$$

where,

$$X_1 = \frac{1}{2}\left(x_0^{(1)} + x_0^{(2)}\right), \quad T_1 = t_0, \tag{16.12}$$

$$X_2 = \frac{1}{2}(\gamma_1 + \gamma_2)\, t_0, \quad T_2 = t_0, \tag{16.13}$$

$$X_3 = \frac{x_0^{(1)} t_0^{(1)} + x_0^{(2)} t_0^{(2)} + \left(x_0^{(1)} + x_0^{(2)}\right) t}{t_0^{(1)} + t_0^{(2)} + 2t}, \; T_3 = \frac{2t_0^{(1)} t_0^{(2)} + \left(t_0^{(1)} + t_0^{(2)}\right) t}{t_0^{(1)} + t_0^{(2)} + 2t}. \tag{16.14}$$

PROOF. By computing $\inf_{\pi \in \mathcal{Q}_j} P(\pi)$ and $\sup_{\pi \in \mathcal{Q}_j} P(\pi)$, $j = 1, 2, 3$, it is simple to obtain the desired result by choosing

$$RP(\pi; \mathcal{Q}_j) = \frac{1}{2}\left(\inf_{\pi \in \mathcal{Q}_j} P(\pi) + \sup_{\pi \in \mathcal{Q}_j} P(\pi)\right).$$

■

Since closed intervals on the real line are connected sets, using Proposition 3.2 in Ríos et al. (1995) we can conclude that $RP(\pi; \mathcal{Q}_j)$, $j = 1, 2, 3$, are Bayes actions.

Corollary 1. *If we assume the single–parameter exponential family (16.6) and the conjugate prior distribution (16.7) with parameters* (X_j, T_j), $j = 1, 2, 3$ *as in (16.12), (16.13) and (16.14) respectively, then the Bayesian premiums* $RP(\pi; \mathcal{Q}_j)$, $j = 1, 2, 3$ *in (16.11) can be rewritten as a credibility formula with the credibility factor as in (16.5).*

PROOF. It is simple. ■

The above study can be extended by using the ε–contaminated class (Ríos et al. (1995), Ríos and Ríos and Ruggeri (2000); Gómez Déniz et al. (2006); among others). If π is the base elicited prior, the ε–contaminated class is given by

$$\Gamma^{\varepsilon} = \{g(\theta) : g(\theta) = (1 - \varepsilon)\pi(\theta) + \varepsilon q(\theta),\ q \in \mathcal{Q}\}, \tag{16.15}$$

where $\mathcal{Q}$ is called the contamination class.

In order to compute PRGM premiums under this class, we first need the following result, which appears in Gómez Déniz et al. (2006).

Theorem 2. *Under the ε–contaminated class Γ^{ε}, the PRGM net premium is given by*

$$RP(\pi; \Gamma^{\varepsilon}) = (1 - \varepsilon) RP(\pi^{\mathbf{x}}) + \varepsilon RP(q^{\mathbf{x}}), \tag{16.16}$$

where $RP(\pi^{\mathbf{x}})$ is the Bayes premium obtained under $\pi^{\mathbf{x}}$, and $RP(q^{\mathbf{x}})$ is the PRGM premium under the class $\mathcal{Q}$ given by

$$RP(q^{\mathbf{x}}) = \frac{1}{2}\left(\inf_{q \in \mathcal{Q}} P(q^{\mathbf{x}}) + \sup_{q \in \mathcal{Q}} P(q^{\mathbf{x}})\right).$$

Consider now the following $\varepsilon-$contaminated class,

$$\Gamma_j^{\varepsilon} = \{g(\theta) : g(\theta) = (1 - \varepsilon)\pi(\theta) + \varepsilon q_j(\theta),\ q_j \in \mathcal{Q}_j\}, \quad j = 1, 2, 3,$$

where $\mathcal{Q}_j$, $j = 1, 2, 3$ as in (16.8), (16.9) and (16.10), respectively. Then, we have the following result.

Theorem 3. *If we assume the single–parameter exponential family (16.6) and the base elicited prior (16.7) and taking the classes* $\Gamma_j^\varepsilon,\ j=1,2,3$ *the PRGM net premium is given by*

$$RP(g;\Gamma_j^\varepsilon)=(1-\varepsilon)\frac{x_0+\sum_{i=1}^t x_i}{t_0+t}+\varepsilon\frac{X_j+\sum_{i=1}^t x_i}{T_j+t}, \tag{16.17}$$

where $X_j, T_j,\ j=1,2,3$, *as in Theorem 1.*

Proof. It is straightforward by using Theorems 1 and 2. ■

Observe that this new situation can be thought of as a compromise between the pure Bayes option ($\varepsilon=0$) and the pure PRGM criterion studied ($\varepsilon=1$). Intermediate situations can be thought of as hybrid positions between the two procedures.

Next proposition is a direct consequence of Proposition 3 and by using the class Γ_1^ε.

Proposition 1. *For* Γ_1^ε *the PRGM net premium in Theorem (3) can be written as*

$$\mathcal{P}_M^{\Gamma_1^\varepsilon}=Z(t)\overline{\mathbf{x}}+[1-Z(t)]\left[(1-\varepsilon)\frac{x_0}{t_0}+\varepsilon\frac{x_0^{(1)}+x_0^{(2)}}{2t_0}\right], \tag{16.18}$$

then is a credibility formula, with credibility factor $Z(t)$ *as in (16.5).*

Proof. First, the risk premium $P(\theta)$ under the single–parameter exponential family (16.6) and the base elicited prior (16.7), see Jewell (1974), is given by $P(\theta)=-c'(\theta)/c(\theta)$. Now, using the fact that under the class Γ_1^ε the contamination distribution is as in (16.7) with parameters $\left(\frac{x_0^{(1)}+x_0^{(2)}}{2},t_0\right)$, we have that the risk premium is given by

$$\int\frac{-c'(\theta)}{c(\theta)}\left[(1-\varepsilon)\pi_0(\theta)+\varepsilon q(\theta)\right]d\theta=(1-\varepsilon)\frac{x_0}{t_0}+\varepsilon\frac{x_0^{(1)}+x_0^{(2)}}{2t_0}.$$

Now, using (16.17) we have that

$$\begin{aligned}P_M^{\Gamma_1^\varepsilon}&=(1-\varepsilon)\frac{x_0+t\bar{\mathbf{x}}}{t_0+t}+\varepsilon\frac{\left(x_0^{(1)}+x_0^{(2)}\right)/2+t\bar{\mathbf{x}}}{t_0+t}\\&=\frac{t\bar{\mathbf{x}}}{t_0+t}+\left[(1-\varepsilon)\frac{x_0}{t_0}+\varepsilon\frac{x_0^{(1)}+x_0^{(2)}}{2t_0}\right]\frac{t_0}{t_0+t}.\end{aligned}$$

■

16.5 Beyond the Loss Function

In this section, generalization of the credibility premiums obtained by Heilmann (1989) are derived by using the weighted balanced loss function (WBLF henceforth),

$$L_2(a,x)=wh(x)(\delta_0-a)^2+(1-w)h(x)(x-a)^2, \tag{16.19}$$

where $0 \leq w \leq 1$ is a weighting factor determined by the practitioner, $h(x)$ is a positive weight function and $\delta_0(X)$ is a function of the observed data.

WBLF is a generalized loss function introduced by Zellner (see Gupta and Berger (1994), p. 371–390, and which appears also in Dey et al. (1999) and Farsipour and Asgharzadhe (2004). This loss includes as a particular case the WLF, L_1, when w is chosen to equal 0.

Proposition 2. *Under WBLF and prior π, the risk and collective balanced premiums are given by*

$$P_{L_2}(\theta) = w\frac{E_{f(x|\theta)}\left[\delta_0(X)h(X)\right]}{E_{f(x|\theta)}\left[h(X)\right]} + (1-w)\frac{E_{f(x|\theta)}\left[Xh(X)\right]}{E_{f(x|\theta)}\left[h(X)\right]}, \tag{16.20}$$

$$P_{L_2}(\pi) = w\delta_0^* + (1-w)\frac{E_{\pi}\left[P_{L_2}(\theta)h(P_{L_2}(\theta))\right]}{E_{\pi}\left[h(P_{L_2}(\theta))\right]}, \tag{16.21}$$

respectively and where δ_0^* is a target estimator for the risk premium P_{L_2}.

Proof. It is simple. ■

Now, the Bayes balanced premium $P_{L_2}(\pi^{\mathbf{x}})$ is obtained replacing in (16.21) π by $\pi^{\mathbf{x}}$.

Now, new credibility expression is derived by using the WBLF as we show in next result.

Theorem 4. *If the Bayes net premium obtained under $L_1(a,x)$ is a credibility formula, the Bayes balanced net premium obtained under WBLF is also a credibility formula in the form:*

$$P_{L_2}(\pi^{\mathbf{x}}) = Z(t)\cdot l\left(P_{L_2}(\pi)\right) + \left[1 - Z(t)\right]\cdot l(\bar{\mathbf{x}}), \tag{16.22}$$

where $Z(t) \in [0,1]$ and $l(x) = (1-w)^2 x + w(1-w)E_{\pi^{\mathbf{x}}(\theta)}\left[E_{f(x|\theta)}\left(\delta_0(X|\theta)\right)\right] + w\delta_0^*$.

Proof. Using (16.20) and (16.21) with $h(x) = 1$ we have that

$$P_{L_2}(\theta) = wE\left[\delta_0(X)|\theta\right] + (1-w)E_{f(x|\theta)}\left(X|\theta\right)$$

and

$$\begin{aligned} P_{L_2}(\pi) &= w\delta_0^* + (1-w)E_{\pi}\left[wE_{f(x|\theta)}\left[\delta_0(X)|\theta\right] + (1-w)E_{f(x|\theta)}\left(X|\theta\right)\right] \\ &= w\delta_0^* + w(1-w)E_{\pi}\left\{E_{f(x|\theta)}\left[\delta_0(X|\theta)\right]\right\} \\ &\quad +(1-w)^2 E_{\pi}\left[E_{f(x|\theta)}\delta_0(X)|\theta\right]. \end{aligned}$$

Therefore

$$P_{L_2}(\pi^{\mathbf{x}}) = w\delta_0^* + w(1-w)E_{\pi^{\mathbf{x}}}\left\{E_{f(x|\theta)}\left[\delta_0(X)|\theta\right] + (1-w)^2 P_{L_1}(\pi^{\mathbf{x}})\right\}.$$

Now, if $P_{L_1}(\pi^{\mathbf{x}})$ is a credibility formula in the form

$$P_{L_1}(\pi^{\mathbf{x}}) = Z(t)P_{L_1}(\pi) + \left[1 - Z(t)\right]\bar{\mathbf{x}},$$

then

$$\begin{aligned} P_{L_2}(\pi^{\mathbf{x}}) &= w\delta_0^* + w(1-w)E_{\pi^{\mathbf{x}}}\left\{E_{f(x|\theta)}\left[\delta_0(X)|\theta\right]\right\} \\ &+ (1-w)^2\left\{Z(t)P_{L_1}(\pi) + \left[1-Z(t)\right]\bar{\mathbf{x}}\right\} \\ &= Z(t)\left[(1-w)^2 P_{L_1}(\pi) + w(1-w)E_{\pi^{\mathbf{x}}}\left\{E_{f(x|\theta)}\left[\delta_0(X)|\theta\right]\right\} + w\delta_0^*\right] \\ &+ \left[1-Z(t)\right]\left[(1-w)^2\bar{\mathbf{x}} + w\delta_0^* + w(1-w)E_{\pi^{\mathbf{x}}}\left\{E_{f(x|\theta)}\left[\delta_0(X)|\theta\right]\right\}\right] \\ &= Z(t)l(P_{L_2}(\pi)) + \left[1-Z(t)\right]l(\bar{\mathbf{x}}). \end{aligned}$$

■

Finally, it is simple to derive the following corollary.

Corollary 2. *If we assume the exponential family of distributions as the likelihood and its conjugate prior, then the Bayes balanced net premium is also a credibility formula.*

To end this section, we merely point out that we can obtain new a credibility formula under WBLF and the posterior regret $\Gamma-$minimax technique.

16.6 Discussion

The results of the work presented here show that the Bayesian procedure is a rich and flexible method to obtain credibility premiums whose results are attractive for the community of actuaries. For decades, standard Bayesian methodology has been used to derive, under appropriate conjugate families, credibility formulae.

In this paper, first we have showed that by combining standard Bayesian and global robust analysis, new credibility formulae can be derived. Obviously, this study can be extended to other classes of distributions instead of the one used here. Second, we have used the WBLF to obtain new credibility premiums richer than the previous ones because they include more parameters than the classical credibility premiums. The methodology used here is very simple, and credibility formulas are straightforwardly obtained.

Obviously, these techniques can be extended to other premium calculation principles, such as the Esscher or variance, see Heilmann (1989) for details. Finally, a distribution free approach similar to the classical Bühlmann's model can be made by using the WBLF.

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17

The Influence of Transport Links on Disaggregation and Regionalization Methods in Interregional Input-Output Models Between Metropolitan and Remote Areas

Fernando Escobedo[1] and Jose M. Ureña[2]

[1] Department of Building and Civil Engineering, University of Castilla-La Mancha, Spain
[2] Department of Geography, City and Regional Planning, University of Cantabria, Spain

Abstract: This paper expounds a new method of regionalization and disaggregation, based on potential methods, which takes into account the Gross Added Value of each economic sector in every region and the transport infrastructure used by those, emphasizing the high speed train and air transport infrastructures. This method is specially suitable for input-output analysis between regions that are linked by a few means of transportation. The method is developed for an Interregional Input-Output Analysis of two regions and then applied for Ciudad Real and Madrid Provinces in Spain. The data come from the Castilla La Mancha (Region which includes Ciudad Real Province) and Madrid Province Input-Output Tables of 1995 and 1996, respectively, and as a result of the contrast between both tables an Interregional Input-Output Table of twenty-seven economic sectors is created. Finally one of the main conclusions is that the method depends largely on the availability of the data of Gross Added Value and its level of disaggregation.

Keywords and phrases: Input-output analysis, regionalization methods, disaggregation methods, peripheral areas, metropolitan areas, high speed transport infrastructures

17.1 Introduction

It is known that the development of interregional input-output models entails many more difficulties than a single region model would. One of the main difficulties is to obtain the non-diagonal submatrixes that express the economic exchanges between the regions that take part in the model. The achievement of those submatrixes usually takes a double process of regionalization and disaggregation of already existing input-output tables, and those processes involve a certain amount of error, Lahr and Stevens (2002). The regionalization process is necessary if the starting input-output tables are of a larger territory, usually the national tables, Jackson and Comer (1993), than the one

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which is studied. The disaggregation process is necessary as it is very rare that there is a specific *Intermediate Demand imported from territory B Table* in the input-output tables of territory A if we are doing the model between territories A and B.

Apart from well known regionalization methods, Comer and Jackson (1997), Rey and Dev (1997), like RAS, Isard et al. (1998), and Location Quotients, Sawyer and Miller (1983), the disaggregation methods are normally based on potential methods, where the flows of goods between the different territories are referred to their relative sizes and the distance between them, Van der Linden (1999). These gravitational models are like this:

$$F_{ij} = k\frac{m_i m_j}{d_{ij}^2} \tag{17.1}$$

Nevertheless, this formula has been generally modified when it has been applied to human and economic interactions, so gravitation is presented as an increasing function with the weight and a decreasing function with the distance, Batten and Boyce (1987). Therefore the formula of these *potential models* is:

$$V_i = k\sum_j \frac{m_j}{d_{ij}} \tag{17.2}$$

From a spatial point of view, the methods of disaggregation are more suitable because they include the distance between the territories that take part in the model, as the distance is one of the most important spatial characteristics of a territorial relation. A debate ensues as to which distance to take if there are different means of transport between the two territories and specially if there are conventional means (i.e., sea transport, two lane highways or normal speed railway lines) and high speed or capacity means (i.e., four lane divided highways, high speed train and air transport).

For that reason it would be very relevant to develop a new method of regionalization that includes the distance as a new parameter. But, even more, it would be very useful to elaborate methods of regionalization and disaggregation that use not only the distance but the type of transport infrastructure used to overcome that distance. Therefore, the main goal of this paper is to develop and evaluate a new method of regionalization and disaggregation applied to intermediate demand tables for achieving the non-diagonal matrixes at interregional input-output models for two regions connected by conventional and high speed transport infrastructures.

17.2 Methodology

The goal of the process is to get an approximation of the purchases of one territory in another one. For this aim the best starting point would be the availability of updated input-output tables of the first territory; nevertheless, this is not very frequent, so it is necessary to make use of the input-output tables of a larger territory, normally the nation which that territory is in. Besides, in the habitual input-output tables, the table of interindustry sales with origin in the rest of the country is not disaggregated so hence a double process has to be carried out: a) disaggregation of the imports with origin in the rest of the country; b) regionalization of the disaggregated value. Therefore the

departure point is that we try to measure the purchases of the economic sectors of a remote subregion C of a region R in metropolitan subregion M of the region Q. That is, the table of interindustry sales of subregion C with origin in the subregion M, z^{MC}, being Z the Interregional Input-Output Transactions Matrix.

$$Z = \begin{pmatrix} z^{CC} & z^{CM} \\ z^{MC} & z^{MM} \end{pmatrix}$$

For this calculation we can use the value of the purchases of the region R to the rest of the country E. The subregions C and M can be linked by different transport infrastructures such as harbors, airports, two lane highways, four lane divided highways, conventional railways, and high speed railways.

These means of transport are much less complex to determine in the generic territorial situation that we are going to study, which consists of a relatively isolated subregion that is well connected only with a metropolitan subregion and not with their intermediate area or the rest of the country. In this situation, the intermediate area between the two regions is not very relevant to appear in the interregional analysis since it is very sparsely populated and since the fast connections between the two regions have no stops in them.

Hence if we take the table of interindustry sales of region R (composed by p subregions) with origins in the rest of the country E (composed by e subregions) , z_{ij} represents the imports that sector j of region R does to sector i of country E. This value may be decomposed in the following way, Escobedo (2005):

$$z_{ij} \Longleftrightarrow \begin{pmatrix} z_{ij}^{11} & z_{ij}^{12} & \dots & z_{ij}^{1C} & \dots & z_{ij}^{1p} \\ z_{ij}^{21} & z_{ij}^{22} & \dots & z_{ij}^{2C} & \dots & z_{ij}^{2p} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ z_{ij}^{M1} & z_{ij}^{M2} & \dots & z_{ij}^{MC} & \dots & z_{ij}^{Mp} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ z_{ij}^{(e-p)1} & z_{ij}^{(e-p)2} & \dots & z_{ij}^{(e-p)C} & \dots & z_{ij}^{(e-p)p} \end{pmatrix} \tag{17.3}$$

Each element z_{ij}^{rs} in this matrix ($r = 1 \dots e-p$; $s = 1 \dots p$) represents the purchases of sector j of subregion s to sector i of subregion r. From these $(e-p)p$ values we need z_{ij}^{MC}, which represents the imports of sector j of subregion C from sector i of subregion M. We propose to obtain these values in two stages trough two matrixes, the Regionalization Location Quotients Matrix and the Disaggregation Location Quotients Matrix.

Regionalization location quotients matrix

In the first stage we assess the total value of the purchases of sector j of subregion C to sector i of the $e-p$ other subregions from the rest of the country E,

$$z_{ij}^{E-R,C} = \sum_{r=1}^{e-p} z_{ij}^{rC}$$

Hence we search a location quotient which expresses the relation

$$l_j^{C,R,E} = \frac{z_{ij}^{E-R,C}}{z_{ij}^{E-R,R}}$$

which considers that there is a relationship between the import potential of sector j of subregion C respect import potential of sector j of region R.

This potential can be expressed using the potential models exposed above. The potential of sector j of subregion C will be expressed in the way $\frac{GAV_j^C}{d_j^{C,E-R}}$, where GAV_j^C is a measure of the economic output such as the *Gross Added Value*, GAV, of sector j of subregion C, and where $d_j^{C,E-R}$ represents the distance from the subregion C to the rest of the country E, $E-R$, for each economic sector j. Each economic sector usually sends its goods or staff by specific means of transport. In this paper we take this fact into account and we classify the economic sectors in two main groups, the heavy and light economic sectors (see table 17.1).

We will allocate the distance by two lane highway (d_{tlh}), conventional railway (d_{cr}), ship (d_s), four lane divided highway (d_{fldh}), high speed railway (d_{hsr}) or airplane (d_a) to the sectors of these groups depending more or less on the suitability of each means of transport for the types of goods of those sectors, which uses to be heavy, low value, etc., in the first group and light, high value, etc., in the second group.

All of those distances can be referred to the most common means of transport: the two lane highway. So in that way we will have

$$d_{cr} = ad_{tlh};\ d_s = bd_{tlh};\ d_{fldh} = cd_{tlh};\ d_{hsr} = ed_{tlh};\ d_a = fd_{tlh} \tag{17.4}$$

if a, b, c, e, f are coefficients that will depend on the spatial features of each case study. For example, in the case of light economic sectors, it will be probably fulfilled that $1 > a > b > c > e > f$.

In a similar way the potential of sector j of region R can be expressed by $\frac{GAV_j^R}{d_j^{R,E-R}}$. But if we want to keep a consistent formulation the potential will be expressed

$$\frac{GAV_j^C}{d_j^{C,E-R}} + \frac{GAV_j^R - GAV_j^C}{d_j^{R-C,E-R}}$$

that is, the potential of region R is the sum of the potential of subregion C and the potential of the rest of region R, $R-C$.

The location quotient of subregion C with respect to region R in sector j with respect to the rest of the country $E-R$ will be as follows:

Table 17.1. Economic sectors based on NAICS-02 divided in heavy and light groups. Source: Paper Authors

Heavy Sectors	*Light Sectors*
Agriculture, Forestry, Fishing and Hunting	Information
Mining	Finance and Insurance
Manufacturing	Real Estate and Rental and Leasing
Utilities	Professional, Scientific, and Technical Services
Construction	Management of Companies and Enterprises
Wholesale and Retail Trade	Administrative and Support Services
Transportation and Warehousing	Educational Services
Accommodation and Food Services	Health Care and Social Assistance
	Arts, Entertainment, and Recreation
	Public Administration

$$l_j^{C,R,E} = \frac{\frac{GAV_j^C}{d_j^{C,E-R}}}{\frac{GAV_j^C}{d_j^{C,E-R}} + \frac{GAV_j^R - GAV_j^C}{d_j^{R-C,E-R}}}. \tag{17.5}$$

As can be seen, there are two different types of distances. First $d_j^{C,E-R}$, which represents the distance from subregion C to the rest of the subregions of country E. This distance is assessed as the arithmetic average of the distances from the capital of subregion C, gravity center of the subregion, to the capitals of the rest of each $e-p$ other subregions of the country E,

$$d_j^{C,E-R} = \frac{\sum_{w=1}^{e-p} d_j^{w,C}}{e-p}. \tag{17.6}$$

The second distance represents the space between the $p-1$ subregions of region R to the rest of $e-p$ other subregions of the country E. We can simplify this distance $d_j^{R-C,E-R}$ as the arithmetic average of the distances between the regional capital of region R with the capitals of the other $t-1$ regions of country E, t being the number of regions of country E. Here this is,

$$d_j^{R-C,E-R} = \frac{\sum_{w=1}^{t-1} d_j^{w,R-C}}{t-1}. \tag{17.7}$$

In this formula $R-C$ is referred to the subregion that hosts the regional capital of region R.

Once we have defined the location quotient $l_j^{C,R,E}$ and the procedure to get it we can establish the first diagonal location quotients matrix, the regionalization location quotients matrix:

$$l^{C,R,E} = \begin{pmatrix} l_1^{C,R,E} & 0 & \dots & 0 \\ 0 & l_2^{C,R,E} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & l_n^{C,R,E} \end{pmatrix}. \tag{17.8}$$

Disaggregation location quotients matrix

In a second stage, the beginning point consists in the purchases of subregion C to the rest of the country E, $z_{ij}^{E-R,C}$. This term has to be divided in two parts: One part is necessary for our model, $z_{ij}^{M,C}$, what subregion C imports from subregion M, and the another part is what subregion C imports from the rest of the country E, region R and subregion M excluded, $z_{ij}^{E-R-M,C}$, so we have

$$z_{ij}^{E-R,C} = z_{ij}^{E-R-M,C} + z_{ij}^{M,C}. \tag{17.9}$$

If we introduce coefficients so all the terms depends on one variable, we have

$$z_{ij}^{E-R,C} = c_i^{E-R-M,C} z_{ij}^{E-R,C} + c_i^{M,C} z_{ij}^{E-R,C} \tag{17.10}$$

when $c_i^{E-R-M,C} + c_i^{M,C} = 1$.

These coefficients have to be proportional to the attractivity of the geographical areas represented, noted like a, and must be normalized. Here this is

$$c_i^{E-R-M,C} = \frac{a_i^{E-R-M,C}}{a_i^{E-R-M,C} + a_i^{M,C}} \text{ and } c_i^{M,C} = \frac{a_i^{M,C}}{a_i^{E-R-M,C} + a_i^{M,C}}. \tag{17.11}$$

These attractivities are going to be assessed in a way similar to former location quotients so

$$a_i^{M,C} = \frac{GAV_i^M}{d_i^{M,C}} \text{ and } a_i^{E-R-M,C} = \frac{GAV_i^E - GAV_i^R - GAV_i^M}{d_i^{E-R-M,C}} \tag{17.12}$$

when GAV_i^E, GAV_i^R, GAV_i^M are the gross added values in sector i in country E, region R and subregion M respectively. So the location quotient needed will be:

$$l_i^{M,C} = \frac{\frac{GAV_i^M}{d_i^{M,C}}}{\frac{GAV_i^M}{d_i^{M,C}} + \frac{GAV_i^E - GAV_i^R - GAV_i^M}{d_i^{E-R-M,C}}}. \tag{17.13}$$

As in former coefficients we have two new distances. First, $d_i^{M,C}$, which represents the distance between M and C subregion capitals. Second, $d_i^{E-R-M,C}$, which represents the distance from subregion C to the rest of subregions of country E excluded subregions belonging to region R and subregion C. This distance is approached by means of an arithmetic average of the distances from subregion C to the mentioned $e - p - 1$ subregions of country E, weighted by the Gross Subregion Output, GSO. In this way

$$d_i^{E-R-M,C} = \frac{\sum_{w=1}^{e-p-1} d_i^{w,C} GSO^w}{GSO^E - GSO^R - GSO^M}. \tag{17.14}$$

So once the location quotient $l_i^{M,C}$ and the procedure to obtain it have been defined, we get the following second location quotients diagonal matrix, the disaggregation matrix:

$$l_i^{M,C} = \begin{pmatrix} l_1^{M,C} & 0 & \dots & 0 \\ 0 & l_2^{M,C} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & l_n^{M,C} \end{pmatrix}. \tag{17.15}$$

Finally, if we want to get the intermediate consumption table with origin in subregion M we must carry out the following procedure:

$$Z^{MC} = l^{M,C} Z^{E,R} l^{C,R,E}. \tag{17.16}$$

17.3 Results and Discussion

This method of regionalization and disaggregation has been tested with the Provinces of Madrid and Ciudad Real in Spain. Their centers are separated by around 185 kilometers and they represent two types of territories, Ureña et al. (2005). Madrid Province and/or its metropolitan area has $8,028\ km^2$, about 5,000,000 inhabitants, and is a very

important tertiary economic center. On the other hand Ciudad Real Province, which is a part of Castilla La Mancha Region, has $19,813\ km^2$ with 487,670 inhabitants and mainly rural features. The capital of this province is Ciudad Real, a small city with 70,000 inhabitants. At the time the study was undertaken there were four main transport infrastructures connecting Ciudad Real and Madrid:

- An electrified conventional railroad line of 261 km
- A road of 184 km (four lane divided highway, 70 km, and two lane highway, 114 km)
- A road of 204 km (four lane divided highway, 171 km, and two lane highway, 33 km)
- A high speed railway line of 171 km, with no intermediate stations

The proposed model uses the 1995 input-output tables of the region of Castilla La Mancha, which includes Ciudad Real Province (there are no I-O tables of this province), and the 1996 input-output tables of the province of Madrid, which includes the metropolitan area of the capital of Spain. These tables were considered more appropriate than national ones, because in the first case the regionalization gap would be smaller, and in the second case there was no need for regionalization.

To generate the interregional input-output model with two regions, and previously to the above mentioned regionalization and disaggregation procedures, an aggregation of economic sectors had to be made. We had to confront the 56 economic sectors of the 1996 I-O Table of Madrid with the 39 economic sectors of the 1995 I-O Table of Castilla La Mancha. This confrontation resulted in a proposal of 27 economic sectors, see table 17.2. This level of disaggregation is acceptable but in the 27^{th} sector, which represents *Professional, and Technical Services* we realize that the aggregation may be too strong, as in one entry there are together economic activities as diverse as Motion Picture and Sound Recording Industries, Real Estate and Rental and Leasing, Computer Systems Design, Investigation and Security Services, Hospitals, etc.

The example that we are going to use to develop and evaluate the proposed method of regionalization and disaggregation is the approximation to the purchases that the economic sectors of Ciudad Real Province carry out in Madrid Province. Our starting data are the purchases that the economic sectors of Castilla La Mancha Region carry out in the rest of Spain, that is, the *Intermediate Demand imported from the rest of Spain Table* of 1995 Castilla La Mancha Input-Output Tables. As seen in Section 17.2, we need to do a double process of Regionalization and Disaggregation and to calculate two location quotients matrixes.

For the regionalization matrix, the first data we need are the GVA of Castilla La Mancha Region and the GVA's of Ciudad Real Province for the 27 economic sectors. The Statistics National Institute of Spain provided the data for Castilla La Mancha with a level of segregation of 30 economic sectors, something suitable for our model, but the data for Ciudad Real Province has a level of segregation of only 6 sectors, INE (2001). So we adopted the hypothesis that the relative distribution of GVA at the provincial level is the same than at the regional level. This involves an additional source of possible error because Castilla La Mancha has five provinces, and every one has two or three main specific and different strong economic sectors, so the regional economic structure is different from the economic structures of the five provinces. In the province of Ciudad Real the main two sectors are Beverage Manufacturing, specially wineries,

and Petrochemical Manufacturing. Therefore, the importance of these two sectors will be reduced with the hypothesis adopted.

On the other hand, we need to estimate two distances. The first one is the distance between the capital of Ciudad Real and the rest of Spain excluding the Region of Castilla La Mancha. Following the methodology expounded we assess the arithmetical average of the distance between Ciudad Real and the capitals of the rest of provinces of Spain in 542 km. Obviously, there should have been different distances for each economic sector, but as Ciudad Real does not have an operating airport at this time and the high speed rail network only links Ciudad Real with three capitals out of forty-six, we realized that their influence on the final value of the arithmetical average would be very small.

The second distance represents the separation between the other four provinces of Castilla La Mancha and the rest of the Spain, Ciudad Real Province excluded. To assess it, we take the distances between the regional capital, Toledo, with the regional capitals of the other sixteen regions of Spain. As Toledo, at the time that this research was undertaken, had neither high-speed rail nor an airport, the distance is the same for all the economic sectors. This distance is 545 km, a very similar value to the first one.

Following the procedure indicated in Section 17.2 we obtain the regionalization locations quotients (see table 17.2). Almost all the values except two are very similar, running from 0.241 to 0.266. This value is normal although maybe less than expected as, for example, the weight of the population and the personal income of Ciudad Real Province in the region is 28% in both cases. On the other hand many sectors have the same location quotient, as the level of disaggregation in the GVA's of the Province of Ciudad Real was low. As a last comment, two sectors have a much higher location quotient than the rest, 0.593, which are the sectors of Mining and Petroleum Manufacturing, reflecting the importance of the petrochemical complex.

The second location quotients matrix is the disaggregation matrix, which in our case will represent the balance between the weight as an exporter of Madrid Province to Ciudad Real Province and the weight as an exporter of Spain minus Castilla La Mancha Region to Ciudad Real Province. The first data we need are the GVA's of Castilla La Mancha Region, Madrid Province and Spain for the 27 economic sectors, data obtained with a level of segregation of 30 economic sectors, something suitable for our model, from INE (2001).

In this case, two types of distances will have to be assessed. The first one is the distance between Madrid and Ciudad Real. We will take for the heavy sectors (see table 17.1) the shorter distance by road, that is, 184 km, as we suppose there is no significant difference for truck transport between two and four lane highways and because conventional railway has larger distances and more scarce services. On the other hand, for the light sectors, we will choose the high speed railway distance. The travel time by this mean of transport between Madrid and Ciudad Real is slightly less than the half than the road trip time, so according to Equation 17.4 we will take the parameter $e = \frac{1}{2}$, that is, $d_{hsr} = 92\ km$.

The second distance represents the separation from Ciudad Real to Spain minus Madrid and Castilla La Mancha Regions. To assess that distance we need the values of the Gross Subregion Output of the provinces of Spain, data that is obtained in INE (2001). On the other hand these GSO weight the distances from Ciudad Real to the

Table 17.2. Disaggregation location quotient, *lme*, and regionalization location quotient, *lcre*, according to economic sectors based on NAICS-02. Source: Paper Authors

	Economic Sectors	*lme*	*lcre*
1	Agriculture, Forestry, Fishing and Hunting (11)	0,03277	0,26614
2	Mining (21)	0,25061	0,59299
3	Animal Slaughtering and Processing (3116)	0,24057	0,24120
4	Dairy Product Manufacturing (3115)	0,24057	0,24119
5	Other Food, Beverage and Tobacco Manufacturing (r311, 312)	0,24057	0,24120
6	Textile Product Mills and Apparel Manufacturing (313-315)	0,22809	0,24120
7	Leather and Allied Product Manufacturing (316)	0,22809	0,24120
8	Wood Product Manufacturing (321)	0,17346	0,24119
9	Paper Manufacturing and Printing Activities (322-323)	0,56222	0,24120
10	Utilities. Petroleum and Coal Manufacturing (22, 324)	0,37680	0,59299
11	Chemical Manufacturing (325)	0,42419	0,24120
12	Plastics and Rubber Products Manufacturing (326)	0,26128	0,24121
13	Nonmetallic Mineral Product Manufacturing (327)	0,26160	0,24120
14	Primary and Fabricated Metal Manufacturing (331-332)	0,21665	0,24120
15	Machinery Manufacturing (333)	0,31472	0,24120
16	Computer, Electronic and Electrical Manufacturing (334-335)	0,59222	0,24120
17	Transportation Equipment Manufacturing (336)	0,33334	0,24120
18	Furniture and Miscellaneous Manufacturing (337-339)	0,34746	0,24119
19	Construction (23)	0,39838	0,31183
20	Wholesale and Retail Trade (42-45)	0,38235	0,26105
21	Accommodation and Food Services (72)	0,38366	0,26105
22	Transportation and Warehousing (48, r49)	0,45894	0,26105
23	Postal Service and Telecommunications (491, 517)	0,45894	0,26105
24	Finance and Insurance (52)	0,69432	0,26105
25	Public Administration (92)	0,64252	0,26041
26	Educational Services (61)	0,53085	0,26051
27	Professional, and Technical Services (r51, 53-56, 62, 71, 81)	0,63979	0,26087

capitals of the rest of provinces of Spain, Madrid and the rest of provinces of Castilla la Mancha excluded. This distances are obtained in DPW (2004), and in this way the final weighted distance is 603 km. As we pointed out above this value is not exact as Ciudad Real Province has some high speed relations with other provinces of Spain, apart from Madrid, such as Sevilla and Cordoba. Nevertheless this would represent a very small difference, so we take the simplification and we do not take into account these two specific relations.

Once we have the different GAV and have calculated the equivalent distances, we can get the disaggregation location quotients (see table 17.2). The highest values, around 64%-69%, come from tertiary activities such as Finance and Insurance, Public Administration, Professional, and Technical Services, which reveal the importance of the capital of Spain as the core of those activities in the country. Several intermediate values are found in Educational Services, High Added Value Manufacturing (Computer, Electronic and Electrical), and Printing Activities, also strong sectors in Madrid Province, whose values are about 53%-59%. Transportation and Warehousing, Postal

Service and Telecommunications and Chemical Manufacturing are in the environs of 45%-42%, the last of these reflecting the administrative dependence of petrochemical complex on Madrid. We can emphasize too the economic sectors of low added value manufacturing, sectors 2-8 in table 17.2, which are mainly in the rank of 23%-25% and therefore, do not show a strong dependence on Madrid. Finally the lowest value comes from Agriculture, Forestry, Fishing and Hunting, which shows a very weak dependence on Madrid, only 3%.

17.4 Conclusions

The accuracy of the regionalization and disaggregation location quotients depends largely (i) on the available disaggregated *Gross Added Values* (GVA) of the territories that are considered in the interregional input-output analysis and (ii) on the level of disaggregation of the economic sectors in the interregional input-output table. If the level of disaggregation of the GVA data of a territory is similar to the number of economic sectors of the Input-Output Table, it may represent more precisely the economic structure of that territory, which means a strengthening to the effectiveness of the model. On the other hand, if there is one main economic sector in every single entry of the interregional input-output table, each location quotient will be applied to one specific economic sector so that the economical significance of the results will be more accurate.

This method is especially suitable to study subregions that have high speed means of transport, such as high speed ground transportation and air transport. Besides, if these subregions are inserted in dense and diverse networks of transport, there will be significant different distances for the different economic sectors, and the influence of the different transport infrastructures on the model will be notorious.

In our case, the highest regionalization location quotients normally show the main economic sectors of underdeveloped or very peripheral regions, which did not used to belong to high technology sectors. On the other hand, the highest disaggregation location quotients correspond to economic sectors of very peripheral regions that show a stronger dependence on metropolitan economic structures. These economic sectors belong to high added value manufacturing and tertiary services, which used to be the main economic sectors of metropolitan areas.

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Part VII

Statistical Methods

18

Jackknife Bias Correction of a Clock Offset Estimator

Daniel R. Jeske

Department of Statistics, University of California, Riverside

Abstract: Internet telephony and wireless geolocation prediction are two examples of many data networking applications that require synchronization among independent network clocks. An approach to estimating the offset between two clocks in the presence of variable network delays involves exchanging timing messages between the clocks. A well known clock offset estimator based on this approach can be interpreted as the maximum likelihood estimator when the underlying network delay distributions are assumed to be exponential. Several studies on network delay characteristics show that no single distribution adequately characterizes delays. Not only are delays highly dependent on the nature of traffic, but they are also time varying. Therefore, robustness with respect to the assumed underlying network delay distribution is an important property for any clock offset estimator.

Previous work used the bootstrap technique to obtain an estimator of the bias of the well known estimator, and a new bias-corrected estimator was proposed. The effectiveness of the new estimator was demonstrated across a wide variety of distribution assumptions. In this paper, the jackknife technique is used to derive an alternative bias-corrected estimator. The effectiveness of the jackknife estimator is compared to the effectiveness of the bootstrap estimator using a variety of distributions. Recent studies of Internet traffic show that delay distributions can be heavy-tailed, and thus special attention is given to the performance of the two estimators in the context of heavy tailed network delays.

Keywords and phrases: Bootstrap, jackknife, heavy tail distributions

18.1 Introduction

A classic sampling scheme to gather data for estimating clock offset is based on a sequence of so-called timing message exchanges. Figure 18.1 illustrates the i-th exchange between two clocks, A and B, that begins with A sending a message to B which includes a time stamp T_i^0 indicating the time as known at A when the message is sent. Immediately upon receipt of this message, B puts a time stamp T_i^1 in the received

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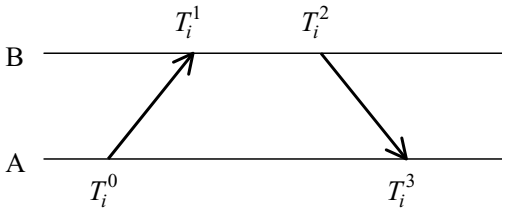

Figure 18.1. Timing message exchange

message. Just before B sends the message back to A it places another time stamp T_i^2 on the message. When A receives the returned message from B, it records another time stamp T_i^3 on the message. After n such exchanges, A has the sequence of observations $\{T_i^0, T_i^1, T_i^2, T_i^3\}_{i=1}^n$ from which to estimate the clock offset between itself and B.

Define θ to be the (unknown) offset of clock B, relative to clock A. It follows that if at a given instant clock B shows time t_B and clock A shows time t_A, then $t_B = t_A + \theta$. The sojourn times for the $A \to B$ and $B \to A$ timing messages are $X_i = T_i^1 - T_i^0$ and $Y_i = T_i^3 - T_i^2$, respectively. Apart from the offset of clock B from clock A, two other components of the message sojourn times are propagation delay and network delay. Propagation delay is the time required for the message to travel across the transmission medium connecting the two clocks if there were no other intervening delays. In general, the propagation delay is quite small, on the order of nanoseconds, for example, and it is typically assumed that the propagation delay is the same in both directions, say d. Network delay arises due to message queuing that occurs at various points along the path that the message takes to get from origin to destination. Network delay can range from milliseconds to seconds, and is the variable component of sojourn times. Let e_i^{AB} and e_i^{BA} denote the network delays associated with the $A \to B$ and $B \to A$ timing messages, respectively.

It follows from the preceding definitions, that $X_i = d + \theta + e_i^{AB}$ and $Y_i = d - \theta + e_i^{BA}$, where both d and θ are unknown. We assume that $\{e_i^{AB}\}_{i=1}^n$ is a sequence of (non-negative) independent and identically distributed random variables from a distribution function $F_{AB}(\cdot)$, and is independent of the sequence $\{e_i^{BA}\}_{i=1}^n$, which are (non-negative) independent and identically distributed random variables from a distribution function $F_{BA}(\cdot)$. In general, $F_{AB} \neq F_{BA}$ since the $A \to B$ and $B \to A$ transmission paths through the network typically have different traffic characteristics and thus the network delays in each path are potentially different [see, for example, Claffy *et al.* (1993)].

Alternative estimators of θ based on timing message exchange samples have been proposed. A frequently used estimator proposed by Paxson (1998) is $\hat{\theta} = (X_{(1)} - Y_{(1)})/2$, where $X_{(1)}$ and $Y_{(1)}$ denote the minimum of the $\{X_i\}_{i=1}^n$ and $\{Y_i\}_{i=1}^n$, respectively. Jeske and Sampath (2003) examined the bias of the Paxson estimator and derived a closed form expression for the bootstrap bias-corrected version, $\hat{\theta}^{BS}$, of the estimator. In the context of exponential network delays, it was shown analytically that $\hat{\theta}^{BS}$ has smaller mean squared error than $\hat{\theta}$. Jeske and Sampath (2003), and Jeske and Chakravartty (2006) examined the robustness of $\hat{\theta}^{BS}$ and several other estimators including the ordered-BLUEs under the exponential and Pareto models for network delays. Under a variety of alternative models, including lognormal, gamma, Weibull and a class of heavy-tail models derived from stable distributions, $\hat{\theta}^{BS}$ emerged as the most robust of all the estimators.

In this paper, the effort to improve the performance of $\hat{\theta}$ using bias-correction techniques is extended to consideration of the jackknife technique. The rest of this paper is organized as follows. In Section 18.2, the derivation of $\hat{\theta}$ and $\hat{\theta}^{BS}$ is reviewed and the jackknife bias-corrected estimator $\hat{\theta}^{JK}$ derived. In Section 18.3, the mean squared error of the three estimators $\hat{\theta}$, $\hat{\theta}^{BS}$ and $\hat{\theta}^{JK}$ is examined under the exponential and Pareto models for network delay. In Section 18.4, the robustness of the estimators is examined more broadly by comparing their MSE under a variety of models for network delay.

