STATISTICAL MODELING AND ANALYSIS FOR COMPLEX DATA PROBLEMS

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STATISTICAL MODELING AND ANALYSIS FOR COMPLEX DATA PROBLEMS

Edited by
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Foreword

GERAD celebrates this year its 25th anniversary. The Center was created in 1980 by a small group of professors and researchers of HEC Montréal, McGill University and of the École Polytechnique de Montréal. GERAD's activities achieved sufficient scope to justify its conversion in June 1988 into a Joint Research Centre of HEC Montréal, the École Polytechnique de Montréal and McGill University. In 1996, the Université du Québec à Montréal joined these three institutions. GERAD has fifty members (professors), more than twenty research associates and post doctoral students and more than two hundreds master and Ph.D. students.

GERAD is a multi-university center and a vital forum for the development of operations research. Its mission is defined around the following four complementarily objectives:

- The original and expert contribution to all research fields in GERAD's area of expertise;

- The dissemination of research results in the best scientific outlets as well as in the society in general;

- The training of graduate students and post doctoral researchers;

- The contribution to the economic community by solving important problems and providing transferable tools.

GERAD's research thrusts and fields of expertise are as follows:

- Development of mathematical analysis tools and techniques to solve the complex problems that arise in management sciences and engineering;

- Development of algorithms to resolve such problems efficiently;

- Application of these techniques and tools to problems posed in related disciplines, such as statistics, financial engineering, game theory and artificial intelligence;

- Application of advanced tools to optimization and planning of large technical and economic systems, such as energy systems, transportation/communication networks, and production systems;

- Integration of scientific findings into software, expert systems and decision-support systems that can be used by industry.

One of the marking events of the celebrations of the 25th anniversary of GERAD is the publication of ten volumes covering most of the Center's research areas of expertise. The list follows: **Essays and Surveys in Global Optimization**, edited by C. Audet, P. Hansen and G. Savard; **Graph Theory and Combinatorial Optimization**, edited by D. Avis, A. Hertz and O. Marcotte; **Numerical Methods in Finance**, edited by H. Ben-Ameur and M. Breton; **Analysis, Control and Optimization of Complex Dynamic Systems**, edited by E.K. Boukas and R. Malhamé; **Column Generation**, edited by G. Desaulniers, J. Desrosiers and M.M. Solomon; **Statistical Modeling and Analysis for Complex Data Problems**, edited by P. Duchesne and B. Rémillard; **Performance Evaluation and Planning Methods for the Next Generation Internet**, edited by A. Girard, B. Sansò and F. Vázquez-Abad: **Dynamic Games: Theory and Applications**, edited by A. Haurie and G. Zaccour; **Logistics Systems: Design and Optimization**, edited by A. Langevin and D. Riopel; **Energy and Environment**, edited by R. Loulou, J.-P. Waaub and G. Zaccour.

I would like to express my gratitude to the Editors of the ten volumes, to the authors who accepted with great enthusiasm to submit their work and to the reviewers for their benevolent work and timely response. I would also like to thank Mrs. Nicole Paradis, Francine Benoît and Louise Letendre and Mr. André Montpetit for their excellent editing work.

The GERAD group has earned its reputation as a worldwide leader in its field. This is certainly due to the enthusiasm and motivation of GERAD's researchers and students, but also to the funding and the infrastructures available. I would like to seize the opportunity to thank the organizations that, from the beginning, believed in the potential and the value of GERAD and have supported it over the years. These are HEC Montréal, École Polytechnique de Montréal, McGill University, Université du Québec à Montréal and, of course, the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Fonds québécois de la recherche sur la nature et les technologies (FQRNT).

Georges Zaccour
Director of GERAD

Avant-propos

Le Groupe d'études et de recherche en analyse des décisions (GERAD) fête cette année son vingt-cinquième anniversaire. Fondé en 1980 par une poignée de professeurs et chercheurs de HEC Montréal engagés dans des recherches en équipe avec des collègues de l'Université McGill et de l'École Polytechnique de Montréal, le Centre comporte maintenant une cinquantaine de membres, plus d'une vingtaine de professionnels de recherche et stagiaires post-doctoraux et plus de 200 étudiants des cycles supérieurs. Les activités du GERAD ont pris suffisamment d'ampleur pour justifier en juin 1988 sa transformation en un Centre de recherche conjoint de HEC Montréal, de l'École Polytechnique de Montréal et de l'Université McGill. En 1996, l'Université du Québec à Montréal s'est jointe à ces institutions pour parrainer le GERAD.

Le GERAD est un regroupement de chercheurs autour de la discipline de la recherche opérationnelle. Sa mission s'articule autour des objectifs complémentaires suivants :

- la contribution originale et experte dans tous les axes de recherche de ses champs de compétence;
- la diffusion des résultats dans les plus grandes revues du domaine ainsi qu'auprès des différents publics qui forment l'environnement du Centre;
- la formation d'étudiants des cycles supérieurs et de stagiaires post-doctoraux;
- la contribution à la communauté économique à travers la résolution de problèmes et le développement de coffres d'outils transférables.

Les principaux axes de recherche du GERAD, en allant du plus théorique au plus appliqué, sont les suivants :

- le développement d'outils et de techniques d'analyse mathématiques de la recherche opérationnelle pour la résolution de problèmes complexes qui se posent dans les sciences de la gestion et du génie;
- la confection d'algorithmes permettant la résolution efficace de ces problèmes;
- l'application de ces outils à des problèmes posés dans des disciplines connexes à la recherche opérationnelle telles que la statistique, l'ingénierie financière, la théorie des jeux et l'intelligence artificielle;
- l'application de ces outils à l'optimisation et à la planification de grands systèmes technico-économiques comme les systèmes énergé-

tiques, les réseaux de télécommunication et de transport, la logistique et la distributique dans les industries manufacturières et de service;

- l'intégration des résultats scientifiques dans des logiciels, des systèmes experts et dans des systèmes d'aide à la décision transférables à l'industrie.

Le fait marquant des célébrations du 25e du GERAD est la publication de dix volumes couvrant les champs d'expertise du Centre. La liste suit : **Essays and Surveys in Global Optimization**, édité par C. Audet, P. Hansen et G. Savard; **Graph Theory and Combinatorial Optimization**, édité par D. Avis, A. Hertz et O. Marcotte; **Numerical Methods in Finance**, édité par H. Ben-Ameur et M. Breton; **Analysis, Control and Optimization of Complex Dynamic Systems**, édité par E.K. Boukas et R. Malhamé; **Column Generation**, édité par G. Desaulniers, J. Desrosiers et M.M. Solomon; **Statistical Modeling and Analysis for Complex Data Problems**, édité par P. Duchesne et B. Rémillard; **Performance Evaluation and Planning Methods for the Next Generation Internet**, édité par A. Girard, B. Sansò et F. Vázquez-Abad; **Dynamic Games: Theory and Applications**, édité par A. Haurie et G. Zaccour; **Logistics Systems: Design and Optimization**, édité par A. Langevin et D. Riopel; **Energy and Environment**, édité par R. Loulou, J.-P. Waaub et G. Zaccour.

Je voudrais remercier très sincèrement les éditeurs de ces volumes, les nombreux auteurs qui ont très volontiers répondu à l'invitation des éditeurs à soumettre leurs travaux, et les évaluateurs pour leur bénévolat et ponctualité. Je voudrais aussi remercier Mmes Nicole Paradis, Francine Benoît et Louise Letendre ainsi que M. André Montpetit pour leur travail expert d'édition.

La place de premier plan qu'occupe le GERAD sur l'échiquier mondial est certes due à la passion qui anime ses chercheurs et ses étudiants, mais aussi au financement et à l'infrastructure disponibles. Je voudrais profiter de cette occasion pour remercier les organisations qui ont cru dès le départ au potentiel et la valeur du GERAD et nous ont soutenus durant ces années. Il s'agit de HEC Montréal, l'École Polytechnique de Montréal, l'Université McGill, l'Université du Québec à Montréal et, bien sûr, le Conseil de recherche en sciences naturelles et en génie du Canada (CRSNG) et le Fonds québécois de la recherche sur la nature et les technologies (FQRNT).