18.2 Candidate Clock Offset Estimators

18.2.1 Paxson's estimator

The Paxson (1998) estimator is $\hat{\theta} = (X_{(1)} - Y_{(1)})/2$. The mean of Paxson's estimator is $E(\hat{\theta}) = \theta + [E(e^{AB}_{(1)}) - E(e^{BA}_{(1)})]/2$. Provided that both of the distributions $F_{AB}(\cdot)$ and $F_{BA}(\cdot)$ have support on the interval $(0, \infty)$, $\hat{\theta}$ is asymptotically unbiased. However, with a finite number of samples, the estimator is biased since, in general $E(e^{AB}_{(1)}) \neq E(e^{BA}_{(1)})$. Jeske (2005) showed that Paxson's estimator is the maximum likelihood estimator under the assumption that network delays are exponentially distributed. As previously discussed, we cannot expect any distribution assumption for network delays to be valid all the time and as such the objective in the search for a good estimator of θ is that it exhibit robustness to whatever the underlying distribution actually is. It is reasonable, therefore, to consider modifications to $\hat{\theta}$ that reduce the bias that will inevitably exist when they are used in 'hostile' contexts.

18.2.2 Bootstrap bias-correction

Consider the class of estimators of the form $T = \sum_{i=1}^{n} w_i[X_{(i)} - Y_{(i)}]$, for a suitable choice of weights $\{w_i\}_{i=1}^{n}$ which have the property $\sum_{i=1}^{n} w_i = 1/2$. Paxson's estimator is clearly of this form where $w_1 = 1/2$ and $w_i = 0$ $(2 \leq i \leq n)$. Jeske and Chakravatty (2006) show that the bootstrap bias-corrected form of T is

$$T^{BS} = \sum_{k=1}^{n} w_k^*[X_{(k)} - Y_{(k)}].$$

Where $w_k^* = 2w_k - \sum_{i=1}^{n} w_i[u_k(i) - u_{k+1}(i)]$ and

$$u_k(i) = \sum_{j=0}^{i-1} C_j^n (k-1)^j (n-k+1)^{n-j}/n^n.$$

The weights for the bias-corrected version of Paxson's estimator are $w_1^* = 1/2 + [(n-1)/n]^n/2$ and $w_k^* = -[(n-k+1)/n]^n/2 + [(n-k)/n]^n/2$, $(2 \leq k \leq n)$, while the estimator itself is $\hat{\theta}^{BS} = \sum_{k=1}^{n} w_k^*[X_{(k)} - Y_{(k)}]$.

18.2.3 Jackknife bias-correction

Given an estimator $\hat{\theta}$ that depends on n observations, the general form of the jackknife bias-corrected estimator is $\hat{\theta}^{JK} = n\hat{\theta} - (n-1)\hat{\theta}_{(\cdot)}$, where $\hat{\theta}_{(\cdot)} = \sum_{i=1}^{n} \hat{\theta}_{(i)}/n$ and where $\hat{\theta}_{(i)}$ is the value of $\hat{\theta}$ using all but the i-th observation. For application to Paxson's estimator, we consider the observations to be the pairs $\{(X_i, Y_i)\}_{i=1}^{n}$. When considering the possible values for $\hat{\theta}_{(i)}$, two cases need to be considered: 1) $X_{(1)}$ and $Y_{(1)}$ appear in the same observation, and 2) $X_{(1)}$ and $Y_{(1)}$ do not appear in the same observation.

In the first case, two possible values among $\{\hat{\theta}_{(i)}\}_{i=1}^{n}$ will arise. When the observation $(X_{(1)}, Y_{(1)})$ is deleted, then the value of $\hat{\theta}_{(i)} = (X_{(2)} - Y_{(2)})/2$ arises. For any of the other $n-1$ observation, the value $\hat{\theta}_{(i)} = \hat{\theta}$ arises. Hence, it follows that $\hat{\theta}_{(\cdot)} = [(n-1)\hat{\theta} + (X_{(2)} - Y_{(2)})/2]/n$. In the second case, three possible values for $\{\hat{\theta}_{(i)}\}_{i=1}^{n}$ will arise. When the deleted observation includes neither $X_{(1)}$ nor $Y_{(1)}$ (which will be the case $n-2$ times), the value $\hat{\theta}_{(i)} = \hat{\theta}$ will arise. When the deleted observation includes $X_{(1)}$, the value $\hat{\theta}_{(i)} = (X_{(2)} - Y_{(1)})/2$ will arise and when it includes $Y_{(1)}$, the value $\hat{\theta}_{(i)} = (X_{(1)} - Y_{(2)})/2$ will arise. Hence, it follows that

$$\begin{aligned}\hat{\theta}_{(\cdot)} &= [(n-2)\hat{\theta} + (X_{(1)} - Y_{(2)})/2 + (X_{(2)} - Y_{(1)})/2]/n \\ &= [(n-1)\hat{\theta} + (X_{(2)} - Y_{(2)})/2]/n\end{aligned}$$

and thus we get the same value for $\hat{\theta}_{(\cdot)}$ in either case. Consequently,

$$\begin{aligned}\hat{\theta}^{JK} &= n\hat{\theta} - (n-1)[(n-1)\hat{\theta} + (X_{(2)} - Y_{(2)})/2]/n \\ &= \frac{2n-1}{2n}(X_{(1)} - Y_{(1)}) - \frac{n-1}{2n}(X_{(2)} - Y_{(2)}).\end{aligned}$$

18.3 Mean Squared Error Under Exponential and Pareto Distributions

18.3.1 Exponential distribution

We now evaluate the mean and variance of $\hat{\theta}$, $\hat{\theta}^{BS}$ and $\hat{\theta}^{JK}$ under the assumption that network delays in the $A \to B$ direction are $Exp(\lambda_{AB})$ and network delays in the $B \to A$ direction are $Exp(\lambda_{BA})$. Using standard results on order statistics of exponential distributions [see, for example, Arnold et al. (1992)] it follows that $E(X_{(i)}) = d + \theta + \mu_i/\lambda_{AB}$, where $\mu_i = \sum_{j=n-i+1}^{n} j^{-1}$, and $Var(X_{(i)}) = \sigma_i^2/\lambda_{AB}^2$, where $\sigma_i^2 = \sum_{j=n-i+1}^{n} j^{-2}$. Similarly, $E(Y_{(i)}) = d - \theta + \mu_i\lambda_{BA}$ and $Var(Y_{(i)}) = \sigma_i^2/\lambda_{BA}^2$. It follows that

$$\begin{aligned}E(\hat{\theta}) &= \theta + \frac{\lambda_{AB}^{-1} - \lambda_{BA}^{-1}}{2n} \\ Var(\hat{\theta}) &= \frac{\lambda_{AB}^{-2} + \lambda_{BA}^{-2}}{4n^2}.\end{aligned}$$

For $\hat{\theta}^{JK}$, we find

$$E(\hat{\theta}^{JK}) = \theta$$
$$Var(\hat{\theta}^{JK}) = \frac{\lambda_{AB}^{-2} + \lambda_{BA}^{-2}}{2n^2}$$

and it can be seen that the jackknife method *eliminates* the bias in $\hat{\theta}$. However, the variance is doubled relative to $\hat{\theta}$ it is easily verified that $MSE(\hat{\theta}) \leq MSE(\hat{\theta}^{JK})$. For $\hat{\theta}^{BS}$, it is convenient to use the representation $\hat{\theta}^{BS} = \sum_{i=1}^{n} w_i^*[X_{(i)} - Y_{(i)}]$ and the results (for $r < s$) $Cov(X_{(r)}, X_{(s)}) = Var(X_{(r)})$ and $Cov(Y_{(r)}, Y_{(s)}) = Var(Y_{(r)})$, to show

$$E(\hat{\theta}^{BS}) = \theta + \Big(\sum_{i=1}^{n} w_i^* \mu_i\Big) \times (\lambda_{AB}^{-1} - \lambda_{BA}^{-1})$$
$$Var(\hat{\theta}^{BS}) = (\lambda_{AB}^{-2} + \lambda_{BA}^{-2}) \times \sum_{i=1}^{n} \Big[(w_i^*)^2 + 2 \sum_{k=i+1}^{n} w_i^* w_k^*\Big]\sigma_i^2.$$

It can be shown that $MSE(\hat{\theta}^{BS}) \leq MSE(\hat{\theta})$, and thus we have the ordering $MSE(\hat{\theta}^{BS}) \leq MSE(\hat{\theta}) \leq MSE(\hat{\theta}^{JK})$. Table 18.1 illustrates this ordering by showing the absolute bias, standard deviation and root mean squared error (RMSE) of the estimators for the case where the mean delay in the $A \to B$ direction is one and the mean delay in the $B \to A$ direction is ten.

18.3.2 Pareto distribution

We now evaluate the mean and variance of $\hat{\theta}$, $\hat{\theta}^{BS}$ and $\hat{\theta}^{JK}$ under the assumption that network delays follow a translated Pareto distribution. The cumulative distribution function of the translated Pareto distribution is $F(x) = 1-(\frac{k}{k+x})^a$, for $k > 0, a > 0, x \geq 0$. We denote this distribution with the notation Pareto(k, a). Provided $a > 1$ the mean of the distribution is $k/(a-1)$, and provided $a > 2$ the variance is $ak^2/[(a-1)^2(a-2)]$, respectively. It follows from results in Arnold et al. (1992) that the mean of the r-th order statistic from a sample of n observations is kv_r, where $v_r = \frac{\Gamma(n+1)\Gamma(n-r+1-1/a)}{\Gamma(n-r+1)\Gamma(n+1-1/a)} - 1$. The variance-covariance matrix of the order statistics is $V = k^2\Sigma$, where Σ is the $n \times n$ symmetric matrix whose (r, s) $(s \geq r)$ element is $u_{rs} - (v_r + 1)(v_s + 1)$, where $u_{rs} = \frac{\Gamma(n+1)\Gamma(n-s+1-1/a)\Gamma(n-r+1-2/a)}{\Gamma(n-s+1)\Gamma(n-r+1-1/a)\Gamma(n+1-2/a)}$. We assume that e_i^{AB} are independent and identically distributed random variables that follow a Pareto(k_{AB}, a) distribution. Similarly, we assume that e_i^{BA} are independent and identically distributed random variables that follow a Pareto(k_{BA}, a) distribution.

Table 18.1. $A \to B$ network delays are Exp(1) and $B \to A$ network delays are Exp(0.1)

n	Absolute Bias			Standard Deviation			Root Mean Squared Error		
	$\hat{\theta}^{BS}$	$\hat{\theta}$	$\hat{\theta}^{JK}$	$\hat{\theta}^{BS}$	$\hat{\theta}$	$\hat{\theta}^{JK}$	$\hat{\theta}^{BS}$	$\hat{\theta}$	$\hat{\theta}^{JK}$
10	.192	.450	0	.543	.502	.711	.576	.675	.711
20	.095	.225	0	.271	.251	.355	.287	.337	.355
40	.047	.113	0	.135	.126	.178	.143	.169	.178

Table 18.2. $A \rightarrow B$ network delays are Pareto(2,3) and $B \rightarrow A$ network delays are Pareto(20,3)

n	Absolute Bias			Standard Deviation			Root Mean Squared Error		
	$\hat{\theta}^{BS}$	$\hat{\theta}$	$\hat{\theta}^{JK}$	$\hat{\theta}^{BS}$	$\hat{\theta}$	$\hat{\theta}^{JK}$	$\hat{\theta}^{BS}$	$\hat{\theta}$	$\hat{\theta}^{JK}$
10	.121	.310	.012	.385	.359	.510	.404	.474	.510
20	.062	.153	.0027	.186	.173	.245	.196	.231	.245
40	.031	.076	.00065	.092	.085	.120	.097	.114	.120

All of the estimators $\hat{\theta}$, $\hat{\theta}^{BS}$ and $\hat{\theta}^{JK}$ are expressible in the form

$$T = \sum_{i=1}^{n} w_i [X_{(i)} - Y_{(i)}]$$

for a suitable choice of weights $\{w_i\}_{i=1}^n$ that have the property $\sum_{i=1}^n w_i = 0.5$. It follows that $E(T) = \theta + (k_{AB} - k_{BA})w'v$ and $Var(T) = (k_{AB}^2 + k_{BA}^2)w'\Sigma w$. Thus, under the translated Pareto assumption for network delays the MSE of each estimator in Section 18.2 can be calculated from the formula $MSE(T) = [(k_{AB} - k_{BA})w'v]^2 + (k_{AB}^2 + k_{BA}^2)w'\Sigma w$ by simply substituting the appropriate weight vector for w.

Table 18.2 shows bias, standard deviation, and root mean squared error (RMSE) for the cases where $(k_{AB}, a) = (2, 3)$ and $(k_{BA}, a) = (20, 3)$, which correspond to mean network delays of 1 and 10 in the $A \rightarrow B$ direction and $B \rightarrow A$ direction, respectively. We can see in this case that $\hat{\theta}^{JK}$ again has achieved greater bias reduction than $\hat{\theta}^{BS}$, and in fact has nearly eliminated it completely once again. But in terms of RMSE, we once again have $MSE(\hat{\theta}^{BS}) \leq MSE(\hat{\theta}) \leq MSE(\hat{\theta}^{JK})$.

18.4 Additional Mean Squared Error Comparisons via Simulation

18.4.1 Lognormal, gamma and Weibull distribution

Let LN(μ, σ) denote the lognormal distribution whose mean is $exp(\mu + \sigma^2/2)$, Gamma(r, λ) denote the gamma distribution whose mean is r/λ, and Weibull(β, θ) denote the Weibull distribution whose mean is $\theta\Gamma(1 + 1/\beta)$. When network delays follow these distributions, the mean squared errors of the estimators do not have simple closed form expressions. Figures 18.2–18.4 show the RMSE of the estimators $\hat{\theta}$, $\hat{\theta}^{BS}$ and $\hat{\theta}^{JK}$ that were obtained by simulating 100,000 sets of n message exchanges. The simulation size of 100,000 was selected based on good agreement between simulation results and analytic calculations that are available in the exponential case. Each message exchange was simulated by generating the pair of one-way sojourn times (X_i, Y_i) from the formulas $X_i = d + \theta + e_i^{AB}$ and $Y_i = d - \theta + e_i^{BA}$, where the $\{e_i^{AB}\}_{i=1}^n$ and $\{e_i^{BA}\}_{i=1}^n$ are simulated from the selected distribution. Since each of the estimators is of the form $T = \sum_{i=1}^n w_i[X_{(i)} - Y_{(i)}]$, we take $d = 0$ and $\theta = 0$ without loss of generality.

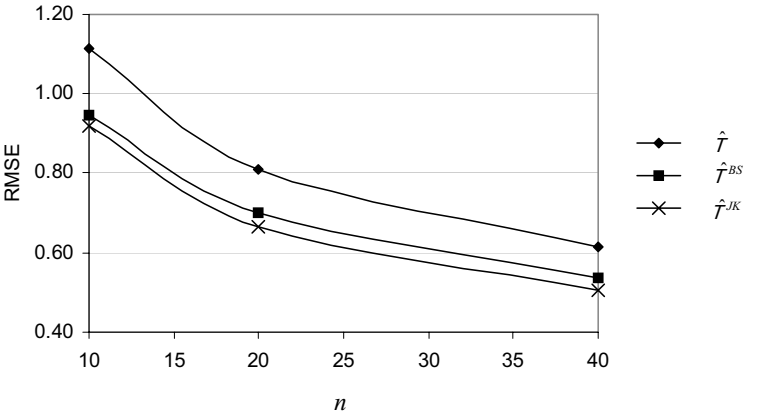

Figure 18.2. RMSE When $A \rightarrow B$ Delays are LN$(-0.35, 0.83)$ and $B \rightarrow A$ Delays are LN$(1.96, 0.83)$

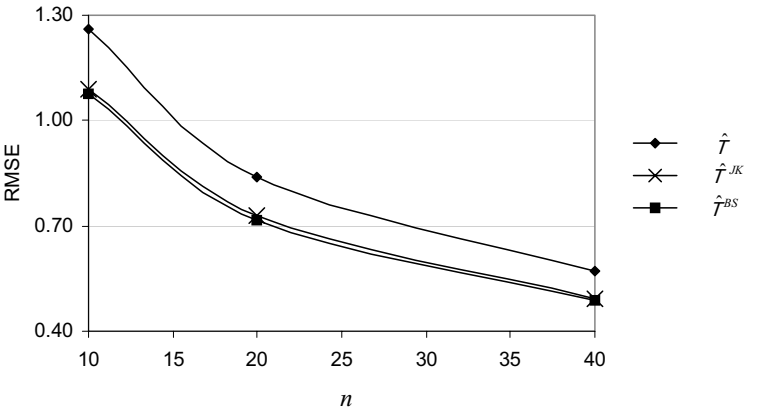

Figure 18.3. RMSE When $A \rightarrow B$ Delays are Gamma$(2, 2)$ and $B \rightarrow A$ Delays are Gamma$(2, 0.2)$

In figures 18.2–18.4, the mean network delays in the $A \rightarrow B$ direction and $B \rightarrow A$ directions are 1 and 10, respectively. For the lognormal distribution, $\sigma = 0.83$ was chosen to make the coefficient of variation unity and μ was then selected to achieve the desired mean. For the gamma distribution, and $r = 2$ was chosen and λ was then selected to achieve the desired mean. Finally, for the Weibull distribution $\beta = 2$ was chosen and θ was then selected to achieve the desired mean. Conclusions drawn from simulations based on other parameter values for the lognormal, gamma and Weibull distributions produce are consistent with what we discuss in light of figures 18.2-18.4.

Figures 18.2–18.4 show that $\hat{\theta}^{BS}$ and $\hat{\theta}^{JK}$ essentially have the same RMSE, and both offer significant improvements over $\hat{\theta}$. Not shown by the figures is the fact that $\hat{\theta}^{JK}$ is significantly more effective at bias reduction than $\hat{\theta}^{BS}$, but those gains are offset in terms of RMSE by the associated increased variance.

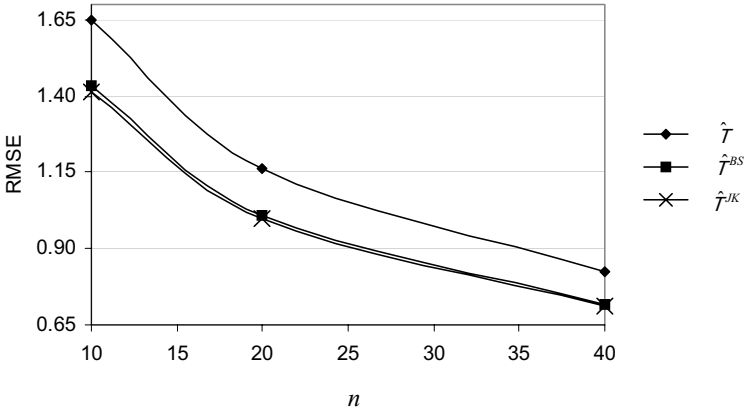

Figure 18.4. RMSE When $A \rightarrow B$ Delays are Weibull$(2, 1.13)$ and $B \rightarrow A$ Delays are Weibull$(2, 11.3)$

18.4.2 Heavy tailed distributions

The network delay model utilized in this section is $|X|$, where X has a Stable $(\alpha, 0, \gamma, 0)$ distribution [see, for example, Nolan (2005)]. Although the distribution of $|X|$ is not stable, it does have a heavy tail provided that $\alpha < 2$. We utilize the absolute value transformation to impose the non-negativity constraint we have for network delays, and select $\beta = 0$ to allow skewness to be solely introduced by the absolute value transformation (avoiding the possibility that the resulting distribution is multimodal). Selecting $\delta = 0$ enables the use of $E|X| = 2\Gamma(1 - 1/\alpha)\gamma/\pi$ and thus γ can be selected to set the mean at a desired level [see, for example, Samorodnitsky (1994)].

A simulation study was used to investigate the bias and mean squared error properties of $\hat{\theta}$, $\hat{\theta}^{BS}$ and $\hat{\theta}^{JK}$ under the proposed heavy tail distribution for network delays. A sample size of $n = 20$ and means of 1 and 10 for network delays in the $A \rightarrow B$ and $B \rightarrow A$ directions, respectively, were selected. The value of α was varied among the values $\{1.5, 1.6, 1.7, 1.8, 1.9, 2.0\}$ with corresponding values of γ chosen from the relation $E|X| = 2\Gamma(1 - 1/\alpha)\gamma/\pi$. The first four choices of α produce a distribution with tails heavier than the Pareto$(20, 3)$ distribution. The choice $\alpha = 2$ corresponds to a folded normal distribution. Observations for X, and hence $|X|$ were simulated using the algorithm described in Chambers et al. (1976, 1987). The number of simulations used was 5 million, and it was verified by using a larger number of simulations that this was sufficient to estimate the bias to within three significant digits.

Figure 18.5 shows the absolute bias of $\hat{\theta}$, $\hat{\theta}^{BS}$ and $\hat{\theta}^{JK}$ as a function of α. In each case the mean network delay in the $A \rightarrow B$ and $B \rightarrow A$ directions are one and ten, respectively. Figure 18.5 shows once again that both $\hat{\theta}^{BS}$ and $\hat{\theta}^{JK}$ are effective at reducing bias, and $\hat{\theta}^{JK}$ again nearly eliminates it. Figure 18.6 shows the RMSE of the estimators and it is evident that $\hat{\theta}^{JK}$ loses its advantage over $\hat{\theta}$ due to the variance increase that comes along with its bias reduction. On the other hand, $\hat{\theta}^{BS}$ continues to outperform $\hat{\theta}$.

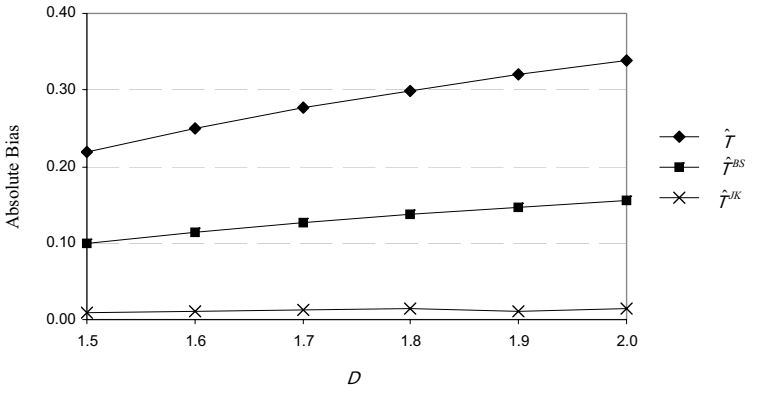

Figure 18.5. Absolute Bias When $A \rightarrow B$ Delays are $|\text{Stable}(\alpha, 0, \gamma, 0)|$ with $\gamma = 0.5\pi\Gamma^{-1}(1 - 1/\alpha)$ and $B \rightarrow A$ Delays are $|\text{Stable}(\alpha, 0, \gamma, 0)|$ with $\gamma = 5\pi\Gamma^{-1}(1 - 1/\alpha)$

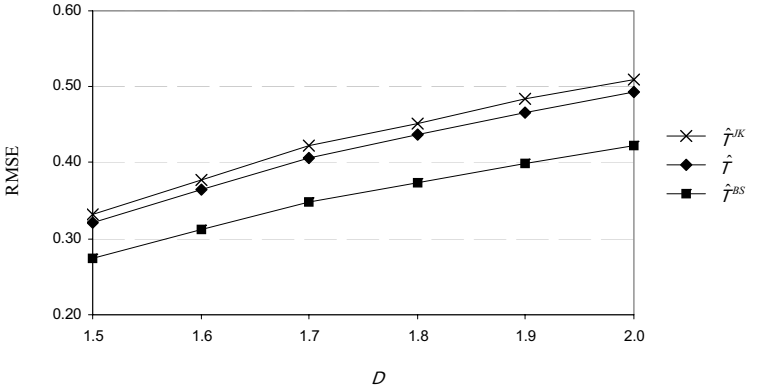

Figure 18.6. RMSE When $A \rightarrow B$ Delays are $|\text{Stable}(\alpha, 0, \gamma, 0)|$ with $\gamma = 0.5\pi\Gamma^{-1}(1 - 1/\alpha)$ and $B \rightarrow A$ Delays are $|\text{Stable}(\alpha, 0, \gamma, 0)|$ with $\gamma = 5\pi\Gamma^{-1}(1 - 1/\alpha)$

18.5 Summary

Previous work identified the bootstrap bias-corrected version of the Paxson (1998) estimator of clock offset to be robust in terms of mean squared error properties over a wide variety of alterative distributions for network delays. In this paper, we explored whether jackknife bias-correction of the Paxson estimator would offer similar, or even better, performance. We have seen that the jackknife bias-corrected estimator does a better job at reducing bias (even eliminating it completely for the case of exponential delays), but that for the most part the gains in reduced absolute bias are eroded by the variance increase. Thus, the recommended estimator from an overall point of view remains the bootstrap bias-corrected version of Paxson's estimator.

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19

Pretesting in Polytomous Logistic Regression Models Based on Phi-divergence Measures

Leandro Pardo[1], María Luisa Menéndez[2], and Nirian Martín[3]

[1] Department of Statistics and Operations Research I, Complutense University of Madrid, Spain
[2] Department of Applied Mathematics, E.T.S.A.M., Technical University of Madrid, Spain
[3] Department of Statistics and Operations Research III, Complutense University of Madrid, Spain

Abstract: In this paper, we study a preliminary test estimator based on phi-divergence measures for the vector of parameters in the Polytomous Logistic Regression Model when additional linear restrictions on the parameter vector are assumed to hold.

Keywords and phrases: Phi-divergence test statistics, unrestricted and restricted minimum phi-divergence estimator, preliminary test estimation

19.1 Introduction

Consider a response random variable Y belonging to one of J distinct categories $C_1, ..., C_J$, which is observed together with $p+1$ explanatory variables $\boldsymbol{x}^T = (1, x_1, ..., x_p) \in \mathbb{R}^{p+1}$. For convenience $x_0 = 1$. Let $\pi_j(\boldsymbol{x}) = \Pr(Y \in C_j \mid \boldsymbol{x})$, $j = 1, ..., J$, denotes the probability that the random variable Y belongs to the category C_j, $j = 1, ..., J$, when the explanatory variable is $\boldsymbol{x}$. More specifically suppose that the dependence between Y and $\boldsymbol{x}$ can be modeled by the multinomial logistic regression model

$$\pi_j(\boldsymbol{x}) = \exp\left(\boldsymbol{\beta}_j^T \boldsymbol{x}\right) \Big/ \sum_{l=1}^{J} \exp\left(\boldsymbol{\beta}_l^T \boldsymbol{x}\right), \ j = 1, ..., J, \tag{19.1}$$

where $\boldsymbol{\beta}_j^T = (\beta_{0j}, ..., \beta_{pj})$, $j = 1, ..., J-1$, is a vector of unknown parameters and $\boldsymbol{\beta}_J$ is a $(p+1)$-dimensional vector of zeros, for convenience. The vector

$$\boldsymbol{\beta}^T = \left(\boldsymbol{\beta}_1^T, ..., \boldsymbol{\beta}_{J-1}^T\right) \tag{19.2}$$

is ν-dimensional with $\nu = (J-1)(p+1)$. The parameters β_{0j}, $j = 1, ..., J-1$, are intercept parameters and $(\beta_{1j}, ..., \beta_{pj})$ are regression parameter vectors, $j = 1, ..., J-1$. The model described in (19.1) is the classical *Polytomous Logistic Regression Model*

B.C. Arnold et al. (eds.), *Advances in Mathematical and Statistical Modeling*,
DOI: 10.1007/978-0-8176-4626-4_19,

(PLRM). For more details about this model see Liu and Agresti (2005) and references there in. In the following we shall denote

$$\begin{aligned}\Theta =&\{\boldsymbol{\beta}:\boldsymbol{\beta}^T=\left(\boldsymbol{\beta}_1^T,...,\boldsymbol{\beta}_{J-1}^T\right),\\ &\boldsymbol{\beta}_j^T=\left(\beta_{0j},...,\beta_{pj}\right),j=1,...,J-1:\beta_{sj}\in\mathbb{R},\ s=0,...,p\},\end{aligned}\tag{19.3}$$

the parameter space associated with the PLRM.

Assume that N different values of the vector of explanatory variables,

$$\boldsymbol{x}_i^T=\left(1,x_{i1},...,x_{ip}\right),\quad i=1,...,N,$$

are available. Let $n\left(\boldsymbol{x}_i\right)$ be the number of observations considered when the explanatory variable $\boldsymbol{x}$ has the value $\boldsymbol{x}_i$, in such a way that if $\boldsymbol{x}$ is fixed at $\boldsymbol{x}_i$ we have a multinomial distribution with parameters

$$\left\{n\left(\boldsymbol{x}_i\right);\pi_1\left(\boldsymbol{x}_i\right),...,\pi_J\left(\boldsymbol{x}_i\right)\right\},\quad i=1,...,N.$$

Vectors of probabilities are denoted by $\pi\left(\boldsymbol{x}_i\right)=\left(\pi_1\left(\boldsymbol{x}_i\right),...,\pi_J\left(\boldsymbol{x}_i\right)\right)^T$ and total sample size by $n=n\left(\boldsymbol{x}_1\right)+...+n\left(\boldsymbol{x}_N\right)$. Given the explanatory variable $\boldsymbol{x}_i$, denote by y_{si} the number of observations in the class C_s, $s=1,...,J$. It is clear that $n\left(\boldsymbol{x}_i\right)=\sum_{s=1}^J y_{si}$. To estimate β_{js} $(j=0,...,p;s=1,...,J-1)$ Gupta et al. (2006) considered the minimum ϕ-divergence estimator defined by

$$\widehat{\boldsymbol{\beta}}^{\phi}\equiv\arg\min_{\boldsymbol{\beta}\in\Theta}D_{\phi}\left(\widehat{\boldsymbol{\beta}},\boldsymbol{p}\left(\boldsymbol{\beta}\right)\right),\tag{19.4}$$

where

$$\begin{aligned}\widehat{\boldsymbol{p}}&=\left(\frac{y_{11}}{n},...,\frac{y_{J1}}{n},\frac{y_{12}}{n},...,\frac{y_{J2}}{n},...,\frac{y_{1N}}{n},...,\frac{y_{JN}}{n}\right)^T,\\ \boldsymbol{p}\left(\boldsymbol{\beta}\right)&=\left(\frac{n(\boldsymbol{x}_1)}{n}\left(\pi_1\left(\boldsymbol{x}_1\right),...,\pi_J\left(\boldsymbol{x}_1\right)\right),...,\frac{n(\boldsymbol{x}_N)}{n}\left(\pi_1\left(\boldsymbol{x}_N\right),...,\pi_J\left(\boldsymbol{x}_N\right)\right)\right)^T\end{aligned}\tag{19.5}$$

and $D_{\phi}\left(\widehat{\boldsymbol{p}},\boldsymbol{p}\left(\boldsymbol{\beta}\right)\right)$ is the ϕ-divergence measure between the probability vectors $\widehat{\boldsymbol{p}}$ and $\boldsymbol{p}\left(\boldsymbol{\beta}\right)$, given by

$$D_{\phi}\left(\widehat{\boldsymbol{p}},\boldsymbol{p}\left(\boldsymbol{\beta}\right)\right)\equiv\sum_{j=1}^{J}\sum_{i=1}^{N}\pi_j\left(\boldsymbol{x}_i\right)\frac{n\left(\boldsymbol{x}_i\right)}{n}\phi\left(\frac{y_{ji}}{\pi_j\left(\boldsymbol{x}_i\right)n\left(\boldsymbol{x}_i\right)}\right);\phi\in\boldsymbol{\Phi}^*,\tag{19.6}$$

where $\boldsymbol{\Phi}^*$ is the class of all convex functions $\phi\left(x\right)$, $x>0$, such that at $x=1,\phi\left(1\right)=\phi'\left(1\right)=0,\phi''\left(1\right)>0$, at $x=0$, $0\phi\left(0/0\right)=0$ and $0\phi\left(p/0\right)=p\lim_{u\to\infty}\phi\left(u\right)/u$. Some properties of ϕ-divergence measures can be found in Cressie and Pardo (2003) and Pardo (2006).

In the particular case of $\phi\left(x\right)=x\log x-x+1$ we obtain the Kullback-Leibler divergence, $D_{Kull}(\widehat{\boldsymbol{p}},\boldsymbol{p}\left(\boldsymbol{\beta}\right))$. It is not difficult to establish that

$$D_{Kull}\left(\widehat{\boldsymbol{p}},\boldsymbol{p}\left(\boldsymbol{\beta}\right)\right)=c-\frac{1}{n}\log\prod_{i=1}^{N}\prod_{l=1}^{J}\pi_l\left(\boldsymbol{x}_i\right)^{y_{li}}\approx-\log L\left(\boldsymbol{\beta}\right),$$

where $L\left(\boldsymbol{\beta}\right)$ is the likelihood function associated with the model under consideration and c is independent of $\boldsymbol{\beta}$. Therefore the maximum likelihood estimator can be seen

as the minimum Kullback-Leibler divergence estimator. In this sense the minimum ϕ-divergence estimator, defined in (19.4), can be considered as a generalization of the maximum likelihood estimator.

In addition to the sample information contained in the model, information in the form of r linear hypotheses about $\boldsymbol{\beta}$ may be denoted as $\boldsymbol{K}^T\boldsymbol{\beta}=\boldsymbol{m}$ or, if the linear hypotheses are incorrect as $\boldsymbol{K}^T\boldsymbol{\beta}-\boldsymbol{m}=\boldsymbol{\delta}$, where $\boldsymbol{m}$ is a known vector, $\boldsymbol{K}^T$ is a $r \times (J-1)(p+1)$ known matrix of rank r and $\boldsymbol{\delta}$ is an unknown $r \times 1$ vector representing specification errors in the linear hypotheses or perceived information. Making use of both the sample and exact prior information in $\boldsymbol{K}^T\boldsymbol{\beta}=\boldsymbol{m}$ we can get the restricted minimum ϕ-divergence estimator,

$$\widehat{\boldsymbol{\beta}}_{\phi}^{H_0} \equiv \arg\min_{\boldsymbol{\beta}\in\Theta_0} D_{\phi}\left(\widehat{\boldsymbol{p}}, \boldsymbol{p}\left(\boldsymbol{\beta}\right)\right), \tag{19.7}$$

being $\Theta_0 = \left\{\boldsymbol{\beta} \in \Theta : \boldsymbol{K}^T\boldsymbol{\beta}=\boldsymbol{m}\right\}$.

In order to test the compatibility of the restricted and unrestricted estimates, $H_0 : \boldsymbol{\beta} \in \Theta_0$ or $H_0 : \boldsymbol{K}^T\boldsymbol{\beta}=\boldsymbol{m}$, we can use a ϕ-divergence test statistic,

$$T_n^{\phi_1,\phi_2} = \frac{2n}{\phi_1''(1)} D_{\phi_1}\left(\boldsymbol{p}\left(\widehat{\boldsymbol{\beta}}_{\phi_2}\right), \boldsymbol{p}\left(\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}\right)\right). \tag{19.8}$$

If the linear hypotheses are correct the ϕ-divergence test statistic has asymptotically a chi-square distribution with r degrees of freedom. Under contiguous alternative hypotheses (see (19.13) or (19.14)) the ϕ-divergence test statistic has asymptotically a non-central chi-square with r degrees of freedom and a given noncentrality parameter (see Theorem 2). A procedure that we can follow is to test the null hypothesis that $\boldsymbol{K}^T\boldsymbol{\beta}=\boldsymbol{m}$ by using a ϕ-divergence test statistic defined in (19.8) and if we accept $\boldsymbol{K}^T\boldsymbol{\beta}=\boldsymbol{m}$, we use the restricted minimum ϕ-divergence estimator as our estimate of $\boldsymbol{\beta}$; otherwise the conventional or unrestricted minimum ϕ-divergence estimator is used. Now we use the test statistic (19.8) as well as the sample information to define an alternative estimator to the estimators $\widehat{\boldsymbol{\beta}}_{\phi_2}$ and $\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}$ for $\boldsymbol{\beta}$. We shall consider the preliminary ϕ-divergence test estimator, defined by

$$\widehat{\boldsymbol{\beta}}_{\phi_1,\phi_2}^{pre} = \widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0} I_{\left(0,\chi^2_{r,\alpha}\right)}(T_n^{\phi_1,\phi_2}) + \widehat{\boldsymbol{\beta}}_{\phi_2} I_{\left[\chi^2_{r,\alpha},\infty\right)}(T_n^{\phi_1,\phi_2}),$$

where $I_A(y)$ denotes the function taking the value 1 if $y \in A$ and 0 if $y \notin A$. Preliminary test estimation was introduced by Bancroft (1944). Since then many papers studying the behaviour of this procedure of estimation have been published. An interesting study about preliminary test estimation in different statistical problems can be seen in Saleh (2006). In Section 19.2 some asymptotic distributional results are given. In Section 19.3 we present the asymptotic distributional quadratic risk for $\widehat{\boldsymbol{\beta}}_{\phi_2}$, $\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}$ and $\widehat{\boldsymbol{\beta}}_{\phi_1,\phi_2}^{pre}$. Finally, Section 19.4 presents a comparison among $\widehat{\boldsymbol{\beta}}_{\phi_2}$, $\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}$ and $\widehat{\boldsymbol{\beta}}_{\phi_1,\phi_2}^{pre}$ under null and contiguous alternative hypotheses.

19.2 Preliminaries and Notation

The expression of the Fisher information matrix in the PLRM is

$$\boldsymbol{I}_{F,n}(\boldsymbol{\beta}) = \boldsymbol{X}^T \boldsymbol{V}_n(\boldsymbol{\beta}) \boldsymbol{X} = \sum_{j=1}^{N} \frac{n(\boldsymbol{x}_j)}{n} \boldsymbol{X}_j^T \boldsymbol{V}_j(\boldsymbol{\beta}) \boldsymbol{X}_j$$

where $\boldsymbol{X}^T = \left(\boldsymbol{X}_1^T, ..., \boldsymbol{X}_N^T\right)_{(p+1)(J-1)\times(J-1)N}$,

$$\boldsymbol{X}_i = \begin{pmatrix} \boldsymbol{x}_i^T & \boldsymbol{0}^T & ... & \boldsymbol{0}^T \\ \boldsymbol{0}^T & \boldsymbol{x}_i^T & ... & \boldsymbol{0}^T \\ . & . & . & . \\ \boldsymbol{0}^T & \boldsymbol{0}^T & ... & \boldsymbol{x}_i^T \end{pmatrix}_{(J-1)\times(J-1)(p+1)} \tag{19.9}$$

and the matrix $\boldsymbol{V}_n(\boldsymbol{\beta})$ is defined by

$$\boldsymbol{V}_n(\boldsymbol{\beta}) = diag\left(\frac{n(\boldsymbol{x}_1)}{n}\boldsymbol{V}_1(\boldsymbol{\beta}), ..., \frac{n(\boldsymbol{x}_N)}{n}\boldsymbol{V}_N(\boldsymbol{\beta})\right)_{N(J-1)\times N(J-1)} \tag{19.10}$$

with

$$\boldsymbol{V}_i(\boldsymbol{\beta})_{(J-1)\times(J-1)} = \left(\pi_s(\boldsymbol{x}_i)\left(\delta_{st} - \pi_t(\boldsymbol{x}_i)\right)\right)_{s,t=1,...,J-1}, \ i = 1, ..., N,$$

where δ_{st} is the Kronecker delta.

We denote

$$\boldsymbol{V}_n^*(\boldsymbol{\beta}) = diag\left(\frac{n(\boldsymbol{x}_1)}{n}\boldsymbol{C}_1(\boldsymbol{\beta}), ..., \frac{n(\boldsymbol{x}_I)}{n}\boldsymbol{C}_I(\boldsymbol{\beta})\right)_{JN\times N(J-1)}$$

with

$$\boldsymbol{C}_i(\boldsymbol{\beta})_{(J-1)\times(J-1)} = \left(\pi_s(\boldsymbol{x}_i)\left(\delta_{st} - \pi_t(\boldsymbol{x}_i)\right)\right)_{\substack{s=1,...,J \\ t=1,...,J-1}}, \ i = 1, ..., I. \tag{19.11}$$

In Gupta et al. (2006) it was established that

$$\widehat{\boldsymbol{\beta}}_{\phi_2} = \boldsymbol{\beta}_0 + \left(\boldsymbol{X}^T \boldsymbol{V}_n(\boldsymbol{\beta}_0) \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \boldsymbol{V}_n^*(\boldsymbol{\beta}_0)^T diag\left(\boldsymbol{p}(\boldsymbol{\beta}_0)^{-1/2}\right)\left(\widehat{\boldsymbol{p}} - \boldsymbol{p}(\boldsymbol{\beta}_0)\right) + \left\|\widehat{\boldsymbol{p}} - \boldsymbol{p}(\boldsymbol{\beta}_0)\right\| \boldsymbol{\alpha}_1\left(\widehat{\boldsymbol{p}}; \widehat{\boldsymbol{p}} - \boldsymbol{p}(\boldsymbol{\beta}_0)\right),$$

where $\boldsymbol{\beta}_0$ is the true value of the parameter and the function $\boldsymbol{\alpha}_1 : \mathbb{R}^{JN} \to \mathbb{R}^{(J-1)(p+1)}$ verifies $\boldsymbol{\alpha}_1(\boldsymbol{p}; \boldsymbol{p} - \boldsymbol{p}(\boldsymbol{\beta}_0)) \to \boldsymbol{0}$ as $\boldsymbol{p} \to \boldsymbol{p}(\boldsymbol{\beta}_0)$. Let $\phi_2(t)$ be twice differentiable function at $t > 0$ and $n(\boldsymbol{x}_i) \to \infty$, $i = 1, ..., N$, such that $n(\boldsymbol{x}_i)/n \to \lambda_i > 0$, $i = 1, ..., N$. In the cited paper of Gupta et al. (2006) it was established that

$$\sqrt{n}\left(\widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_0\right) \underset{n\to\infty}{\overset{L}{\to}} N\left(\boldsymbol{0}, \left(\boldsymbol{X}^T \boldsymbol{V}_\lambda(\boldsymbol{\beta}_0) \boldsymbol{X}\right)^{-1}\right),$$

being

$$\boldsymbol{V}_\lambda(\boldsymbol{\beta}_0) = diag\left(\lambda_1 \boldsymbol{V}_1(\boldsymbol{\beta}_0), ..., \lambda_N \boldsymbol{V}_N(\boldsymbol{\beta}_0)\right) = \lim_{n\to\infty} \boldsymbol{V}_n(\boldsymbol{\beta}_0).$$

Based on Pardo et al. (2002) we get the following expansion for the restricted minimum ϕ_2-divergence estimator $\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}$,

$$\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0} = \boldsymbol{\beta}_0 + \boldsymbol{H}_n(\boldsymbol{\beta}_0)\left(\boldsymbol{X}^T\boldsymbol{V}_n(\boldsymbol{\beta}_0)\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{V}_n^*(\boldsymbol{\beta}_0)$$
$$\times diag\left(\boldsymbol{p}(\boldsymbol{\beta}_0)^{-1/2}\right)(\widehat{\boldsymbol{p}} - \boldsymbol{p}(\boldsymbol{\beta}_0)) + \|\widehat{\boldsymbol{p}} - \boldsymbol{p}(\boldsymbol{\beta}_0)\|\,\boldsymbol{\alpha}_2(\widehat{\boldsymbol{p}};\widehat{\boldsymbol{p}}-\boldsymbol{p}(\boldsymbol{\beta}_0)), \quad (19.12)$$

where

$$\boldsymbol{H}_n(\boldsymbol{\beta}_0) = \boldsymbol{I} - \left(\boldsymbol{X}^T\boldsymbol{V}_n(\boldsymbol{\beta}_0)\boldsymbol{X}\right)^{-1}\boldsymbol{K}\left(\boldsymbol{K}^T\left(\boldsymbol{X}^T\boldsymbol{V}_n(\boldsymbol{\beta}_0)\boldsymbol{X}\right)^{-1}\boldsymbol{K}\right)^{-1}\boldsymbol{K}^T$$

and $\boldsymbol{\alpha}_2$ is a function verifying $\boldsymbol{\alpha}_2(\boldsymbol{p};\boldsymbol{p}-\boldsymbol{p}(\boldsymbol{\beta}_0)) \to \boldsymbol{0}$ as $\boldsymbol{p} \to \boldsymbol{p}(\boldsymbol{\beta}_0)$.