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Preface

The GERAD is a well-established multi-university center and a vital forum for the development of analysis tools required for solving complex problems. Traditionally, realizations of the GERAD concerned mainly Operations Research. In recent years, Statistical Sciences also emerged within GERAD, with members specializing in both theoretical and applied statistics, probability theory and stochastic processes. One objective of the present book is to present contributions to some important directions of research in the fields of interest of the statistics group at GERAD.

In Abdous, Genest and Rémillard, the authors study the properties of copulas, such as stochastic orders and dependence measure, in the context of elliptical distributions. Andrews and Feuerverger analyze complex survey data. They discuss the controversial result of the 2000 American election in Florida County. Functional estimation is the main topic of two articles. In Angers and MacGibbon, the authors develop Fourier expansion for the hazard rates in a Bayesian framework, while Berlinet and Rouvière consider the estimation of multivariate densities, with special attention to the resulting computational problems. Croteau, Cléroux and Léger present an example of the application of bootstrap interval estimation to parameters of a complex process in a periodic replacement problem. Three papers explore statistical testing in various contexts, and two of them deal with dependent data. Dabrowski proposes a statistical test of comparisons to detect difference between genes. Bellavance and Tardif study the validity of F-ratio tests in the case of dependent errors due to cross-over designs. In Larocque, the author establishes properties of a signed rank test of Wilcoxon for correlated cluster data. The analysis of time series is a common feature of four articles. Bou-Hamad and Duchesne study asymptotic properties of robust estimators to outliers, for autoregressive models with exogenous variables. Dufour and Jouini establish the asymptotic behavior for multivariate autoregressive moving-average time series models. In Francq and Zakoian, linear models with dependent but uncorrelated innovations are reviewed. Hallin and Lofti investigate the detection of periodicities in vectorial autoregressive models. Data mining is covered by one article, in which Bengio and Grandvalet consider the estimation of uncertainty for machine learning algorithms. Finally, interacting stochastic processes are covered in two papers. In Dawson and Del Moral, the authors prove a result of large deviation for interactive processes when the strong topol-

ogy is used, and Gentil, Rémillard and Del Moral present an efficient non linear filtering algorithm for the position detection of multiple targets.

We would like to thank all authors of the present volume for their contribution to the successful realization of this project. We would also like to express our gratitude to Nicole Paradis for her efficient editorial coordination.

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PIERRE DUCHESNE
BRUNO RÉMILLARD

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Chapter 1

DEPENDENCE PROPERTIES OF META-ELLIPTICAL DISTRIBUTIONS

Belkacem Abdous
Christian Genest
Bruno Rémillard

Abstract A distribution is said to be meta-elliptical if its associated copula is elliptical. Various properties of these copulas are critically reviewed in terms of association measures, concepts, and stochastic orderings, including tail dependence Most results pertain to the bivariate case.

1.   Introduction

The study of meta-elliptical multivariate distributions was recently launched by Fang, Fang and Kotz (2002), and their extension of the meta-Gaussian family of distributions due to Krzysztofowicz and Kelly (1996) is sure to find its way gradually into statistical, actuarial, economic and financial applications, where elliptically contoured distributions are already in common use. A forerunner example is provided by the work of Frey, McNeil and Nyfeler (2001), who use multivariate Student and generalized hyperbolic distributions to model credit portfolio losses.

A vector $Z = (Z_1, \ldots, Z_p)$ is said to be elliptically contoured if it admits the stochastic representation $Z = \mu + RAU$, where $\mu \in \mathbb{R}^p$, R and U are independent random variables, R is non-negative, U is uniformly distributed on the unit sphere in $\mathbb{R}^p$, and A is a fixed $p \times p$ matrix such that $AA^\top = \Sigma$ is non-singular. In particular when $\mu = 0$ and R is absolutely continuous, the density of Z is of the form

$$ h(z) = |\Sigma|^{-1/2} g\left(z^\top \Sigma^{-1} z \right), \quad z \in \mathbb{R}^p $$