19.3 Contiguous Alternative Hypotheses

Let $\boldsymbol{\beta}_n \in \Theta - \Theta_0$ be a given alternative and let $\boldsymbol{\beta}$ be the element in Θ_0 closest to $\boldsymbol{\beta}_n$ in the Euclidean distance sense. A first possibility to introduce contiguous alternative hypotheses is to consider a fixed $\boldsymbol{\Delta}^T \in \mathbb{R}^{(J-1)(p+1)}$ and allowing $\boldsymbol{\beta}_n$ to move towards $\boldsymbol{\beta}$ as n increases in the following way

$$H_{1,n} : \boldsymbol{\beta}_n = \boldsymbol{\beta} + n^{-1/2}\boldsymbol{\Delta}. \quad (19.13)$$

A second approach is to relax the condition $g(\boldsymbol{\beta}) = \boldsymbol{K}^T\boldsymbol{\beta} - \boldsymbol{m} = \boldsymbol{0}$ defining Θ_0. Let $\boldsymbol{\delta}^T \in \mathbb{R}^r$ be and consider the following sequence, $\boldsymbol{\beta}_n$, of parameters approaching Θ_0 according to

$$H_{1,n}^* : g(\boldsymbol{\beta}_n) = n^{-1/2}\boldsymbol{\delta}. \quad (19.14)$$

Note that a Taylor series expansion of $g(\boldsymbol{\beta}_n)$ around $\boldsymbol{\beta} \in \Theta_0$ yields

$$g(\boldsymbol{\beta}_n) = g(\boldsymbol{\beta}) + \boldsymbol{K}^T(\boldsymbol{\beta}_n - \boldsymbol{\beta}) + \|\boldsymbol{\beta}_n - \boldsymbol{\beta}\|\,\boldsymbol{\alpha}_3(\boldsymbol{\beta}_n;\boldsymbol{\beta}_n - \boldsymbol{\beta}), \quad (19.15)$$

being $\boldsymbol{\alpha}_3$ a function verifying $\boldsymbol{\alpha}_3(\boldsymbol{\beta}_n;\boldsymbol{\beta}_n - \boldsymbol{\beta}) \to \boldsymbol{0}$ as $\boldsymbol{\beta}_n \to \boldsymbol{\beta}$. By substituting $\boldsymbol{\beta}_n = \boldsymbol{\beta} + n^{-1/2}\boldsymbol{\Delta}$ in (19.15) and taking into account that $g(\boldsymbol{\beta}) = 0$, we obtain

$$g(\boldsymbol{\beta}_n) = n^{-1/2}\boldsymbol{K}^T\boldsymbol{\Delta} + \|\boldsymbol{\beta}_n - \boldsymbol{\beta}\|\,\boldsymbol{\alpha}_3(\boldsymbol{\beta}_n;\boldsymbol{\beta}_n - \boldsymbol{\beta}),$$

so that the equivalence in the limit is obtained for $\boldsymbol{\delta} = \boldsymbol{K}^T\boldsymbol{\Delta}$.

The following result will be important in the next section.

Theorem 1. *Under* $H_{1,n}^*$ *we have*

$$\sqrt{n}g\left(\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}\right) \xrightarrow[n\to\infty]{L} N\left(\boldsymbol{\delta},\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\right)$$

and under $H_{1,n}$

$$\sqrt{n}g\left(\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}\right) \xrightarrow[n\to\infty]{L} N\left(\boldsymbol{K}^T\boldsymbol{\Delta},\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\right),$$

where $\boldsymbol{\Sigma}_{\boldsymbol{U}} = \left(\boldsymbol{X}^T\boldsymbol{V}_\lambda(\boldsymbol{\beta}_0)\boldsymbol{X}\right)^{-1}$.

PROOF. A Taylor series expansion of $g\left(\widehat{\boldsymbol{\beta}}_{\phi_2}\right)$ around $\boldsymbol{\beta}_n$ yields

$$g\left(\widehat{\boldsymbol{\beta}}_{\phi_2}\right) = g\left(\boldsymbol{\beta}_n\right) + \boldsymbol{K}^T\left(\widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_n\right) + \left\|\widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_n\right\| \boldsymbol{\alpha}_4\left(\widehat{\boldsymbol{\beta}}_{\phi_2}; \widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_n\right),$$

where $\boldsymbol{\alpha}_4\left(\boldsymbol{\beta}^*; \boldsymbol{\beta}^* - \boldsymbol{\beta}_n\right) \to \mathbf{0}$ as $\boldsymbol{\beta}^* \to \boldsymbol{\beta}_n$. From (19.15) we have

$$\begin{aligned} g\left(\widehat{\boldsymbol{\beta}}_{\phi_2}\right) = n^{-1/2}\boldsymbol{K}^T\boldsymbol{\Delta} + \boldsymbol{K}^T\left(\widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_n\right) + \left\|\widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_n\right\| \boldsymbol{\alpha}_4\left(\widehat{\boldsymbol{\beta}}_{\phi_2}; \widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_n\right) \\ + \left\|\boldsymbol{\beta}_n - \boldsymbol{\beta}\right\| \boldsymbol{\alpha}_3\left(\boldsymbol{\beta}_n; \boldsymbol{\beta}_n - \boldsymbol{\beta}\right). \end{aligned}$$

As $n^{1/2}\left\|\widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_n\right\|$ is bounded in probability and, under $H_{1,n}$, $\widehat{\boldsymbol{\beta}}_{\phi_2} \xrightarrow[n\to\infty]{P} \boldsymbol{\beta}_n$ we have,

$$n^{1/2}\left\|\widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_n\right\| \boldsymbol{\alpha}_4\left(\widehat{\boldsymbol{\beta}}_{\phi_2}; \widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_n\right) \xrightarrow[n\to\infty]{P} \mathbf{0}.$$

Similarly $n^{1/2}\left\|\boldsymbol{\beta}_n - \boldsymbol{\beta}\right\| \boldsymbol{\alpha}_3\left(\boldsymbol{\beta}_n; \boldsymbol{\beta}_n - \boldsymbol{\beta}\right) \xrightarrow[n\to\infty]{P} \mathbf{0}$. Therefore,

$$\sqrt{n}g\left(\widehat{\boldsymbol{\beta}}_{\phi_2}\right) \xrightarrow[n\to\infty]{L} N\left(\boldsymbol{K}^T\boldsymbol{\Delta}, \boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\right),$$

because under $H_{1,n}^*$

$$\sqrt{n}\left(\widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_n\right) \xrightarrow[n\to\infty]{L} N\left(\mathbf{0}, \boldsymbol{\Sigma}_{\boldsymbol{U}}\right).$$

Now from the relationship $\boldsymbol{\delta} = \boldsymbol{K}^T\boldsymbol{\Delta}$, if $g\left(\boldsymbol{\beta}_n\right) = n^{-1/2}\boldsymbol{\delta}$, then

$$\sqrt{n}g\left(\widehat{\boldsymbol{\beta}}_{\phi_2}\right) \xrightarrow[n\to\infty]{L} N\left(\boldsymbol{\delta}, \boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\right).$$

■

The following theorem presents the asymptotic distribution of $T_n^{\phi_1,\phi_2}$, given in (19.8), under $H_{1,n}^*$.

Theorem 2. *Under $H_{1,n}^*$ the asymptotic distribution of $T_n^{\phi_1,\phi_2}$ is chi-squared with r degrees of freedom and noncentrality parameter*

$$\mu = \boldsymbol{\delta}^T\left(\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\right)^{-1}\boldsymbol{\delta}. \tag{19.16}$$

PROOF. It is not difficult to establish that

$$T_n^{\phi_1,\phi_2} = \sqrt{n}\left(\widehat{\boldsymbol{\beta}}_{\phi_2} - \widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}\right)^T \boldsymbol{I}_{F,n}\left(\boldsymbol{\beta}_0\right)\sqrt{n}\left(\widehat{\boldsymbol{\beta}}_{\phi_2} - \widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}\right) + o_p(1).$$

Now we are going to look for another expression for $\widehat{\boldsymbol{\beta}}_{\phi_2} - \widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}$. By (19.12) we have,

$$
\begin{aligned}
\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0} &= \boldsymbol{\beta}_0 + \boldsymbol{H}_n\left(\boldsymbol{\beta}_0\right)\left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{V}_n^*\left(\boldsymbol{\beta}_0\right) diag\left(\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)^{-1/2}\right)\left(\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right) \\
&\quad + \left\|\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right\|\boldsymbol{\alpha}_2\left(\widehat{\boldsymbol{p}};\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right) \\
&= \boldsymbol{\beta}_0 + \left(\boldsymbol{I}-\left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{K}\left(\boldsymbol{K}^T\left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{K}\right)^{-1}\boldsymbol{K}^T\right) \\
&\quad \times\left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{V}_n^*\left(\boldsymbol{\beta}_0\right) diag\left(\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)^{-1/2}\right)\left(\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right) \\
&\quad + \left\|\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right\|\boldsymbol{\alpha}_2\left(\widehat{\boldsymbol{p}};\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right) \\
&= \boldsymbol{\beta}_0 + \left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{V}_n^*\left(\boldsymbol{\beta}_0\right) diag\left(\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)^{-1/2}\right)\left(\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right) \\
&\quad - \left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{K}\left(\boldsymbol{K}^T\left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{K}\right)^{-1}\boldsymbol{K}^T\left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1} \\
&\quad \times\boldsymbol{X}^T\boldsymbol{V}_n^*\left(\boldsymbol{\beta}_0\right) diag\left(\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)^{-1/2}\right)\left(\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right) + \left\|\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right\|\boldsymbol{\alpha}_2\left(\widehat{\boldsymbol{p}};\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right) \\
&= \widehat{\boldsymbol{\beta}}_{\phi_2} - \left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{K}\left(\boldsymbol{K}^T\left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{K}\right)^{-1}\boldsymbol{K}^T\left(\widehat{\boldsymbol{\beta}}_{\phi_2}-\boldsymbol{\beta}_0\right) \\
&\quad + \left\|\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right\|\left(\boldsymbol{\alpha}_2\left(\widehat{\boldsymbol{p}};\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right)-\boldsymbol{\alpha}_1\left(\widehat{\boldsymbol{p}};\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right)\right) \\
&= \widehat{\boldsymbol{\beta}}_{\phi_2} - \left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{K}\left(\boldsymbol{K}^T\left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{K}\right)^{-1}\left(\boldsymbol{K}^T\widehat{\boldsymbol{\beta}}_{\phi_2}-\boldsymbol{m}\right) \\
&\quad + \left\|\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right\|\left(\boldsymbol{\alpha}_2\left(\widehat{\boldsymbol{p}};\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right)-\boldsymbol{\alpha}_1\left(\widehat{\boldsymbol{p}};\widehat{\boldsymbol{p}}-\boldsymbol{p}\left(\boldsymbol{\beta}_0\right)\right)\right).
\end{aligned}
$$

Therefore we get,

$$
\begin{aligned}
T_n^{\phi_1,\phi_2} &= \sqrt{n}\left(\boldsymbol{K}^T\widehat{\boldsymbol{\beta}}_{\phi_2}-\boldsymbol{m}\right)^T\left(\boldsymbol{K}^T\left(\boldsymbol{X}^T\boldsymbol{V}_n\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1}\boldsymbol{K}\right)^{-1}\sqrt{n}\left(\boldsymbol{K}^T\widehat{\boldsymbol{\beta}}_{\phi_2}-\boldsymbol{m}\right) \\
&\quad + o_p(1).
\end{aligned}
$$

Now the result follows from Theorem 1 and Lemma in (Ferguson (1996), p. 63). ■

Remark 1. We denote

$$
\boldsymbol{U}_n = \sqrt{n}\left(\widehat{\boldsymbol{\beta}}_{\phi_2}-\boldsymbol{\beta}_n\right) \text{ and } \boldsymbol{Z}_n = \sqrt{n}\left(\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}-\boldsymbol{\beta}_n\right).
$$

The random vectors $\boldsymbol{U}$ and $\boldsymbol{Z}$ obtained as

$$
\boldsymbol{U}_n \xrightarrow[n\to\infty]{L} \boldsymbol{U} \quad \text{and } \boldsymbol{Z}_n \xrightarrow[n\to\infty]{L} \boldsymbol{Z},
$$

respectively, are distributed normally with mean vectors and variance covariance matrices given by

$$
\boldsymbol{\mu}_{\boldsymbol{U}} = \boldsymbol{0}, \qquad \boldsymbol{\Sigma}_{\boldsymbol{U}} = \left(\boldsymbol{X}^T\boldsymbol{V}_\lambda\left(\boldsymbol{\beta}_0\right)\boldsymbol{X}\right)^{-1} \tag{19.17}
$$

and

$$
\boldsymbol{\mu}_{\boldsymbol{Z}} = -\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\left(\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\right)^{-1}\boldsymbol{\delta}, \qquad \boldsymbol{\Sigma}_{\boldsymbol{Z}} = \boldsymbol{\Sigma}_{\boldsymbol{U}} - \boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\left(\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\right)^{-1}\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}, \tag{19.18}
$$

respectively.

If we denote $\boldsymbol{Y}_n = \sqrt{n}\left(\boldsymbol{K}^T\widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{m}\right)$, the random vector $\left(\boldsymbol{U}_n^T, \boldsymbol{Y}_n^T\right)^T$ converges in law to a normal distribution with mean vector $\left(\boldsymbol{0}^T, \boldsymbol{\delta}^T\right)^T$ and variance-covariance matrix

$$\begin{pmatrix} \boldsymbol{\Sigma_U} & \boldsymbol{\Sigma_U K} \\ \boldsymbol{K}^T\boldsymbol{\Sigma_U} & \boldsymbol{K}^T\boldsymbol{\Sigma_U K} \end{pmatrix}.$$

Therefore the asymptotic distribution of the random vector $\boldsymbol{U}$ conditioned to $\boldsymbol{Y} = \boldsymbol{y}$ is normal with mean vector

$$\boldsymbol{\mu_{U/Y=y}} = \boldsymbol{\Sigma_U K}\left(\boldsymbol{K}^T\boldsymbol{\Sigma_U K}\right)^{-1}(\boldsymbol{y}-\boldsymbol{\delta})$$

and variance-covariance matrix

$$\boldsymbol{\Sigma_U} = \boldsymbol{\Sigma_U} - \boldsymbol{\Sigma_U K}\left(\boldsymbol{K}^T\boldsymbol{\Sigma_U K}\right)^{-1}\boldsymbol{K}^T\boldsymbol{\Sigma_U} = \boldsymbol{\Sigma_Z}.$$

19.4 Asymptotic Distributional Quadratic Risk of $\widehat{\boldsymbol{\beta}}_{\boldsymbol{\phi_2}}$, $\widehat{\boldsymbol{\beta}}_{\boldsymbol{\phi_2}}^{\boldsymbol{H_0}}$ and $\widehat{\boldsymbol{\beta}}_{\boldsymbol{\phi_1,\phi_2}}^{\boldsymbol{pre}}$

In the following theorem we are going to get the asymptotic distribution of the random vector

$$\boldsymbol{W}_n = \sqrt{n}\left(\widehat{\boldsymbol{\beta}}_{\phi_1,\phi_2}^{pre} - \boldsymbol{\beta}_n\right).$$

By $G_r(x;\mu)$ we shall denote the distribution function of a noncentral chi-square random variable with r degrees of freedom and noncentrality parameter μ evaluated at x and by $\Phi_{N(\boldsymbol{a},\boldsymbol{\Sigma})}(\boldsymbol{x})$ the distribution function of a normal random variable with mean vector $\boldsymbol{a}$ and variance-covariance matrix $\boldsymbol{\Sigma}$ evaluated at $\boldsymbol{x}$.

Theorem 3. *Under $H_{1,n}^*$ the random vector $\boldsymbol{W}_n$ converges in law to the random vector $\boldsymbol{W}$ whose distribution function is given by*

$$F_{\boldsymbol{W}}(\boldsymbol{x}) = \Phi_{N(\boldsymbol{0},\boldsymbol{\Sigma_Z})}(\boldsymbol{x}+\boldsymbol{L\delta})\,G_r\left(\chi_{r,\alpha}^2;\mu\right) + \int\limits_{E(\boldsymbol{\delta})} \Phi_{N(\boldsymbol{0},\boldsymbol{\Sigma_Z})}(\boldsymbol{x}-\boldsymbol{Ls})\,d\Phi_{N\left(\boldsymbol{0},\boldsymbol{K}^T\boldsymbol{\Sigma_U K}\right)}(\boldsymbol{s}),$$

where

$$\boldsymbol{L} = \boldsymbol{\Sigma_U K}\left(\boldsymbol{K}^T\boldsymbol{\Sigma_U K}\right)^{-1} \tag{19.19}$$

and

$$E(\boldsymbol{\delta}) = \left\{\boldsymbol{s} : (\boldsymbol{s}+\boldsymbol{\delta})^T\left(\boldsymbol{K}^T\boldsymbol{\Sigma_U K}\right)^{-1}(\boldsymbol{s}+\boldsymbol{\delta}) > \chi_{r,\alpha}^2\right\}.$$

By $\chi_{r,\alpha}^2$ we are denoting the value verifying $\Pr\left(\chi_r^2 \le \chi_{r,\alpha}^2\right) = \alpha$ and χ_r^2 is a chi-square random variable with "r" degrees of freedom.

PROOF. The result follows by Remark 1. ■

Let $\widehat{\boldsymbol{\beta}}^*$ be a suitable estimator of $\boldsymbol{\beta}$, and $\boldsymbol{M}$ a given positive semi-definite matrix. The standard quadratic loss function is

$$L\left(\widehat{\boldsymbol{\beta}}^*, \boldsymbol{\beta}\right) = \left(\widehat{\boldsymbol{\beta}}^* - \boldsymbol{\beta}\right)^T \boldsymbol{M} \left(\widehat{\boldsymbol{\beta}}^* - \boldsymbol{\beta}\right)$$

and the asymptotic distributional quadratic risk (ADQR), $R\left(\widehat{\boldsymbol{\beta}}^*; \boldsymbol{M}\right)$, of $\widehat{\boldsymbol{\beta}}^*$, under $H_{1,n}^*$, is defined by

$$\lim_{n\to\infty} E\left[\sqrt{n}\left(\widehat{\boldsymbol{\beta}}^* - \boldsymbol{\beta}_n\right)^T \boldsymbol{M}\sqrt{n}\left(\widehat{\boldsymbol{\beta}}^* - \boldsymbol{\beta}_n\right)\right].$$

The following theorem presents the ADQR for $\widehat{\boldsymbol{\beta}}_{\phi_2}$, $\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}$ and $\widehat{\boldsymbol{\beta}}_{\phi_1,\phi_2}^{pre}$.

Theorem 4. *Under $H_{1,n}^*$ and assuming that ϕ_1 and ϕ_2 are twice differentiable continuously at $x > 0$, we have:*

$$R\left(\widehat{\boldsymbol{\beta}}_{\phi_2}; \boldsymbol{M}\right) = tr\left(\boldsymbol{M}\boldsymbol{\Sigma}_{\boldsymbol{U}}\right),$$

$$R\left(\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}; \boldsymbol{M}\right) = tr\left(\boldsymbol{M}\boldsymbol{\Sigma}_{\boldsymbol{Z}}\right) + \boldsymbol{\delta}^T\boldsymbol{L}^T\boldsymbol{M}\boldsymbol{L}\boldsymbol{\delta}$$

and

$$R\left(\widehat{\boldsymbol{\beta}}_{\phi_1,\phi_2}^{pre}; \boldsymbol{M}\right) = tr\left(\boldsymbol{M}\boldsymbol{\Sigma}_{\boldsymbol{U}}\right) - tr\left(\boldsymbol{M}\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\left(\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\right)^{-1}\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\right) G_{r+2}\left(\chi_{r,\alpha}^2; \mu\right)$$
$$+ \boldsymbol{\delta}^T\boldsymbol{L}^T\boldsymbol{M}\boldsymbol{L}\boldsymbol{\delta}\left[-G_{r+4}\left(\chi_{r,\alpha}^2; \mu\right) + 2G_{r+2}\left(\chi_{r,\alpha}^2; \mu\right)\right].$$

PROOF. Under $H_{1,n}^*$ the random vector $\boldsymbol{U}_n = \sqrt{n}\left(\widehat{\boldsymbol{\beta}}_{\phi_2} - \boldsymbol{\beta}_n\right)$ is asymptotically normal with mean vector $\mathbf{0}$ and variance-covariance matrix $\boldsymbol{\Sigma}_{\boldsymbol{U}}$. Therefore the result for $\widehat{\boldsymbol{\beta}}_{\phi_2}$ follows immediately.

The asymptotic distribution of the random vector $\boldsymbol{Z}_n = \sqrt{n}\left(\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0} - \boldsymbol{\beta}_0\right)$ is normal with mean vector $\boldsymbol{\mu}_{\boldsymbol{Z}}$ and variance-covariance matrix $\boldsymbol{\Sigma}_{\boldsymbol{Z}}$, given in (19.18). Therefore,

$$R\left(\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}; \boldsymbol{M}\right) = tr\left(\boldsymbol{M}\boldsymbol{\Sigma}_{\boldsymbol{Z}}\right) + \boldsymbol{\mu}_{\boldsymbol{Z}}^T\boldsymbol{M}\boldsymbol{\mu}_{\boldsymbol{Z}},$$

and $\boldsymbol{\mu}_{\boldsymbol{Z}}^T\boldsymbol{M}\boldsymbol{\mu}_{\boldsymbol{Z}} = \boldsymbol{\delta}^T\boldsymbol{L}^T\boldsymbol{M}\boldsymbol{L}\boldsymbol{\delta}$. The result follows for $\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}$.

In relation with $\widehat{\boldsymbol{\beta}}_{\phi_1,\phi_2}^{pre}$we have,

$$
\begin{aligned}
R\left(\widehat{\boldsymbol{\beta}}^{pre}_{\phi_1,\phi_2};\boldsymbol{M}\right) &= \int \boldsymbol{x}^T\boldsymbol{M}\boldsymbol{x}dF_{\boldsymbol{W}}\left(\boldsymbol{x}\right)\\
&= G_r\left(\chi^2_{r,\alpha};\mu\right)\left(tr\left(\boldsymbol{M}\boldsymbol{\Sigma}_{\boldsymbol{Z}}\right)+\boldsymbol{\delta}^T\boldsymbol{L}^T\boldsymbol{M}\boldsymbol{L}\boldsymbol{\delta}\right)\\
&+ \int\limits_{E(\boldsymbol{\delta})}\left(\int \boldsymbol{x}^T\boldsymbol{M}\boldsymbol{x}\phi_{N(\boldsymbol{0},\boldsymbol{\Sigma}_{\boldsymbol{Z}})}\left(\boldsymbol{x}-\boldsymbol{L}\boldsymbol{s}\right)d\boldsymbol{x}\right)d\Phi_{N\left(\boldsymbol{0},\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\right)}\left(\boldsymbol{s}\right)\\
&= G_r\left(\chi^2_{r,\alpha};\mu\right)\left(tr\left(\boldsymbol{M}\boldsymbol{\Sigma}_{\boldsymbol{Z}}\right)+\boldsymbol{\delta}^T\boldsymbol{L}^T\boldsymbol{M}\boldsymbol{L}\boldsymbol{\delta}\right)\\
&+ \int\limits_{E(\boldsymbol{\delta})}\left(tr\left(\boldsymbol{M}\boldsymbol{\Sigma}_{\boldsymbol{Z}}\right)+\boldsymbol{s}^T\boldsymbol{L}^T\boldsymbol{M}\boldsymbol{L}\boldsymbol{s}\right)d\Phi_{N\left(\boldsymbol{0},\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\right)}\left(\boldsymbol{s}\right).
\end{aligned}
$$

By Sen (1979), we have

$$
\int\limits_{E(\boldsymbol{\delta})} tr\left(\boldsymbol{M}\boldsymbol{\Sigma}_{\boldsymbol{Z}}\right)d\Phi_{N\left(\boldsymbol{0},\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}\right)}\left(\boldsymbol{s}\right) = tr\left(\boldsymbol{M}\boldsymbol{\Sigma}_{\boldsymbol{Z}}\right)\left(1-G_r\left(\chi^2_{r,\alpha};\mu\right)\right)
$$

and

$$
\begin{aligned}
\textstyle\int_{E(\boldsymbol{\delta})}\boldsymbol{s}^T\boldsymbol{L}^T\boldsymbol{M}\boldsymbol{L}\boldsymbol{s}d\Phi_{N(\boldsymbol{0},\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K})}(\boldsymbol{z}) &= \left(1-G_{r+2}\left(\chi^2_{r,\alpha};\mu\right)\right)\\
&\times tr(\boldsymbol{M}\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K}(\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}}\boldsymbol{K})^{-1}\boldsymbol{K}^T\boldsymbol{\Sigma}_{\boldsymbol{U}})\\
&- \boldsymbol{\delta}^T\boldsymbol{L}^T\boldsymbol{M}\boldsymbol{L}\boldsymbol{\delta}\{G_r\left(\chi^2_{r,\alpha};\mu\right)-2G_{r+2}\left(\chi^2_{r,\alpha};\mu\right)\\
&+ G_{r+4}\left(\chi^2_{r,\alpha};\mu\right)\}.
\end{aligned}
$$

Now the result follows for $\widehat{\boldsymbol{\beta}}^{pre}_{\phi_2}$. ■

19.5 Comparison of $\widehat{\boldsymbol{\beta}}_{\boldsymbol{\phi_2}}$, $\widehat{\boldsymbol{\beta}}^{\boldsymbol{H_0}}_{\boldsymbol{\phi_2}}$ and $\widehat{\boldsymbol{\beta}}^{\boldsymbol{pre}}_{\boldsymbol{\phi_1},\boldsymbol{\phi_2}}$

Under $H_0 : \boldsymbol{K}^T\boldsymbol{\beta}=\boldsymbol{m}$ it is immediate to get

$$
R\left(\widehat{\boldsymbol{\beta}}^{H_0}_{\phi_2};\boldsymbol{M}\right) < R\left(\widehat{\boldsymbol{\beta}}^{pre}_{\phi_1,\phi_2};\boldsymbol{M}\right) < R\left(\widehat{\boldsymbol{\beta}}_{\phi_2};\boldsymbol{M}\right),
$$

because $\boldsymbol{\delta}=\boldsymbol{0}$.

In order to study the behavior of the ADQR's under contiguous alternative hypotheses we are going to assume that $\boldsymbol{M}=\boldsymbol{X}^T\boldsymbol{V}_\lambda(\boldsymbol{\beta}_0)\boldsymbol{X}$. In this case we have

$$
R\left(\widehat{\boldsymbol{\beta}}_{\phi_2};\boldsymbol{M}\right) = (p+1)(J-1)
$$

and

$$
R\left(\widehat{\boldsymbol{\beta}}^{H_0}_{\phi_2};\boldsymbol{M}\right) = (p+1)(J-1)-r+\mu,
$$

where μ was defined in (19.16). Therefore

$$R\left(\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0};\boldsymbol{M}\right) \leq R\left(\widehat{\boldsymbol{\beta}}_{\phi_2};\boldsymbol{M}\right)$$

if $\mu < r$, i.e., if the noncentrality parameter, μ, is less than r the estimator $\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}$ performs better than $\widehat{\boldsymbol{\beta}}_{\phi}$.

On the other hand

$$R\left(\widehat{\boldsymbol{\beta}}_{\phi_1,\phi_2}^{pre};\boldsymbol{M}\right) = (p+1)(J-1) - r\left\{G_{r+2}(\chi^2_{r,\alpha};\mu) + \mu\left[G_{r+4}(\chi^2_{r,\alpha};\mu) - 2G_{r+2}(\chi^2_{r,\alpha};\mu)\right]\frac{1}{r}\right\}.$$

Therefore

$$R\left(\widehat{\boldsymbol{\beta}}_{\phi_1,\phi_2}^{pre};\boldsymbol{M}\right) \leq R\left(\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0};\boldsymbol{M}\right),$$

i.e., $\widehat{\boldsymbol{\beta}}_{\phi_1,\phi_2}^{pre}$ performs better than $\widehat{\boldsymbol{\beta}}_{\phi_2}^{H_0}$ if the noncentrality parameter μ verifies,

$$\mu > \frac{r\left(1 - G_{r+2}(\chi^2_{r,\alpha};\mu)\right)}{1 - G_{r+4}(\chi^2_{r,\alpha};\mu) + 2G_{r+2}(\chi^2_{r,\alpha};\mu)}.$$

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20

A Unified Approach to Model Selection, Discrimination, Goodness of Fit and Outliers in Time Series

Daniel Peña[1] and Pedro Galeano[2]

[1] Department of Statistics, Carlos III University of Madrid, Spain
[2] Department of Statistics and Operations Research, University of Santiago de Compostela, Spain

Abstract: This article presents a unifying approach of several procedures in time series. First, we show that quadratic discrimination provides a framework for deriving model selection criteria for time series. Second, we establish a connection between model selection criteria and goodness of fit tests. Finally, we show that the outlier detection problem in ARIMA models can be seen as a particular case of model selection. Therefore, the problems of model selection, discrimination, goodness of fit tests and outliers in time series can be treated under the same principles.

Keywords and phrases: Akaike information criterion, ARIMA models, Bayesian information criterion, discrimination, portmanteau tests, robust estimation

20.1 Introduction

Model selection criteria are widely used for selecting the model that better fits the data among a set of candidates. These criteria have been derived from different points of view, and it is usual to classify them into two different groups. The first one is formed by the consistent criteria, which, under certain conditions and the assumption that the true model is in the set of candidates, asymptotically select the true one. Two consistent criteria are the Bayesian information criterion (BIC), derived by Schwarz (1978), which selects the model with highest posterior probability, and the Hannan-Quinn criterion (HQC), derived by Hannan and Quinn (1979), which was designed to have the fastest convergence rate to the true model. The second group is formed by the efficient criteria, which, under certain conditions, asymptotically select the model that produces the least mean square prediction error. Three efficient criteria are the final prediction error criterion (FPE), derived by Akaike (1969), which selects the model that minimizes the one step ahead square prediction error; the Akaike information criterion (AIC), derived by Akaike (1973), which is an estimator of the expected Kullback-Leibler divergence between the true and the fitted model; and the corrected Akaike information

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criterion (AICc), derived by Hurvich and Tsai (1989), which is a bias correction form of the AIC that appears to work better in small samples.

All these criteria have the general form:

$$MSC = -2 \times (\text{maximized log-likelihood}) + r \times C(T, r),$$

where r is the number of estimated parameters in the prediction function of the model, T is the sample size, and $C(T, r) = \log(T)$, for the BIC, $C(T, r) = 2c \log\log(T)$ with $c > 1$, for the HQC, $C(T, r) = (T/r)\log((T + r)/(T - r))$ for the FPE, $C(T, r) = 2$ for the AIC, and $C(T, r) = 2T/(T - r - 1)$ for the AICc.

The discrimination problem appears when it is known that the data have been generated by one of the members of a set of models and the objective is to classify the data into the generating population. When the data are Gaussian distributed, the classification is usually made by using either the quadratic discrimination rule or the Bayesian posterior probabilities. The first purpose of this paper is to show the connection between discrimination and model selection in linear Gaussian time series.

Goodness of fit tests are a useful tool for checking whether the data are well fitted by a chosen model. These tests proceed by using a test statistic and some cut-off value that takes into account the potential loss incurred if the model is wrongly rejected. Some authors (see Pukilla, Koreisha and Kallinen, 1990, and Koreisha and Pukilla (1995)) have proposed to substitute goodness of fit tests for model selection procedures, but the relationship between these two approaches is not well understood. We show that there is a close connection between model selection criteria and the powerful goodness of fit test proposed by Peña and Rodríguez (2006).

Real data are often affected by the presence of outliers, which may have serious effects on the statistical analysis of the data. Usual methods to detect the presence of outliers are based on a likelihood ratio test and the distribution of the test statistic is computed by Monte Carlo and depends on the model and the sample size. The third contribution of this paper is to show that the detection of outliers in a linear Gaussian time series can be seen as a model selection problem, and thus model selection criteria provide objective rules for outlier detection.

The rest of this paper is organized as follows. Section 20.2 briefly presents the notation and some estimation results for the class of autoregressive moving average Gaussian time series models. Section 20.3 discusses the connection between the quadratic discriminant rules in linear Gaussian time series and model selection criteria, from both the maximum likelihood and the Bayesian approach. Section 6.4 proves the connection between the goodness of fit test proposed by Peña and Rodríguez (2006) and model selection criteria. Finally, Section 20.5 shows that the problem of outlier detection in time series can be seen as a model selection problem and suggests new suitable solutions to this problem.

20.2 Estimating ARMA Time Series Models

In what follows we assume that a time series given by $x = (x_1, ..., x_T)'$ has been generated by the autoregressive moving average Gaussian process, ARMA(p, q), given by the equation:

$$x_t - \phi_1 x_{t-1} - \ldots - \phi_p x_{t-p} = a_t - \theta_1 a_{t-1} - \ldots - \theta_q a_{t-q}, \tag{20.1}$$

where a_t is a sequence of independent Gaussian distributed random variables with zero mean and variance $\sigma^2_{p,q}$. The ARMA(p,q) model, denoted by $M_{p,q}$, has the $(p+q+1)\times 1$ vector of parameters $\alpha_{p,q} = \left(\beta'_{p,q}, \sigma^2_{p,q}\right)'$ where $\beta_{p,q} = (\phi_1, \ldots, \phi_p, \theta_1, \ldots, \theta_q)'$, and is assumed to be causal, invertible, stationary and such that the polynomials $1 - \phi_1 B - \ldots - \phi_p B^p$ and $1 - \theta_1 B - \ldots - \theta_q B^q$ have no common roots.

The likelihood function of x under the model $M_{p,q}$ is given by:

$$p\left(x \mid M_{p,q}\right) = (2\pi)^{-\frac{T}{2}} \left|\Sigma_{p,q}\right|^{-\frac{1}{2}} \exp\left(-\frac{1}{2} x' \Sigma^{-1}_{p,q} x\right), \tag{20.2}$$

where $\Sigma_{p,q}$ is the $T \times T$ covariance matrix of x under the model $M_{p,q}$, which can be written as $\Sigma_{p,q} = \sigma^2_{p,q} Q_{p,q}$, where $Q_{p,q}$ is a $T \times T$ matrix which only depends on the parameters $\beta_{p,q}$. The vector of innovations can be written as $a_{p,q} = L^{-1}_{p,q} x$, where $Q_{p,q} = L_{p,q} L'_{p,q}$ is the Cholesky decomposition of $Q_{p,q}$.

The maximum likelihood estimators of the parameters $\alpha_{p,q}$ in the model $M_{p,q}$ are denoted by $\widehat{\alpha}_{p,q} = \left(\widehat{\beta}'_{p,q}, \widehat{\sigma}^2_{p,q}\right)'$ and are obtained after maximizing the log-likelihood of x under model $M_{p,q}$, given by:

$$\log p\left(x \mid M_{p,q}\right) = -\frac{T}{2} \log 2\pi - \frac{1}{2} \log \left|\Sigma_{p,q}\right| - \frac{1}{2} x' \Sigma^{-1}_{p,q} x.$$

The estimated covariance matrix of x under the model $M_{p,q}$ is written as $\widehat{\Sigma}_{p,q} = \widehat{\sigma}^2_{p,q} \widehat{Q}_{p,q}$, where $\widehat{Q}_{p,q}$ is the matrix $Q_{p,q}$ with $\beta_{p,q}$ replaced by $\widehat{\beta}_{p,q}$. The vector of residuals of the fit can be written as $\widehat{a}_{p,q} = \widehat{L}^{-1}_{p,q} x$, where $\widehat{Q}_{p,q} = \widehat{L}_{p,q} \widehat{L}'_{p,q}$ is the Cholesky decomposition of $\widehat{Q}_{p,q}$.

20.3 Quadratic Discrimination of ARMA Time Series Models

The discrimination problem in time series can be stated as follows (see, Galeano and Peña (2000)). Suppose it is known that the time series $x = (x_1, \ldots, x_T)'$ has been generated by one of the models $M_{p,q}$, in which $p \in \{0, \ldots, p_{\max}\}$ and $q \in \{0, \ldots, q_{\max}\}$, where $p_{\max}$ and $q_{\max}$ are some fixed upper bounds. The objective of discrimination is to select the true data generating model of the time series x, which is denoted by M_{p_0,q_0} and has the $(p_0 + q_0 + 1) \times 1$ vector of parameters $\alpha_{p_0,q_0} = \left(\beta'_{p_0,q_0}, \sigma^2_{p_0,q_0}\right)'$. This is equivalent to consider the set of hypothesis $M_{p,q} : x \in N_T\left(0, \Sigma_{p,q}\right)$. The standard quadratic classification rule will select the model which maximizes the likelihood (20.2), while the Bayesian classification rule will select the model which maximizes the posterior probability $p\left(M_{p,q} \mid x\right) = cp\left(M_{p,q}\right) p\left(x \mid M_{p,q}\right)$, where $p\left(M_{p,q}\right)$ is the prior probability of the model $M_{p,q}$ and c is a constant.

In practice, the vector of parameters $\alpha_{p,q}$ is unknown. Following the maximum likelihood approach, if the unknown parameters, $\alpha_{p,q}$, are replaced by its maximum likelihood estimates, $\widehat{\alpha}_{p,q} = \widehat{\alpha}_{p,q}(x)$, the rule (20.2) will always choose the model with the largest number of parameters. A first attempt to avoid this problem is to compute

the expected likelihood rather than the observed likelihood. Thus, we may select the model that maximizes the expectation with respect to a new realization of the process, y, of the same size than x, and generated by the true model with parameters α_{p_0,q_0}, given by:

$$E_{\alpha_{p_0,q_0}}\left[\log p(y|\widehat{\alpha}_{p,q})\right] = \int \log p(y|\widehat{\alpha}_{p,q}) p(y|\alpha_{p_0,q_0}) dy.$$

Note that this approach takes into account the uncertainty about new observations but not the uncertainty in the parameter estimates. Galeano and Peña (2007a) showed that this expectation can be computed as:

$$E_{\alpha_{p_0,q_0}}\left[\log p(y|\widehat{\alpha}_{p,q})\right] = -\frac{T}{2}\left(\log 2\pi + 1\right) - \frac{1}{2}\log\left|\widehat{\Sigma}_{p,q}\right| - \frac{T\left(p+q+1\right)}{T-(p+q+1)-1} + O_p(1),$$

and includes terms that have the same order, $O_p(1)$, as the penalty term, and can not be avoided. Suppose then that we also include in the expectation the uncertainty about the parameter estimates, that is, we also take the expectation with respect to the distribution of the estimate, $\widehat{\alpha}_{p,q}$. This leads us to select the model that attains the largest value of:

$$E_{\widehat{\alpha}_{p,q}}\left[E_{\alpha_{p_0,q_0}}\left[\log p(y|\widehat{\alpha}_{p,q})\right]\right] = \int\int \log p(y|\widehat{\alpha}_{p,q}) p(y|\alpha_{p_0,q_0}) f(\widehat{\alpha}_{p,q}|\alpha_{p_0,q_0}) dy d\widehat{\alpha}_{p,q} \tag{20.3}$$

where $f(\widehat{\alpha}_{p,q}|\alpha_{p_0,q_0})$ is the distribution of the estimate and $\widehat{\alpha}_{p,q}$ and y are assumed to be independent. Therefore, this rule selects the model that maximizes the expected value with respect to the two sources of uncertainty: the distribution of future observations and the distribution of the estimate. The rule (20.3) can be written as follows (see, Galeano and Peña (2000)):

$$E_{\widehat{\alpha}_{p,q}}\left[E_{\alpha_{p_0,q_0}}\left[\log p(y|\widehat{\alpha}_{p,q})\right]\right] = -\frac{T}{2}\left(\log 2\pi + 1\right) - \frac{1}{2}\log\left|\widehat{\Sigma}_{p,q}\right| - \frac{T\left(p+q+1\right)}{T-(p+q+1)-1} + o(1),$$

which is equivalent to the expression of the AICc criterion for ARMA models derived by Hurvich et al. (1990). Note also that the rule (20.3) selects the model that minimizes the expected Kullback-Leibler divergence of a new realization of the process to the true one, which is given by:

$$E_{\widehat{\alpha}_{p,q}}\left[E_{\alpha_{p_0,q_0}}\left[\log\frac{p(y|\alpha_{p_0,q_0})}{p(y|\widehat{\alpha}_{p,q})}\right]\right] = \int\int \log\frac{p(y|\alpha_{p_0,q_0})}{p(y|\widehat{\alpha}_{p,q})} p(y|\alpha_{p_0,q_0}) f(\widehat{\alpha}_{p,q}|\alpha_{p_0,q_0}) dy d\widehat{\alpha}_{p,q},$$

and this was the approach followed by Akaike (1973) to derive the AIC criterion. Thus, both the AIC and the AICc may be derived by the standard quadratic discriminant rule.

On the other hand, the Bayesian approach of computing the posterior probabilities of each model automatically takes into account the two sources of uncertainty previously discussed. In fact, the logarithm of the posterior probability of the model $M_{p,q}$ can be written, by using the Laplace approximation (see, Galeano and Peña (2007b)), as follows:

$$\begin{aligned}\log p(M_{p,q}|x) = &-\frac{p+q+1}{2}\log\left(\frac{T}{2\pi}\right) - \frac{T}{2}\left(\log 2\pi + 1\right) - \frac{1}{2}\log\left|\widehat{\Sigma}_{p,q}\right| \\ &+ \log\left\{p(\widehat{\alpha}_{p,q}|M_{p,q})\left|H\left(\widehat{\alpha}_{p,q}\right)\right| + O_p(T^{-\frac{p+q+1}{2}-1})\right\} \\ &+ \log p\left(M_{p,q}\right) - \log p\left(x\right), \end{aligned} \tag{20.4}$$

where $p(\widehat{\alpha}_{p,q}|M_{p,q})$ and $\left|H\left(\widehat{\alpha}_{p,q}\right)\right|$ are the prior probability of the parameters and the Hessian of the log-likelihood at the maximum likelihood parameters, respectively. Now, deleting constants and terms that are $o_p\left(1\right)$ and taking the same prior probabilities for all the set of candidate models, (20.4) leads to the expression of the BIC criterion proposed by Schwarz (1978).

In summary, it has been shown that the quadratic discriminant rules lead to model selection criteria, such as the AIC, AICc and BIC. Thus, model selection problems and discrimination problems are solving the same problem and can be analyzed by using the same procedures.

20.4 Goodness of Fit for ARMA Time Series Models

The goodness of fit tests in time series work as follows. After selecting a model to fit the time series $x = (x_1, \ldots, x_T)'$, a goodness of fit test checks whether the data are reasonable well fitted by the chosen model by using a test statistic which measures the quality of the fit. The more often used goodness of fit test for linear time series uses a function of a statistic of the form:

$$t_s = T\left\{\delta\sum_{i=1}^{s} w_i g(\hat{r}_i^2) + (1-\delta)\sum_{i=1}^{s}\omega_i g(\widehat{\pi}_i^2)\right\} \tag{20.5}$$

where $\widehat{r}_i$ and $\widehat{\pi}_i$ are the autocorrelation and partial autocorrelation coefficients of the residuals and δ, w_i and ω_i are some constant weights. See Ljung and Box (1978), Monti (1994), Velilla (1994) and Peña and Rodríguez (2002). In this section, we analyze the connection between these goodness of fit tests and model selection criteria. We will use the test proposed by Peña and Rodríguez (2006), which is of the form (20.5) with $g(x) = -\log(1-x)$, $\delta = 0$ and $\omega_i = (s+1-i)/(s+1)$ and seems to be the most powerful test of this family. The test can also be presented as a test of the log of the determinant of the s autocorrelation matrix of the residuals. This matrix is an estimation of the autocorrelation matrix of the estimated residuals $\widehat{a}_{p,q}$ assuming that the largest possible autocorrelation different from zero appears at lag s.