where g is a scale function uniquely determined by the distribution of R. If σ_i^2 denotes the (i,i)th entry of Σ, the variables Z_i/σ_i are then identically distributed with density

$$f(z) = \frac{\pi^{(p-1)/2}}{\Gamma\{(p-1)/2\}} \int_{z^2}^{\infty} \left(t - z^2\right)^{(p-1)/2-1} g(t)dt, \quad z \in \mathbb{R}$$

and cumulative distribution function

$$F(z) = \frac{1}{2} + \frac{\pi^{(p-1)/2}}{\Gamma\{(p-1)/2\}} \int_0^z \int_{s^2}^{\infty} \left(t - s^2\right)^{(p-1)/2-1} g(t)dtds, \quad z \in \mathbb{R}.$$

The special case $g(t) \propto e^{-at}$ with $a \in \mathbb{R}_+$ corresponds to Z being multivariate Gaussian. Other examples include the multivariate Cauchy, Student and logistic, as well as generalized multivariate hyperbolic, Kotz and symmetric Pearson type-VII distributions. See Cambanis, Huang and Simons (1981) or Fang, Kotz and Ng (1987), among others, for theory and applications of elliptically contoured distributions.

Paraphrasing Fang, Fang and Kotz (2002), a random vector $X = (X_1, \ldots, X_p)$ with cumulative distribution function K and continuous marginals $K_i(x) = \mathrm{P}(X_i \leq x)$ is said to be meta-elliptically distributed if the joint distribution of the variables $Z_i = F^{-1}\{K_i(X_i)\}$ is elliptical with scale function g and matrix Σ whose main diagonal entries are equal to unity. In other words, the dependence structure of the vectors X and Z is characterized by the same copula. The latter is termed meta-elliptical, to avoid possible confusion with the elliptical copulas recently introduced and studied by Kurowicka and Cooke (2001), and Kurowicka, Misiewicz and Cooke (2001).

The purpose of this note is to review critically some of the elementary dependence properties of meta-elliptical distributions, mostly in the bivariate case. All measures, concepts and orders of dependence to be considered here are defined in terms of the distribution's underlying copula. However, as noted by Joe (1997), Nelsen (1999) or Drouet–Mari and Kotz (2001) and references therein, these various notions are invariant under monotone increasing transformations of the components. Thus when comparing two bivariate meta-elliptical copulas with the same scale function g, it will often prove more convenient to work directly from the associated elliptical vectors, whose distribution will only then differ by their value of r, the off-diagonal entry of Σ.

The most common association measures, concepts and stochastic orderings characterizing bivariate dependence are considered in turn in Sections 2–4. Recent results pertaining to tail dependence are also referenced in the concluding section.

Before proceeding, it should be noted that contrary to formulas (2.2)–(2.4) in Fang, Fang and Kotz (2002), the joint density and marginals of an elliptical vector (Z_1, Z_2) with scale function g and matrix

$$\Sigma = \begin{pmatrix} 1 & r \\ r & 1 \end{pmatrix}$$

are given respectively by

$$h(x, y) = \frac{1}{\sqrt{1 - r^2}} g\left(\frac{x^2 + y^2 - 2rxy}{1 - r^2}\right) \tag{1.1}$$

and

$$F(z) = \begin{cases} \displaystyle\int_{z^2}^{\infty} \arccos\left(-z/\sqrt{t}\right) g(t)dt & \text{for } z \leq 0, \\[3mm] 1 - \displaystyle\int_{z^2}^{\infty} \arccos\left(z/\sqrt{t}\right) g(t)dt & \text{for } z > 0. \end{cases} \tag{1.2}$$

Note also that $r = \text{corr}(Z_1, Z_2)$ whenever the latter exists, that is, when $\int_0^\infty tg(t)dt < \infty$.