Let $\widehat{R}_{p,q}$ be the autocorrelation matrix of the residuals defined as:

$$\widehat{R}_{p,q} = \frac{\widehat{a}_{p,q}\widehat{a}'_{p,q}}{T\widehat{\sigma}^2_{p,q}},$$

and taking into account that $x = \widehat{L}_{p,q}\widehat{a}_{p,q}$, the sample covariance matrix of x can be written as:

$$\frac{xx'}{T} = \frac{\widehat{L}_{p,q}\widehat{a}_{p,q}\widehat{a}'_{p,q}\widehat{L}'_{p,q}}{T} = \widehat{\sigma}^2_{p,q}\widehat{L}_{p,q}\widehat{R}_{p,q}\widehat{L}'_{p,q},$$

which shows that,

$$\left|\frac{xx'}{T}\right| = \left|\widehat{\sigma}^2_{p,q}\widehat{L}_{p,q}\widehat{R}_{p,q}\widehat{L}'_{p,q}\right| = \left|\widehat{\Sigma}_{p,q}\right|\left|\widehat{R}_{p,q}\right|, \tag{20.6}$$

because $\left|\widehat{\Sigma}_{p,q}\right| = \left|\widehat{\sigma}^2_{p,q}\widehat{L}_{p,q}\widehat{L}'_{p,q}\right|$. Now, taking logs in (20.6), the following expression holds:

$$\log\left|\frac{xx'}{T}\right| = \log\left|\widehat{\Sigma}_{p,q}\right| + \log\left|\widehat{R}_{p,q}\right|,$$

and the model selection criteria can be written in terms of this matrix as follows:

$$MSC\left(M_{p,q}\right) = \log\left|\frac{xx'}{T}\right| - \log\left|\widehat{R}_{p,q}\right| + (p+q+1)\,C\left(T, p+q+1\right).$$

Therefore, taking into account that the sample covariance matrix of the time series x is constant for all the candidate models, any of the model selection criteria will select the models that have a significatively larger value of the estimated correlation determinant of the residuals, which is the goodness of fit test statistic proposed by Peña and Rodríguez (2006). In practice the test is made by approximating $|\widehat{R}_{p,q}|$, which is squared of order T and cannot be computed, by $|\widehat{R}_s|$, which is of order s and includes the first s autocorrelation coefficients of the residuals.

It is important to stress that model selection criteria is penalized by the number of parameters, whereas goodness of fit criteria do not introduce this correction. However, as we have shown, the same measures of fitting appear in a natural way in model selection and model checking. This results in two interesting implications. First, the model chosen by a model selection criterion is not always the model with the most significant goodness of fit statistic. Second, the term $\log|\widehat{\Sigma}_{p,q}|$ can also be seen as a measure of the goodness of fit of the model $M_{p,q}$ to the series x.

This analysis clarifies the connection between model checking and model selection. Some authors (see Pukkila et al. (1990)) have proposed to check the fitted model by finding the order of the best autoregressive model fitted to the residuals. If the selected order is zero, it can be assumed that the residuals are white noise. Koreisha and Pukilla (1995) showed that the BIC criterion worked well for this objective. However, in general, both model selection and model checking are needed. First the model selected may not be an acceptable model by the goodness of fit test. This may happen when the model chosen is the best in a given family of models, but the data have been generated by a model that does not belong to the class considered. Second, several models may be acceptable by a goodness of fit test. Then the values of the goodness of fit statistic do not provide a good ground for selecting the model, which should be chosen by model selection criteria, accounting for the number of fitted parameters.

20.5 Outliers in ARMA Time Series Models

Outliers in time series can arise for several reasons. First, outliers may be gross errors such as measurement, recording and typing mistakes. Second, outliers may be real data generated by a different pattern than the rest of observations, for instance, caused for unknown intervention events. The presence of outliers in time series can seriously affect the estimation of the parameters of the model and produce poor forecasts. Since the seminal paper of Fox (1972), outliers in time series have received considerable attention, and several papers have analyzed their effects and proposed methods for their detection in univariate linear time series. See for instance, Tsay (1986), Chang et al. (1988), Chen and Liu (1993), Le et al. (1996), Luceño (1998), and Sánchez and Peña (2003), among others. Much of these works have been focused on the framework of statistical hypothesis testing. In particular, the procedure proposed by Chen and Liu (1993) is widely used and has been implemented in several time series packages, such as TRAMO and SCA. This and other procedures rely on the use of likelihood ratio tests with critical values obtained via simulation, and which depend on the sample size and the model. In this section we show that the outlier detection problem can be formulated as a model selection problem and can be solved by using model selection criteria. These criteria provide objective rules to decide whether a set of observations are outliers or not, avoiding the use of simulation to obtain critical values.

Let $x = (x_1, \ldots, x_T)'$ be a time series generated by an ARMA(p, q) process as in (20.1), where, for simplicity, the orders p and q are assumed known. Assume that instead of observing x, we observe a time series $y = (y_1, \ldots, y_T)'$ defined as follows:

$$y_t = \begin{cases} x_t & t \neq t_1, \ldots, t_m \\ x_t + z_t & t = t_1, \ldots, t_m \end{cases},$$

where m is the number of outliers in the time series, $t_1, \ldots, t_m$ are their locations, which verify $1 \leq t_1 < \cdots < t_m \leq T$, and $z_{t_1}, \ldots, z_{t_m}$ are their sizes. For simplicity we will only consider additive outliers in this section.

In practice, the parameters of the ARMA(p, q) model and the number, locations and sizes of the outliers are unknown, and have to be estimated from the data. In this section, it is shown that the outlier detection problem can be stated as a model selection problem, for which model selection criteria can be applied. For that, let M_{τ_m} be the ARMA(p, q) model with m outliers with locations at the vector time indices $\tau_m = (t_1, \ldots, t_m)'$. The problem of joint estimation of the model parameters, number of outliers, their locations and their sizes can be now stated as the selection of the true model among the set of candidate ones. This set includes the model without outliers, denoted by M_{τ_0}, the T models with one outlier, denoted by M_{τ_1}, where $\tau_1 = 1, \ldots, T$, and so on. In general, there are $\binom{T}{m}$ candidate models with m outliers with all the possible $\binom{T}{m}$ locations of the m outliers, and calling $m_{\max} \leq T/2$ the maximum number of outliers, the total number of candidate models is $k_{m_{\max}} = \binom{T}{0} + \cdots + \binom{T}{m_{\max}}$, which is of order $T^{m_{\max}}$. As it is assumed that the set of candidate models includes the true one, the BIC criterion, which is the most widely used consistent criteria, is adequate. Therefore, given the model M_{τ_m}, which assumes m outliers at locations $\tau_m = (t_1, \ldots, t_m)'$, the parameters to estimate are the $(p + q + 1) \times 1$ vector of unknown

parameters of the ARMA(p,q) model, $\alpha_{p,q}$, and the $m \times 1$ vector of unknown sizes of the outliers, $\mu_{\tau_m} = (z_{t_1}, \ldots, z_{t_m})'$. In summary, the model has $p+q+m+1$ unknown parameters, which are included in the $(p+q+m+1) \times 1$ vector $\gamma_{\tau_m} = \left(\alpha'_{p,q}, \mu'_{\tau_m}\right)'$. The maximum likelihood estimators of the vector of parameters γ_{τ_m} of the model M_{τ_m} are denoted by $\widehat{\gamma}_{\tau_m} = \left(\widehat{\alpha}'_{p,q}, \widehat{\mu}'_{\tau_m}\right)'$ and are obtained after maximizing the log-likelihood given by:

$$\log p\left(y \mid M_{\tau_m}\right) = -\frac{T}{2}\log 2\pi - \frac{1}{2}\log\left|\Sigma_{\tau_m}\right| - \frac{1}{2}\left(y - \delta_{\tau_m}\right)' \Sigma_{\tau_m}^{-1}\left(y - \delta_{\tau_m}\right),$$

where Σ_{τ_m} is the $T \times T$ covariance matrix of y under the model M_{τ_m} and δ_{τ_m} is a $T \times 1$ vector whose components are, the outliers sizes, $z_{t_1}, \ldots, z_{t_m}$, at the components $t_1, \ldots, t_m$, and are 0, elsewhere. The posterior probability of the model M_{τ_m} can be written as follows by using the Laplace approximation (see, Galeano and Peña (2007b)):

$$\begin{aligned}\log p(M_{\tau_m}|y) = \log p\left(y \mid \widehat{\gamma}_{\tau_m}\right) - \frac{p+q+m+1}{2}\log\frac{T}{2\pi} + \log p\left(M_{\tau_m}\right) \\ - \log p\left(y\right) + \log\left\{p(\widehat{\gamma}_{\tau_m}|M_{\tau_m})\left|H\left(\widehat{\gamma}_{\tau_m}\right)\right| + O_p(T^{-\frac{p+q+1}{2}-1})\right\} \quad (20.7)\end{aligned}$$

where $\log p\left(y \mid \widehat{\gamma}_{\tau_m}\right)$ is the maximized log-likelihood of y under the M_{τ_m} model, and $p(\widehat{\gamma}_{p,q}|M_{p,q})$ and $\left|H\left(\widehat{\gamma}_{p,q}\right)\right|$ are the prior probability of the parameters and the Hessian of the log-likelihood at the maximum likelihood parameters, respectively.

We consider three alternative approaches to the outlier problem based on the approximation (20.7). The first approach assumes that all the models are equally probable and therefore, $p\left(M_{\tau_m}\right) = 1/(k_{m_{\max}}+1)$. Thus, after deleting constants and terms that are $o_p\left(1\right)$, (20.7) leads to the BIC criterion for this first approach, denoted by BIC_1:

$$BIC_1\left(M_{\tau_m}\right) = -2\log p\left(y \mid \widehat{\gamma}_{\tau_m}\right) + (p+q+m+1)\log T. \quad (20.8)$$

From (20.8), we can obtain the BIC_1 approximations of the posterior probabilities $p(M_{\tau_m}|y)$ which are given by:

$$p_1\left(M_{\tau_m}|y\right) = \frac{\exp\left(-\frac{BIC_1(M_{\tau_m})}{2}\right)}{\sum_{i=0}^{m_{\max}}\sum_{\tau_i}\exp\left(-\frac{BIC_1(M_{\tau_i})}{2}\right)} = \frac{p\left(y \mid \widehat{\gamma}_{\tau_m}\right)T^{-\frac{p+q+m+1}{2}}}{\sum_{i=0}^{m_{\max}}\sum_{\tau_i}p\left(y \mid \widehat{\gamma}_{\tau_i}\right)T^{-\frac{p+q+i+1}{2}}}. \quad (20.9)$$

The second approach assumes that all the possible numbers of outliers are equally probable. Thus, taking equal prior probabilities for the $m_{\max}+1$ models with $0, 1, \ldots,$ $m_{\max}$ outliers, respectively, and equal prior probabilities for all the models with m outliers, the prior probabilities of the models M_{τ_m} are given by:

$$p\left(M_{\tau_m}\right) = \frac{1}{m_{\max}+1}\frac{1}{\binom{T}{m}},$$

while its logarithm can be written as follows:

$$\log p\left(M_{\tau_m}\right) = -\log\left(m_{\max}+1\right) + \sum_{j=1}^{m}\log j - \sum_{j=T-m+1}^{T}\log j.$$

Replacing this term and deleting constants and terms that are $o_p(1)$, (20.7) leads to the BIC criterion for this second approach, which is denoted by BIC_2:

$$BIC_2(M_{\tau_m}) = -2\log p(y \mid \widehat{\gamma}_{\tau_m}) + (p+q+m+1)\log T + 2\left(\sum_{j=T-m+1}^{T} \log j - \sum_{j=1}^{m} \log j\right).$$

Note that BIC_1 and BIC_2 are related by the expression:

$$BIC_2(M_{\tau_m}) = BIC_1(M_{\tau_m}) + 2\left(\sum_{j=T-m+1}^{T} \log j - \sum_{j=1}^{m} \log j\right),$$

which shows that $BIC_2(M_{\tau_m})$ can be written as $BIC_1(M_{\tau_m})$ plus an additional penalization term by the number of outliers. Thus, BIC_2 will select models with less number of outliers than BIC_1.

In this case, the BIC_2 approximations to the posterior probabilities $p(M_{\tau_m}|y)$ are given by:

$$\begin{aligned} p_2(M_{\tau_m}|y) &= \frac{\exp\left(-\frac{BIC_2(M_{\tau_m})}{2}\right)}{\sum_{i=0}^{m_{\max}} \sum_{\tau_i} \exp\left(-\frac{BIC_2(M_{\tau_i})}{2}\right)} \\ &= \frac{p(y \mid \widehat{\gamma}_{\tau_m}) T^{-\frac{p+q+m+1}{2}} m!(T-m)!}{\sum_{i=0}^{m_{\max}} \sum_{\tau_i} p(y \mid \widehat{\gamma}_{\tau_i}) T^{-\frac{p+q+i+1}{2}} i!(T-i)!}. \end{aligned} \tag{20.10}$$

The third possibility takes into account the hierarchical structure of the problem. In other words, the idea is to derive a BIC criterion for selecting the number of outliers, m, and then make inference on: (1) the outlier locations given m, τ_m, and, (2) the parameters given m and τ_m. To do that, note that the marginal distribution of the number of outliers and the posterior probability of the model M_{τ_m} given the series are given by:

$$p(m|y) = \frac{\sum_{\tau_m} p(M_{\tau_m}) p(y|M_{\tau_m})}{\sum_{i=0}^{m_{\max}} \sum_{\tau_i} p(M_{\tau_i}) p(y|M_{\tau_i})},$$

and

$$p(M_{\tau_m}|y) = \frac{p(M_{\tau_m}) p(y|M_{\tau_m})}{\sum_{i=0}^{m_{\max}} \sum_{\tau_i} p(M_{\tau_i}) p(y|M_{\tau_i})},$$

respectively. Thus, the posterior probability of the number of outliers, $p(m|y)$, can be written as follows:

$$p(m|y) = \sum_{\tau_m} p(M_{\tau_m}|y),$$

which is independent of the prior probabilities $p(M_{\tau_m})$. Now, the posterior probabilities $p(M_{\tau_m}|y)$ can be approached by either (20.9) or (20.10), providing two alternative approximations of $\log p(m|y)$ given by:

$$\log p\left(m|y\right) \simeq \log\left(\sum_{\tau_m} p\left(y \mid \widehat{\gamma}_{\tau_m}\right)\right) - \frac{p+q+m+1}{2}\log T - \log\left(\sum_{i=0}^{m_{\max}}\sum_{\tau_i} p\left(y \mid \widehat{\gamma}_{\tau_i}\right) T^{-\frac{p+q+i+1}{2}}\right),$$

and

$$\log p\left(m|y\right) \simeq \log\left(\sum_{\tau_m} p\left(y \mid \widehat{\gamma}_{\tau_m}\right)\right) - \frac{p+q+m+1}{2}\log T - \left(\sum_{j=T-m+1}^{T}\log j - \sum_{j=1}^{m}\log j\right) - \log\left(\sum_{i=0}^{m_{\max}}\sum_{\tau_i} p\left(y \mid \widehat{\gamma}_{\tau_i}\right) T^{-\frac{p+q+i+1}{2}}\right),$$

which, after deleting constants and terms that are $o_p\left(1\right)$, leads to us define two new BIC criteria for the number of outliers in the time series given by:

$$BIC_1\left(m\right) = -2\log\left(\sum_{\tau_m} p\left(y \mid \widehat{\gamma}_{\tau_m}\right)\right) + \left(p+q+m+1\right)\log T,$$

and

$$BIC_2\left(m\right) = -2\log\left(\sum_{\tau_m} p\left(y \mid \widehat{\gamma}_{\tau_m}\right)\right) + \left(p+q+m+1\right)\log T + 2\left(\sum_{j=T-m+1}^{T}\log j - \sum_{j=1}^{m}\log j\right),$$

respectively. In summary, the number of outliers is selected as the value that provides the minimum value of either the criterion $BIC_1\left(m\right)$ or the criterion $BIC_2\left(m\right)$. Note that as in the previous approaches, BIC_1 and BIC_2 are related as follows:

$$BIC_2\left(m\right) = BIC_1\left(m\right) + 2\left(\sum_{j=T-m+1}^{T}\log j - \sum_{j=1}^{m}\log j\right),$$

and thus, $BIC_1\left(m\right)$ is expected to select a smaller number of outliers than $BIC_2\left(m\right)$.

After selecting the number of outliers, m, inference on the vector of unknown locations, τ_m, is done by comparing the values of the likelihood of the models M_{τ_m} with m outliers, $p\left(y \mid \widehat{\gamma}_{\tau_m}\right)$. In other words, the estimates of the unknown locations, τ_m, are the ones that attain the largest value of $p\left(y \mid \widehat{\gamma}_{\tau_m}\right)$. Finally, estimation of the vector of parameters once that m and τ_m have been selected is carried out with the maximum likelihood estimates $\widehat{\gamma}_{\tau_m} = \left(\widehat{\alpha}'_{p,q}, \widehat{\mu}'_{\tau_m}\right)'$.

Galeano and Peña (2007b) provide an extensive analysis of the behavior of these alternative approaches. Also, in order to avoid the computation of the maximum likelihood estimates of all the models involved in the analysis, these authors proposed an algorithm that only requires to compute the maximum likelihood estimates of the models with largest posterior probabilities.

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21

Generalized Linear Models Diagnostics for Binary Data using Divergence Measures

J. A. Pardo and M. C. Pardo

Department of Statistics and Operations Research I, Complutense University of Madrid, Spain

Abstract: The binary data appears often in different situations, and generally they can be modeled according to a generalized linear model. In this work we focus on checking a generalized linear model after fitting it to the data. The most common goodness-of-fit tests to do it are the Pearson chi-square and the deviance tests. We propose a new family of test statistics based on a divergence measure that contains the above test statistics whose significance level and power are evaluated in small and moderate sample situations. Finally, we introduce new diagnostic methods based on divergences.

Keywords and phrases: Generalized linear model, binary data, divergence measures

21.1 Introduction

In many areas of application of statistical principles and procedures, from agronomy through to zoology, one encounters observations made on individual experimental units that take one of two possible forms. For example, a seed may germinate or fail to germinate under certain experimental conditions; an integrated circuit manufactured by an electronics company may be defective or non-defective; a patient in a clinical trial to compare alternative forms of treatment may or may not experience relief from symptoms; an insect in an insecticidal trial may survive or die when exposed to a particular dose of the insecticide. Such data are said to be binary wherein a binomial model may be assumed for the independent response variables $Y_1, ..., Y_I$. The individual level sample sizes are denoted by n_i and the unknown probabilities of response by π_i. We assume that π_i depends on $k+1$ explanatory variables $\boldsymbol{x}_i = (x_{i0}, ..., x_{ik})$ through the linear predictor

$$\eta_i \equiv g(\pi_i) = \sum_{j=0}^{k} x_{ij}\beta_j, i = 1, ..., I. \tag{21.1}$$

Here g is the link function (any monotonic and differentiable function) and $\boldsymbol{\beta} = (\beta_0, ..., \beta_k)$ is a $(k+1) \times 1$ vector of unknown parameters. Unless restrictions are

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imposed on $\boldsymbol{\beta} = (\beta_0, ..., \beta_k)$ we have -$\infty < \eta_i < \infty$, $i = 1, ..., I$. We will assume $x_{i0} = 1$, $i = 1, ..., I$ and we denote by $\boldsymbol{X}$ the $I \times (k+1)$ matrix with rows $\boldsymbol{x}_i$, $i = 1, .., I$. We also shall assume that $rank(\boldsymbol{X}) = k+1$. So we consider generalized linear models with binary data (GLM). As $\eta_i \equiv g(\pi_i)$ can be any monotonic, differentiable function, a wide choice of link functions $g(\pi_i)$, $i = 1, ..., I$ is available. However, in practice, only a small set of link functions are actually used. In particular, links are chosen such that the inverse link

$$\pi_i = g^{-1}(\eta_i)$$

is easily computed. Some of them can be seen in Nelder and Wedderburn (1972) and McCullagh and Nelder (1989). The two most well-known are the logistic function,

$$g_1(\pi_i) = \log\left(\frac{\pi_i}{1-\pi_i}\right)$$

and the probit or inverse normal function,

$$g_2(\pi_i) = \psi^{-1}(\pi_i),$$

where ψ is the distribution function of a normal distribution with mean 0 and variance 1. For more details of these models see Agresti (2002). All of them share the feature that they map the unit interval onto the real line. Pregibon (1980) defined a family of link functions, including the logit link as a particular case. Aranda-Ordaz (1981) introduced two separate one-parameter families of models for symmetric and asymmetric departures, respectively, from the logistic model. Some family members of models considered for symmetric departures approximate the probit model closely. Guerrero and Johnson (1982) considered a one-parameter family of link functions that also contains the logit link as a particular case. Morgan (1988) introduced two separate families of links functions that contain the families introduced by Pregibon and Aranda-Ordaz. Other families of link functions that contain or approximate the traditional logit and probit link functions can be seen in Stukel (1988).

To fit model (21.1) to our binary data, for any given link function, is equivalent to estimate the unknown parameter $\boldsymbol{\beta}$. For this we consider, as a natural generalization of the maximum likelihood estimator (MLE) for the GLM, the minimum ϕ-divergence estimator given by,

$$\widehat{\boldsymbol{\beta}}_\phi \equiv \arg \min_{\beta_0, \beta_1, ..., \beta_k} D_\phi\left(\widehat{\boldsymbol{p}}, \boldsymbol{p}(\boldsymbol{\beta})\right), \tag{21.2}$$

where

$$\widehat{\boldsymbol{p}} \equiv (\hat{p}_{11}, \hat{p}_{12}, ..., \hat{p}_{I1}, \hat{p}_{I2})^T = \left(\frac{n_{11}}{N}, \frac{n_{12}}{N}, \frac{n_{21}}{N}, \frac{n_{22}}{N}, ..., \frac{n_{I1}}{N}, \frac{n_{I2}}{N}\right)^T$$

and

$$\begin{aligned} \boldsymbol{p}(\boldsymbol{\beta}) &\equiv (p_{11}(\boldsymbol{\beta}), p_{12}(\boldsymbol{\beta}), ..., p_{I1}(\boldsymbol{\beta}), p_{I2}(\boldsymbol{\beta}))^T \\ &= \left(\pi\left(\boldsymbol{x}_1^T\boldsymbol{\beta}\right)\frac{n_1}{N}, \left(1-\pi\left(\boldsymbol{x}_1^T\boldsymbol{\beta}\right)\right)\frac{n_1}{N}, ..., \pi\left(\boldsymbol{x}_I^T\boldsymbol{\beta}\right)\frac{n_I}{N}, \left(1-\pi\left(\boldsymbol{x}_I^T\boldsymbol{\beta}\right)\right)\frac{n_I}{N}\right)^T \end{aligned} \tag{21.3}$$

with $n_{11}, ..., n_{I1}$ the observed values of the random variables $Y_1, ..., Y_I, n_{i2} = n_i - n_{i1}, N = \sum_{j=1}^{2}\sum_{i=1}^{I} n_{ij}$ and $\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}\right) = \pi_i$. The $\phi-$divergence is defined by,

$$D_\phi\left(\widehat{\boldsymbol{p}},\boldsymbol{p}\left(\boldsymbol{\beta}\right)\right)\equiv\sum_{j=1}^{2}\sum_{i=1}^{I}p_{ij}\left(\boldsymbol{\beta}\right)\phi\left(\frac{\widehat{p}_{ij}}{p_{ij}\left(\boldsymbol{\beta}\right)}\right);\phi\in\boldsymbol{\Phi},$$

where $\boldsymbol{\Phi}$ is the class of all convex functions such that $\phi\left(1\right)=\phi'\left(1\right)=0,\phi''\left(1\right)>0$, $0\phi\left(0/0\right)=0$ and $0\phi\left(p/0\right)=p\lim_{u\to\infty}\phi\left(u\right)/u$. For more details about $\phi-$ divergence see Vajda (1989) and Pardo (2006).

For $\phi\left(x\right)\equiv\phi_{(\lambda)}\left(x\right)=\left(\lambda\left(\lambda+1\right)\right)^{-1}\left(x^{\lambda+1}-x\right);\ \lambda\neq0,\lambda\neq-1$, with $\phi_{(0)}\left(x\right)=\lim_{\lambda\to0}\phi_{(\lambda)}\left(x\right)=x\log x-x+1$ and $\phi_{(-1)}\left(x\right)=\lim_{\lambda\to-1}\phi_{(\lambda)}\left(x\right)=-\log x+x-1$, we obtain the power-divergence family (see Cressie and Read (1984)).

An important step in the modeling process is assessing how well the data are described by the model. The tests that are used to evaluate fit in this manner are referred to as "goodness-of-fit tests". The most common goodness-of-fit tests for generalized linear models include the Pearson χ^2 -test and the deviance test. In Section 21.2, we propose a new family of test statistics based on the ϕ -divergence that contains the above test statistics. Furthermore, we estimate the unknown parameters of the model using the extension of the maximum likelihood estimator, the minimum ϕ-divergence estimator given in (21.2). In Section 21.3 a computational study is carried out in order to find good alternatives to the classical goodness-of-fit tests belonging to this new family of test statistics. Finally, diagnostic tools based on the $\phi-$divergence are introduced in Section 21.4 to identify the nature of one lack of fit.

21.2 Checking Goodness-of-fit

After fitting the GLM, it would be useful to have a single measure that would indicate how well these observations are explained. The Pearson chi-square and the likelihood ratio statistics perform this role.

The Pearson chi-square statistic is defined by

$$X^2=\sum_{i=1}^{I}\frac{\left(n_{i1}-n_i\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}\right)\right)^2}{n_i\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}\right)\left(1-\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}\right)\right)}\tag{21.4}$$

where $\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}\right)$ is obtained from $\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}\right)$ replacing $\boldsymbol{\beta}$ by its MLE. The other classical test statistic for goodness-of-fit in a GLM is the likelihood ratio test defined by

$$D=\sum_{i=1}^{I}2\left\{n_{i1}\log\frac{n_{i1}}{n_i\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}\right)}+\left(n_i-n_{i1}\right)\log\frac{n_i-n_{i1}}{n_i\left(1-\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}\right)\right)}\right\}.\tag{21.5}$$

Therefore, we propose, for testing a GLM with binary data, i.e.

$$H_0:\boldsymbol{p}=\boldsymbol{p}\left(\boldsymbol{\beta}^0\right)\in\left\{\boldsymbol{p}\left(\boldsymbol{\beta}\right):\boldsymbol{\beta}=\left(\beta_0,...,\beta_k\right),-\infty<\beta_j<\infty,j=0,...,k\right\}\tag{21.6}$$

where $\boldsymbol{p}\left(\boldsymbol{\beta}\right)$ is given in (21.3) and β^0 is the true value of parameter, the family of tests statistics,

$$T_{\phi_1,\phi_2} = \frac{2N}{\phi_1''(1)} D_{\phi_1}\left(\widehat{\boldsymbol{p}}, \boldsymbol{p}\left(\widehat{\boldsymbol{\beta}}^{\phi_2}\right)\right) \tag{21.7}$$

which contains as particular cases the test statistics given in (21.4) and (21.5) for $\phi_2(x) = x\log x - x - 1$, $\phi_1(x) = \frac{1}{2}(x-1)^2$ and $\phi_1(x) = x\log x - x - 1$, respectively. We shall establish in the following theorem the asymptotic distribution of (21.7) under (21.6). This distribution is known to be a chi-square with $I-(k+1)$ degrees of freedom for (21.4) and (21.5).

Theorem 1. *We consider the GLM given by* $\eta_i \equiv g(\pi_i) = \sum_{j=0}^{k} x_{ij}\beta_j, i = 1,...,I$. *Choose functions* ϕ_1 *and* $\phi_2 \in \Phi$ *and twice continuously differentiable. Then, under the hypothesis given in (21.6), the test statistic* T_{ϕ_1,ϕ_2} *has a chi-squared distribution with* $I-(k+1)$ *degrees of freedom.*

Proof. Denoting by

$$\boldsymbol{L} = \boldsymbol{S}_{2I\times I}\boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T Diag\left(\left(\boldsymbol{C}_i^T\right)_{i=1,...,I}\right) Diag\left(\boldsymbol{p}\left(\boldsymbol{\beta}^0\right)^{-1/2}\right) \tag{21.8}$$

where

$$\boldsymbol{W} = Diag\left(\left(\frac{n_i}{N\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)\left(1-\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)\right)}\left(\frac{\partial\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)}{\partial\eta_i}\right)^2\right)_{i=1,...,I}\right), \tag{21.9}$$

$$\boldsymbol{C}_i = \left(\frac{n_i}{N}\right)^{1/2}\frac{\partial\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)}{\partial\eta_i}\begin{pmatrix}\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)^{-1/2}\\ -\left(1-\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)\right)^{-1/2}\end{pmatrix},\ i = 1,...,I$$

and

$$\boldsymbol{S}_{2I\times I} = Diag\left(\left(\frac{n_i}{N}\frac{\partial\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)}{\partial\eta_i}\begin{pmatrix}-1\\1\end{pmatrix}\right)_{i=1,...,I}\right). \tag{21.10}$$

The result is obtained following the same steps that in Theorem 1 of Pardo et al. (2006). ■

By this theorem the GLM is rejected as a description of the data if the level of significance $p = P\left(\chi^2_{I-(k+1)} \geq c\right)$, with c the value of T_{ϕ_1,ϕ_2}, is sufficiently small.

Remark 1. If we consider the power-divergence of Cressie and Read, i.e., if we consider

$$\phi(x) \equiv \phi_{(\lambda)}(x) = \left(\lambda(\lambda+1)\right)^{-1}\left(x^{\lambda+1} - x\right);\ \lambda \neq 0, \lambda \neq -1,$$

with

$$\phi_{(0)}(x) = \lim_{\lambda\to 0}\phi_{(\lambda)}(x) = x\log x - x + 1$$
$$\phi_{(-1)}(x) = \lim_{\lambda\to -1}\phi_{(\lambda)}(x) = -\log x + x - 1.$$

we have the power family of test statistic,

$$T_{\lambda_1,\lambda_2} = \frac{2}{\lambda_1(\lambda_1+1)} \left\{ \sum_{j=1}^{2} \sum_{i=1}^{I} \frac{n_{ij}^{\lambda_1+1}}{\left(n_i \widehat{\pi}_{ij}^{\phi(\lambda_2)}\right)^{\lambda_1}} - 1 \right\},$$

where $\widehat{\pi}_{i1}^{\phi(\lambda_2)} = \pi\left(\boldsymbol{x}_i^T \widehat{\beta}_{\phi(\lambda_2)}\right)$ and $\widehat{\pi}_{i2}^{\phi(\lambda_2)} = 1 - \pi\left(\boldsymbol{x}_i^T \widehat{\beta}_{\phi(\lambda_2)}\right)$, that under the hypothesis given in (21.6), has a chi-squared distribution with $I - (k+1)$ degrees of freedom.

To compare, on one hand, the classic test statistics with the new family of test statistics (21.7) and, on the other hand, to find the best member of our family of test statistics we have carried out a simulation study that we present in the next section. We consider the power-divergence family that includes the classic test statistics, i.e., the test statistics given in Remark 1. The type I error rates and the powers of some members of this family are obtained for a probit model. Alternative test statistics to the classic ones emerge as the best.

21.3 Simulation Study

The members of the family of test statistics T_{λ_1,λ_2} given in Remark 1 according Theorem 1 are asymptotically equivalent, but for small and moderate samples this is not necessary true. For this reason we present a simulation study for size as well as for power of the test statistics T_{λ_1,λ_2} for testing the hypothesis given in (21.6) with $\boldsymbol{p}(\beta)$ defined in (21.3) for the probit model, with

$$\psi^{-1}\left(\pi\left(\boldsymbol{x}_i^T \beta\right)\right) = \beta_0 + \beta_1 x_i$$

where $\beta = (\beta_0, \beta_1)^T$ with $\beta_0 = -1$ and $\beta_1 = 2$, and $x_i = -1(0.2)1$, $i = 1, ..., 11$, against the alternative hypothesis $\boldsymbol{p} = \boldsymbol{p}(\beta)$ with $\boldsymbol{p}(\beta)$ defined in (21.3) for the different models given in table 21.1.

All the computations presented here are based on $M = 10000$ random samples of sizes $n = (n_1, ..., n_{11})^T \in \mathcal{N} = \{n^1, n^2, n^3\}$ with

$$\begin{aligned} n^1 &= (20, 20, 20, 20, 20, 20, 20, 20, 20, 20, 20), \\ n^2 &= (40, 40, 40, 40, 40, 40, 40, 40, 40, 40, 40), \\ n^3 &= (60, 60, 60, 60, 60, 60, 60, 60, 60, 60, 60). \end{aligned}$$

We choose $\lambda_2 = 0, 2/3$ and 1 for estimation since Pardo and Pardo (2007) found that, for the probit model, the power-divergence estimators corresponding to these values of λ_2 have the best behavior. For testing we consider $\lambda_1 = -1/2$, 0, 2/3, 1 and 2.

Table 21.1. Alternative hypothesis

$A_1 \equiv \pi\left(\boldsymbol{x}_i^T \beta\right) = 0.9 - 0.2x_i^2$	$A_4 \equiv \pi\left(\boldsymbol{x}_i^T \beta\right) = 0.3 + 0.2x_i^2 + 0.4x_i^3$
$A_2 \equiv \pi\left(\boldsymbol{x}_i^T \beta\right) = 0.9 - 0.4x_i^2$	$A_5 \equiv \pi\left(\boldsymbol{x}_i^T \beta\right) = 0.3 + 0.2x_i^2 + 0.1x_i^3$
$A_3 \equiv \pi\left(\boldsymbol{x}_i^T \beta\right) = 0.4x_i^2$	

Firstly, the simulated exact size at a level α for the population of size n, $\widehat{\alpha}_n$, is obtained by

$$\widehat{\alpha}_n = \frac{\text{Number of } T^j_{\lambda_1,\lambda_2} > \chi^2_{9,1-\alpha}}{M}$$

where $T^j_{\lambda_1,\lambda_2}$, $j = 1, ..., M$ is the test statistic T_{λ_1,λ_2} for the jth random sample. Simulated exact sizes corresponding to the test statistics T_{λ_1,λ_2} are provided in table 21.2.

To study the closeness of the simulated exact size $\widehat{\alpha}_n$ to the nominal size $\alpha = 0.05$, we consider the inequality proposed by Dale (1986)

$$|\text{logit } (1 - \widehat{\alpha}_n) - \text{logit } (1 - \alpha)| \leq d, \tag{21.11}$$

where logit $(p) = \ln(p/(1-p))$ and $\widehat{\alpha}_n$ is the simulated exact size by a sample of size n. Dale consider that the nominal size is "close" to the simulated exact size if they satisfy (21.11) with $d = 0.35$ and "fairly close" if they satisfy (21.11) with $d = 0.7$. Note that for $\alpha = 0.05, d = 0.35$ corresponds to $\widehat{\alpha}_n \in [0.0357, 0.0695]$, and $d = 0.7$ corresponds with $\widehat{\alpha}_n \in [0.0254, 0.0959]$. The "bold numbers" in table 21.2 correspond to the values of the simulated size verifying the criterion to be "close", and the values verifying the criterion to be "fairly close" are "bold numbers" jointly with "italic numbers".

In table 21.3, we present the powers of the test statistics corresponding to the criterion to be "close" in relation to their sizes. To obtain the powers we consider the data generated from the models of table 21.1. From each one of these M generated random samples, $\widehat{\beta}_{\phi(0)}$, $\widehat{\beta}_{\phi(2/3)}$ and $\widehat{\beta}_{\phi(1)}$ are calculated under the probit model. After this, $T^j_{\lambda_1,\lambda_2}$, $j = 1, ..., M$ is calculated. The simulated exact power at a level α for a population of size n is given by the proportion of $T^j_{\lambda_1,\lambda_2}$ that is greater than $\chi^2_{9,1-\alpha}$.

From table 21.3, we can observe that the best is $T_{0,1}$ and the second best is $T_{0,2/3}$. This means to use the Kullback divergence for testing but the members of the power-divergence corresponding to $\lambda_2 = 1$ or $2/3$ for estimating. If we consider the criterion "fairly close" the results are quite similar. We have considered in our study samples with equal size but if we consider samples with different size we obtain the same results.

Table 21.2. Simulated exact sizes when β is estimated for $\widehat{\beta}_{\phi(0)}$, $\widehat{\beta}_{\phi(2/3)}$ or $\widehat{\beta}_{\phi(1)}$

n	λ_1	$\lambda_2 = 0$	$\lambda_2 = 2/3$	$\lambda_2 = 1$
	$-.5$	*.0887*	.1490	.1755
	0	*.0270*	**.0373**	**.0456**
n^1	2/3	*.0327*	.0150	.0157
	1	**.0518**	.0130	.0122
	2	.1358	*.0268*	.0117
	$-.5$	*.0810*	.1350	.1610
	0	*.0305*	**.0414**	**.0514**
n^2	2/3	**.0402**	.0231	.0241
	1	**.0599**	.0231	.0212
	2	.1450	**.0490**	*.0263*
	$-.5$	*.0803*	.1275	.1502
	0	*.0324*	**.0424**	**.0531**
n^3	2/3	**.0419**	*.0266*	*.0278*
	1	**.0602**	*.0266*	.0248
	2	.1404	**.0615**	**.0370**

Table 21.3. Simulated exact powers of T_{λ_1,λ_2} for the alternative hypothesis A_1, A_2, A_3, A_4 and A_5

	λ_2	λ_1	A_1	A_2	A_3	A_4	A_5
	0	1	.3888	.9410	.9966	.5867	.2609
n^1	2/3	0	.4848	.9553	.9996	.6665	.2949
	1	0	.5013	.9571	.9998	.6721	.2969
	0	2/3	.7509	1.000	1.000	.9381	.5397
	0	1	.7475	1.000	1.000	.9329	.5367
n^2	2/3	0.	.7727	.9997	1.000	.9489	.5522
	2/3	2	.7172	.9994	1.000	.9170	.5327
	1	0	.7810	.9998	1.000	.9496	.5531
	0	2/3	.9272	1.000	1.000	.9948	.7641
	0	1	.9264	1.000	1.000	.9945	.7623
n^3	2/3	0	.9340	1.000	1.000	.9963	.7697
	2/3	2	.9164	1.000	1.000	.9934	.7613
	1	0	.9372	1.000	1.000	.9963	.7703
	1	2	.9108	1.000	1.000	.9932	.7604

This conclusion coincides with the results obtained in Pardo et al. (2006) for the logistic regression models.

21.4 "Outlying" Detection Procedures

In Section 21.2 we introduced statistics for checking model fit in a global sense. The disadvantage of these single overall test statistics of goodness-of-fit is that it will not usually give constructive guidance on how to deal with any failure of the original model and is likely to be insensitive in detecting specific types of departure. Therefore, more specific tools to check models are considered such as diagnostic methods based on residuals. These measures should readily identify observations that are not well explained by the model. These observations are called "outlying" observations. For a binary GLM, the most well known residuals for the fits are

$$e_i = \frac{n_{i1} - n_i \pi\left(\boldsymbol{x}_i^T \widehat{\boldsymbol{\beta}}\right)}{\sqrt{n_i \pi\left(\boldsymbol{x}_i^T \widehat{\boldsymbol{\beta}}\right)\left(1 - \pi\left(\boldsymbol{x}_i^T \widehat{\boldsymbol{\beta}}\right)\right)}}.$$

These residuals are known as Pearson residuals, since $X^2 = \sum_{i=1}^{I} e_i^2$ is the Pearson chi-square statistic given in (21.4). These residuals therefore measure the contribution that each observation makes to a statistic that is a summary measure of goodness-of-fit of the fitted GLM. For this reason, they are intuitively appealing as measures of model adequacy.

Another type of residual can be constructed from the likelihood ratio test statistic, D, given in (21.5). The signed square root of the contribution of the ith observation to this overall deviance is

$$d_i = sig\left(n_{i1} - n_i\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}\right)\right) \times \sqrt{2}\left[\left(n_{i1}\log\frac{n_{i1}}{n_i\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}\right)}\right) + (n_i - n_{i1})\log\frac{n_i - n_{i1}}{n_i\left(1-\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}\right)\right)}\right]^{1/2}.$$

The quantity d_i is known as a deviance residual and is such that the overall deviance is $D = \sum_{i=1}^{I} d_i^2$.

The residuals e_i and d_i can be obtained as particular cases of the family of residuals,

$$c_i^{\phi_1,\phi_2} = sig\left(n_{i1} - n_i\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}_{\phi_2}\right)\right) \times \sqrt{\frac{2n_i}{\phi_1''(1)}}\left\{\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}_{\phi_2}\right)\phi_1\left(\frac{n_{i1}}{\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}_{\phi_2}\right)n_i}\right) + \left(1-\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}_{\phi_2}\right)\right)\phi_1\left(\frac{n_{i2}}{\left(1-\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}_{\phi_2}\right)\right)n_i}\right)\right\}^{1/2},$$

where $\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}_{\phi_2}\right)$ is obtained from $\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}\right)$ replacing $\boldsymbol{\beta}$ by its minimum ϕ_2-divergence estimator $\widehat{\boldsymbol{\beta}}_{\phi_2}$. We obtain e_i considering $\phi_1(x) = \frac{1}{2}(x-1)^2$ and d_i considering $\phi_1(x) = x\log x - x + 1$ when $\phi_2(x) = x\log x - x + 1$.

As same as the Pearson chi-square and the deviance statistics are obtained adding the squares of the residuals e_i and d_i, respectively, the statistic proposes in (21.7) is obtained adding the squares of the residual $c_i^{\phi_1,\phi_2}$.

However, the standardization used in the construction of the Pearson residuals does not yield residuals that have even approximate unit variance, since the true variance of $n_{i1} - \pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}\right)n_i$ can be different from $n_i\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)\left(1-\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)\right)$. This variance does not take into account the variability of $\pi\left(\boldsymbol{x}_i^T\widehat{\boldsymbol{\beta}}\right)$. The same happens in general for $c_i^{\phi_1,\phi_2}$. A better procedure is to divide $c_i^{\phi_1,\phi_2}$ by their asymptotic standard error, $SE\left(c_i^{\phi_1,\phi_2}\right)$. In Theorem 2 we derive it.

Theorem 2. *We consider the GLM given by* $\eta_i \equiv g(\pi_i) = \sum_{j=0}^{k} x_{ij}\beta_j, i = 1,...,I$. *Choose functions* ϕ_1 *and* $\phi_2 \in \Phi$ *and twice continuously differentiable. Then,*

$$SE\left(c_i^{\phi_1,\phi_2}\right) \approx \sqrt{1-h_{ii}}$$

where h_{ii} *are the diagonal elements of the hat matrix (Pregibon , 1981),*

$$\boldsymbol{H} = \boldsymbol{W}^{1/2}\boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{W}^{1/2}$$

with W given in (21.9).

PROOF. Following the same steps used in the proof of Theorem 3 in Pardo et al. (2006) it can be proved that

$$c_i^{\phi_1,\phi_2} \underset{N\to\infty}{\overset{L}{\longrightarrow}} \mathcal{N}\left(0,\tau_i^2\right)$$

where

$$\tau_i^2 = 1 - \frac{\alpha_i}{\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)\left(1-\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)\right)}\left(\frac{\partial\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)}{\partial\eta_i}\right)^2 \boldsymbol{x}_i I_F\left(\boldsymbol{\beta}^0\right)^{-1}\boldsymbol{x}_i^T$$

being $I_F\left(\boldsymbol{\beta}^0\right) = \boldsymbol{X}^T\boldsymbol{W}^*\boldsymbol{X}$ the Fisher information matrix with $\boldsymbol{W}^* = \lim_{N\to\infty} W$ with $\boldsymbol{W}$ is given in (21.9) and $\alpha_i = \lim_{N\to\infty} n_i/N$.

Taking into account that

$$Var\left(n_{i1}\right) = n_i\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)\left(1-\pi\left(\boldsymbol{x}_i^T\boldsymbol{\beta}^0\right)\right), \quad i = 1,...,I$$

we have the result. ■

Remark 2. The standardized residual based on $c_i^{\phi_1,\phi_2}$ is given by

$$\left(c_i^{\phi_1,\phi_2}\right)^* = \frac{c_i^{\phi_1,\phi_2}}{\sqrt{1-\widehat{h}_{ii}^{\phi_2}}},$$

where $\widehat{h}_{ii}^{\phi_2}$ is obtained replacing $\boldsymbol{\beta}^0$ by the minimum ϕ_2-divergence estimator in h_{ii}.