2. Measures of association

The two most common nonparametric measures of dependence are Spearman's rho and Kendall's tau. In dimension $p = 2$, their respective values can either be expressed as

$$\rho = 12 \, \text{E}\{K_1(X_1)K_2(X_2)\} - 3 \quad \text{and} \quad \tau = 4 \, \text{E}\{K(X_1, X_2)\} - 1$$

in terms of expectations involving the pair (X_1, X_2) with joint distribution K and marginals K_1 and K_2, or equivalently as

$$\rho = 12 \, \text{E}\{F(Z_1)F(Z_2)\} - 3 \quad \text{and} \quad \tau = 4 \, \text{E}\{H(Z_1, Z_2)\} - 1$$

in terms of the transformed variables $Z_i = F^{-1}\{K_i(X_i)\}$ with joint cumulative distribution function H and common marginal F.

Fang, Fang and Kotz (2002) show that

$$\tau = \frac{2}{\pi} \arcsin(r)$$

is independent of g. This result is reported also by Lindskog, McNeil and Schmock (2001) and Frahm, Junker and Szimayer (2003). Curiously, however, these various authors omit to mention that

$$\tau = 4 \, \text{P}\left(Z_1 \leq 0, Z_2 \leq 0\right) - 1$$

also corresponds to Blomqvist's medial correlation coefficient, since the median of F is zero. These observations extend at once to any bivariate marginal from a multivariate meta-elliptical distribution.

In contrast, ρ generally depends on both g and r. Indeed, a simple change of variables yields

$$\rho = 12 \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} F(x) F\left(xr + y\sqrt{1-r^2}\right) g\left(x^2 + y^2\right) dy dx - 3.$$

Note that while this formula does involve F, as stated by Fang, Fang and Kotz (2002), the dependence of ρ on this marginal distribution is only apparent, as the latter is entirely determined by g through (1.2).

Closed-form expressions for ρ rarely seem possible. A well-known exception is the bivariate normal distribution, for which Kruskal (1958) established that $\rho = 6 \arcsin(r/2)/\pi$. See Hult and Lindskog (2002) for another example of explicit calculation.

For fixed scale function g, it is obvious that τ is a continuous, strictly increasing function of r that ranges from -1 to 1. To show that ρ enjoys the same properties, one can call on the continuity of F and Lebesgue's Dominated Convergence Theorem; its strict monotonicity follows from Proposition 1.4, to be established in Section 4.

The extreme cases where $r = \pm 1$ describe situations of perfect functional dependence, namely Fréchet's upper and lower bound; one then has $\tau = \rho = \pm 1$. It is important, however, to realize that $r = 0$ does *not* correspond to stochastic independence, except in the meta-Gaussian case.

PROPOSITION 1.1 *If (X_1, X_2) is a meta-elliptical random pair with scale function g and dependence parameter r, then*

$$\rho(X_1, X_2) = \tau(X_1, X_2) = 0 \Leftrightarrow r = 0.$$

Furthermore if X_1 and X_2 are independent, then $g(t) = e^{-t/2}/(2\pi)$.

Proof. That $\tau(X_1, X_2) = 0 \Leftrightarrow r = 0$ is immediate from the formula for Kendall's tau. Furthermore, stochastic independence between X_1 and X_2 implies $\tau = r = 0$, in which case it follows from Lemma 5 of Kelker (1970) that the variables $Z_i = F^{-1}\{K_i(X_i)\}$ are Gaussian.

Now when $r = 0$, the pairs $(\pm Z_1, \pm Z_2)$ all have the same joint distribution, whose common marginal F is also symmetric with respect to the origin. Thus if Z_1', Z_2' are independent observations from F, one has

$$P\left(Z_1' \le Z_1, Z_2' \le Z_2\right) = P\left(\epsilon_1 Z_1' \le \epsilon_1 Z_1, \epsilon_2 Z_2' \le \epsilon_2 Z_2\right)$$

with $\epsilon_1, \epsilon_2 \in \{-1, 1\}$. Since the probabilities of the four possible events on the right sum up to one, it follows that

$$E\{F(Z_1)F(Z_2)\} = P\left(Z_1' \le Z_1, Z_2' \le Z_2\right) = 1/4$$

and hence $\rho = 0$.

To establish the reverse implication, observe that if $\rho(r_0) = 0$ held true for some $r_0 > 0$, say, one would then have $\rho(r) \equiv 0$ on $[0, r_0]$, contradicting the strictly increasing nature of Spearman's rho as a function of r, for fixed g. □

Because it is based on a symmetry property of elliptically contoured vectors with $r = 0$, the chain of implications in Proposition 1.1 can be verified for other copula-based measures of association such as Gini's coefficient or the asymmetric and symmetric versions of Blest's index of association, respectively studied by Blest (2000) and Genest and Plante (2003). Although these additional nonparametric measures of association cannot be expressed explicitly, they too are increasing in r and sweep all degrees of dependence between -1 and 1.

3.   Concepts of dependence

In the classical work of Lehmann (1966), the weakest notion of association between the components of a random pair (X_1, X_2) with distribution K and marginals K_1 and K_2 is that of positive quadrant dependence. This condition, which is met whenever $K(x, y) \geq K_1(x) K_2(y)$ for all $x, y \in \mathbb{R}$, guarantees that ρ, τ and the other above-mentioned nonparametric measures of dependence are non-negative.

A stronger notion, alternatively called monotone regression dependence or stochastic monotonicity of X_2 in X_1, requires $P(X_2 > y | X_1 = x)$ to be increasing in x for every fixed value of $y \in \mathbb{R}$. However, the most stringent condition considered by Lehmann (1966) is likelihood ratio dependence, which is verified if K is absolutely continuous and if its density k is TP_2 in the sense of Karlin (1968), namely

$$k\left(x, y'\right) k\left(x', y\right) \leq k\left(x, y\right) k\left(x', y'\right) \tag{1.3}$$

for all $x \leq x'$ and $y \leq y'$. The latter requirement implies monotone regression dependence, but also several other notions of dependence, such as association, left-tail decreasingness, right-tail increasingness, etc.

In their paper, Fang, Fang and Kotz (2002) claim that every pair of meta-elliptically contoured random variables with $r \geq 0$ is likelihood ratio dependent. As the property is really an attribute of the copula associated with K, their Theorem 3.3 amounts to saying that the density (1.1) of any absolutely continuous elliptical vector (Z_1, Z_2) should satisfy condition (1.3). This is well known to hold true in the bivariate Gaussian case; see Rüschendorf (1981) for a multivariate extension of this result. Unfortunately, the claim turns out to be *false* in general, as stated next.

PROPOSITION 1.2 *Assume that an elliptically contoured distribution has a scale function g such that $\phi(t) = \log\{g(t)\}$ is twice differentiable. In*

order that this elliptically contoured distribution be likelihood ratio de-
pendent for a given $r \in [0, 1)$, *it is necessary and sufficient that* $\phi''(t) = 0$
whenever $\phi'(t) = 0$ *and that*

$$-\frac{r}{1+r} \leq \inf_{t \in T} \frac{t\phi''(t)}{\phi'(t)} \leq \sup_{t \in T} \frac{t\phi''(t)}{\phi'(t)} \leq \frac{r}{1-r},$$

where $T = \{t \in \mathbb{R}_+ : \phi'(t) < 0\}$. *In particular, if this elliptically*
contoured distribution is likelihood ratio dependent for $r = 0$, *then it is*
Gaussian.

Proof. If h denotes the density of the elliptically contoured distribution
with scale function g and dependence parameter $r \geq 0$, the assumed
conditions on ϕ imply that property (1.3) holds true if and only if

$$\frac{\partial^2}{\partial x \partial y} \log \{h(x, y)\} \geq 0$$

everywhere on $\mathbb{R}^2$. Introduce the change of variables

$$x = \sqrt{t}\sin(\theta), \quad \frac{y - rx}{\sqrt{1 - r^2}} = \sqrt{t}\cos(\theta),$$

so that $(x^2 + y^2 - 2rxy)/(1 - r^2) = t$. The condition on h is then satisfied
if and only if

$$2\cos\theta\left(\sqrt{1 - r^2}\sin\theta - r\cos\theta\right)t\phi''(t) \geq r\phi'(t) \qquad (1.4)$$

for every $t \in \mathbb{R}_+$ and $\theta \in [0, 2\pi]$. Letting $r = \sin\alpha$ for some $\alpha \in [0, \pi/2)$,
and in view of the trigonometric identity

$$\cos\theta\left(\sqrt{1 - r^2}\sin\theta - r\cos\theta\right) = \cos\theta\sin(\theta - \alpha),$$

one may then reexpress (1.4) in the form

$$2\cos\theta\sin(\theta - \alpha)t\phi''(t) \geq r\phi'(t), \qquad (1.5)$$

which again must be valid for every $t \in \mathbb{R}_+$ and $\theta \in [0, 2\pi]$.