From the above theorem, it is clear that $\left(c_i^{\phi_1,\phi_2}\right)^* \approx \mathcal{N}\left(0,1\right)$ and $\left(c_i^{\phi_1,\phi_2}\right)^*$ are useful as diagnostics for detecting model deviations in GLM analysis. Their role as diagnostics are primarily to indicate which of the observed responses contribute most to a significant test statistics.

An alternative way for identifying an "outlying" at a designated case, say i, consists in considering the model,

$$\eta_s = \begin{cases} \sum_{j=0}^k x_{sj}\beta_j + \gamma_s & \text{if } s = i \\ \sum_{j=0}^k x_{sj}\beta_j & \text{if } s \neq i \end{cases}, \quad s = 1...,I. \tag{21.12}$$

This model is an analogue of the mean slippage model commonly used for outlying detection in linear regression (Cook and Weisberg (1982), p. 20). A test that observation $\mathbf{x}_i$ is an "outlying" is equivalent to

$$H_0 : \gamma_i = 0 \quad \text{against} \quad H_{1,i} : \gamma_i \neq 0. \tag{21.13}$$

If the null hypothesis is rejected, the ith observation will be an "outlying,"or if we express the GLM given in (21.12) as the GLM binary response

$$\eta_s \equiv g\left(\pi_s\right) = \textstyle\sum_{j=0}^{k+1} x_{sj}^*\beta_j^*, s = 1,...,I,$$

where $x_{sj}^* = x_{sj}$ for $j \neq k+1$, $x_{ik+1}^* = 1$ and $x_{sk+1}^* = 0$ for $s \neq i$. The vector of parameters for this model is $\beta^* = \left(\beta_0,...,\beta_k,\gamma_i\right)$. Then, to test the hypothesis given in (21.13) is equivalent to test

$$H_0 : K^T\beta^* = 0 \quad \text{against} \quad H_{1,i} : K^T\beta^* \neq 0. \tag{21.14}$$

where,

$$K^T = (\mathbf{0}_{k+1}, 1)\,.$$

A test statistics for testing (21.14) is given by

$$T_{N,i}^{\phi_1,\phi_2} = \frac{2N}{\phi''(1)} D_{\phi_1}\left(p\left(\widehat{\beta}_{\phi_2}^{H_{1,i}}\right), p\left(\widehat{\beta}_{\phi_2}^{H_0}\right)\right) \tag{21.15}$$

where $\widehat{\beta}_{\phi_2}^{H_{1,i}}$ and $\widehat{\beta}_{\phi_2}^{H_0}$ are the minimum ϕ_2-divergence estimator under the alternative hypothesis and under the null hypothesis, respectively. The asymptotic distribution of this statistic can be seen in the following Theorem.

Theorem 3. *We consider the GLM given by (21.1). Under the null hypothesis given in (21.14) the asymptotic distribution of the $\phi-$divergence test statistic given in (21.15) is a chi-squared with 1 degree of freedom.*

Proof. We omit the proof because follows the same steps that Theorem 1 considered in Menéndez et al. (2006) for a binary logit model. ■

When the candidate case for an "outlying" is unknown, a multiple testing procedure, such as one based on the first Bonferroni inequality (Miller, 1966), must be used to find significance levels. In our case, we will say that $\mathbf{x}_i$ is an "outlying" if

$$T_{N,i}^{\phi_1,\phi_2} \geq \chi^2_{1,\alpha/I}$$

and the probability to reject incorrectly an observation is given by

$$P_r\left(\bigcup_{i=1}^{I}\left(T_{N,i}^{\phi_1,\phi_2} \geq \chi^2_{1,\alpha/I}\right)\right) \leq \sum_{i=1}^{I} P_r\left(T_{N,i}^{\phi_1,\phi_2} \geq \chi^2_{1,\alpha/I}\right) = \alpha.$$

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Part VIII

Applied Mathematics

22

Some Problems in Geometric Processing of Surfaces

Jaime Puig-Pey, Akemi Gálvez, Andrés Iglesias, Pedro Corcuera, and José Rodríguez

Department of Applied Mathematics and Computational Sciences, University of Cantabria, Spain

Abstract: This paper addresses two interesting problems in geometric processing of surfaces: (1) the determination of the curves on a surface having a constant angle with a prescribed constant direction (helical curves) and (2) the construction of the curve of contact between the surface and the cone circumscribing the surface, with its vertex at the observation point (silhouette curves). Both problems are formulated by using geometric and differential arguments leading to initial value problems of systems of explicit first-order ordinary differential equations that can be efficiently solved through standard step-by-step numerical integration methods. For each problem, the interesting cases of surfaces given in implicit and parametric form are discussed. Some illustrative examples show the good performance of the proposed methods.

Keywords and phrases: Geometric processing, differential geometry, parametric surfaces, implicit surfaces, helical curves, silhouette curves

22.1 Introduction

During the last few years, geometric processing has become a very important and widely researched issue in Mathematical Modeling. In its most comprehensive meaning, geometric processing usually refers to the calculation of geometric properties of entities such as curves, surfaces and solids (Barnhill, 1992). These geometric problems are represented as equations or systems, nonlinear in general, which are often solved by means of algebraic techniques as made by Bajaj et al. (1988), Krishnan and Manocha (1997). But other methods based on differential equations are receiving increasing attention during the last few years. Thus, Grandine (2000) formulates geometric problems as boundary problems in systems of algebraic-differential equations. Patrikalakis and Maekawa (2002) also apply algebraic and differential methods to some issues related to curves and surfaces. In this paper, we also follow a geometric-differential approach to solve two interesting problems in geometric processing of surfaces:

1. the determination of the curves on a surface having a constant angle with a prescribed constant direction (*helical curves*) and

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2. the construction of the curve of contact between the surface and the cone circumscribing the surface, with its vertex at the observation point (*silhouette curves*).

Our approach is quite similar to that in our previous papers in Gálvez et al. (2004), Puig-Pey et al. (2003, 2004) and Puig-Pey et al. (2005). The problems are formulated by using geometric and differential arguments, leading in most cases to initial value problems of systems of explicit first-order ordinary differential equations (ODEs), which can be solved efficiently by standard step-by-step numerical integration methods, available in most numerical libraries (Press et al. (1992), The Mathworks Inc (1999), The Netlib Repository at `http://www.netlib.org`). Basic definitions and properties from classical Differential Geometry, see Struik (1988), are very important tools in this work. We apply them to surfaces expressed in implicit form, $f(x, y, z) = 0$, and also to parametric surfaces, $\mathbf{S}(u, v) = (x(u, v), y(u, v), z(u, v))$, in particular NURBS (Non Uniform Rational B-Splines), a rational piecewise model very common for the definition of free form curves and surfaces in Computer Aided Geometric Design (see a recent overview of CAGD in Farin et al. (2002)). Efficient algorithms for evaluation of functions and derivatives associated to NURBS curves and surfaces can be found in the book by Piegl and Tiller (1997). We make use of them throughout this work.

The guidelines of this paper are as follows: Firstly, some mathematical preliminaries on parametric and implicit surfaces are given in Section 22.2. Section 22.3 deals with the calculation of helical curves, which maintain a constant angle with a prescribed constant direction. The cases of helical curves on implicit and parametric surfaces are discussed. Then, in Section 22.4 we provide an efficient method for computing the silhouette curves (the curves of contact between the surface and the cone circumscribing the surface, with vertex at the observation point). The method is also presented for both the implicit and parametric surfaces. The chapter closes with the conclusions of this work and some further remarks.

22.2 Mathematical Preliminaries

In this work we will consider differentiable surfaces given in parametric and implicit forms. In the first case, they are described by a vector-valued function of two variables:

$$\mathbf{S}(u, v) = (x(u, v), y(u, v), z(u, v)), \qquad u, v \in \Omega \subset \mathbb{R}^2 \tag{22.1}$$

where u and v are the surface parameters and Ω represents the surface domain. Expression (22.1) is called a parameterization of the surface $\mathbf{S}$. We shall use the notation:

$$\mathbf{S}_u(u, v) = \frac{\partial \mathbf{S}(u, v)}{\partial u} \quad , \quad \mathbf{S}_v(u, v) = \frac{\partial \mathbf{S}(u, v)}{\partial v}$$

to denote the first derivatives of $\mathbf{S}$, which depend on the specific parameterization adopted. However, all the differential geometric characteristics of the surface employed in this paper are independent of the chosen parameterization.

At regular points, the partial derivatives $\mathbf{S}_u(u, v)$ and $\mathbf{S}_v(u, v)$ do not vanish simultaneously. For $\{u = u_0, v = v_0\}$, $\mathbf{S}_u$ and $\mathbf{S}_v$ are vectors on the tangent plane to the surface at the point $\mathbf{S}(u_0, v_0)$, each being tangent to the parametric or coordinate curve

$v = v_0$ and $u = u_0$, respectively. These vectors define the *unit normal vector* $\mathbf{N}$ to the surface $\mathbf{S}$:

$$\mathbf{N} = \frac{\mathbf{S}_u \times \mathbf{S}_v}{||\mathbf{S}_u \times \mathbf{S}_v||_2} \tag{22.2}$$

where the symbol "$\times$" is used to indicate the cross product and $||.||_2$ denotes the Euclidean norm.

Any arbitrary curve $\mathbf{C}$ on the surface can be described in parametric form on the surface domain Ω by $\{u = u(t), v = v(t)\}$. This expression defines a three-dimensional curve on the surface $\mathbf{S}$ given by $\mathbf{C}(t) = \mathbf{S}(u(t), v(t))$. Applying the chain rule, the tangent vector of the curve $\mathbf{C}$ at a point $\mathbf{C}(t)$ becomes:

$$\frac{d\mathbf{C}(t)}{dt} = \mathbf{S}_u \ \frac{du}{dt} + \mathbf{S}_v \ \frac{dv}{dt} \tag{22.3}$$

or, as a differential arc of $\mathbf{C}(t)$:

$$d\mathbf{C} = \mathbf{S}_u \ du + \mathbf{S}_v \ dv. \tag{22.4}$$

It is useful to consider the case in which the curve $\mathbf{C}$ is parameterized by the arc-length on the surface. Its geometric interpretation is that a constant step traces a constant distance along an arc-length parameterized curve. A practical application in computer controlled milling operations is that the curve path followed by the milling machine must be parameterized such that the cutter neither speeds up nor slows down along the path. Consequently, the optimal path is that parameterized by the arc-length s on the surface $\mathbf{S}$, given by the First Fundamental Form:

$$E \ \left(\frac{du}{ds}\right)^2 + 2 \ F \ \frac{du}{ds} \ \frac{dv}{ds} + G \ \left(\frac{dv}{ds}\right)^2 = 1 \tag{22.5}$$

or, in differential form:

$$ds^2 = E \ du^2 + 2F \ du \ dv + G dv^2 \tag{22.6}$$

where the coefficients E, F and G are given by:

$$E = \mathbf{S}_u.\mathbf{S}_u \ , \ F = \mathbf{S}_u.\mathbf{S}_v \ , \ G = \mathbf{S}_v.\mathbf{S}_v \tag{22.7}$$

and "." is used to indicate the *dot* product (see Struik (1988) for details). In some cases, it can be useful to consider s as the arc-length measured in the parametric domain for (u, v). Then the differential relation is:

$$ds^2 = du^2 + dv^2 \tag{22.8}$$

For a surface given in implicit form, $f(x, y, z) = 0$, calling f_x, f_y, f_z to the corresponding partial derivatives, the unit normal vector at a nonsingular point (i.e., a point at which the three partial derivatives do not vanish simultaneously) is:

$$\mathbf{N} = \frac{(f_x, f_y, f_z)}{||(f_x, f_y, f_z)||_2} \tag{22.9}$$

A parametrically defined curve $\mathbf{C}(s) = (x(s), y(s), z(s))$, has tangent vector:

$$\frac{d\mathbf{C}(s)}{ds} = \left(\frac{dx}{ds}, \frac{dy}{ds}, \frac{dz}{ds}\right). \tag{22.10}$$

If $\mathbf{C}(s)$ is lying on $f(x, y, z) = 0$, the tangent vector is orthogonal to the surface normal $\mathbf{N}$, and then, from (22.9) and (22.10):

$$f_x \ \frac{dx}{ds} + f_y \ \frac{dy}{ds} + f_z \ \frac{dz}{ds} = 0 \tag{22.11}$$

or, calling $d\mathbf{C} = (dx, dy, dz)$ to the differential arc of $\mathbf{C}$, one has the following differential expression:

$$f_x \ dx + f_y \ dy + f_z \ dz = 0. \tag{22.12}$$

Further, the elementary arc-length ds of differential arc $d\mathbf{C}$ and its components are related by the Pythagorean relationship:

$$ds^2 = dx^2 + dy^2 + dz^2 \tag{22.13}$$

or equivalently (the tangent vector $\dfrac{d\mathbf{C}}{ds}$ is unitary):

$$\left(\frac{dx}{ds}\right)^2 + \left(\frac{dy}{ds}\right)^2 + \left(\frac{dz}{ds}\right)^2 = 1. \tag{22.14}$$

22.3 Helical Curves on Surfaces

Helical curves are curves whose tangent vector maintains a constant angle ϕ with a given constant direction $\mathbf{D}$. As shown by several authors, the helical topology is important in the generation of tool-paths for numerical controlled machining, particularly for high-speed machining processes (see, for instance, Choi and Jerard (1998) or Patrikalakis and Maekawa (2002)). Helical curves are also relevant for designing curves on surfaces where the control of slopes is important, like in railways, roads, etc.

In this section we show how to obtain a helical curve $\mathbf{C}$ lying on a surface $\mathbf{S}$ and defined by a parametric representation, $\mathbf{C}(s) = (x(s), y(s), z(s))$, where s is the 3D arc-length on $\mathbf{S}$. For $\mathbf{C}(s)$ to be a helical curve, it must exhibit a constant angle ϕ with an arbitrary given vector $\mathbf{D}$, which will be the axis of such a helical curve. Since $\left|\left|\dfrac{d\mathbf{C}}{ds}\right|\right|_2 = 1$ and, without loss of generality, we can assume that $||\mathbf{D}||_2 = 1$, we get:

$$\frac{d\mathbf{C}}{ds}.\mathbf{D} = cos(\phi) \tag{22.15}$$

The cases of helical curves on implicit and parametric surfaces are discussed in the following paragraphs.

22.3.1 Implicit surfaces

Let $\mathbf{S}$ be a surface given in implicit form by $f(x, y, z) = 0$. In this case, we take as unknows the components of the unit tangent vector to $\mathbf{C}(s)$, given by (22.10). Without loss of generality, we can assume that $\mathbf{D} = (0, 0, 1)$ (the discussion is quite similar for any other choice of the unit vector $\mathbf{D}$), so from (22.15) we get:

$$\frac{dz}{ds} = cos(\phi). \tag{22.16}$$

Substituting (22.16) into (22.13), combining the resulting equation with (22.12) and making some calculations, we finally obtain:

$$\begin{cases} \dfrac{dx}{ds} = \dfrac{-f_x\, f_z cos(\phi) \pm f_y \sqrt{\left(f_x^2 + f_y^2\right) sin^2(\phi) - f_z^2\, cos^2(\phi)}}{f_x^2 + f_y^2} \\ \\ \dfrac{dy}{ds} = \dfrac{-f_y\, f_z cos(\phi) \mp f_x \sqrt{\left(f_x^2 + f_y^2\right) sin^2(\phi) - f_z^2\, cos^2(\phi)}}{f_x^2 + f_y^2} \\ \\ \dfrac{dz}{ds} = cos(\phi) \end{cases} . \tag{22.17}$$

Equations (22.17) together with an initial point:

$$\begin{cases} x(0) = u_0 \\ y(0) = v_0 \\ z(0) = z_0 \end{cases} \tag{22.18}$$

constitute an initial-value problem for an explicit first-order system of ordinary differential equations. Note that there are two different systems of differential equations, associated with the signs $\pm$ and $\mp$ in (22.17), respectively. They correspond to the two different helical curves passing through a given point on the surface $\mathbf{S}$ for which the value of the expression $\Delta = \left(f_x^2 + f_y^2\right) sin^2(\phi) - f_z^2\, cos^2(\phi)$ is positive, $\Delta > 0$. On the contrary, a value $\Delta < 0$ at a point $\mathbf{P}$ means that there is no helical curve at that point for the chosen direction $\mathbf{D}$ and the angle ϕ.

Example 1. Figure 22.1 shows two examples of helical curves on implicit surfaces. The figure on the left is given by the implicit equation $\alpha(z-1) + (x^2 + y^2)z = 0$ (for $\alpha = 0.04$) while the figure on the right is comprised of two spheres and a cylinder. The helical curves correspond to angles $\phi = 80^o$ and $\phi = 85^o$ respectively for the vector $\mathbf{D} = (0, 0, 1)$ in both cases. As the reader can see, the method exhibits a good performance even when the curve moves on a piece comprised of several surfaces (see Section 22.5 for a more detailed discussion).

22.3.2 Parametric surfaces

In the case of a parametric surface $\mathbf{S}(u, v)$ given by Eq. (22.1), we obtain the helical curve $\mathbf{C}(s)$ in parametric form by taking as unknowns the derivatives $\dfrac{du}{ds}, \dfrac{dv}{ds}$ and

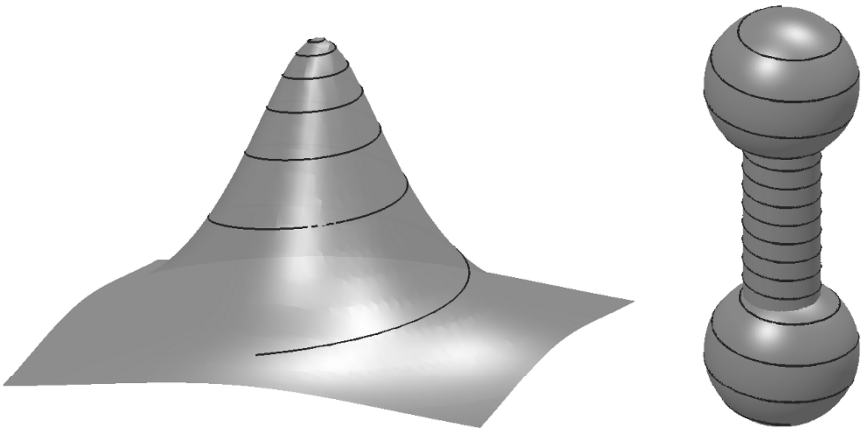

Figure 22.1. Examples of helical curves on implicit surfaces

calculating $u(s)$, $v(s)$. The procedure is as follows: Firstly, we insert (22.3) into (22.15) and get:

$$(\mathbf{S}_u.\mathbf{D})\ \frac{du}{ds} + (\mathbf{S}_v.\mathbf{D})\ \frac{dv}{ds} = cos(\phi). \tag{22.19}$$

Combining Eqs. (22.5) and (22.19) and making some calculations, we obtain:

$$\begin{cases} \dfrac{du}{ds} = \dfrac{-B \pm 2(\mathbf{S}_v.\mathbf{D})\sqrt{(F^2 - EG)\,cos^2(\phi) + A}}{2A} \\ \dfrac{dv}{ds} = \dfrac{-C \mp 2(\mathbf{S}_u.\mathbf{D})\sqrt{(F^2 - EG)\,cos^2(\phi) + A}}{2A} \end{cases} \tag{22.20}$$

where the values A, B and C are given by

$$A = E\,(\mathbf{S}_v.\mathbf{D})^2 - 2F\,(\mathbf{S}_u.\mathbf{D})\,(\mathbf{S}_v.\mathbf{D}) + G\,(\mathbf{S}_u.\mathbf{D})^2$$
$$B = 2\,cos(\phi)\ [F(\mathbf{S}_v.\mathbf{D}) - G(\mathbf{S}_u.\mathbf{D})]$$
$$C = 2\,cos(\phi)\,[F\,(\mathbf{S}_u.\mathbf{D}) - E\,(\mathbf{S}_v.\mathbf{D})]$$

and E, F and G are defined by (22.7). For system (22.20) to be completely determined we need to consider an initial point:

$$\begin{cases} u(0) = u_0 \\ v(0) = v_0 \end{cases} \tag{22.21}$$

on the surface domain. System (22.20)–(22.21) constitutes an initial-value problem of explicit first-order ordinary differential equations. The signs $\pm$ and $\mp$ in (22.20) mean that there are two helical curves starting at (u_0, v_0) associated with the two possible ϕ directions at this point, provided that the discriminant $(F^2 - EG)\,cos^2(\phi) + A$ is positive at this point, and no solution otherwise. Once the system (22.20)–(22.21) is solved for u and v, the x, y and z coordinates of the helical curve can be automatically determined by a simple substitution of u and v into the surface equation $\mathbf{S}(u, v)$.

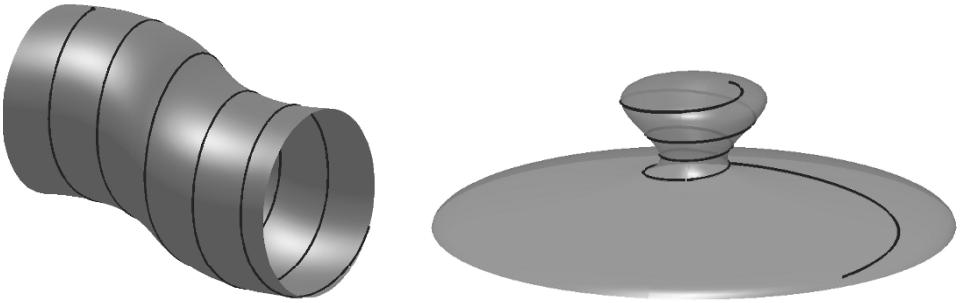

Figure 22.2. Examples of helical curves on parametric surfaces

Example 2. Figure 22.2 shows two examples of helical curves on parametric surfaces. The figure on the left is a NURBS surface of order $(3, 3)$ defined by a mesh of 4×4 control points and non-periodic knot vectors for both variables u and v. The helical curve corresponds to $\phi = 70^o$ and $\mathbf{D} = (1, 0, 0)$. The figure on the right is the top part of a teapot comprised of 8 bicubic Bézier surfaces. In this example, $\phi = 85^o$ and $\mathbf{D} = (0, 0, 1)$.

22.4 Silhouette Curve on a Surface

The general problem is equivalent to the construction of the curve of contact between the surface and the cone circumscribing the surface, with its vertex at the observation point. This problem appears in robotics and computer vision for control of visibility, etc. An efficient method for calculating the silhouette of a canal surface is presented by Kim and Lee (2003). If the vision is parallel, similar statements can be made, referring to the cylinder circumscribing the surface, with its axis in the direction of the observation. In the case of conic vision, the condition is that the line joining each point of the silhouette curve with the cone vertex, must be orthogonal to the surface normal at the considered silhouette point. The formulation for this case of conic vision is presented in the following paragraphs.

22.4.1 Surface in implicit form

Let $f(x, y, z) = 0$ be the implicit equation of a surface $\mathbf{S}$. At a point (x, y, z) of $\mathbf{S}$ placed on the silhouette curve, with the vision point $\mathbf{Q} = (Q_1, Q_2, Q_3)$, the two following conditions must be verified:

$$f(x, y, z) = 0 \tag{22.22}$$

$$\begin{aligned} &((x, y, z) - \mathbf{Q}).(f_x, f_y, f_z) = 0 \\ &\equiv (x - Q_1)f_x + (y - Q_2)f_y + (z - Q_3)f_z = 0 \\ &\equiv g(x, y, z) = 0. \end{aligned} \tag{22.23}$$

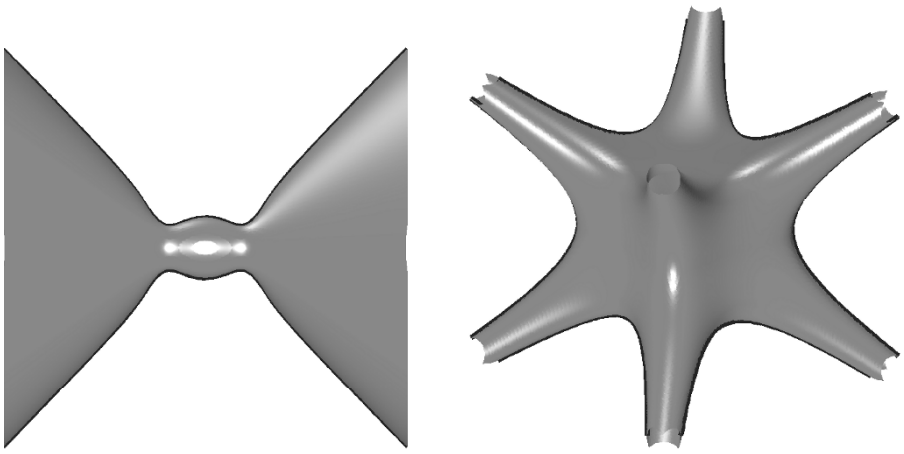

Figure 22.3. Examples of silhouette curves on implicit surfaces

This system (22.22)–(22.23) of 2 equations with 3 unknowns, represents the silhouette, and can be understood as the intersection of two surfaces given in implicit form, namely, $f(x, y, z) = 0$ and $g(x, y, z) = 0$. If $\mathbf{N}_1 = (f_x, f_y, f_z)$ and $\mathbf{N}_2 = (g_x, g_y, g_z)$ denote the respective normals at an intersection point, the differential of arc of the intersection curve, $d\mathbf{C} = (dx, dy, dz)$, follows the direction of the vector:

$$\mathbf{W} = (W_1, W_2, W_3) = (\mathbf{N}_1 \times \mathbf{N}_2) = (f_y g_z - f_z g_y, f_z g_x - f_x g_z, f_x g_y - f_y g_x)$$

provided that the surfaces are not tangent. Consequently:

$$\frac{dx}{W_1} = \frac{dy}{W_2} = \frac{dz}{W_3}.$$

Combining these equations with Eq. (22.13) we obtain the following first-order explicit system of ODEs that represents the silhouette curve $\mathbf{C}$:

$$\begin{cases} \dfrac{dx}{ds} = \pm \dfrac{f_y g_z - f_z g_y}{\sqrt{(f_y g_z - f_z g_y)^2 + (f_z g_x - f_x g_z)^2 + (f_x g_y - f_y g_x)^2}} \\ \dfrac{dy}{ds} = \pm \dfrac{f_z g_x - f_x g_z}{\sqrt{(f_y g_z - f_z g_y)^2 + (f_z g_x - f_x g_z)^2 + (f_x g_y - f_y g_x)^2}} \\ \dfrac{dz}{ds} = \pm \dfrac{f_x g_y - f_y g_x}{\sqrt{(f_y g_z - f_z g_y)^2 + (f_z g_x - f_x g_z)^2 + (f_x g_y - f_y g_x)^2}} \end{cases} . \tag{22.24}$$

From (22.23) the partial derivatives can be obtained as:

$$\begin{pmatrix} g_x \\ g_y \\ g_z \end{pmatrix} = \begin{pmatrix} f_{xx} & f_{yx} & f_{zx} \\ f_{xy} & f_{yy} & f_{zy} \\ f_{xz} & f_{yz} & f_{zz} \end{pmatrix} \begin{pmatrix} x - Q_1 \\ y - Q_2 \\ z - Q_3 \end{pmatrix} + \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix} \tag{22.25}$$

Taking as the initial condition $(x(0), y(0), z(0)) = (x_0, y_0, z_0)$ for (22.24), we have an initial value problem of ODEs. In order to obtain an initial point $\mathbf{P}_0$ of the intersection

curve of $f = 0$ and $g = 0$ a combination of scalar and vector fields can be applied (see Puig-Pey et al. (2005) for details).

Example 3. Figure 22.3 shows two examples of silhouette curves on implicit surfaces. The figures are given by $x^4 + 2x^2z^2 - 0.36x^2 - y^4 + \frac{y^2}{4} + z^4 = 0$ (on the left) and $x^4 + y^4 + z^4 - x^2y^2 - x^2z^2 - y^2z^2 - 1 = 0$ (on the right). The observation points for these examples are $(-3, 0, 0)$ and $(2, -2, 0)$ respectively.

22.4.2 Surfaces in parametric form

If the surface is in parametric form, $\mathbf{S}(u, v) = (x(u, v), y(u, v), z(u, v))$, the points on the silhouette hold:

$$(\mathbf{S}(u, v) - \mathbf{Q})(\mathbf{S}_u(u, v) \times \mathbf{S}_v(u, v)) = 0 \equiv c(u, v) = 0, \tag{22.26}$$

that is, the silhouette appears as an implicit equation denoted by $c(u, v) = 0$. Its graphical representation is a plane curve in the parametric domain of the u, v parameters of $\mathbf{S}$. If $c(u, v)$ is algebraic, González-Vega and Necula (2002) introduce a method for deducting precisely the topology of this curve. To trace the curve we use a differential formulation. In particular, two equations with the three differential unknowns du, dv and ds are considered. The first one is $c_u\ du + c_v\ dv = 0$, which represents the orthogonality between the differential arc of curve $c(u, v) = 0$ and its normal vector, both in the domain u, v. Combining this expression with Eq. (22.8) we get the first-order explicit system of ODEs:

$$\begin{cases} \dfrac{du}{ds} = \pm \dfrac{c_v}{\sqrt{c_u^2 + c_v^2}} \\ \dfrac{dv}{ds} = \mp \dfrac{c_u}{\sqrt{c_u^2 + c_v^2}} \end{cases} \tag{22.27}$$

where:

$$c_u = \mathbf{S}_u.(\mathbf{S}_u \times \mathbf{S}_v) + (\mathbf{S} - \mathbf{Q}).(\mathbf{S}_{uu} \times \mathbf{S}_u + \mathbf{S}_u \times \mathbf{S}_{vu})$$
$$c_v = \mathbf{S}_v.(\mathbf{S}_u \times \mathbf{S}_v) + (\mathbf{S} - \mathbf{Q}).(\mathbf{S}_{uv} \times \mathbf{S}_v + \mathbf{S}_u \times \mathbf{S}_{vv}).$$

An initial point is needed, and it can be obtained by solving the scalar equation (22.26) when a value is assigned to u or v. As an alternative, the idea of scalar and vector fields can be fruitful. The scalar function $c(u, v)$ in the (u, v) domain plays the role of a scalar field $\boldsymbol{\Phi}$; a gradient curve is obtained in a step by step integration process, advancing in the gradient direction, $\nabla\boldsymbol{\Phi}$, with the adequate orientation, starting at a "freely chosen" initial point (recommended to be not far from the expected silhouette curve) in the (u, v) domain, until detecting a change in the sign of the value of $c(u, v)$ and, hence, getting the point verifying $c(u, v) = 0$, the initial point for tracing the silhouette curve.

Example 4. Figure 22.4 shows two examples of silhouette curves on parametric surfaces. The figure on the left is a NURBS surface of order $(5, 4)$ defined by a mesh of 8×6 control points, while the surface on the right is a NURBS surface of order $(3, 4)$ and

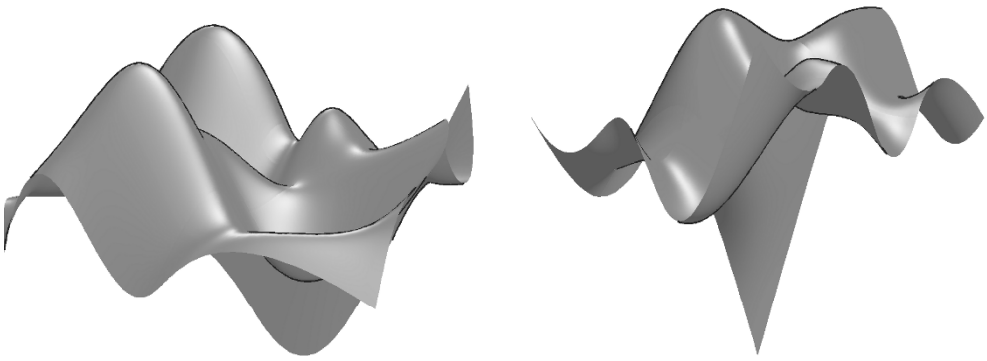

Figure 22.4. Examples of silhouette curves on parametric surfaces

6×6 control points. The observation points are $\left(-20, \frac{15}{4}, 1\right)$ and $\left(-10, -10, \frac{5}{4}\right)$ respectively.

22.5 Conclusions and Further Remarks

In this chapter the problem of the computation of helical and silhouette curves on surfaces have been addressed. The presented methods are obtained by using geometric and differential arguments that characterize the problem to be solved. In addition, the methods can deal with surfaces given in implicit or in parametric form. The methodology presented here has the advantage of being quite general because it is valid for any type of smooth functions involved in the surface equations, and it does not depend on being polynomial, or rational or other. For the formulation to have sense, it is merely necessary that they can be differentiated. In the case of surfaces consisting of several patches, the ODEs are valid inside each patch, and special attention has to be paid in the transition from one patch to another, taking into account the continuity between them. If there are not strong discontinuities, one can progress smoothly between patches, because only low order derivatives appear in the ODEs. Otherwise, the border crossing point must be carefully identified, with the integration of the ODEs starting from it as the initial point for traversing the next patch.

The first order explicit ODEs systems associated with initial value problems can be treated numerically with methods that are widely available, fast and reliable. In our case we have used the integrator function `ode45` of MATLAB (The Mathworks Inc, 1999), which is based on an adaptive step-by-step technique combining 4th- and 5th-order Runge-Kutta methods for controlling the error and the step integration size. Values for absolute and relative error tolerances can be specified by the user. The routine allows for using stopping criteria in simple ways, controlling common conditions for values of the variables or for certain functions appearing in the problem. There is no

perfect numerical procedure for solving all cases of initial value ODEs problems, but to our experience this integrator function has shown a very good behaviour. Let us mention too the routines `odeint`, `rkqs` and `rkck` in the book Numerical Recipes by Press et al. (1992) that are available in C and C++, Fortran 77 and 90 languages. They are adaptive step size integration procedures based on Runge-Kutta technique as well. In the Netlib Repository one can find a wide variety of tested computer codes for different numerical problems, including ODEs.

Regarding stopping criteria for the step-by-step integration processes in the problems included here, one case will appear when going beyond some limit in the domain of definition of the x, y, z variables or for the u, v parameters. The presence of singular points on a surface (zero values for partial derivatives, undefined normals) introduces singularities in the ODEs. Although floating point calculations make it more difficult to obtain exact zero values, this could actually happen, leading to numerical instabilities when the integration arrives in the neighbourhood of such points.

The explained methods are deduced from the analysis of a local behaviour at differential level. In the case of a solution curve with several components, these techniques are not sufficient for an automatic identification of all the simple components. Any criteria for generating different trajectories in the associated initial value problem will be useful for approaching the different components.

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23

Generalized Inverse Computation Based on an Orthogonal Decomposition Methodology

Patricia Gómez[1], Beatriz Lacruz[2], and Rosa Eva Pruneda[3]

[1] Department of Applied Mathematics, University of Cantabria, Spain
[2] Department of Statistical Methods, University of Zaragoza, Spain
[3] Department of Mathematics, University of Castilla-La Mancha, Spain

Abstract: The need to compute the generalized inverse of a matrix appears in several statistical, mathematical and engineering problems, such as the estimation of linear classification and regression functions, electrical circuits estimation, calculus of structures, etc. In this paper, we propose to apply an orthogonal decomposition methodology to compute a weak generalized inverse, based on the calculus of a non-singular submatrix of the given matrix. Special attention will be focussed on the updating of the generalized inverse when some of the elements of the original matrix are modified. The proposed method allows us to perform this updating without starting the process from scratch. The proposed procedures will be illustrated with some examples and their application to the estimation of linear regression coefficients when a problem of multicollinearity is present.

Keywords and phrases: Generalized inverse updating, non full rank matrix, linear regression, multicollinearity

23.1 Introduction

Castillo et al. (1999) have introduced a pivoting transformation for obtaining the orthogonal of a given linear subspace. This process decomposes the Euclidean Space in a direct sum of the orthogonal linear subspace and its complement. This method is applied to solve a long list of problems in linear algebra, including the resolution of linear systems of equations. Some of these applications can be found in Castillo et al. (2006a,b). The direct methods that arise from this transformation have a complexity identical to that associated with the Gaussian Elimination Method (see Castillo et al. (1999)). However, they are specially suitable for updating solutions when changes in rows, columns, or variables are done. In fact, when changing a row, column or variable, a single step of the process allows us to obtain (to update) the new solution, without needing to start from scratch.

In this paper we propose to apply the pivoting transformation based on the orthogonal decomposition to obtain the generalized inverse $\mathbf{A}^-$ of a matrix $\mathbf{A} \in \mathcal{M}_{m\times n}$

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which verifies $\mathbf{A}\mathbf{A}^{-}\mathbf{A} = \mathbf{A}$. The method is based on the calculus of the inverse of a maximum rank submatrix of the given matrix $\mathbf{A}$. We also extend this methodology to update the generalized inverse when a row of the given matrix is modified.

The paper is structured as follows. In Section 23.2, the definition of a generalized inverse and the theoretical calculus to obtain it are introduced. In Section 23.3, we present the algorithm to calculate a generalized inverse of a given matrix. In Section 23.4 we present the algorithm to update the generalized inverse when a row of the original matrix is modified. Both algorithms are illustrated with an example. In Section 23.5 we present the application of this technique to estimate the parameters of a lineal model where multicollinearity is present. Finally, some conclusions are reported in Section 23.6.

23.2 Generalized Inverse

In case of a rectangular matrix or a non full rank matrix, the concept of inverse matrix must be generalized. In this paper we consider a weak generalized inverse, $\mathbf{A}^{-}$, called simply *generalized inverse of* $\mathbf{A}$ or $\{1\}$-*inverse*. It is called weak since it must verify just one condition (given in the following definition) in order to generalize the inverse of a given matrix.

Definition 1 ($\{1\}$-inverse). *Given $\mathbf{A} \in \mathcal{M}_{m\times n}$, the matrix $\mathbf{A}^{-} \in \mathcal{M}_{n\times m}$ is a $\{1\}$-inverse of $\mathbf{A}$ if and only if $\mathbf{A}\mathbf{A}^{-}\mathbf{A} = \mathbf{A}$.*

There is not a unique $\{1\}$-inverse, but at least one always exists. There are different methods to compute it, see for example Schott (2005). In particular, we will use the following result:

Theorem 1 ($\{1\}$-inverse computation). *Let $\mathbf{A} \in \mathcal{M}_{m\times n}$ be a matrix with $rank(\mathbf{A}) = k \leq min(m, n)$. If $rank(\mathbf{A}) = k$, there exist permutation matrices $\mathbf{R}$ and $\mathbf{C}$, such that, the matrix $\mathbf{A}$ can be reordered as*

$$\mathbf{RAC} = \mathbf{B} = \left(\begin{array}{c|c} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \hline \mathbf{B}_{21} & \mathbf{B}_{22} \end{array}\right), \tag{23.1}$$

where $\mathbf{B}_{11}$ is a non singular submatrix of order k. Then, a generalized inverse of the matrix $\mathbf{B}$ can be calculated as

$$\mathbf{B}^{-} = \left(\begin{array}{c|c} \mathbf{B}_{11}^{-1} & \mathbf{0}_{k\times(m-k)} \\ \hline \mathbf{0}_{(n-k)\times k} & \mathbf{0}_{(n-k)\times(m-k)} \end{array}\right) \tag{23.2}$$

where $\mathbf{B}_{11}^{-1}$ is the inverse of the submatrix $\mathbf{B}_{11}$ and $\mathbf{0}$ stands for the zero matrix. Consequently, a generalized inverse of the matrix $\mathbf{A}$ is attained and it is computed as:

$$\mathbf{A}^{-} = \mathbf{C}\mathbf{B}^{-}\mathbf{R}. \tag{23.3}$$

23.3 The Algorithm to Obtain a Generalized Inverse

We adapt the algorithm given in Castillo et al. (1998, 2000), based on the orthogonal decomposition of the Euclidian space, to compute the inverse of a maximum rank submatrix in order to obtain the {1}-inverse in Eq. (23.3). The algorithm works as follows:

Algorithm 1

Input: A matrix $\mathbf{A}$ of dimension $m \times n$. The starting matrix $\mathbf{W} = \mathbf{I}_n$ (the identity matrix of dimension n) and the starting vector $\mathbf{u} = \mathbf{0}_n$ (the null vector of dimension n).

Output: A vector $\mathbf{u}$ that indicates which rows and columns of $\mathbf{A}$ form the submatrix $\mathbf{B}_{11}$ and a matrix $\mathbf{W}$ that contains its inverse $\mathbf{B}_{11}^{-1}$.

Step 1: Initial step. Set $\mathbf{W} = \mathbf{I}_n$. Set $\mathbf{u} = \mathbf{0}_n$. Let $i = 1$.

Step 2: Dot products. Calculate the dot products $t_j = \mathbf{a}_i^T \mathbf{w}_j,\ j = 1, \ldots, n$, that is, the dot products of the i-th row of $\mathbf{A}$ by each column of $\mathbf{W}$.

Step 3: Select a pivoting column. Locate the first non null t_p corresponding to a null element in the p-th position of $\mathbf{u}$, which indicates the p-th column of the $\mathbf{W}$ to be used as pivot. Replace the p-th component of $\mathbf{u}$ by i and continue with Step 4. If there is not such a column, go to Step 6.

Step 4: Modify the pivoting column. Divide the p-th column of $\mathbf{W}$ by t_p.

Step 5: Pivoting. For $j = 1$ to n, $j \neq p$ and $t_j \neq 0$ do $w_{kj} = w_{kj} - t_j w_{kp}$ for $k = 1, \ldots, n$.

Step 6: If $i = m$, continue with Step 7. Otherwise, increase i in one unit and go back to Step 2.

Step 7: Output. The matrix $\mathbf{W}$ which contains the inverse of a submatrix of maximum rank of $\mathbf{A}$. This maximum rank submatrix is composed by the intersection of the rows of $\mathbf{A}$ whose indices are the non null elements of $\mathbf{u}$ and the columns given by the position of these indices in $\mathbf{u}$. The inverse of this submatrix is composed by the columns of $\mathbf{W}$ corresponding to the non null elements in $\mathbf{u}$ and the same rows. The rank of $\mathbf{A}$ is equal to the number of non null elements in $\mathbf{u}$.

In Step 3, not to find the pivot means that the row $\mathbf{a}_i^T$ of matrix $\mathbf{A}$, introduced in the previous step, is linearly dependent of the rows given by the non null elements of $\mathbf{u}$. Furthermore, the coefficients of such linear combination are given by the corresponding dot products in vector $\mathbf{t}$.

The iterations of the algorithm can be organized in tabular form. Table 23.1 shows the elements of the i-th iteration. The vector $\mathbf{u}$ is in the first row of the tableau and the row of $\mathbf{A}$ introduced in the pivoting process is in the first column. The last row corresponds to the dot products computed in Step 2 and $\mathbf{W}$ is inside the tableau.

Example 1. We apply algorithm 1 to obtain the generalized inverse of

$$\mathbf{A} = \begin{pmatrix} -1 & 1 & 0 & 1 \\ 3 & -1 & 2 & 2 \\ 2 & 0 & 2 & 3 \\ 1 & -1 & 0 & 1 \\ 3 & -1 & 2 & 4 \end{pmatrix}. \tag{23.4}$$

Table 23.1. i-th iteration of Algorithm 1

Iteration i				
	u_1	u_2	...	u_n
a_{i1}	w_{11}	w_{12}	...	w_{1n}
a_{i2}	w_{21}	w_{22}	...	w_{2n}
⋮	⋮	⋮	⋮	⋮
a_{in}	w_{n1}	w_{n2}	...	w_{nn}
t	t_1	t_2	...	t_n

The iterations in tabular form are shown in table 23.2. We proceed as follows:

Step 1: Initial step. The first tableau shows **u** equal to the null vector of dimension 4 and **W** equal to the identity matrix of order 4. Since $i = 1$, the first column in the tableau is the first row of **A**, that is, $\mathbf{a}_1^T = (-1, 1, 0, 1)$.

Step 2: Dot products. The last row in the first tableau contains the vector $\mathbf{t} = \mathbf{a}_1^T \cdot \mathbf{I}_4 = (-1, 1, 0, 1)$.

Step 3: Select a pivoting column. Since $t_1 = -1$ is the first non null component of **t** corresponding to a null element in vector **u**, select $p = 1$ and the first column of **W** is the pivoting column. It is given in boldface. For the same reason, the second tableau shows that $u_1 = 1$ and the rest of the components of **u** remain unchanged.

Step 4: Modify the pivoting column. The second tableau shows the first column of $\mathbf{W} = \mathbf{I}_4$ divided by $t_1 = -1$.

Step 5: Pivoting. Since $p = 1$ and $t_3 = 0$, for $j = 2$ and $j = 4$ we compute the new w_{kj}, $k = 1, \ldots, 4$. For example, $w_{12} = w_{14} = 0 - (-1) \cdot 1 = 1$. The rest of elements of **W** remains unchanged as it is shown in the second tableau.

Step 6: Now we go back to Step 2 and after five iterations we stop and go to Step 7.

Step 7: Output. The final tableau shows $\mathbf{u} = (1, 2, 0, 4)$, which means that the submatrix of **A** composed by the intersection of its first, second and forth rows and the same columns,

Table 23.2. Iterations in tabular form to obtain the inverse of a maximum rank submatrix of **A** in example 1. B_{11}^{-1} is boldfaced in the Final Tableau

Iteration 1				
	0	**0**	**0**	**0**
−1	**1**	0	0	0
1	**0**	1	0	0
0	**0**	0	1	0
1	**0**	0	0	1
t	**−1**	1	0	1

Iteration 2				
	1	**0**	**0**	**0**
3	−1	**1**	0	1
−1	0	**1**	0	0
2	0	**0**	1	0
2	0	**0**	0	1
t	−3	**2**	2	5

Iteration 3				
	1	**2**	**0**	**0**
2	1/2	1/2	−1	−3/2
0	3/2	1/2	−1	−5/2
2	0	0	1	0
3	0	0	0	1
t	1	1	0	0

Iteration 4				
	1	**2**	**0**	**0**
1	1/2	1/2	−1	**−3/2**
−1	3/2	1/2	−1	**−5/2**
0	0	0	1	**0**
1	0	0	0	**1**
t	−1	0	0	**2**

Iteration 5				
	1	**2**	**0**	**4**
3	−1/4	1/2	−1	−3/4
−1	1/4	1/2	−1	−5/4
2	0	0	1	0
4	1/2	0	0	1/2
t	1	1	0	1

Final Tableau			
1	**2**	**0**	**4**
−1/4	**1/2**	−1	**−3/4**
1/4	**1/2**	−1	**−5/4**
0	0	1	0
1/2	**0**	0	**1/2**

$$\mathbf{B}_{11} = \begin{pmatrix} -1 & 1 & 1 \\ 3 & -1 & 2 \\ 1 & -1 & 1 \end{pmatrix}, \tag{23.5}$$

is a maximum rank submatrix. Note that the rows are determined by the non null elements of **u**, that is, 1, 2 and 4, and the columns by their positions in the vector, that is, first, second and forth. Finally, choosing the first, second, and forth rows and columns of the matrix **W** in that tableau, we obtain $\mathbf{B}_{11}^{-1}$.

All the tableaux show the pivoting column in boldface. Note that it does not occur in iterations 3 and 5, since no pivot is found. This is because the third row of matrix **A** is linearly dependent on the first and second rows. The coefficients of the linear combination are the components of **t** associated with the non null components of vector **u** in Iteration 3. That is, $\mathbf{a}_3 = 1 \cdot \mathbf{a}_1 + 1 \cdot \mathbf{a}_2$. Analogously, the fifth row of matrix **A** is $\mathbf{a}_5 = 1 \cdot \mathbf{a}_1 + 1 \cdot \mathbf{a}_2 + 1 \cdot \mathbf{a}_4$.

Note that, in this case, the generalized inverse is reached without performing any permutation of the original matrix. After placing zeros as it is indicated in Theorem 1, we get the generalized inverse

$$\mathbf{A}^- = \begin{pmatrix} -1/4 & 1/2 & 0 & -3/4 & 0 \\ 1/4 & 1/2 & 0 & -5/4 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 & 0 \end{pmatrix}. \tag{23.6}$$

23.4 Generalized Inverse Updating Algorithm

This algorithm provides a method for updating a generalized inverse obtained by Algorithm 1 (given in Section 23.3) when a row of the initial matrix **A** is modified. The main advantage of this method is that we do not need to start the process from the beginning.

Let $\mathbf{A}^*$ be the new matrix. Under some conditions we will only need an extra iteration to obtain the generalized inverse of $\mathbf{A}^*$.

Algorithm 1

Input: The matrix **W** and the vector **u** resulting after the application of Algorithm 1 to obtain the generalized inverse of **A**. The modified row $\mathbf{a}_i^*$ of **A**

Output: The new matrix **W** and a new vector **u**

Step 1: Initialize. Let **W** and **u** be the output of Algorithm 1 applied to matrix **A**.

Step 2: Dot products. Calculate the dot products $t_j = \mathbf{a}_i^{*T}\mathbf{w}_j,\ j = 1, \ldots, n$, that is, the dot products of the new row of **A** by the columns of **W**.

(i) If i is a component of **u** and the dot product associated with this column is non null, replace i by i^* in **u**, select the corresponding column as pivot and go to Step 4.

(ii) If i is a component of **u** and the dot product associated with this column is null or if i is not in vector **u**, continue with Step 3.

Step 3: Find the pivoting column. Locate the first non null t_p corresponding to a null element in the p-th position of vector $\mathbf{u}$, which indicates that this is the pivoting column of $\mathbf{W}$. Replace the p-th zero component of $\mathbf{u}$ by i^* and continue with Step 4. If there is not such a column, go to Step 7.
Step 4: Modify the pivoting column. Divide the p-th column of matrix $\mathbf{W}$ by t_p.
Step 5: Pivoting. For $j = 1$ to n, $j \neq p$ and $t_j \neq 0$ do $w_{kj} = w_{kj} - t_j w_{kp}$ for $k = 1, \ldots, n$.
Step 6: Cancel the pivoting column associated with index i. If i and i^* are in $\mathbf{u}$ we need an extra iteration to obtain the updated generalized inverse. Consider the canonical vector $\mathbf{e}_s$, where s is the position of the index i in vector $\mathbf{u}$. Calculate the dot products $t_j = \mathbf{e}_s^T \mathbf{w}_j$, $j = 1, \ldots, n$. Divide the s-th column of $\mathbf{W}$ by t_s. For $j = 1$ to n, $j \neq s$ and $t_j \neq 0$, do $w_{kj} = w_{kj} - t_j w_{ks}$ for $k = 1, \ldots, n$.
Step 7: Check redundant rows of $\mathbf{A}$. If the row $\mathbf{a}_i$ is involved in the linear combinations of redundant rows of the initial matrix $\mathbf{A}$, apply Algorithm 1 to the redundant rows of matrix $\mathbf{A}$ starting from the matrix $\mathbf{W}$ and vector $\mathbf{u}$ obtained in Step 6.
Step 8: Output. The rows and columns in matrix $\mathbf{W}$ corresponding to the non null components of $\mathbf{u}$ contains the inverse of a non singular submatrix of $\mathbf{A}^*$.

An exception occurs in Step 6, when t_s is zero. We can proceed, without loss of generality, by reordering the initial matrix in order to avoid this situation.

Example 2. Suppose that the second row of matrix $\mathbf{A}$ in (23.4) is modified as follows:

$$\mathbf{A}^* = \begin{pmatrix} -1 & 1 & 0 & 1 \\ \mathbf{1} & \mathbf{-1} & \mathbf{1} & \mathbf{0} \\ 2 & 0 & 2 & 3 \\ 1 & -1 & 0 & 1 \\ 3 & -1 & 2 & 4 \end{pmatrix}. \tag{23.7}$$

Algorithm 2 is applied and the extra iteration is shown in table 23.3.

Step 1: Initial step. Let $\mathbf{W}$ and $\mathbf{u}$ those given in the Final Tableau of Table 23.2.
Step 2: Dot products. Since $i = 2$ is in $\mathbf{u}$ but its corresponding dot product is equal to 0, $t_2 = 0$, this column is not available for pivoting process. We continue with Step 3.
Step 3: Find the pivoting column. Third column of $\mathbf{W}$ is selected as pivot.
Step 4: Modify the pivoting column. Divide the third column of $\mathbf{W}$ by $t_3 = 1$.
Step 5: Pivoting. Complete the pivoting process with the rest of the columns of $\mathbf{W}$.
Step 6: Cancel the pivoting column associated with index 2. Since $i = 2$ and $i = 2^*$ are in $\mathbf{u}$ we introduce $\mathbf{e}_2 = (0, 1, 0, 0)^T$ in a new tableau and we select the second column of matrix $\mathbf{W}$ as pivot, as it is shown in table 23.4.

Table 23.3. Extra iteration to obtain the generalized inverse of matrix $\mathbf{A}^*$ in (23.7)

Extra Iteration					**Final Tableau**			
	1	**2**	**0**	**4**	**1**	**2**	**2***	**4**
1	−1/4	1/2	**−1**	−3/4	**−3/4**	1/2	**−1**	**−1/4**
−1	1/4	1/2	**−1**	−5/4	−1/4	1/2	−1	−3/4
1	0	0	**1**	0	**1/2**	0	**1**	**−1/2**
0	1/2	0	**0**	1/2	**1/2**	0	**0**	**1/2**
t	−1/2	0	**1**	1/2				

Table 23.4. Extra iteration to cancel the second column of matrix **W** in the Final Tableau of table 23.3

Extra Iteration				
	1	**2**	**2***	**4**
0	−3/4	**1/2**	−1	−1/4
1	−1/4	**1/2**	−1	−3/4
0	1/2	**0**	1	−1/2
0	1/2	**0**	0	1/2
t	−1/4	**1/2**	−1	−3/4

Final Tableau			
1	**0**	**2***	**4**
−1/2	1	**0**	**1/2**
0	1	0	0
1/2	0	**1**	**−1/2**
1/2	0	**0**	**1/2**

Step 7: Check redundant rows of **A**. The row $\mathbf{a}_2$ is involved in the linear combination of the redundant rows $\mathbf{a}_3$ and $\mathbf{a}_5$ (see Example 1). Then, starting with **W** and **u** obtained in the previous step, first, we make the pivoting process with $\mathbf{a}_3$, as it is shown in table 23.5. Pivot is found and the pivoting transformation is shown in the Final Tableau. Since vector **u** has non null components, the process is finished. Otherwise, we would proceed to pivot with the fifth row $\mathbf{a}_5$.

Step 8: Output. In the Final Tableau of table 23.5 the inverse of a non singular submatrix of matrix $\mathbf{A}^*$ in (23.7) is boldfaced. This non singular submatrix is composed by the intersection of the first, second, third and forth rows and the same columns, as indicated by the non null elements of **u** and its positions.

Finally, reordering the columns of matrix **W** as indicated by the components of **u**, the generalized inverse of $\mathbf{A}^*$ in (23.7) is:

$$\mathbf{A}^{*-} = \begin{pmatrix} -5/4 & -1 & 1/2 & -1/4 & 0 \\ -3/4 & -1 & 1/2 & -3/4 & 0 \\ 1/2 & 1 & 0 & -1/2 & 0 \\ 1/2 & 0 & 0 & 1/2 & 0 \end{pmatrix}. \tag{23.8}$$

Table 23.5. Extra iteration to pivot with the third row of matrix $\mathbf{A}^*$ in (23.4)

Extra Iteration				
	1	**0**	**2***	**4**
2	−1/2	**1**	0	1/2
0	0	**1**	0	0
2	1/2	**0**	1	−1/2
3	1/2	**0**	0	1/2
t	3/2	**2**	2	3/2

Final Tableau			
1	**3**	**2***	**4**
−5/4	**1/2**	**−1**	**−1/4**
−3/4	**1/2**	**−1**	**−3/4**
1/2	**0**	**1**	**−1/2**
1/2	**0**	**0**	**1/2**

23.5 Least Squares Estimation for Less than Full Rank Models

In this section we apply the calculus of the generalized inverse and the updating algorithm proposed in this paper to estimate the parameters in less than full rank linear regression models.

The linear regression model can be written as:

$$\mathbf{y} = \mathbf{X}\beta + \epsilon, \tag{23.9}$$

where $\mathbf{y}$ is the $n \times 1$ vector of observations of the response variable, $\mathbf{X}$ a $n \times k$, $n > k$, matrix of observations of the regressor variables, β is the $k \times 1$ vector of unknown parameters, and ϵ the $n \times 1$ vector of random errors with $E(\epsilon) = \mathbf{0}$ and $Var(\epsilon) = \sigma^2\mathbf{I}_n$. The problem is to estimate the unknown parameters β. The method of least squares is typically used to this aim. If rank($\mathbf{X}$)=k, the least squares estimator is $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$. But, if rank($\mathbf{X}$) $< k$ a particular solution must be given in terms of the generalized inverse. That is, $\tilde{\beta} = (\mathbf{X}^T\mathbf{X})^{-}\ \mathbf{X}^T\mathbf{y}$.

Example 3. To illustrate the estimation of parameters in case of non full rank matrix, consider a regression problem with five explanatory variables, $X_1, \ldots, X_5$, where X_4 is linearly dependent of X_1 and X_3 as follows

$$X_4 = 2X_1 - 3X_3 + \delta, \tag{23.10}$$

with $\delta \sim N(0, 0.01)$ since non exact linear combinations are found in real cases. Let $\mathbf{A} = \mathbf{X}^T\mathbf{X}$ the matrix:

$$\mathbf{A} = \begin{pmatrix} 36.9971 & -4.0667 & 0.9487 & 71.1471 & -3.0860 \\ -4.0667 & 29.2428 & 1.0520 & -11.2894 & -3.2536 \\ 0.9487 & 1.0520 & 35.8975 & -105.7943 & 1.8359 \\ 71.1471 & -11.2894 & -105.7943 & 459.6730 & -11.6790 \\ -3.0860 & -3.2536 & 1.8359 & -11.6790 & 39.1338 \end{pmatrix}. \tag{23.11}$$

To calculate the generalized inverse, Algorithm 1 is applied. The iterations in tabular form are shown in table 23.6. It can be noticed that in Iteration 4, no pivot is found and the dot products associated with first and third columns are the coefficients of the linear combination assumed in (23.10).

The inverse of the non singular submatrix of $\mathbf{A}$ is composed by the intersection of the first, second, third and fifth rows and columns as is shown in the Last Tableau of table 23.6. Finally, the generalized inverse of $\mathbf{A}$ is:

$$\mathbf{A}^{-} = \begin{pmatrix} 0.0277 & 0.0042 & -0.0010 & 0.0000 & 0.0026 \\ 0.0042 & 0.0352 & -0.0013 & 0.0000 & 0.0033 \\ -0.0010 & -0.0013 & 0.0280 & 0.0000 & -0.0015 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0026 & 0.0033 & -0.0015 & 0.0000 & 0.0261 \end{pmatrix}. \tag{23.12}$$

Table 23.6. Iterations in tabular form to obtain the inverse of a maximum full rank submatrix of matrix **A** in (23.11)

Iteration 1					
	0	**0**	**0**	**0**	**0**
36.9971	**1.0000**	0.0000	0.0000	0.0000	0.0000
-4.0667	**0.0000**	1.0000	0.0000	0.0000	0.0000
0.9487	**0.0000**	0.0000	1.0000	0.0000	0.0000
71.1471	**0.0000**	0.0000	0.0000	1.0000	0.0000
-3.0860	**0.0000**	0.0000	0.0000	0.0000	1.0000
t	**36.9971**	-4.0667	0.9487	71.1471	-3.0860

Iteration 2					
	1	**0**	**0**	**0**	**0**
-4.0667	0.0270	**0.1099**	-0.0256	-1.9230	0.0834
29.2428	0.0000	**1.0000**	0.0000	0.0000	0.0000
1.0520	0.0000	**0.0000**	1.0000	0.0000	0.0000
-11.2894	0.0000	**0.0000**	0.0000	1.0000	0.0000
-3.2536	0.0000	**0.0000**	0.0000	0.0000	1.0000
t	-0.1099	**28.7957**	1.1563	-3.4689	-3.5928

Iteration 3					
	1	**2**	**0**	**0**	**0**
0.9487	0.0274	0.0038	**-0.0301**	-1.9098	0.0971
1.0520	0.0038	0.0347	**-0.0402**	0.1205	0.1248
35.8975	0.0000	0.0000	**1.0000**	0.0000	0.0000
-105.7943	0.0000	0.0000	**0.0000**	1.0000	0.0000
1.8359	0.0000	0.0000	**0.0000**	0.0000	1.0000
t	0.0301	0.0402	**35.8267**	-107.4794	2.0593

Iteration 4					
	1	**2**	**3**	**0**	**0**
71.1471	0.0275	0.0039	-0.0008	-2.0000	0.0989
-11.2894	0.0039	0.0348	-0.0011	0.0000	0.1271
-105.7943	-0.0008	-0.0011	0.0279	3.0000	-0.0575
459.6730	0.0000	0.0000	0.0000	1.0000	0.0000
-11.6790	0.0000	0.0000	0.0000	0.0000	1.0000
t	2.0000	-0.0000	-3.0000	0.0000	0.0004

Iteration 5					
	1	**2**	**3**	**0**	**0**
-3.0860	0.0275	0.0039	-0.0008	-2.0000	**0.0989**
-3.2536	0.0039	0.0348	-0.0011	0.0000	**0.1271**
1.8359	-0.0008	-0.0011	0.0279	3.0000	**-0.0575**
-11.6790	0.0000	0.0000	0.0000	1.0000	**0.0000**
39.1338	0.0000	0.0000	0.0000	0.0000	**1.0000**
t	-0.0989	-0.1271	0.0575	0.0004	**38.3098**

Final Tableau				
1	**2**	**3**	**0**	**5**
0.0277	**0.0042**	**-0.0010**	-2.0000	**0.0026**
0.0042	**0.0352**	**-0.0013**	0.0000	**0.0033**
-0.0010	**-0.0013**	**0.0280**	3.0000	**-0.0015**
0.0000	0.0000	0.0000	1.0000	0.0000
0.0026	**0.0033**	**-0.0015**	0.0000	**0.0261**

Example 4. Suppose now that the second variable is substituted by $2X_2$, which implies that the second row and the second column of matrix **A** have been modified. Then, the new matrix is $\mathbf{A}^* = \mathbf{X}^{*T}\mathbf{X}^*$,

$$\mathbf{A}^* = \begin{pmatrix} 36.9971 & \mathbf{-8.1335} & 0.9487 & 71.1471 & -3.0860 \\ \mathbf{-8.1335} & \mathbf{116.9710} & \mathbf{2.1040} & \mathbf{-22.5788} & \mathbf{-6.5072} \\ 0.9487 & \mathbf{2.1040} & 35.8975 & -105.7943 & 1.8359 \\ 71.1471 & \mathbf{-22.5788} & -105.7943 & 459.6730 & -11.6790 \\ -3.0860 & \mathbf{-6.5072} & 1.8359 & -11.6790 & 39.1338 \end{pmatrix}. \tag{23.13}$$

Starting from the last tableau in table 23.6, the generalized inverse of $\mathbf{A}^*$ in (23.13) is achieved in two steps.

- First, we consider that only the second row of matrix **A** has been modified as follows

$$\mathbf{A}^{*r} = \begin{pmatrix} 36.9971 & -4.0667 & 0.9487 & 71.1471 & -3.0860 \\ \mathbf{-8.1335} & \mathbf{116.9710} & \mathbf{2.1040} & \mathbf{-22.5788} & \mathbf{-6.5072} \\ 0.9487 & 1.0520 & 35.8975 & -105.7943 & 1.8359 \\ 71.1471 & -11.2894 & -105.7943 & 459.6730 & -11.6790 \\ -3.0860 & -3.2536 & 1.8359 & -11.6790 & 39.1338 \end{pmatrix}. \tag{23.14}$$

  Then, we apply Algorithm 2 to update the generalized inverse (see the iterations in tabular form in table 23.7). The maximum rank submatrix of matrix $\mathbf{A}^{*r}$ is composed by its first, second, third and fifth rows and columns. That is,

$$\mathbf{B}_{11}^{*r} = \begin{pmatrix} 36.9971 & -4.0667 & 0.9487 & -3.0860 \\ \mathbf{-8.1335} & \mathbf{116.9710} & \mathbf{2.1040} & \mathbf{-6.5072} \\ 0.9487 & 1.0520 & 35.8975 & 1.8359 \\ -3.0860 & -3.2536 & 1.8359 & 39.1338 \end{pmatrix}. \tag{23.15}$$

Table 23.7. Extra iteration for updating the generalized inverse after the modification of one row

Extra Iteration					
	1	**2**	**3**	**0**	**5**
-8.1335	0.0277	**0.0042**	-0.0010	-2.0000	0.0026
116.9710	0.0042	**0.0352**	-0.0013	0.0000	0.0033
2.1040	-0.0010	**-0.0013**	0.0280	3.0000	-0.0015
-22.5788	0.0000	**0.0000**	0.0000	1.0000	0.0000
-6.5072	0.0026	**0.0033**	-0.0015	0.0000	0.0261
t	0.2444	**4.0583**	-0.0767	0.0002	0.1940

Final Tableau				
1	**2***	**3**	**0**	**5**
0.0275	**0.0010**	**-0.0009**	-2.0000	**0.0024**
0.0021	**0.0087**	**-0.0006**	0.0000	**0.0016**
-0.0009	**-0.0003**	**0.0280**	3.0000	**-0.0014**
0.0000	0.0000	0.0000	1.0000	0.0000
0.0024	**0.0008**	**-0.0014**	0.0000	**0.0259**

Its inverse is composed by the first, second, third and fifth rows and columns of **W** (given in boldface in the Final Tableau of table 23.7).

- Second, the maximum rank submatrix $\mathbf{B}_{11}^{*r}$ is modified by the corresponding components of the second column of matrix $\mathbf{A}^*$. The result is the following

$$\mathbf{B}_{11}^{*} = \begin{pmatrix} 36.9971 & \mathbf{-8.1335} & 0.9487 & -3.0860 \\ -8.1335 & \mathbf{116.9710} & 2.1040 & -6.5072 \\ 0.9487 & \mathbf{2.1040} & 35.8975 & 1.8359 \\ -3.0860 & \mathbf{-6.5072} & 1.8359 & 39.1338 \end{pmatrix}. \tag{23.16}$$

Then, we apply the updating inverse matrix algorithm in Castillo et al. (1999) and the inverse is attained in the Final Tableau of table 23.8.
Finally, the generalized inverse is:

$$\mathbf{A}^{*-} = \begin{pmatrix} 0.0277 & 0.0021 & -0.0010 & 0.0000 & 0.0026 \\ 0.0021 & 0.0088 & -0.0007 & 0.0000 & 0.0017 \\ -0.0010 & -0.0007 & 0.0280 & 0.0000 & -0.0015 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0026 & 0.0017 & -0.0015 & 0.0000 & 0.0261 \end{pmatrix}. \tag{23.17}$$

Table 23.8. Extra iteration for updating the inverse matrix of matrix $\mathbf{B}_{11}^{*r}$ after modify its second column

Extra Iteration				
	1	**0**	**3**	**5**
-8.1335	0.0275	**0.0021**	-0.0009	0.0024
116.9710	0.0010	**0.0087**	-0.0003	0.0008
2.1040	-0.0009	**-0.0006**	0.0280	-0.0014
-6.5072	0.0024	**0.0016**	-0.0014	0.0259
t	-0.1204	**0.9856**	0.0378	-0.0956

Final Tableau			
1	**2**	**3**	**5**
0.0277	**0.0021**	**-0.0010**	**0.0026**
0.0021	**0.0088**	**-0.0007**	**0.0017**
-0.0010	**-0.0007**	**0.0280**	**-0.0015**
0.0026	**0.0017**	**-0.0015**	**0.0261**

23.6 Conclusions

We present an algorithm to calculate a generalized inverse using the methodology based on obtaining a decomposition of the Euclidian space given in Castillo et al. (1998, 2000). Our algorithm provides simultaneously the inverse of a maximum rank submatrix of the given matrix **A** and the rows and columns of **A** which form that maximum rank submatrix. Moreover, we obtain the coefficients of the linear dependencies of the rows of **A**.

We also introduce an algorithm to update the generalized inverse when one row of the initial matrix is modified. Finally, we apply both methods to the estimation of the coefficients in linear regression when collinear data are used.

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24

Single and Ensemble Fault Classifiers Based on Features Selected by Multi-Objective Genetic Algorithms

Enrico Zio, Piero Baraldi, Giulio Golam, and Nicola Pedroni

Dipartimento di Ingegneria Nucleare, Politecnico di Milano, Milan, Italy

Abstract: The problem of identifying faults in systems and processes can be formulated as a problem of partitioning objects (i.e., the measured data patterns representing the symptoms) into classes (i.e., the types of faults causing the symptoms). In this view, two main steps need to be carried out in order to effectively perform the fault identification: i) the selection of the features carrying information relevant for the identification; ii) the classification of the measured data patterns of features into the different fault types. In this work, the two tasks are tackled by combining a multi-objective genetic algorithm search with a Fuzzy K-Nearest Neighbors classification. Two different approaches to the development of the fault classification model are considered: a single classifier based on a feature subset chosen a posteriori on the Pareto-front identified by the multi-objective genetic search and an ensemble of classifiers, each one built on a different feature subset taken from the genetic algorithm population at convergence. Examples of application of the proposed approaches are given with reference to two different industrial processes: the classification of simulated nuclear transients in the feedwater system of a Boiling Water Reactor and of multiple faults in rotating machinery.

Keywords and phrases: Fault classification, feature selection, multi-objective genetic algorithms, fuzzy K-nearest neighbors, ensemble, diversity

24.1 Introduction

In this paper, the issue of fault diagnosis in complex engineering systems and processes is framed as a pattern classification problem. The basis for the classification is that different faults and anomalies lead to different patterns of evolution of the involved process variables, hereafter called features.

The pattern classification is performed by the following two tasks: 1) the selection of the features relevant for the classification; 2) the classification of the patterns into different fault classes.

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The first step of feature selection is motivated by the fact that irrelevant or noisy features are found to unnecessarily increase the complexity of the diagnostic problem and degrade the modeling performance (Kohavi and John, 1997).

On the other hand, hundreds of parameters are monitored for operation and safety reasons in modern industrial plants so that expert judgment alone cannot effectively drive the feature selection.

The feature selection technique proposed in this work combines a Multi-Objective Genetic Algorithm (MOGA) search (Holland (1975); Goldberg (1989)) with a Fuzzy K-Nearest Neighbors (FKNN) classification algorithm (Keller et al., 1985). The performance achieved by the latter is used as criterion for comparing the different feature subsets searched by the former.

The success of the genetic algorithm search depends largely on the ability of maintaining diversity in the population (Holland (1975); Goldberg (1989)). In this respect, a modified Niched Pareto MOGA (Horn et al., 1994) is adopted to evolve the population towards alternative, equivalent solutions of feature subsets which give a well distributed, representative description of the Pareto front of non-dominated solutions.

The second task of pattern classification is carried out exploring two possible approaches: a single FKNN classifier based on a chosen best Pareto-front feature subset and an ensemble of FKNN classifiers working on the different feature subsets contained in the MOGA population at convergence.

With respect to the latter approach, the motivation for developing ensembles of classifiers is that in many instances they have been shown capable of providing accuracies higher than any of the single base classifiers which constitute them (Tsymbal et al., 2001, 2005). Furthermore, reliance on different classifiers renders the classification more robust. In fact, sensor failures or de-calibration may not permit us to trust some of the measured features.

An important property for an ensemble to be effective is the diversity in the class assignments of the base classifiers which constitute it, i.e., their capability of erring on different sub-regions of the pattern space. In order to obtain diversity among classifiers, a properly defined diversity function is added to the MOGA search as objective function. A voting technique is used to effectively combine the assignments of the base classifiers to construct the ensemble output (Tsymbal et al., 2005).

The effectiveness of the feature selection and fault classification approach is tested on a diagnostic problem regarding the classification of simulated transients in the feedwater system of a nuclear Boiling Water Reactor (Puska and Normann, 2002) and on a case of multiple fault classification in rotating machinery (Kilundu and Dehombreaux, 2005).

24.2 Feature Selection for Pattern Classification

The fault identification task may be viewed as a problem of partitioning of objects (the measured data patterns) into classes (the faults). From a mathematical point of view, a classifier is a mapping function $\Phi(\cdot)$ that assigns an object $\mathbf{x}$ in an n-dimensional domain $\Omega \subset \Re^n$ to a given class l. If one knew the exact expression of $\Phi(\cdot)$, the question of which features of $\mathbf{x}$ to use would not be of interest. In fact, in such situations adding

features does not decrease the accuracy of the classifier, and hence, restricting to a subset of features is never advised. However, as it is often the case in engineering, it is not possible to determine the exact analytical expression of the function $\Phi(\cdot)$ due to the complexity of the systems under analysis. Hence, one resorts to empirical classification techniques in which the classifier is built through a process based on a set of classification example pairs $\{(\mathbf{x}, l)\}$, each one constituted by a pattern $\mathbf{x}$ in the feature space labelled by the corresponding class l.

In practice, the number of measured features is quite large and various reasons suggest a reduction of this number for use in the classification model. First of all, irrelevant, non informative features result in a classification model which is not robust (Na et al. (2002); Verikas and Bacauskiene (2002)). Second, when the model handles many features, a large number of observation data are required to properly span the high-dimensional feature space for accurate multivariable interpolation (Na et al. (2002); Emmanouilidis et al. (1999)). Third, by eliminating unimportant features the cost and time of collecting the data and developing the classifier can be reduced (Na et al. (2002); Emmanouilidis et al. (1999)). Finally, reducing the number of selected features permits achievement of more transparent and easily interpretable models (Kohavi and John, 1997).

Given a labeled dataset, the objective of feature selection is that of finding a subset of the features such that the classifier built on these features classifies the available data with the highest possible accuracy (Kohavi and John, 1997).

24.2.1 An overview of feature selection techniques

Feature selection involves conducting a search for an optimal feature subset in the space of possible features. The inclusion or not of a feature in the subset can be encoded in terms of a binary variable that takes value 1 or 0, respectively. For n features, the size of the binary vector search space is 2^n. Thus, an exhaustive search is impractical unless n is small, which is rarely the case.

Each feature subset selected during the search must be evaluated with respect to the objective functions characteristics of the classification problem at hand, e.g., classification performance and number of features. In this respect, either a filter or a wrapper approach can be undertaken (Kohavi and John, 1997).

In filter methods, the feature selector algorithm is independent of the specific algorithm used for the classification and acts as a filter discarding irrelevant features, a priori of the construction of the classifier. A numerical evaluation function quantifying the clustering properties of the features is used to compare the feature subsets proposed by the search algorithm. Under a conjecture that such properties govern the classification capabilities of the features, the subset with the highest value of the evaluation function is kept as basis for the classification.

Contrary to filter methods, in wrapper methods the feature selector behaves as a "wrapper" around the specific algorithm used to construct the classifier, whose performance is directly used to compare the different feature subsets (Kohavi and John, 1997).

The filter approach is generally computationally more efficient than the wrapper one because for each feature subset of trial tested during the search for the optimal, the computation of an evaluation function is less time consuming than the development

of a complete classification model. Hence, for many practical applications the wrapper approach is feasible only if the classifier is a fast-computing algorithm, e.g., the K-Nearest Neighbor (KNN) (Duran and Odell, 1974) algorithm or its fuzzy extension (FKNN) (Keller et al. (1985); Marcelloni (2003)). On the other hand, wrapper approaches are more performing than the filter ones since the former ensure the selection of the features more suitable for the specific classification algorithm used, whereas the latter totally ignore the effects of the selected feature subspace on the performance of the classifier that will actually be used.

With respect to the search algorithms, three approaches are commonly adopted: complete, heuristic and probabilistic (Kohavi and John, 1997).

In the complete approach, the properties of a pre-defined evaluation function are used to prune the feature space to a manageable size, thus avoiding that the complete search is also exhaustive (Narendra and Fukunaga, 1977). Only some evaluation functions give rise to a search that guarantees the optimum feature subset selection without being exhaustive.

The heuristic approach does not guarantee that the best feature subset is achieved, but it is less time consuming than the complete one and may be employed in combination with any evaluation function (Zio et al., 2005). At present, the most employed heuristic methods are greedy search strategies such as the sequential forward selection (SFS) or the sequential backward elimination (SBE) "hill climbing" methods, which iteratively add or subtract features and at each iteration the evaluation function is evaluated (Kohavi and John, 1997). The hill-climbing search is usually stopped when adding or removing new features does not increase the value of the evaluation function or when the number of features has reached a predefined threshold.

The hill climbing methods suffer from the so called "nesting effect": if the features added cannot be removed, a local minimum of the evaluation function may be found. To reduce this effect, it is possible to use the so called plus-t-take-away-r method (PTA) (Kohavi and John, 1997). In this method, after t steps of the forward selection, r steps of the backward elimination are applied so as to allow escaping from local minima. Still, there is no guarantee of obtaining the absolute optimum.

The probabilistic approach is based on population-based metaheuristics guided by the goodness of the solutions iteratively explored, such as the genetic algorithms presented in this paper, or on methods like simulated annealing and tabu search algorithms (Zhang and Sun, 2002).

24.3 GA-based Feature Selection for Pattern Classification

Genetic Algorithms (GAs) are optimization methods aiming at finding the global optimum of a set of real objective functions of one or more decision variables, possibly subject to various linear or non linear constraints. Their main properties are that the search is conducted i) using a population of multiple solution points or candidates, called chromosomes, which are strings of numbers, generally sequences of binary digits 0 and 1, ii) using operations inspired by the evolution of species, such as breeding and genetic mutation, iii) using probabilistic operations, iv) using only information on the objective or search function (fitness) and not on its derivatives (Goldberg, 1989).

In this section, a Multi-Objective Genetic Algorithm (MOGA) is adopted for searching the optimal feature subset to be used as the basis for the classification of patterns into classes. Two objective functions (fitnesses) are used for evaluating and comparing the feature subsets during the search: the fraction of patterns correctly classified (recognition rate) by a Fuzzy K-Nearest Neighbors classifier (to be maximized) and the number m of features forming the subsets (to be minimized). During the search, the evolving feature subsets are compared in terms of dominance with respect to these two objective functions. At convergence, this leads to the identification of the so called Pareto optimal set or front of non-dominated feature subsets (Goldberg (1989); Sawaragy et al. (1985)).

The generic chromosome representative of a given feature subset is made of n bits, each one associated with one of the n features constituting the patterns: If the i-th bit equals 1, then the i-th feature is included in the subset and viceversa if the bit is 0. Thus, the number m of features in the subset is the total number of 1's in the chromosome.

The efficiency of the search depends on the ability to maintain genetic diversity through the generations so as to arrive at a population of individuals that uniformly represents the real nondominated solutions of the Pareto set (Goldberg, 1989). This can be achieved by resorting to niching techniques, e.g., sharing (Goldberg (1989); Horn et al. (1994)), which apply a "controlled niched pressure" in the parents selection step of the algorithm, so that those individuals with less crowded neighborhoods (niches) in the objective functions space are preferentially selected as parents and thus allowed to create more offsprings in the following generations. This action spreads out the population in the search space so that convergence is shared on different niches of the Pareto front, which is thus evenly covered.

Regarding the evaluation of the objective function related to the FKNN classification performance, the available labelled patterns are randomly subdivided into a set containing 75% of the data, which are used for the classifier construction, and a tuning set of 25% of the data, which are used to compute the performance of the classifier in terms of its accuracy. By trial and error, a number $K = 5$ of neighbors has been found to produce good classification results by the FKNN. The obtained fuzzy partition $\{\mu_l(\mathbf{x}_k)\}$ of the tuning data set, where $0 \leq \mu_l(\mathbf{x}_k) \leq 1$ is the membership function of pattern $\mathbf{x}_k$ to class l, is converted into a hard partition by assigning each pattern to the class with highest membership value.

The subdivision of the available patterns in training and tuning sets is randomly repeated 10 times (tenfold cross-validation) and for each tuning set the accuracy of the FKNN classifier operating on the generic subset of features S_q is evaluated in terms of the recognition rate (the fraction of tuning patterns correctly classified). Then, the mean recognition rate is calculated and sent back to the GA as the fitness value of the chromosome representative of feature subset S_q.

At convergence, a family of non-dominated chromosomes (i.e., feature subsets) with different trade-offs of classification performance (FKNN recognition rate) and complexity (number of features) is obtained. Based on these results, an informed choice can be made on the features to be actually monitored for the pattern classification task considering also practical issues of costs, ease of data acquisition and data interpretability. Eventually, the analyst must select the preferred solution according to some subjective preference values.

Finally, a validation data set, separate from the training and tuning sets used for the feature selection task, is processed by the classifier based on the optimal feature subset to verify the classification accuracy on new patterns (never used during the feature selection process). This validation procedure is of paramount importance for safety applications in critical technologies such as the nuclear one.

24.4 Classification of Transients in the Feedwater System of a Boiling Water Reactor

As an example of application, the identification of a predefined set of 18 simulated faults in a Boiling Water Reactor (BWR) is considered (Puska and Normann, 2002), based on $n = 369$ wavelet coefficients extracted from the time measurements collected on the plant (Strang and Nguyen, 1996). Two power levels, 50% and 80% of full power, have been considered: the transients at 50% of full power are used for the feature selection task, whereas the transients at 80% of full power are left out for validation of the resulting classifier.

Given the large number of possible solutions (2^{369}), the task of maintaining genetic diversity in the population in order to explore more accurately the search space is sought by using a Niched Pareto-Based Genetic Algorithm (NPGA) (Zio et al., 2002a).

Figure 24.1 shows the Pareto front and the final population found by the NPGA at convergence. The "niching pressure" applied by the equivalence class sharing method succeeds in spreading the population out along the Pareto optimal front: indeed, the NPGA Pareto solutions cover from $m = 0$ to $m = 22$, with only individuals with $m = 8, 9, 15$ not present.

In the present case, the optimization results for the non-dominated subset with 7 features show a good compromise between high classification accuracy and low number of features (pointing arrow in figure 24.1).

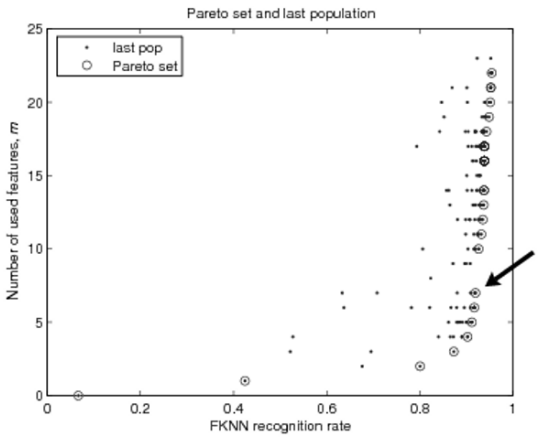

Figure 24.1. Pareto front and final population found by the NPGA at convergence

A set of patterns taken from transients at 80% power level, never employed during the feature selection phase, has then been used to cross-validate the performance of the FKNN classifier resting upon the selected 7-features subset. The resulting recognition rate of 0.9190 ± 0.0301 is significantly higher than that obtained by using all the 369 features (0.647 ± 0.055) and by using the features arbitrarily selected by a plant expert (0.789 ± 0.029).

24.5 The Ensemble Approach to Pattern Classification

An alternative technique to develop a pattern classification model is to use an ensemble of classifiers. The motivation for developing ensembles is that in many application domains they have been shown to provide accuracies higher than any of the single base classifiers that constitute them (Tsymbal et al., 2001, 2005). Furthermore, reliance on different classifiers renders the classification more robust. In fact, sensor failures or de-calibration may not permit to trust some of the measured features. This problem can be overcome by basing the classification, through the assignment of appropriate weights, only on those classifiers of the ensemble whose features are correctly measured.

The development of an ensemble of classifiers entails addressing two issues: the construction of the base classifiers that constitute the ensemble and the integration of their class assignments to construct the ensemble output.

24.5.1 The construction of the ensemble

A possible approach for generating an ensemble of diverse classifiers h_1,...,h_S from a set X of labelled patterns of the form $\{(\mathbf{x}_k,l_k)\}$, k=1,2,...,N, is to base each of them on a different feature subset (Tsymbal et al., 2001, 2005). Whereas the goal of traditional feature selection (Holland (1975); Goldberg (1989); Chambers (1995); Sawaragi, Nakayama and Tanino (1985); Raymer et al. (2000); Bozdogan (2003)) for a single classifier (see Sections 24.2 and 24.3) is to find the feature subset that gives the optimal performance of the classifier, ensemble feature selection aims instead at finding many feature subsets upon which to construct a set of diverse base classifiers (Tsymbal et al., 2001).

The problem of multiple feature subsets selection for generating diverse base classifiers is here tackled by means of a combination of a MOGA technique and Fuzzy K-Nearest Neighbours (FKNN) classification (Zio et al., 2002b). Besides the two objectives previously adopted, of maximizing the classification accuracy and minimizing the number of features forming the subsets, the maximization of the diversity among the base classifiers is a third optimization criterion added.

In this paper, a popular pairwise diversity measure based on the correlation between the performances of the two classifiers, i.e., the numbers of patterns correctly/wrongly classified, is adopted. Let h_1 and h_2 be a pair of base classifiers: The correlation between the outputs can be measured as (Tsymbal et al., 2005):

$$corr_{h_1,h_2} = \frac{N^{11}N^{00} - N^{01}N^{10}}{\sqrt{(N^{11}+N^{10})(N^{01}+N^{00})(N^{11}+N^{01})(N^{10}+N^{00})}} \tag{24.1}$$

where N^{ab} is the number of test patterns classified correctly (a=1) or incorrectly (a=0) by the classifier h_1 and correctly (b=1) or incorrectly (b=0) by the classifier h_2. The value of $corr_{h_1,h_2}$ varies from -1 to 1 and for statistically independent classifiers, the expected value of $corr_{h_1,h_2}$ is 0. Classifiers that tend to recognize the same patterns correctly will have positive values of $corr_{h_1,h_2}$, whereas those which commit errors on different patterns will render $corr_{h_1,h_2}$ negative. A correlation-based diversity measure between classifiers h_1 and h_2 can then be defined based on the correlation coefficient of Eq. (24.1) as (Tsymbal et al., 2005):

$$div_{h_1,h_2} = \frac{1 - corr_{h_1,h_2}}{2} \tag{24.2}$$

This measure varies between 0 and 1. Obviously, classifiers that are statistically correlated are considered less diverse and viceversa.

At convergence of the MOGA search, the S chromosomes of the last population are used as feature subsets S_1,S_2,...,S_S to build S diverse base classifiers h_1,h_2,...,h_S (figure 24.2).

Again, for validating the performance of the ensemble of classifiers, a test is made with respect to a validation data set, different from the data set used for the MOGA feature selection. Each base classifier h_q , q=1,2,...,S, is asked to classify the specific validation data set whose patterns are constituted by the particular features used by that classifier to perform the classification task.

24.5.2 Integration of class assignments

The integration of the class assignments of the multiple classifiers is crucial for improving the classification performance of the single classifiers. In this paper, this is handled by means of a so-called Static Weighted Voting (SWV) combination approach. The validation set is partitioned into a training set and a test set. According to the SWV, a unitary vote is assigned to each base classifier h_q and multiplied by a weight $w_q \in [0, 1]$ proportional to the accuracy of the classifier measured in terms of the Mean Recognition Rate (MRR), i.e. the fraction of patterns of the training set it correctly classifies (figure 24.3).