Now it is easy to check that $A_r(\theta) \equiv 2\cos\theta\sin(\theta - \alpha)$ takes all possi-
ble values in the interval $[-1 - r, 1 - r]$ as θ varies in $[0, 2\pi]$. In particular
if $r = \alpha = 0$, it follows at once that $\phi''(t) = 0$ for all $t > 0$, because this
is the only way that the left-hand side of (1.5) can be non-negative for
all choices of θ. Accordingly, one then has $\phi(t) = -at + b$ and hence
$g(t) \propto e^{-at}$ for some $a \in \mathbb{R}_+$, which entails that h is Gaussian.

Next, for fixed $r \in (0,1)$, letting $\theta = \alpha$ in (1.5) shows that $\phi'(t)$ is necessarily non-positive on its entire domain. Consequently, the condition on ϕ is met if and only if $\phi''(t) = 0$ whenever $\phi'(t) = 0$ and, in addition,

$$A_r(\theta) \frac{t\phi''(t)}{\phi'(t)} \leq r$$

for all $t \in T$, which may be reformulated as in the statement of the proposition. $\qquad\square$

As an illustration, take $g(t) \propto \exp(-\beta t^\alpha)$ with $\alpha, \beta \in \mathbb{R}_+$. Then $t\phi''(t)/\phi'(t) = \alpha - 1$. The elliptically contoured distribution generated by g is thus likelihood ratio dependent whenever $r \geq \max(1 - 1/\alpha, 1/\alpha - 1)$ and $r \neq 0$, which can happen only when $\alpha > 1/2$. As another example, note that when $g(t) \propto t^{\gamma - 1} \exp(-\beta t^\alpha)$ with $\alpha, \beta, \gamma \in \mathbb{R}_+$, and $\gamma \neq 1$, the corresponding Kotz-type elliptically contoured distribution is not likelihood ratio dependent for any $r \in [0,1)$, since $\lim_{t \to 0} t\phi''(t)/\phi'(t) = -1 < -r/(1+r)$ for any such value of r.

The following result represents a strengthening of Proposition 1.2 in the special case where $r = 0$.

PROPOSITION 1.3 *If an elliptically contoured distribution is positive quadrant dependent at $r = 0$, then it is Gaussian.*

Proof. It was observed earlier (see the proof of Proposition 1.1) that when $r = 0$, the four pairs $(\pm Z_1, \pm Z_2)$ have the same distribution. Thus in particular

$$
\begin{aligned}
H(x,y) &= \mathrm{P}\left(Z_1 \leq x, Z_2 \leq y\right) \\
&= \mathrm{P}\left(-Z_1 \leq x, Z_2 \leq y\right) = F(y) - H(-x,y)
\end{aligned}
$$

for arbitrary $x, y \in \mathbb{R}$, so that if the pair (Z_1, Z_2) is positive quadrant dependent, then

$$
\begin{aligned}
F(x)F(y) &\leq H(x,y) = F(y) - H(-x,y) \\
&\leq F(y) - F(-x)F(y) = F(x)F(y),
\end{aligned}
$$

whence $H(x,y) = F(x)F(y)$ for all $x, y \in \mathbb{R}$. In other words, Z_1 and Z_2 are independent and hence Gaussian by Lemma 5 of Kelker (1970). $\quad\square$

The identification of general conditions under which meta-elliptical copulas are positive quadrant dependent poses an interesting challenge. Until this open problem has been solved, caution should be exerted in modelling association with structures of this sort. For fixed scale function g, it will nevertheless be seen below that the association parameter

r orders meta-elliptical distributions by their relative degree of dependence, as characterized by various stochastic orderings. These facts may serve to justify the use of meta-elliptical distributions in robustness and power studies.