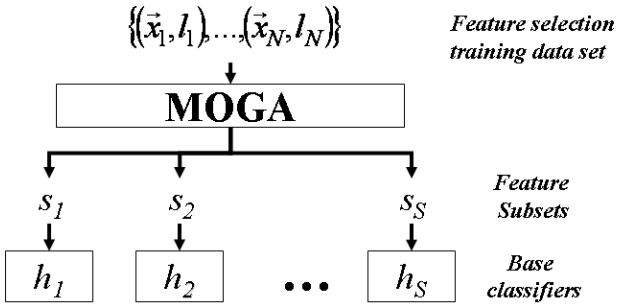

Figure 24.2. Generation of base classifiers

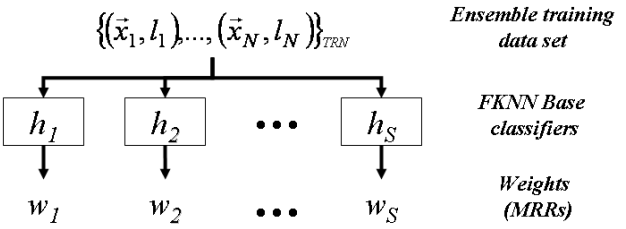

Figure 24.3. Computation of base classifiers' weights (MRRs)

Once the base classifiers weights are computed, the classification of the patterns of the test set is performed. When the generic base classifier h_q assigns the generic k-th test pattern to the class l, its weight w_q is added to the ensemble vote for that class. By doing so, each class l of the k-th test pattern receives an ensemble vote v_l^k given by the sum of all weights assigned to that class, viz.:

$$v_l^k = \sum_{q=1}^{S} w_q \cdot \delta_{l,l_{h_q}} \tag{24.3}$$

where $\delta_{l,l_{h_q}}$ is 1 only if the classifier h_q assigns the k-th pattern to class l. Finally, the k-th test pattern is assigned to the class l_k with the highest ensemble vote (figure 24.4):

$$l_k = \arg(\max_{1 \le l \le c} v_l^k) \tag{24.4}$$

where c is the total number of classes.

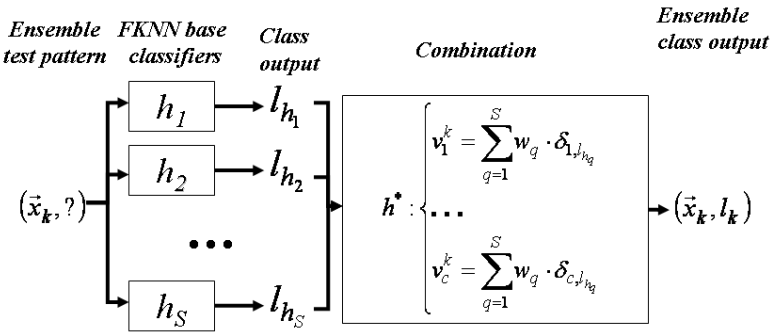

Figure 24.4. Ensemble classification of test patterns

24.6 Application to Multiple Fault Classification

Some numerical experiments of ensemble classification have been conducted on a case of multiple faults in rotating machinery. Literature-available time domain vibration signals (Kilundu and Dehombreaux, 2005) are considered bases to build an ensemble of classifiers for fault diagnosis. The combination of 4 fault types of different intensity levels is considered. Fault 1 is characterized by 3 intensity levels, whereas the other 3 faults by 3 intensity levels each (Kilundu and Dehombreaux, 2005). A total amount of 648 experimental labelled patterns are available for constructing, validating and testing the ensemble of classifiers. The input part of each pattern consists of the values of the 48 measured features (f_1,...,f_{48}) upon which to base the classification of the four intensity levels of fault. With respect to the classification output part of the pattern, a 1 is placed in correspondence of the intensity level of the given fault (possibly more than one) affecting the bearing. Level 0 denotes the situation where there is no fault (Kilundu and Dehombreaux, 2005).

The data have been split into two subsets of equal size: 324 patterns for the ensemble feature selection procedure to generate the base classifiers and 324 patterns for building and validating the ensemble of classifiers.

Four classification models have been developed, each one devoted to the recognition of the intensity of a particular fault. The population of 100 chromosomes (Feature Subsets) obtained at the last generation of the MOGA search is used to build the ensemble of 100 base classifiers. The 400-generation MOGA search is performed separately for each of the 4 faults and correspondingly 4 ensembles of base classifiers are built on the 4 final populations of 100 chromosomes (figure 24.5).

The classifications of the four ensembles, one for each fault, must then be combined to obtain the global classification accuracy. Correct classification is achieved when the input pattern under analysis is assigned by each ensemble to the correct intensity class of the fault for which it is specialized. The FKNN classification performances obtained

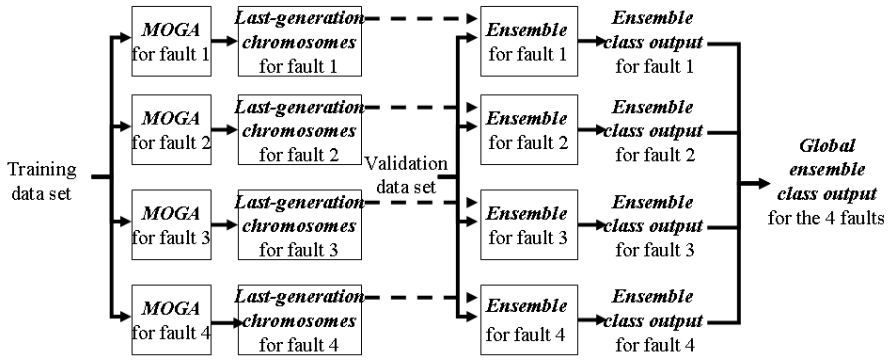

Figure 24.5. Sketch of the multiple-fault classification procedure: For each fault, a MOGA search is performed using the training data set; the 4 last-generation populations of chromosomes thereby obtained constitute the 4 ensembles for the classification of the validation data set

Table 24.1. Classification results obtained by the ensemble compared with those obtained using one single optimal classifier

	Ensemble		*Single optimal classifier*
	Accuracy (MRR)	*Diversity*	*Accuracy (MRR)*
Global	0.8468 ± 0.0430	/	0.7895 ± 0.0517
Fault 1	0.8882 ± 0.0358	0.3748	0.8363 ± 0.0501
Fault 2	0.9661 ± 0.0255	0.3701	0.9613 ± 0.0301
Fault 3	0.9701 ± 0.0201	0.3629	0.9405 ± 0.0299
Fault 4	0.9853 ± 0.0162	0.4017	0.9680 ± 0.0231

by the ensemble are presented in table 24.1 in terms of the Global Mean Recognition Rate (GMRR) of the ensemble on the four faults, and of the MRR and diversity of the ensemble of base classifiers specific for each single fault. The ensemble diversity is computed as the mean of the diversities of the base classifiers. The performances of the ensemble are compared with those achieved on the same validation set by the four Pareto-front chromosomes (one for each fault) with the highest MRRs, resulting from four specific, two-objective MOGA searches for each single fault classification.

The advantage of adopting an ensemble approach is readily demonstrated by the obtained results: with respect to using single classifiers, a marked increase of the GMRR is achieved by the ensemble, mostly due to a significant increase of the MRR of fault 1 which presents critical classification difficulties inherent in its data structure.

24.7 Conclusions

Fault identification is a matter of paramount importance for the safety and operation of modern industrial plants. In this paper, this issue has been framed as a pattern classification problem.

First of all, the problem of discerning among the several measured plant parameters those features to be used for fault identification has been tackled. This is a crucial issue to be resolved for the application of advanced diagnostic techniques to complex plants where hundreds of parameters are measured. A wrapper approach which combines a Niched Pareto genetic algorithm search with a Fuzzy K-Nearest Neighbors (FKNN) classification algorithm has been embraced. The proposed search scheme has been applied to a task of classification of simulated transients in the feedwater system of a Boiling Water Reactor.

Then, two different techniques for using the results obtained by the feature selector have been compared: a single classifier based on the best Pareto-front feature subset and an ensembles of classifiers working on the different feature subsets corresponding to the final population of the MOGA search. The results obtained in an application of multiple fault classification in rotating machinery show that the ensemble is more accurate than the single best Pareto-front classifier. This is due to the fact that the maximization of diversity among the base classifiers allows exploiting the classification capabilities of each base classifier in a specific sub-region of the pattern space.

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25

Feasibility Conditions in Engineering Problems Involving a Parametric System of Linear Inequalities

Cristina Solares[1] and Eduardo W. V. Chaves[2]

[1] Department of Mathematics, University of Castilla-La Mancha, Spain
[2] Department of Applied Mechanics and Engineering Design, University of Castilla-La Mancha, Spain

Abstract: In this paper we apply the Γ-algorithm to obtain the feasibility conditions in different engineering problems involving a parametric system of linear inequalities. The feasibility conditions are the conditions for which the original system of linear inequalities has a solution. The Γ-algorithm is applied to solve the following problems: a heat transfer problem related to the finite difference method, various beam problems related to the finite difference method and a fracture mechanics problem related to numerical integration. Working with the $\Gamma-$algorithm, the feasibility conditions problem can be reduced to find the dual of a cone.

Keywords and phrases: Feasibility conditions, dual cone, parametric systems of linear inequalities, fracture mechanics, heat transfer, beam problem

25.1 Introduction

In this paper we study systems of linear inequalities in the following form

$$\begin{array}{rrrrr} a_{11}x_1 & +a_{12}x_2 & +\cdots & +a_{1n}x_n & \leq b_1, \\ a_{21}x_1 & +a_{22}x_2 & +\cdots & +a_{2n}x_n & \leq b_2, \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{m1}x_1 & +a_{m2}x_2 & +\cdots & +a_{mn}x_n & \leq b_m, \end{array} \tag{25.1}$$

where a_{ij} are numerical coefficients, x_j are variables and b_i are parameters (in some problems a part of the b_i values are numbers).

The study of the above systems, in the sense of obtaining the feasibility conditions in numerical-symbolic problems of applied mechanics and engineering, has been introduced by Ioakimidis (2000). In that work, the author applies the Fourier elimination algorithm (see Duffin (1974)) to obtain the feasibility conditions of numerical problems involving a parametric system of linear inequalities. The Fourier algorithm extends the idea of the Gaussian elimination algorithm to systems of inequalities. Fourier treated a system of inequalities by a method of elimination of variables; each variable is eliminated by adding each pair of inequalities having coefficients of opposite sign (pairwise

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elimination). Duffin:74 did some modifications on that algorithm to study the compatibility of a parametric system of linear inequalities. Ioakimidis (2001), proposes the Weispfenning computational quantifier elimination algorithms (implemented in REDLOG), as an alternative to the Fourier elimination algorithm, to obtain the above feasibility conditions. In this paper, our study is restricted to the $\Gamma-$algorithm as an alternative to the Fourier algorithm.

The application of the $\Gamma-$algorithm (see Castillo et al. (1999); Castillo and Jubete (2004) and Castillo et al. (2006)) as an alternative to the Fourier algorithm, to analyze a simple one dimensional heat transfer problem, has been introduced in Solares and Chaves (2006). Working with the $\Gamma-$algorithm, the feasibility conditions problem can be reduced to find the dual of a cone (see Castillo and Jubete (2004)). The $\Gamma-$algorithm uses a pivoting transformation (see Castillo et al. (1999)) to obtain the dual of the cone generated by the columns of the system matrix. This method is specially suitable for updating dual cones when new generators are incorporated (i.e. new columns are inserted in the matrix of the system). In fact, when adding a new generator only one step of the process allows one to obtain the new dual cone without the need of starting again from scratch. The $\Gamma-$algorithm is also useful to obtain the dual cone of cones generated by some subsets of generators of the initial cone (i.e. cones generated by some columns of the system matrix). The above are important advantages of using the $\Gamma-$algorithm instead of the Fourier algorithm. In addition, once we obtain the feasibility conditions with the $\Gamma-$algorithm, if we make a change in the independent terms vector in (25.1), we can obtain directly the new feasibility conditions.

In this paper, we apply the $\Gamma-$algorithm to obtain the feasibility conditions in the following engineering problems involving a parametric system of linear inequalities: a heat transfer problem related to the finite difference method, a fracture mechanical problem related to numerical integration and various beam problems related to the finite difference method. Some of these problems have been previously studied by Ioakimidis (2000, 2001). The results provide us with the feasibility conditions for which the satisfaction of the original system of linear inequalities is possible.

The paper is structured as follows. Section 25.2 introduces the heat transfer problem. Section 25.3 introduces the fracture mechanical problem. Section 25.4 introduces various beam problems. In Section 25.5 some conclusions are given.

25.2 The Heat Transfer Problem

In this section, we apply the $\Gamma-$algorithm in a one-dimensional boundary value problem of the heat transfer problem. This problem has been introduced by Ioakimidis (2000). We apply the finite difference method to the steady-state, one dimensional differential equation for the temperature distribution $\phi(x)$ through the slab, $x \in [0, L]$, of thickness L and thermal conductivity k (see figure 25.1). We suppose that the temperature at $x = 0$ takes a constant value $\phi(x_0) = \Phi_0$, the heat flow takes the constant value D at $x = L$, $\frac{d\phi}{dx}(L) = D$, and we consider the heat generation at a rate $Q(x)$ per unit length of the slab (see Ioakimidis (2000)). The differential equation for this problem is

$$-k\frac{d^2\phi}{dx^2} = Q(x),\ \phi(0) = \Phi_0,\ \frac{d\phi}{dx}(L) = D. \tag{25.2}$$

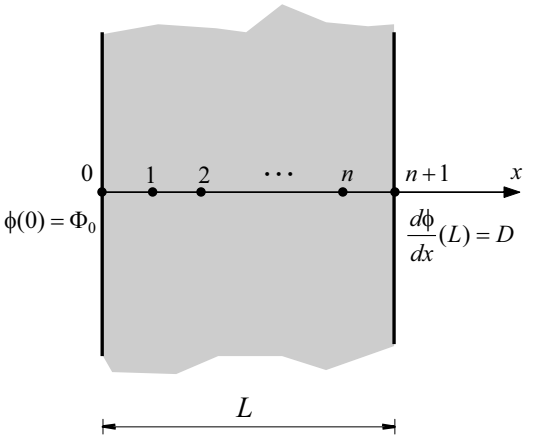

Figure 25.1. Interval partition in the finite difference method applied to the heat transfer problem in Section 25.2

We approximate the second order differential equation and the boundary condition in Eq. (25.2) by the finite difference method (central difference approximation) generating a set of $n+2$ equally spaced points $x_i = hi, i = 0, \ldots, n+1$ where $h = L/(n+1)$ (see figure 25.1). From the above, we get the approximate system of linear equations

$$\left.\begin{aligned} -\phi_2 + 2\phi_1 &= \Phi_0 + h^2 Q_1/k, \\ -\phi_{i+1} + 2\phi_i - \phi_{i-1} &= h^2 Q_i/k,\ i = 2, \ldots, n, \\ \phi_{n+1} - \phi_n &= h\ D, \end{aligned}\right\} \tag{25.3}$$

where $\phi_i = \phi(x_i)$ and $Q_i = Q(x_i)$.

Following Ioakimidis (2000), we consider that the heat generation $Q_i/k \geq Q_0$ $(i = 1, \ldots, n)$, the temperature $\phi_i \leq T_0$ $(i = 1, \ldots, n)$ and the heat flow $D \geq D_0$, where D_0, Q_0 and T_0 are constant values. We obtain the following system of linear inequalities

$$\left.\begin{aligned} -\phi_2 + 2\phi_1 &\geq \Phi_0 + h^2 Q_0, & \\ -\phi_{i+1} + 2\phi_i - \phi_{i-1} &\geq h^2 Q_0, & i = 2, \ldots, n, \\ \phi_{n+1} - \phi_n &\geq D_0 h, & \\ \phi_i &\leq T_0, & i = 1, \ldots, n+1. \end{aligned}\right\} \tag{25.4}$$

We study the system (25.4) in the particular case $n = 2$ and $L = 1$. Using slack variables to convert the inequalities into equalities and one more artificial variable to convert the arbitrary variables into non negative variables, we get the equivalent system of linear equalities

$$\begin{pmatrix} -1 & 2 & -1 & 0 & -1 & 0 & 0\,0\,0\,0 \\ 0 & -1 & 2 & -1 & 0 & -1 & 0\,0\,0\,0 \\ 0 & 0 & -1 & 1 & 0 & 0 & -1\,0\,0\,0 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0\,1\,0\,0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0\,0\,1\,0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0\,0\,0\,1 \end{pmatrix} \begin{pmatrix} \phi_1^* \\ \phi_2^* \\ \phi_3^* \\ \phi_4^* \\ \phi_5^* \\ \phi_6^* \\ \phi_7^* \\ \phi_8^* \\ \phi_9^* \\ \phi_{10}^* \end{pmatrix} = \begin{pmatrix} \Phi_0 + h^2 Q_0 \\ h^2 Q_0 \\ D_0 h \\ T_0 \\ T_0 \\ T_0 \end{pmatrix} \tag{25.5}$$

with $\phi_i^* \geq 0, i = 1, \ldots, 10$. Applying the $\Gamma-$algorithm to the columns of the system matrix $\mathbf{A}$ in Eq. (25.5), we obtain the dual of the cone generated by that columns, $\mathbf{A}_\pi^p = \mathbf{W}_\pi$, where

$$\mathbf{W} = \begin{pmatrix} 1 & 3 & 6 \\ 2 & 6 & 6 \\ 3 & 6 & 6 \\ 0 & 0 & -6 \\ 0 & -3 & 0 \\ -1 & 0 & 0 \end{pmatrix}. \tag{25.6}$$

The product of the dual cone generators (columns of $\mathbf{W}$ in Eq. (25.6)) and the parametric independent terms vector $\mathbf{b}^T = (\Phi_0 + h^2 Q_0, h^2 Q_0, D_0 h, T_0, T_0, T_0)$ with $h = 1/3$, gives us the feasibility conditions

$$\begin{pmatrix} \Phi_0 + (1/9)Q_0 & (1/9)Q_0 & D_0(1/3) & T_0 & T_0 & T_0 \end{pmatrix} \begin{pmatrix} 1 & 3 & 6 \\ 2 & 6 & 6 \\ 3 & 6 & 6 \\ 0 & 0 & -6 \\ 0 & -3 & 0 \\ -1 & 0 & 0 \end{pmatrix} \leq \mathbf{0} \tag{25.7}$$

which can be written as

$$\begin{aligned} &T_0 \geq \Phi_0 + (1/3)Q_0 + (3/3)D_0, \\ &T_0 \geq \Phi_0 + (1/3)Q_0 + (2/3)D_0, \\ &T_0 \geq \Phi_0 + (1/9)Q_0 + (1/3)D_0. \end{aligned} \tag{25.8}$$

Analogously, we obtain the feasibility conditions for other n values in (25.4). We study the system (25.4) in the particular case $n = 10$, obtaining so the feasibility conditions

$$\begin{aligned} &T_0 \geq \Phi_0 + (10/121)Q_0 + (11/11)D_0, \\ &T_0 \geq \Phi_0 + (19/121)Q_0 + (10/11)D_0, \\ &T_0 \geq \Phi_0 + (54/121)Q_0 + (9/11)D_0, \\ &T_0 \geq \Phi_0 + (52/121)Q_0 + (8/11)D_0, \\ &T_0 \geq \Phi_0 + (49/121)Q_0 + (7/11)D_0, \\ &T_0 \geq \Phi_0 + (45/121)Q_0 + (6/11)D_0, \\ &T_0 \geq \Phi_0 + (40/121)Q_0 + (5/11)D_0, \\ &T_0 \geq \Phi_0 + (34/121)Q_0 + (4/11)D_0, \\ &T_0 \geq \Phi_0 + (27/121)Q_0 + (3/11)D_0, \\ &T_0 \geq \Phi_0 + (19/121)Q_0 + (2/11)D_0, \\ &T_0 \geq \Phi_0 + (10/121)Q_0 + (1/11)D_0. \end{aligned} \tag{25.9}$$

The above conditions are related with the exact values of the temperature $\phi(x_i)$ at each node of the partition, $x_i = hi, i = 1, \ldots, 11$ where $h = 1/11$. The feasibility conditions in Eq. (25.9) are the same conditions obtained by Ioakimidis (2000) using the Fourier algorithm.

25.3 A Fracture Mechanical Problem

In this section, we consider the problem of a through crack in an infinite plane under uniform tension, which has been analyzed by Ioakimidis (2000). Both crack edges are assumed loaded by a tension distribution $p(t)$. We are interested in the values of the mode-I stress intensity factors $k_{1,2}$. The stress intensity factors are used in fracture mechanics to more accurately predict the stress state near the tip of the crack caused by a remote load. When this stress state becomes critical a small crack grows and the material fails.

Following Ioakimidis (2000), we will use the formula for the stress intensity factors

$$k_{1,2} = \frac{1}{\pi} \int_{-1}^{1} \frac{1 \mp t}{\sqrt{1-t^2}}\, p(t)dt, \tag{25.10}$$

and we approximate the integral (25.10) by the Gauss-Chebyshev quadrature rule (with n nodes) with respect to the weight function $w(t) = 1/\sqrt{1-t^2}$ on the interval $[-1, 1]$

$$k_{1,2} \approx \frac{1}{n} \sum_{i=1}^{n} (1 \mp t_{in}) p(t_{in}) \text{ where } t_{in} = \cos \frac{(2i-1)\pi}{2n}. \tag{25.11}$$

Following Ioakimidis (2000), we consider the bounds for the loading values $p_i = p(t_{in}), i = 1, \ldots, n$

$$p_i \geq P_i,\ i = 1, \ldots, n \tag{25.12}$$

and for the fracture coefficients

$$k_1 \leq K_1 \text{ and } k_2 \leq K_2. \tag{25.13}$$

The aim of this work is to obtain the feasibility conditions of the system of linear inequalities (25.12)-(25.13), which can be written as

$$\left.\begin{array}{l} \sum\limits_{i=1}^{n} (1 - t_{in}) p_i \leq K_1, \\ \sum\limits_{i=1}^{n} (1 + t_{in}) p_i \leq K_2, \\ p_i \geq P_i, i = 1, \ldots, n, \end{array}\right\} \tag{25.14}$$

where $t_{in} = \cos \frac{(2i-1)\pi}{2n}, i = 1, \ldots, n$. We study the above system for different n values. In the case $n = 2$, the system (25.14) can be written as

$$\left.\begin{array}{rl} 0.1464\, p_1 + 0.8535\, p_2 \leq & K_1, \\ 0.8535\, p_1 + 0.1464\, p_2 \leq & K_2, \\ p_1 \geq & P_1, \\ p_2 \geq & P_2. \end{array}\right\} \tag{25.15}$$

Using slack variables to convert the inequalities into equalities and one more artificial variable to convert the arbitrary variables into non negative variables, the system (25.15) is equivalent to the system of linear equalities

$$\begin{pmatrix} 1 & 0.1464 & 0.8535 & 1 & 0 & 0 & 0 \\ 1 & 0.8535 & 0.1464 & 0 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & -1 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} p_1^* \\ p_2^* \\ p_3^* \\ p_4^* \\ p_5^* \\ p_6^* \\ p_7^* \end{pmatrix} = \begin{pmatrix} K_1 \\ K_2 \\ P_1 \\ P_2 \end{pmatrix} \tag{25.16}$$

with $p_1^*, p_2^*, p_3^*, p_4^*, p_5^*, p_6^*, p_7^* \geq 0$.

Applying the $\Gamma-$algorithm to the columns of the system matrix in Eq. (25.16) we obtain the feasibility conditions

$$\begin{pmatrix} K_1 & K_2 & P_1 & P_2 \end{pmatrix} \begin{pmatrix} -1.1716 & 0.0 \\ 0.0 & -6.8284 \\ 0.1716 & 5.8284 \\ 1.0 & 1.0 \end{pmatrix} \leq \mathbf{0} \tag{25.17}$$

which can be written as

$$\begin{aligned} 0.1464\, P_1 + 0.8535\, P_2 &\leq K_1, \\ 0.8535\, P_1 + 0.1464\, P_2 &\leq K_2. \end{aligned} \tag{25.18}$$

Analogously, we obtain the feasibility conditions for other n values. As an example, in the case $n = 10$ we obtain the feasibility conditions

$$\begin{aligned} K_1 \geq\ & 0.0012\, P_1 + 0.0109\, P_2 + 0.0293\, P_3 + \\ & 0.0546\, P_4 + 0.0844\, P_5 + 0.1156\, P_6 + \\ & 0.1454\, P_7 + 0.1707\, P_8 + 0.1891\, P_9 + \\ & 0.1988\, P_{10}, \\ K_2 \geq\ & 0.1988\, P_1 + 0.1891\, P_2 + 0.1707\, P_3 + \\ & 0.1454\, P_4 + 0.1156\, P_5 + 0.0844\, P_6 + \\ & 0.0546\, P_7 + 0.0293\, P_8 + 0.0109\, P_9 + \\ & 0.0012\, P_{10}. \end{aligned} \tag{25.19}$$

The above are the same feasibility conditions obtained by Ioakimidis (2000), applying the Fourier algorithm. The feasibility conditions (25.19) are obviously related with the expression of k_1 (and k_2) in (25.11).

25.4 The Beam Problem

In this section, we consider a one-dimensional case of beam on $[0, L]$, which is simply supported (roller) at $x = 0$ and simply supported at $x = L$ (see figure 25.2).

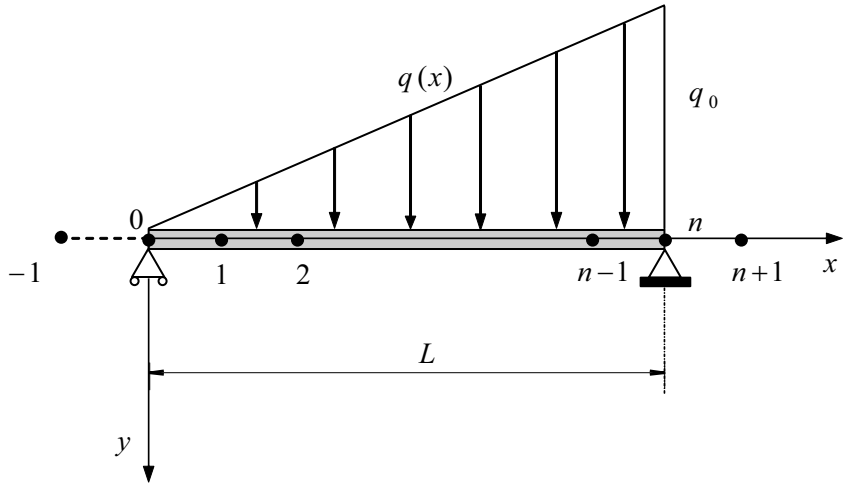

Figure 25.2. Interval partition in the finite difference method applied to the beam simply supported (roller) at $x = 0$ and simply supported at $x = L$ in Section 25.3. The load $q(x)$ is a linear function, $q(x) = q_0 x/L,\ 0 \le x \le L$

The fourth-order ordinary differential equation for this problem is

$$EI\frac{d^4y}{dx^4} = q(x),\ 0 \le x \le L \tag{25.20}$$

where y is the deflection of the beam (positive upward), $q(x)$ is intensity of the load (positive upward), E is the modulus of elasticity and I is the moment of inertia of a cross section of the beam. In this example we consider that $q(x) = q(x)/(EI)$. The boundary conditions for the above problem are $y(0) = y(L) = 0$, $\frac{d^2y}{dx^2}(0) = 0$ and $\frac{d^2y}{dx^2}(L) = 0$. Following Ioakimidis (2000), we approximate the fourth order differential equation and the boundary conditions in Eq. (25.20), by the finite difference method. Taking $n + 1$ equally spaced points $x_i = hi, i = 0, \ldots, n$ where $h = L/n$, we get the approximate system of linear equations

$$\frac{y_{i+2} - 4y_{i+1} + 6y_i - 4y_{i-1} + y_{i-2}}{h^4} = q_i, \tag{25.21}$$

where $y_i = y(x_i)$ and $q_i = q(x_i),\ i = 1, 2, \ldots, n-1$. The boundary conditions can be approximated as

$$\begin{aligned} y(0) = 0,\ \frac{d^2y}{dx^2}(0) &= \frac{y_1 - 2\,y_0 + y_{-1}}{h^2} = 0, \\ y(L) = 0,\ \frac{d^2y}{dx^2}(L) &= \frac{y_{n+1} - 2\,y_n + y_{n-1}}{h^2} = 0. \end{aligned} \tag{25.22}$$

Firstly, we suppose that the load $q(x)$ on the beam is a linear function, $q(x) = q_0 x/L,\ 0 \le x \le L$ (see figure 25.2). From (25.21) and (25.22) we get the system of linear equations

$$\left.\begin{array}{l} \dfrac{y_{i+2}-4y_{i+1}+6y_i-4y_{i-1}+y_{i-2}}{h^4} = c\,x_i,\ i=1,\ldots,n-1 \\ y_0 = 0, \\ y_n = 0, \\ y_1 - 2y_0 + y_{-1} = 0, \\ y_{n+1} - 2\,y_n + y_{n-1} = 0 \end{array}\right\} \tag{25.23}$$

where $c = q_0/L$, $h = L/n$, $x_i = hi, i = 0,\ldots,n$ and $y_i = y(x_i), i = 1,\ldots,n-1$.

Following Ioakimidis (2000), we suppose that q_0 is large enough and $c = q_0/L \geq 1$, then we should impose that the deflection of the beam $y_i \leq H_0, i = 1,\ldots,n-1$. We study the feasibility conditions of the system (25.23) with the inequality constraints $y_i \leq H_0, i = 1,\ldots,n-1$, for different n values.

In the case $n = 4$, $L = 1$ and $h = 1/4$, we study the feasibility conditions of the system

$$\left.\begin{array}{rrrrrrrrrr} y_{-1} & -4\,y_0 & +6\,y_1 & -4\,y_2 & +y_3 & & & & \geq h^4/4 \\ & y_0 & -4\,y_1 & +6\,y_2 & -4\,y_3 & +y_4 & & & \geq h^4/2 \\ & & y_1 & -4\,y_2 & +6\,y_3 & -4\,y_4 & +y_5 & & \geq 3h^4/4 \\ & y_0 & & & & & & & = 0 \\ y_{-1} & -2\,y_0 & +y_1 & & & & & & = 0 \\ & & & & & & y_4 & & = 0 \\ & & & & & y_3 & -2y_4 & +y_5 & = 0 \end{array}\right\} \tag{25.24}$$

together with $y_1, y_2, y_3 \leq H_0$.

In this example, we show how the $\Gamma-$algorithm can be applied to obtain the feasibility conditions in a mixed problem with linear equalities and inequalities. Using slack variables in (25.24) to convert the inequalities into equalities and one more artificial variable to convert the arbitrary variables into non negative variables, we get the equivalent system of linear equalities with matrix

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & -4 & 6 & -4 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -4 & 6 & -4 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -4 & 6 & -4 & 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{25.25}$$

Applying the $\Gamma-$algorithm to the columns of the matrix $\mathbf{A}$, we obtain the dual cone $\mathbf{A}_\pi^p = \mathbf{W}_\pi$, where

$$\mathbf{W} = \begin{pmatrix} 0.625 & 1. & 0.875 & 0.25 & -0.625 & 0.75 & -0.875 & 0. & 0. & -1. \\ 0.666 & 1. & 0.666 & 0.333 & -0.666 & 0.333 & -0.666 & 0. & -0.666 & 0. \\ 0.875 & 1. & 0.625 & 0.75 & -0.875 & 0.25 & -0.625 & -1. & 0. & 0. \end{pmatrix}. \tag{25.26}$$

The product of the dual cone generators (columns of $\mathbf{W}$ in Eq. (25.26)) and the parametric independent terms vector

$$\mathbf{b}^T = (h^4(1/4), h^4(1/2), h^4(3/4), 0, 0, 0, 0, H_0, H_0, H_0)$$

gives us the feasibility conditions

$$H_0 \geq \{0.00512695, 0.00683594, 0.00463867\}. \tag{25.27}$$

The conditions in Eq. (25.27) are approximations of the exact values of the deflection of the beam, $y_i = y(x_i),\ i = 1, 2, 3$, at each point of the partition. Taking the maximum value in Eq. (25.27), we obtain that $H_0 \geq 0.00683594$. Working analogously in the cases $n = 6$, $n = 8$ and $n = 10$, we obtain that $H_0 \geq 0.00665509$, $H_0 \geq 0.0065918$ and $H_0 \geq 0.0065625$, respectively. We can see that there is a convergence to the exact maximum value of the deflection $y(x)$ which obtained analytically is 0.00652218.

Consider now that we make a change in the load expression. We consider the problem (25.21)-(25.22) and suppose that the load takes a constant value $q_i = q$ along the interval $[0, L]$. We suppose that q is large enough $q \geq 1$, and impose that the deflection of the beam $y_i \leq H_0, i = 1, \ldots, n-1$. The only differences with the previous problem are in the independent terms vector. Then, we don't have to apply again the $\Gamma-$algorithm to obtain the new feasibility conditions. To obtain the new feasibility conditions in the case $n = 4$, we consider the product of the $\mathbf{W}$ matrix in (25.26) and the new independent terms vector $\mathbf{b}^T = (h^4, h^4, h^4, 0, 0, 0, 0, H_0, H_0, H_0)$, obtaining the feasibility conditions $H_0 \geq 0.0136719$. Analogously, in the cases $n = 6$, $n = 8$ and $n = 10$, we obtain the feasibility conditions $H_0 \geq 0.0133102$, $H_0 \geq 0.0131836$ and $H_0 \geq 0.013125$, respectively. The exact maximum value of the deflection $y(x)$, obtained analytically, is 0.0130208.

Working with the $\Gamma-$algorithm is easy to update the feasibility conditions when we take a subset of the initial cone generators (columns of matrix $\mathbf{A}$ in Eq. (25.25)) or if we add new generators to the cone $\mathbf{A}_\pi$. Suppose that we make a change in the above beam problem; we consider that the beam is simple supported (roller) at $x = 0$ and fixed at $x = L$. The load takes a constant value $q_i = q$ along the interval $[0, L]$ (see figure 25.3). The new boundary conditions are $y(0) = y(L) = 0$, $\frac{d^2y}{dx^2}(0) = 0$ and $\frac{dy}{dx}(L) = 0$. We only need two more iterations in the $\Gamma-$algorithm to obtain the new

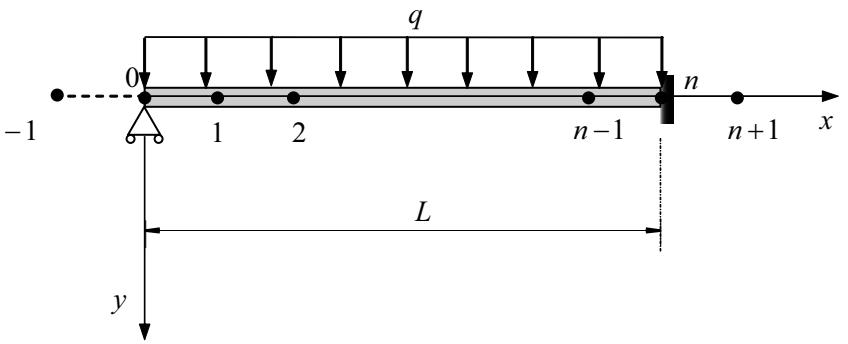

Figure 25.3. Interval partition in the finite difference method applied to the beam simply supported (roller) at $x = 0$ and fixed at $x = L$ in Section 25.3. The load $q(x)$ is a constant function, $q(x) = q,\ 0 \leq x \leq L$

feasibility conditions in the cases $n = 4$ ($H_0 \geq 0.0065696$), $n = 8$ ($H_0 \geq 0.0056493$) and $n = 10$ ($H_0 \geq 0.00560448$). The exact maximum value of the deflection $y(x)$, obtained analytically, is 0.00541612.

25.5 Conclusions

In this paper, we show how the $\Gamma-$algorithm can be applied in computational mechanics problems involving a parametric system of linear equalities and inequalities, to obtain the feasibility conditions. The $\Gamma-$algorithm is presented as an alternative to the Fourier algorithm previously studied by Ioakimidis (2000). Three different problems are analyzed to show the capabilities of the $\Gamma-$algorithm: a heat transfer problem related to the finite differences method, a fracture mechanics problem related to numerical integration and various classical beam problems related to the finite difference method. We show the application of the $\Gamma-$algorithm to obtain the feasibility conditions in one-dimensional problems approximated by the finite difference method, but it could be applied to problems with other dimensions, such as the two-dimensional Saint-Venant torsion problem, or to problems approximated by the finite element method.

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26

Forecasting Nonlinear Systems with Neural Networks via Anticipated Synchronization

Sixto Herrera, Daniel San-Martín, Antonio S. Cofiño, and José M. Gutiérrez

Department of Applied Mathematics and Computational Sciences, University of Cantabria, Spain

Abstract: Predictability of chaotic nonlinear systems is limited by the exponential propagation of errors characteristic of chaotic behavior. In this paper we analyze a new nonlinear prediction scheme considering a chain of identical neural networks synchronized to the original system using an anticipated setting. The neural models are fitted to a time series obtained from an embedding of a scalar observable of the original system (e.g., a single variable). The spatiotemporal dynamics of the resulting chain model are analyzed and the maximum prediction horizons attainable with this scheme are estimated. Although it is possible in theory to obtain arbitrary long forecast horizons with this methodology, we show that even tiny errors (e.g., the errors introduced in the modeling phase) limit severely the attainable prediction horizons in practical applications.

Keywords and phrases: Predictability, nonlinear time series analysis, neural networks, anticipated synchronization, spatiotemporal dynamics, forecast horizon

26.1 Introduction

Forecasting the dynamics of nonlinear chaotic systems is a challenging problem with important applications (Fan and Yao, 2005; Kantz and Schreiber, 2003). Although chaotic behavior implies long-term unpredictability, the underlying deterministic nature of these systems allows the prediction of their dynamics to some extent. From a theoretical point of view, the inverse of the Lyapunov exponent gives a theoretical limit for the prediction horizon attainable for a particular system. However, in practice, the original system is unknown, and approximate models fitted to the available data have to be used to model and forecast its nonlinear dynamics (e.g., neural networks). In this situation, the attainable forecast horizon depends not only on the dynamics of the original system, but also on the error of the approximate model.

Among the different methodologies introduced in the literature to forecast nonlinear systems, anticipated synchronization has become a popular and intriguing methodology (Voss, 2000). Synchronization of chaos refers to a process wherein a common dynamical

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behavior is imposed in two chaotic systems (either identical or approximate) using an appropriate coupling or forcing (see, e.g., Pikovsky et al., 2001). Unidirectional master-slave coupling is a typical synchronization framework where a slave system is forced to follow the master dynamics after an initial transient. Anticipated synchronization is a recently discovered master-slave synchronization regime that occurs when the slave becomes synchronized with the master but, additionally, its signal is shifted in time; i.e., the slave system anticipates the future dynamics of the master. This scheme provides a natural method for nonlinear system forecasting, since approximate models fitted to the available data (local linear techniques, neural networks, etc., see Kantz and Schreiber (2003)) can be synchronized to the original master model to anticipate its future dynamics. Moreover, this synchronization regime can be obtained in cascade (the first slave can act as the master for a second slave system, and so on), thus extending the anticipation time.

In this paper we analyze the mechanism underlying this synchronization cascade phenomenon and describe its limitations for practical applications, showing that even negligible errors limit severely the attainable prediction horizons. This is an important result for practical applications since, theoretically, in total absence of errors it is possible to obtain arbitrarily long forecast horizons using this methodology.

This paper is organized as follows. Section 26.2 describes a synchronization methodology that allows us to anticipate the dynamics of nonlinear systems using chains of a master and several slave coupled models. Section 26.3 analyzes the application of neural networks to model nonlinear time series based on an embedding framework. Section 26.4 combines anticipated synchronization and neural networks to provide a practical setup for time series forecast. Finally, some conclusions are given in Section 26.5.

26.2 Anticipated Synchronization

Synchronization of chaos refers to a process wherein two (or many) chaotic systems (either identical or approximate) adjust a given property of their motion to a common behavior due to a coupling or to a forcing. Several schemes have been presented in the literature to synchronize chaotic systems (Pikovsky et al., 2001). For instance, given a couple of identical chaotic systems, $\mathbf{u_0}'(t) = f(\mathbf{u_0}(t))$ and $\mathbf{u_1}'(t) = f(\mathbf{u_1}(t))$, identical chaotic synchronization can be achieved with a dissipative coupling of the form

$$\begin{aligned} \mathbf{u_0}'(t) &= \mathbf{f}(\mathbf{u_0}(t)) \\ \mathbf{u_1}'(t) &= f(\mathbf{u_1}(t)) + K(\mathbf{u_0}(t) - \mathbf{u_1}(t)), \end{aligned} \tag{26.1}$$

when the fixed point $\mathbf{\Delta} = \mathbf{0}$ is globally asymptotically stable for the transversal system $\mathbf{\Delta} = \mathbf{u_0} - \mathbf{u_1}$; K is a coupling parameter and the range of feasible values is given by the above condition. In this case, the dynamics of both systems will restrict to the synchronization manifold $\mathbf{u_0}(t) = \mathbf{u_1}(t)$, $t > T$, after some transient time T and, hence, they will exhibit identical dynamical behavior. $\mathbf{u_1}$ is the slave system and $\mathbf{u_0}$ the master, or drive. In most of the cases, no analytical results about stability are possible, and synchronization regimes have to be numerically obtained.

The phenomenon of anticipated synchronization, proposed recently by Voss (2000), has attracted a lot of attention because of its counterintuitive features as well as its

potential applications. As has been shown, anticipated synchronization appears when the slave system becomes synchronized with the output of the master system, but additionally its signal is shifted in time, i.e., the slave system starts to follow the future dynamics of the master system. This is achieved using a dissipative coupling as in (26.1) but with a delay component:

$$\begin{aligned} \mathbf{u_0}'(t) &= \mathbf{f}(\mathbf{u_0}(t)) \\ \mathbf{u_1}'(t) &= \mathbf{f}(\mathbf{u_1}(t)) + K\,(\mathbf{u_0}(t) - \mathbf{u_1}(t-\tau)) \end{aligned} \tag{26.2}$$

where K is a coupling parameter and τ is a delay time (which gives the anticipation time in this case). This achronal synchronization occurs for some bounded region of coupling parameters.

To illustrate the above concepts we consider a benchmark chaotic system, the Rössler model, which is given by the set of differential equations (Rossler, 1976):

$$(x', y', z') = (-y - z, x + a\,y, b + z\,(x - c)) \tag{26.3}$$

with $a = 0.15$, $b = 0.2$ and $c = 10$, and leading Lyapunov exponent $\lambda = 0.09$, which gives a theoretical prediction time of $t = 1/\lambda = 11.1$. In this case we used a fourth-order Runge-Kutta algorithm with a fixed time step $\tau = 10^{-2}$ to integrate the model, recording a time series consisting of 5000 sample points. This set was divided in two parts; the first one was used for training whereas the second one was reserved for testing the models.

For instance, figures 26.1(a)–(c) show the dynamics (time series of variable x) of a master and a slave Rossler systems for different anticipation times $\tau = 0$, 0.7 and 1.2, respectively, for a coupling strength $K = 0.5$. From these figures, it can be shown that for small values of τ the slave follows (figure 26.1a) or anticipates (figure 26.1b) the master dynamics after an initial transient time. However, for large anticipation times the dynamics of the synchronization manifold are unstable and each system evolves differently (figure 26.1c).

To have a global vision of the combination of K and τ parameters which lead to a synchronized behavior, figure 26.2(a) shows the stability region of the anticipated manifold in the $K - \tau$ space by plotting in a gray scale the maximum of the cross-correlation function between $x_1(t - \tau)$ and $x_0(t)$. From this figure, we estimate that the maximum anticipation time $\tau = 0.91$ is reached for $K = 0.5$. This maximum anticipation time is shorter than the inverse of the largest Lyapunov exponent and, in fact, it is similar to the linear prediction time of the original system: 0.95 (obtained as the time where the error of a linear prediction is larger than 5% of the systems range).

This anticipated sychronization can be also applied to a chain of slave systems, where each of them acts as the slave of the previous one, and the master of the following one. For instance, figure 26.2(b) shows the stability region for a chain of 20 slaves; in this case, the figure shows the maximum of the cross-correlation function between $x_{20}(t - 20\tau)$ and $x_0(t)$. Similarly, figure 26.2(c) shows the stability region for a chain of 200 slave systems. From these figures, it can be shown that as the length of the chain grows, the maximum individual anticipation times are smaller due to the amplification of errors through the chain. However, the total anticipation time is substantially incremented and, theoretically, arbitrarily long forecast times can be obtained with this cascading approach (using identical systems and in the absence of errors).

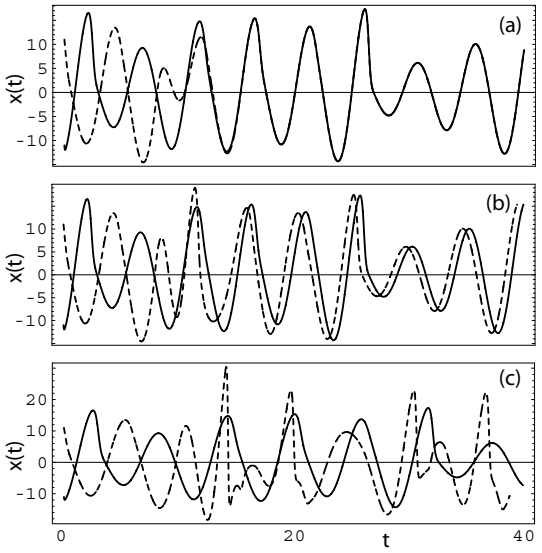

Figure 26.1. Time series of the master x_0 (solid) and slave x_1 (dashed) Rossler models for $K = 0.5$ and $\tau = 0$ (a), 0.7 (b), and 1.2 (c)

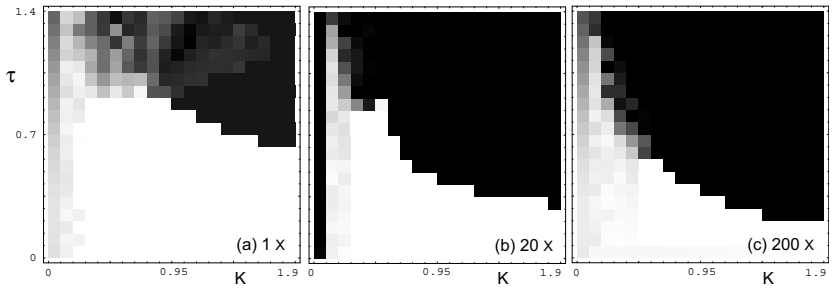

Figure 26.2. Stability regions in the parameter space K and τ for anticipated synchronization scheme with identical copies of (a) one Rossler slave, (b) ten slaves, (c) twenty slaves (black indicates zero and white one correlation values)

Figure 26.3 shows the dynamics of a synchronization chain consisting of $n = 100$ Rossler models.

Once the synchronization coupling is switched on, the slaves progressively become synchronized to the master, following an approximate linear front (thin solid line) until all systems become synchronized in an anticipated form following oblique lines (such as the thick solid line). Note that figure 26.3(b) is similar to (a) but with the times sifted to have identical behavior in the vertical lines; moreover, the white areas in figure 26.3(c) correspond to synchronization regions in the spatiotemporal space.

Therefore, in principle, arbitrary anticipation times could be obtained using an appropriate chain of identical models. However, in practical settings there is a lack of information and, usually, the only information available is in the form of a time series of some system's observable. Therefore, using a identical copy of the master as a

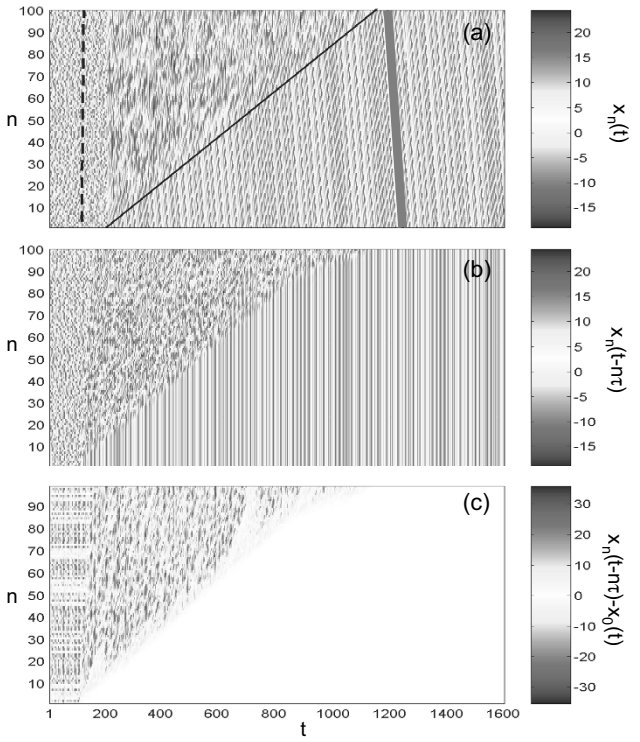

Figure 26.3. Anticipated synchronization of a chain of $n = 100$ Rossler systems. The dashed line shows the time where synchronization is switched on

slave model is not a realistic assumption in practise. To overcome this limitation, an approximate replica of the original model can be obtained applying appropriate nonlinear time series techniques to the available data. Thus, a synchronization cascade could be obtained using the observed models as the master and the inferred approximated models as slaves.

26.3 Nonlinear Time Series Modeling with Neural Networks

The deterministic nature of a nonlinear system allows extracting its functional structure from observed data using appropriate nonlinear techniques (Kantz and Schreiber, 2003; Fan and Yao, 2005). Artificial Neural Networks (NNs) have been successfully applied to this task when complete information of the systems variables is available (Ciszak et al., 2005). In this case, the neural network approximates the functional form of the corresponding differential equations (26.3). However, this is not a realistic situation in practise, since usually only a particular magnitude of the system is observable (e.g., a single variable x) in the form of a scalar time series x_n, $n = 0, 1, 2, \ldots$.

In this situation, according to the embedding theorem, x_n is functionally related to a delayed vector $\mathbf{x}_{n,\delta} = (x_{n-\delta}, \ldots, x_{n-m\,\delta})$, where δ is the embedding delay and m the dimension of the embedding space. Therefore, a neural network can be trained with input-output samples from the time series of the form $\mathbf{x}_{n,\delta}$-x_n. It has been shown that the resulting approximate neural models can also reproduce the dynamical behavior and the nonlinear characteristics of the original model, such as similar Lyapunov exponents or fractal dimension (Cheng et al., 1997), etc.

We have considered different neural networks with increasing complexity (number of parameters) to fit the nonlinear dynamics of the Roosler model considering a time series x_n, $n = 1, \ldots, 5000$, sampled from the original model with a sampling time $\Delta = 0.01$. First, an appropriate embedding delay $\delta = 0.3$ (corresponding to $n = 30$) was obtained from the time series (see figure 26.4(a)) and an optimal embedding dimension $m = 6$ was experimentally computed by increasing the number of input units in the neural networks until no further improvement was achieved. Different neural network topologies were trained dividing the available data in two equal parts; the first one was used for training the model using the Levenberg-Marquad algorithm, whereas the second one was reserved for testing the resulting models. The networks considered were standard feed-forward neural networks (FFNN) with sigmoidal logistic and linear activation functions for hidden and output layers, respectively. Figures 26.4(b) and (c) show the errors obtained with a three layer 6:6:1 network (6 input, 6 hidden and a single output). These figures show that the prediction errors for an anticipation time of $\tau = 0.3$ are, in average, less than 0.1% of the system's amplitude.

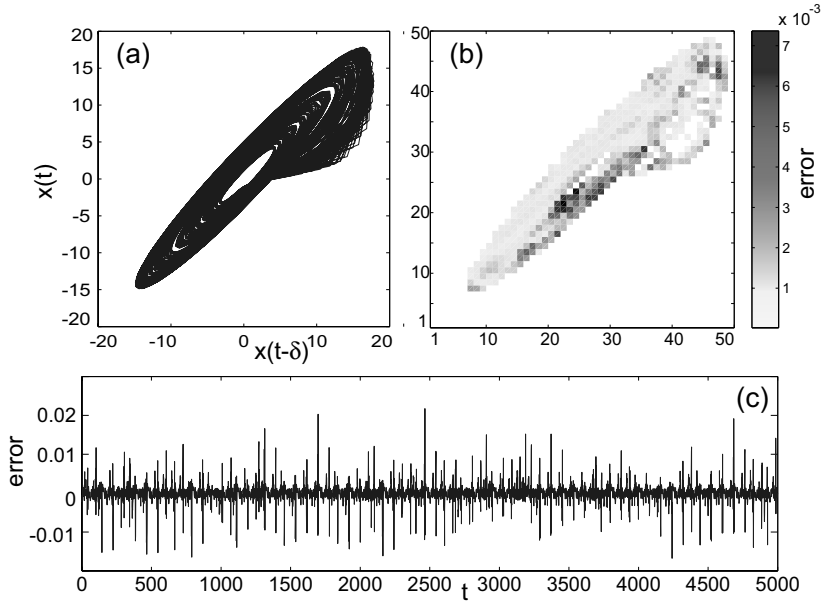

Figure 26.4. (a) Projection in the first two dimensions of the embedding phase space ($\delta = 0.3$) for the x series of the Rossler system. (b) Average error obtained with a 6:6:1 neural network in different regions of the phase space; (c) temporal series of the error

26.4 Error Growth in Synchronized Chains

Once an approximate neural model has been obtained, it can be used as a slave system applying the anticipated synchronization framework to predict the future evolution of the mater system (the observed time series). However, in this case it is not clear how the resulting approximation error (see figure 26.4c) will affect the dynamics of the synchronization chain.

First, we need to adapt the synchronization scheme given in (26.2) to consider a master system given by a time series $x_0, x_1, \ldots$. In this case, we modify the synchronization algorithm as follows:

- We first define $u_k = x_k$, $k = 0, \ldots, m-1$, and the delay vector $\mathbf{v} = (u_{m-1}, \ldots, u_0)$;
- then we proceed as follows for $n = m, m+1, \ldots$

$$\epsilon = K\,(x_n - u_{n-1}), \tag{26.4}$$

$$u_n = NNet(\mathbf{v}) + \epsilon \tag{26.5}$$

$$\mathbf{v} = [u_n, \mathbf{v}_{[1:m-1]} + \epsilon] \tag{26.6}$$

  where $NNet$ is the neural function and $\mathbf{v}_{[1:m-1]}$ is the vector with the first $m-1$ components of $\mathbf{v}$.

As in the original case, K is a coupling parameter and, in this case, the anticipation time reduces to $n = 1$ (which is equivalent to $\tau = 0.3$ due to the sampling time used to obtain the time series).

Figure 26.5(a) shows how the error of the neural network affects the synchronization capabilities of the chain (similar to figure 26.3(a), but in logarithmic scale). This figure shows that the errors obtained in the chain increase from 10^{-2} to 10^{2}, aproximately; moreover, the number of slave systems synchronized at each time step varies dynamically. Thus, the total anticipation time attainable with this approach varies from time to time due to the interplay between error growth and synchronization.

In order to understand the nature of this error dynamics we have also considered a chain of perturbed Rossler slave systems. To this aim, random gaussian values with standard deviation 10^{-2} and 10^{-4} were introduced in the parameters of the master Rossler system (26.3) and the resulting perturbed slaves were synchronized with the master using the synchronization approach (26.2). The evolution of the resulting synchronized chains are shown in figures 26.5(b) and (c), respectively. These figures show that the behavior of the neural chain is in between both cases, indicating that the impact of the neural approximated models in the synchronization dynamics is similar to the impact produced by a small difference between the master and slave systems.

Finally, we analyze the practical anticipation horizons attainable with this approach. To this aim, an error threshold is fixed (1% of the system range) and the first slave in the chain, N, with larger synchronization error is identified. Figure 26.6 shows the histograms of the values N obtained from a time series of 50000 values using both neural and perturbed Rossler slaves. This figure shows that the mean anticipation time with the neural model is $\tau = 3$, but it varies between $\tau = 1.5$ and $\tau = 6$. This distribution of errors characterizes the practical forecast horizon attainable with this anticipation approach.

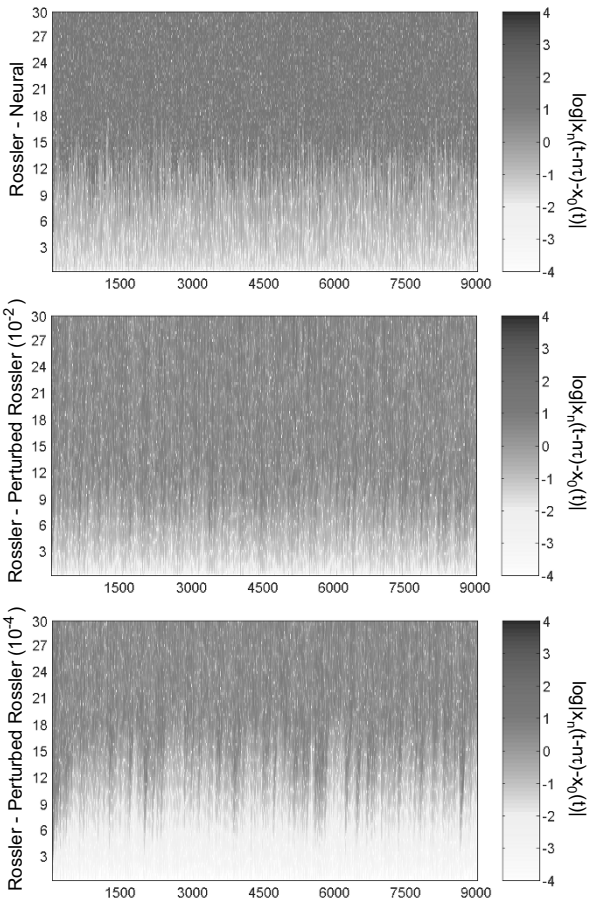

Figure 26.5. (a) Error (in logarithmic scale) between the n-th neural slave system x_n and the Rossler master x_0. (b), (c) Errors considering perturbed Rossler models as slave models

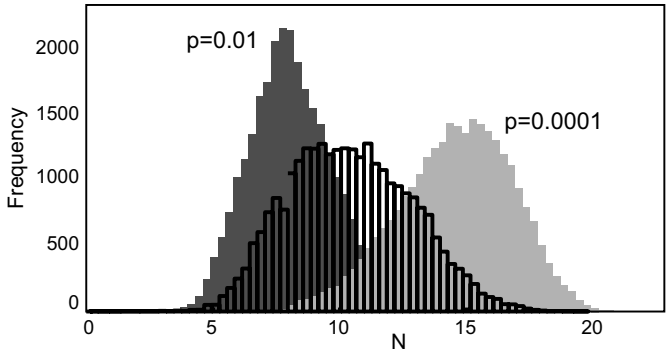

Figure 26.6. Histograms of the anticipation times $\tau = 0.3N$ attained with the neural (front) and perturbed Rossler models (gray shading) using the anticipated synchronization chain scheme

26.5 Conclusions

We have analyzed a practical technique to anticipate the dynamics of chaotic systems using a chain of neural network replicas of a master system combined with the anticipated synchronization scheme. Theoretically, it is possible to obtain arbitrarily long anticipation times using perfect neural network replicas; however, in practice, it is not possible to build identical models and, hence, the anticipation time obtained with this approach are limited. Moreover, the anticipation times vary from time to time. Thus, a statistical characterization is required.

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Part IX

Discrete Distributions

27

The Discrete Half-Normal Distribution

Adrienne W. Kemp

School of Mathematics and Statistics, University of St. Andrews, Scotland

Abstract: The discrete half-normal distribution is derived as the maximum entropy distribution on 0,1,... with specified mean and variance. It is a limiting q-hyper-Poisson-I distribution that arises from the Morse M/M/1 queue with service-dependent balking. Success runs models are reviewed. A new derivation as a mixture of Heine distributions is given. Finally the moment and other properties are examined.

Keywords and phrases: Maximum entropy distribution, confluent q-series distribution, Morse M/M/1 queue with balking, success runs models, Heine mixture, unimodality, logconcavity, increasing failure rate

27.1 Introduction

The (continuous) half-normal distribution is $N(0, \sigma^2)$ folded about the origin; it can therefore be obtained by left-truncating $N(0, \sigma^2)$ below zero. The discrete normal distribution of Lisman and van Zuylen (1972), Kemp (1997), Liang (1999), Szablowski (2001), Navarro and Ruiz (2005) and Johnson et al. (2005) with probability mass function (pmf)

$$\Pr[X = x] = p_x = \frac{\theta^x q^{x(x-1)/2}}{\sum_{x=-\infty}^{\infty} \theta^x q^{x(x-1)/2}}, \quad x = \ldots, -2, -1, 0, 1, 2, \ldots \tag{27.1}$$

is not symmetric however. The discrete half-normal distribution studied here has the pmf

$$\Pr[X = x] = p_x = \frac{\theta^x q^{x(x-1)/2}}{\sum_{x=0}^{\infty} \theta^x q^{x(x-1)/2}}, \quad x = 0, 1, 2, \ldots, \tag{27.2}$$

$0 < q < 1,\ 0 < \theta$. It is (27.1) left-truncated below zero. The probability generating function (pgf) is

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$$G(z) = \sum_{x=0}^{\infty} q^{x(x-1)/2}\theta^x z^x \Big/ \sum_{x=0}^{\infty} q^{x(x-1)/2}\theta^x$$
$$= {}_1\phi_1(q;0;q,-\theta z)/\,{}_1\phi_1(q;0;q,-\theta), \quad 0<q<1,\ 0<\theta, \tag{27.3}$$

using the Gasper and Rahman (2004) q-series notation.

$${}_A\phi_B(a_1,\ldots,a_A;b_1,\ldots,b_B;q,z) = \sum_{j=0}^{\infty} \frac{(a_1;q)_j\ldots(a_A;q)_j z^j}{(b_1;q)_j\ldots(b_B;q)_j(q;q)_j}\left[(-1)^j q^{\binom{j}{2}}\right]^{B-A+1},$$

where $(u;q)_0 = 1$ and $(u;q)_j = (1-u)(1-uq)\ldots(1-uq^{j-1})$ for $j = 1, 2, \ldots$. When $|q|<1$ and $A = B$ this series converges for all z.

The representation (27.3) of the pgf shows that the distribution is a member of the q-confluent family with pgf

$$G(z) = {}_1\phi_1(b;c;q,-\theta z)/\,{}_1\phi_1(b;c;q,-\theta),\ 0<q<1,\ b<1,\ c<1,\ 0<\theta,$$

(see Kemp (2005)), and hence it is a generalization of the Heine distribution of Benkherouf and Bather (1988), Kemp (1992a,b) and Johnson et al. (2005) with pgf

$$G(z) = {}_0\phi_0(-;-;q,-\theta z)/\,{}_0\phi_0(-;-;q,-\theta),$$
$$= {}_1\phi_1(0;0;q,-\theta z)/\,{}_1\phi_1(0;0;q,-\theta), \quad 0<q<1,\ 0<\theta,$$

Section 27.2 explains the rationale for the name "discrete half-normal". The (continuous) half-normal distribution is the maximum entropy distribution on the nonnegative half-line with specified mean and variance; see Kapur (1989), §3.2.2. The discrete half-normal distribution is shown in Section 27.2 to be the analogous maximum entropy distribution with specified mean and variance but with integer support 0,1, ... Its derivation as a limiting form of C. D. Kemp's (Kemp, 2002) q-hyper-Poisson-I distribution is explained in Section 6.3. Section 27.4 relates the distribution to the Morse (1958) M/M/1 queue with service-dependent balking. Success runs models are described in Section 27.5. Section 27.6 gives a new derivation as a mixture of Heine distributions; the distribution is therefore a q-analogue of a mixed Poisson distribution. Moment and other properties are examined in Section 27.7.

27.2 The Maximum Entropy Derivation

The maximum entropy principle implies that if only partial information about a probability distribution is available, then it should be modelled as the distribution with maximum entropy that satisfies the known constraints. Lisman and van Zuylen (1972) termed this "the most probable distribution" subject to the known constraints. The abbreviation "MED" is used.

In Kemp (1997) the discrete normal distribution with pmf (27.1) was characterized as the discrete distribution with integer support on $(-\infty, \infty)$ and specified mean and

variance. Adopting Kapur's method (Kapur, 1989) of undetermined multipliers for the discrete half-normal distribution, we have the Lagrangian

$$L \equiv \sum_{x=0}^{\infty} p_x \ln p_x - c_1 \left[\sum_{x=0}^{\infty} p_x - 1 \right] - c_2 \left[\sum_{x=0}^{\infty} x p_x - \mu \right] - c_3 \left[\sum_{x=0}^{\infty} (x-\mu)^2 p_x - \sigma^2 \right].$$

Hence

$$0 = -\ln p_x - 1 - c_1 - c_2 x - c_3 (x-\mu)^2.$$

Therefore the MED with support $0, 1, 2, \ldots$ and specified mean and variance has the pmf

$$\begin{aligned} p_x &= e^{-1-c_1-c_3\mu^2} e^{(-c_2+2c_3\mu-c_3)x} e^{-c_3 x(x-1)} \\ &= A\theta^x q^{x(x-1)/2}, \quad x = 0, 1, 2. \ldots, \end{aligned}$$

where $\theta = e^{(-c_2+2c_3\mu-c_3)}$, $q = e^{-2c_3}$ and A is the normalizing constant.

27.3 The Limiting *q*-hyper-Poisson-I Derivation

The pgf of C. D. Kemp's (Kemp, 2002) q-hyper-Poisson-I distribution is the special case of (27.3) with $b = q$, $c = q^r$, $\theta = q^{r-1}\lambda$, $0 < q < 1$, $0 < \lambda$. He obtained it by truncating the first $(r-1)$ probabilities of the Heine distribution with parameters (q, λ), normalizing the remaining probabilities and shifting the start of the distribution to the origin. This gives the pgf

$$G(z) = {}_1\phi_1(q; q^r; q, -q^{r-1}\lambda z) / {}_1\phi_1(q; q^r; q, -q^{r-1}\lambda), \quad 0 < q < 1,\ 0 < \lambda,$$

r an integer (the distribution also exists for all $r > 0$). The discrete half-normal distribution is the limiting case as $r \to \infty$.

27.4 The Morse M/M/1 Queue with Balking

The Heine distribution can be derived by assuming an M/M/1 queue with exponential arrival rate α, service rate β and the restriction that when the queue length X has the value x, then arrivals join with probability q^x and the server idles with probability q^x for an exponentially distributed service period (Kemp, 1992b). The transition probabilities are thus assumed to be

$$p_{x,x-1} = \frac{\beta(1-q^x)}{\alpha+\beta}, \quad p_{x,x} = \frac{\alpha(1-q^x)+\beta q^x}{\alpha+\beta}, \quad p_{x,x+1} = \frac{\alpha q^x}{\alpha+\beta},$$

for $x \geq 0$, $\alpha > 0$, $\beta > 0$, $0 < q < 1$. Taking $\alpha/\beta = \theta$ gives the Heine pmf

$$p_x = p_0 \frac{\theta^x q^{x(x-1)/2}}{(1-q)\cdots(1-q^x)}, \quad \alpha/\beta > 0,\ 0 < q < 1,$$

for the stationary queue size. Note that the intensity rate θ can be greater than unity, whereas $0 < \theta < 1$ for the M/M/1 queue without balking.

When arrivals balk as above but there is no server balking, i.e., when

$$\begin{aligned} p_{0,0} &= \frac{\beta}{\alpha+\beta}, \quad p_{0,1} = \frac{\alpha}{\alpha+\beta}, \\ p_{x,x-1} &= \frac{\beta}{\alpha+\beta}, \quad p_{x,x} = \frac{\alpha(1-q^x)}{\alpha+\beta}, \quad p_{x,x+1} = \frac{\alpha q^x}{\alpha+\beta}, \qquad x \geq 1, \end{aligned}$$

and $p_{x,j} = 0$ otherwise, then the stationary outcome has the pmf (27.2)

$$p_x = p_0 \theta^x q^{x(x-1)/2}, \quad \theta = \alpha/\beta.$$

The parameterization $\rho = \theta$, $\gamma = \sqrt{q}$, gives the M/M/1 queue with balking studied in depth by Morse (1958). Here the service rate is constant but the effect of arrival balking is to reduce the arrival rate; this will happen if new arrivals are increasingly reluctant to join the queue as it gets longer.

In Kemp (2005) it was reinterpreted as an M/M/1 queue in which arrivals are only allowed to join the queue when all the existing members of the queue agree; if one or more disagree then the new arrival is not allowed to join.

27.5 Success Run Processes

Kemp (2005) also investigated stationary success run processes giving rise to the distribution. Consider the Markov chain with transition probabilities

$$p_{i,0} = 1 - \lambda q^i, \quad p_{i,i+1} = \lambda q^i, \quad i \geq 0, \quad p_{i,j} = 0 \text{ otherwise.}$$

A necessary condition for the existence of a stationary success run process is

$$\sum_{k=1}^{\infty} \prod_{i=0}^{k-1} p_{i,i+1} < \infty$$

and also the outcome probabilities must decrease monotonically. As shown in Kemp (2005) these conditions are satisfied provided that the extra parameter restriction $0 < \lambda < 1$ is made.

Distributions arising in this way can be reinterpreted as the current age distribution for the lifetime distribution with pgf $\sum_{i=1}^{\infty} a_i z^i$ when

$$(1-a_1) = p_{0,1} = \frac{p_1}{p_0}, \quad \frac{(1-a_1-\cdots-a_{x+1})}{(1-a_1\cdots-a_x)} = p_{x,x+1} = \frac{p_{x+1}}{p_x},\ x > 1.$$

The discrete half-normal distribution was shown to be the current age distribution for the lifetime distribution with pgf

$$G(z) = (1-\theta)z\ {}_2\phi_2(q, \theta q; \theta, 0; q, -\theta z).$$

Kemp (2005) also showed that the following success run process with stagnation yields the discrete half-normal distribution. Consider a transition probability matrix for a Markov chain with $p_{i,j} = 0$ except when $j = 0$, $j = i$, or $j = i+1$, i.e., there is the possibility that trials may result neither in a success nor in a failure. A career scheme in which each year employees are either promoted to the next higher level, remain at the same level, or leave the company was put forward by Kemp (1992b) as a possible scenario. The steady-state probabilities are given by

$$p_{x+1} = p_{x,x+1}p_x + p_{x+1,x+1}p_{x+1}, \quad x \geq 0.$$

The discrete half-normal distribution is the outcome when

$$\begin{aligned} &p_{0,0} = 1-\theta(1-q), && p_{0,1} = \theta(1-q), \\ &p_{i,0} = 1-q^i(1+\theta-\theta q^{i+1}), && p_{i,i} = q^i, \qquad p_{i,i+1} = \theta q^i(1-q^{i+1}), \quad i \geq 1, \end{aligned}$$

provided that $0 < \theta(1-q) < 1$ and $0 < q(1+\theta-\theta q^2) < 1$. These inequalities hold when $0 < q < 1$, $0 < \theta < \min[1, (5-3q)/4]$.

27.6 Mixed Heine Distribution

Using the Heine transformation

$${}_2\phi_1(a, b; c; q, u) = \frac{(a;q)_\infty (bu;q)_\infty}{(c;q)_\infty (u;q)_\infty} {}_2\phi_1(c/a, u; bu; q, a),$$

Gasper and Rahman (2004), p. 13, the discrete half-normal pgf (27.3) becomes

$$\begin{aligned} G(z) &= {}_1\phi_1(q; 0; q, -\theta z)/{}_1\phi_1(q; 0; q, -\theta) \\ &= \lim_{\epsilon \to 0} {}_2\phi_1(q; 1/\epsilon; 0; q, -\theta z\epsilon)/{}_2\phi_1(q; 1/\epsilon; 0; q, -\theta\epsilon) \\ &= \frac{(-\theta z; q)_\infty {}_2\phi_1(0, 0; -\theta z; q; q)}{(-\theta; q)_\infty {}_2\phi_1(0, 0; -\theta; q; q)} \end{aligned} \tag{27.4}$$

where

$$G_H(z|\eta, q) = \frac{{}_0\phi_0(-; -; q, \eta z)}{{}_0\phi_0(-; -; q, \eta)} = \frac{(-\eta z; q)_\infty}{(-\eta; q)_\infty} = \frac{E_q(\eta z)}{E_q(\eta)}.$$

is the pgf for the Heine (η, q) distribution and $E_q(\eta)$ is a q-exponential function. The Heine distribution is a q-analog of the Poisson distribution.

Reformulating (27.4) in terms of the q-integral

$$\int_0^1 f(t) d_q t = (1-q) \sum_{n=0}^{\infty} f(q^n) q^n$$

gives

$$G(z) = \int_0^1 (qt;q)_\infty(-\theta t;q)_\infty \frac{(-\theta zt;q)_\infty}{(-\theta t;q)_\infty} d_q t \Big/ \int_0^1 (qt;q)_\infty(-\theta t;q)_\infty d_q t \qquad (27.5)$$

since

$${}_2\phi_1(a,b;c;q,q^y) = \frac{(a;q)_\infty(b;q)_\infty}{(1-q)(q;q)_\infty(c;q)_\infty} \int_0^1 t^{y-1} \frac{(qt;q)_\infty(ct;q)_\infty}{(at;q)_\infty(bt;q)_\infty} d_q t;$$

see Gasper and Rahman (2004), Ex.1.4.iii. This shows that the discrete half-normal distribution is a mixture of Heine distributions and therefore a q-analog of a Poisson mixture. The nature of the mixture is clarified by expanding the ${}_2\phi_1(\cdot)$ series in the numerator of (27.4). After some algebra

$$G(z) = \sum_{j=0}^{\infty} \frac{q^j}{(q;q)_j\,(-\theta;q)_j} G_H(z|\theta q^j, q) \Big/ \sum_{j=0}^{\infty} \frac{q^j}{(q;q)_j\,(-\theta;q)_j}\,. \qquad (27.6)$$

27.7 Properties

From (27.4)

$$\mu = \sum_{x=0}^{\infty} x p_x = \sum_{x=0}^{\infty} x\theta^x q^{x(x-1)/2} \Big/ \sum_{x=0}^{\infty} \theta^x q^{x(x-1)/2}\,, \qquad (27.7)$$

$$\mu_2^{'} = \sum_{x=0}^{\infty} x^2 p_x = \sum_{x=0}^{\infty} x^2\theta^x q^{x(x-1)/2} \Big/ \sum_{x=0}^{\infty} \theta^x q^{x(x-1)/2}\,. \qquad (27.8)$$

and the variance is

$$\mu_2 = \frac{\sum_{x=0}^{\infty} x^2\theta^x q^{x(x-1)/2}}{\sum_{x=0}^{\infty} \theta^x q^{x(x-1)/2}} - \left[\frac{\sum_{x=0}^{\infty} x\theta^x q^{x(x-1)/2}}{\sum_{x=0}^{\infty} \theta^x q^{x(x-1)/2}}\right]^2. \qquad (27.9)$$

For numerical work the probabilities can be computed recursively, using an assumed value C for p_0 and the recurrence relation $p_{x+1} = \theta q^x p_x$, giving

$$C,\ C\theta,\ (C\theta)\theta q,\ (C\theta^2 q)\theta q^2,\ (C\theta^3 q^3)\theta q^3, \cdots$$

with $C + C\theta + C\theta^2 q + C\theta^3 q^3 + C\theta^4 q^6 + \cdots = T$. Normalization gives

$$p_0 = C/T,\ p_1 = C\theta/T,\ p_2 = C\theta^2 q/T,\ p_3 = C\theta^3 q^3/T,\ p_4 = C\theta^4 q^6/T, \cdots .$$

The mean and variance can then be obtained from the calculated probabilities. If θ is large and q is close to 1 then double or even quadruple precision may be needed.

The shape properties of the discrete half-normal distribution follow from those of the (untruncated) discrete normal distribution (Kemp, 1997). The ratio of successive probabilities is

$$p_{x+1}/p_x = \theta q^x, \quad x = 0, 1, \ldots.$$

As x increases this decreases and hence the distribution is unimodal. If $\theta < 1$, the mode is at the origin. For $\theta > 1$, the mode is at $[-\ln(\theta)/\ln(q)]$ where $[\cdot]$ denotes the integer part. If $-\ln(\theta)/\ln(q)$ is an integer, then there are joint modes at $-\ln(\theta)/\ln(q)$ and $1 - \ln(\theta)/\ln(q)$.

The geometric distribution with $p_x = (1-q)q^x$, $x = 0, 1, \ldots$, is the MED with constrained mean only (Kapur, 1989). For this distribution $p_{x+2}p_x/p_{x+1}^2 = 1$, so it is neither logconcave nor logconvex; it has a constant failure rate. The discrete half-normal distribution (the MED for $x = 0, 1, \ldots$, with constrained mean and variance) has

$$p_{x+2}p_x/p_{x+1}^2 = q < 1.$$

This is constant and so the distribution can be regarded as a generalization of the geometric distribution. Its probabilities are logconcave and therefore, as Gupta et al. (1997) have shown, it has an increasing failure rate.

When $q \to 0$, the distribution tends to the Bernoulli distribution with mean $\theta/(1+\theta)$ and variance $\theta/(1+\theta)^2$. For $\theta < 1$ and $q \to 1$, the limiting distribution is geometric with mean $\theta/(1-\theta)$ and variance $\theta/(1-\theta)^2$. When $\theta \geq 1$ and $q = 1$ the pgf does not converge; for $\theta \geq 1$ and $q \to 1$ the mean and second factorial moment become infinite.

Two open questions remain. Firstly, for what region of the parameter space is the variance greater than the mean? Secondly, whilst logconvexity implies infinite divisibility, logconcavity does not imply the converse (consider for example the Poisson distribution). Is there any region of the parameter space for which the distribution is infinitely divisible?

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28

Parameter Estimation for Certain q-Hypergeometric Distributions

David Kemp

School of Mathematics and Statistics, University of St. Andrews, Scotland

Abstract: Various q-hypergeometric distributions have recently been described and examined in some detail in both the statistics and the quantum physics literatures. The q-hypergeometric distributions are of interest as q-analogues of a wide class of discrete distributions (the generalized hypergeometric probability distributions) which includes, for example, the Poisson, binomial, negative binomial and logarithmic distributions. The additional parameter q can be viewed as modifying the related standard distribution (the term deforming is used in the physics literature). Parameter estimation for the q-distributions has not received much attention. This paper examines the estimation problem with special reference to q-distributions related to the logarithmic distribution. Some simulation results for maximum-likelihood estimation are given.

Keywords and phrases: Probability distributions, q-hypergeometric distributions, q-logarithmic distributions, parameter estimation

28.1 Introduction

Over the past decade, there has been increasing interest in distributions that are q-analogs of standard discrete distributions. q-distributions contain a parameter q $(0 < q < 1)$ such that as $q \to 1$ the q-distribution tends to the related standard distribution.

The main q-distributions that have been researched in both the statistics and physics literature have been the q-analogs of classical distributions, such as the binomial, Poisson, negative binomial, and logarithmic, that are members of A. W. Kemp's broad class of generalized hypergeometric probability distributions (Kemp, 1968).

The probability generating functions (pgfs) for the Kemp class of hypergeometric distributions have the form

$$g(z) = \frac{{}_AF_B[\lambda z]}{{}_AF_B[\lambda]} \tag{28.1}$$

where ${}_AF_B[\cdot]$ denotes the generalized hypergeometric function

$${}_AF_B(a_1, \ldots, a_A; b_1, \ldots, b_B; z) = \sum_{n=0}^{\infty} \frac{(a_1)_n \ldots (a_A)_n}{(b_1)_n \ldots (b_B)_n} \frac{z^n}{n!} \quad , \tag{28.2}$$

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and

$$(a)_n = \begin{cases} 1 & n = 0 \\ a(a+1)\dots(a+n-1) & n = 1, 2, \dots \end{cases} . \tag{28.3}$$

The q-hypergeometric analogs have pgfs of the form

$$g(z) = \frac{{}_A\phi_B[\lambda z]}{{}_A\phi_B[\lambda]} \tag{28.4}$$

where ${}_A\phi_B[\cdot]$ denotes the q-hypergeometric (basic hypergeometric) function

$$\begin{aligned} &{}_A\phi_B(a_1, \dots, a_A; b_1, \dots, b_B; q, z) \\ &= \sum_{n=0}^{\infty} \frac{(a_1; q)_n \dots (a_A; q)_n z^n}{(b_1; q)_n \dots (b_B; q)_n (q; q)_n} \left[(-1)^n q^{\binom{n}{2}}\right]^{B-A+1}, \end{aligned} \tag{28.5}$$

where

$$(a; q)_n = \begin{cases} 1 & n = 0 \\ (1-a)(1-aq)\dots(1-aq^{n-1}) & n = 1, 2, \dots \end{cases} . \tag{28.6}$$

Since

$$\lim_{q \to 1} \frac{(q^a; q)_n}{(1-q)^n} = a(a+1)\dots(a+n-1) = (a)_n , \tag{28.7}$$

it follows that, for example,

$$\lim_{q \to 1} {}_2\phi_1(q^a, q^b; q^c; q, z) = {}_2F_1(a, b; c; z) \tag{28.8}$$

(the usual Gaussian hypergeometric function).

There may be more than one q-analog of a distribution (e.g. there are three q-Poisson distributions).

For basic information on the hypergeometric and q-hypergeometric functions, together with detailed information on individual q-series distributions, see Johnson et al. (2005).

28.2 Special Cases and Properties

For many classical distributions it is easy to obtain simple expressions for various features of the distribution such as the probabilities, moments, factorial moments, cumulants. Unfortunately these are frequently not available for the q-analogs. This is true of the q-distributions related to the logarithmic distribution that we now concentrate on.

The classical logarithmic distribution has pgf

$$\begin{aligned} G(z) &= \frac{\log(1-\theta z)}{\log(1-\theta)} = z \frac{{}_2F_1(1, 1; 2; \theta z)}{{}_2F_1(1, 1; 2; \theta)} \\ &= a\left\{\theta z + \frac{\theta^2 z^2}{2} + \frac{\theta^3 z^3}{3} + \dots\right\}, \end{aligned} \tag{28.9}$$

where $0 < \theta < 1$ and $a = -[\log(1-\theta)]^{-1}$.

Kemp (1997) replaced ${}_2F_1(1,1;2;\theta z)$ by ${}_2\phi_1(q,q;q^2;q,\theta z)$ to obtain a q-logarithmic distribution with pmf

$$p_x = \begin{cases} C\,\theta^x \Big/ \sum_{j=0}^{x-1} q^j & x = 1,2,3,\cdots \\ 0 & \text{elsewhere} \end{cases}, \quad 0 < q < 1,\ 0 < \theta < 1, \tag{28.10}$$

where the normalizing constant $C = [\theta\,{}_2\phi_1(q,q;q^2;q,\theta)]^{-1}$.

As $q \to 1$ it approaches the logarithmic distribution, and as $q \to 0$ it approaches the geometric distribution.

However, whereas the normalizing constant a for the logarithmic distribution is the simple expression $-[\log(1-\theta)]^{-1}$, there is no simple summation formula for the q-logarithmic normalizing constant C.

Similarly, no closed expressions are available for the moments.

The Euler distribution is an infinitely divisible q-analog of the Poisson distribution; its pgf is

$$G(s) = \frac{{}_1\phi_0(0;-;q,\theta s)}{{}_1\phi_0(0;-;q,\theta)}, \qquad 0 < q < 1, \qquad 0 < \theta < 1, \tag{28.11}$$

$$= \sum_{n=0}^{\infty} \frac{\theta^n s^n}{(1-q)\cdots(1-q^n)} \Big/ \sum_{n=0}^{\infty} \frac{\theta^n}{(1-q)\cdots(1-q^n)} \tag{28.12}$$

Viewing it as a Poisson distribution of clusters, with pgf of the form

$$G(z) = \exp(\lambda(h(z)-1)),$$

its cluster size distribution has pgf

$$h(z) = \frac{\sum_0^\infty \theta^i z^i/[i(1-q^i)]}{\sum_0^\infty \theta^i/[i(1-q^i)]}, \qquad 0 < \theta < 1, \qquad 0 < q < 1. \tag{28.13}$$

This has the property that as $q \to 0$ it tends to the logarithmic distribution, so it is a q-analog in a different sense.

The generalized Euler distribution has pgf

$$G(z) = \prod_{j=0}^{\infty} \left(\frac{1-a\theta q^j z}{1-a\theta q^j}\right)\left(\frac{1-\theta q^j}{1-\theta q^j z}\right) = \frac{{}_1\phi_0(a;-;q,\theta z)}{{}_1\phi_0(a;-;q,\theta)}, \tag{28.14}$$

where $0 < q < 1$, $0 \le a < 1$, $0 < \theta < 1$.

Kemp and Kemp (2006) have investigated the cluster distribution of the generalized Euler distribution. This distribution, which they named the q-cluster distribution, has pgf

$$h(z) = \sum_{i=1}^{\infty} \frac{(1-a^i)\theta^i z^i}{i(1-q^i)} \Big/ \sum_{i=1}^{\infty} \frac{(1-a^i)\theta^i}{i(1-q^i)}\ , \tag{28.15}$$

$0 \le q \le 1$, $0 \le a \le 1$, $0 < \theta < 1$.

It is a q-generalization of the logarithmic distribution, which it becomes when $a = q$. As $a \to 1$ it tends to Kemp's q-logarithmic distribution (28.10), and when $a \to 0$ it becomes the Euler cluster distribution (28.13).

28.3 Estimation

Estimating θ for the logarithmic distribution is relatively straightforward. Moment and maximum-likelihood estimation are equivalent. The ML equation has to be solved iteratively, but this not very difficult. There is a considerable literature on the topic. Bounds for the estimator have been found. Various alternative estimators have been proposed. A particularly simple one is $1 - f_1/\bar{x}$. This estimator has been shown to be an approximation to the ML estimator.

The position for the q-analogs of the logarithmic distribution discussed in Section (28.2) is far less satisfactory. No closed expressions for moments are available, so the method of moments cannot be applied. Standard differentation techniques cannot be applied successfully. There are no known explicit estimators. Similarly, bounds are unknown.

We have therefore used an optimization algorithm to maximize the likelihood function. The rest of the paper is devoted to some results from an ongoing simulation project to study the behaviour of this approach.

For any given set of parameters computation of the probabilities by use of a recurrence relation is the only feasible choice. An arbitrary p_1 (θ is a convenient choice) is used to start the process, which is stopped when $p_x < \epsilon$, and the probabilities are then normalized by summation. We used $\epsilon = 10^{-10}$.

N pseudo-random samples, each of size n were taken from the computed distribution. For each of the N samples the negative log-likelihood was then calculated, and the parameters were estimated by the R function nlminb. Various sizes of N were tried; in general, $N = 50$ seemed a reasonable choice.

Logarithmic distributions are normally fitted to long-tailed data and hence θ is large. Once θ starts to exceed .95 the tail starts to lengthen very rapidly. So care has to be taken in choosing the upper bound for possible θ in the optimization procedure.

Table 1 gives results for the Kemp q-logarithmic distribution. The sample size was 100, and 50 samples were taken for each of nine sets of parameter values. The results presented are the means and standard deviations of the 50 estimates of θ and q for each of the 9 sets. Overall, θ seems to be estimated well with means reasonably close to

Table 28.1. Means and standard deviations of estimates from 50 samples of size 100 from the Kemp q-logarithmic distribution

	$\theta = 0.5$			
q	mean($\hat{\theta}$)	sd($\hat{\theta}$)	mean($\hat{q}$)	sd($\hat{q}$)
0.1	0.503	0.056	0.158	0.205
0.5	0.493	0.091	0.454	0.349
0.9	0.403	0.087	0.492	0.379

	$\theta = 0.9$			
q	mean($\hat{\theta}$)	sd($\hat{\theta}$)	mean($\hat{q}$)	sd($\hat{q}$)
0.1	0.901	0.011	0.179	0.165
0.5	0.897	0.039	0.439	0.196
0.9	0.900	0.026	0.884	0.105

	$\theta = 0.95$			
q	mean($\hat{\theta}$)	sd($\hat{\theta}$)	mean($\hat{q}$)	sd($\hat{q}$)
0.1	0.950	0.006	0.185	0.204
0.5	0.947	0.011	0.383	0.212
0.9	0.934	0.056	0.829	0.200

the parameter value and low standard deviations. Estimation of q gives disappointing results. A particularly poor result is that for $\theta = 0.5, q = 0.9$. Larger sample sizes improve the estimates but even $n = 1000$ still gives a standard deviation of 0.160 for the estimator (0.779) of q.

Results for the q-cluster distribution indicate that, as in the case of the Euler cluster distribution, the θ estimator is reasonable but the q estimator poor. The estimator of a also seems to have an unsatisfactorily high standard deviation.

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Index