4.   Stochastic orderings

Two random vectors X and X^* with respective joint distributions K and K^* and the same univariate marginals are said to be ordered by a dependence ordering $\prec$ whenever the relation $X \prec X^*$ implies that the degree of association among the components of X^* is higher than between the components of X. Generally, $\prec$ reduces to a concept of positive dependence when K is the product of the marginals.

In dimension $p = 2$, the standard extension of Lehmann's notion of monotone regression dependence is the ordering $\prec_1$ of Yanagimoto and Okamoto (1969). Let $K_x(y) = \mathrm{P}(X_2 \leq y | X_1 = x)$ and write $K_{x',x} = K_{x'} \circ K_x^{-1}$. Define K_x^* and $K_{x',x}^*$ *mutatis mutandis* for another pair (X_1^*, X_2^*) with distribution K^* having the same marginals as K. Following Capéraà and Genest (1990), $(X_1, X_2) \prec_1 (X_1^*, X_2^*)$ if and only if the implication

$$x \leq x' \Rightarrow K_{x',x}^*(u) \leq K_{x',x}(u) \tag{1.6}$$

is valid for all $u \in (0,1)$. The choice of marginals is immaterial, so long as they are the same for both distributions. As it is actually the copulas that are being compared through $\prec_1$, the relation $X \prec_1 X^*$ implies that $\rho \leq \rho^*$ and $\tau \leq \tau^*$, and likewise for the indices of Gini, Blest (2000) or Genest and Plante (2003), among others.

It is a simple matter to see that if two meta-elliptical distributions correspond to the same scale function g, they are then ordered by their parameter r in Yanagimoto and Okamoto's relation $\prec_1$. Equivalently, one has the following result.

PROPOSITION 1.4 *Let (Z_1, Z_2), (Z_1^*, Z_2^*) be observations from two elliptically contoured distributions with the same scale function g but different parameters r and r^*, respectively. Then $(Z_1, Z_2) \prec_1 (Z_1^*, Z_2^*) \Leftrightarrow r \leq r^*$.*

Proof. Introduce

$$L_x(y) = \int_{-\infty}^y g\left(x^2 + t^2\right) dt \Big/ \int_{-\infty}^\infty g\left(x^2 + t^2\right) dt,$$

which is nothing but the cumulative distribution function of Z_2 given $Z_1 = x$ when $r = 0$. Note that more generally,

$$H_x(y) = \mathrm{P}\left(Z_2 \le y | Z_1 = x\right) = L_x\left(\frac{y - rx}{\sqrt{1 - r^2}}\right),$$

so that

$$H_{x',x}(u) = H_{x'}\left\{H_x^{-1}(u)\right\} = L_{x'}\left\{L_x^{-1}(u) + (x - x')q(r)\right\}$$

with $q(r) = r/\sqrt{1 - r^2}$. Implication (1.6) is then immediate from the fact that $q(r)$ is monotone increasing on $(0, 1)$.   □

As a consequence of this proposition, meta-elliptical distributions H_r generated by the same scale function g are ordered by their values of r in the positive quadrant dependence ordering $\prec_0$, defined by $H \prec_0 H^*$ if and only $H(x, y) \le H^*(x, y)$ for all $x, y \in \mathbb{R}$. Thus if $r \le r^*$, one has $H_r \le H_{r^*}$ and hence by Hoeffding's identity,

$$\rho(r^*) - \rho(r) = 12 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left\{H_{r^*}(x, y) - H_r(x, y)\right\} dF(y) dF(x) \ge 0,$$

with equality if and only if $r = r^*$, which shows the strict increasingness of ρ as a function of r.

In Capéraà and Genest (1990), a stronger ordering than $\prec_1$ was proposed which extends the notion of likelihood ratio dependence to the comparison of two arbitrary copulas. Specifically, write $(Z_1, Z_2) \prec_3 (Z_1^*, Z_2^*)$ if and only if

$$J(u) = \left(x' - x\right) \frac{d}{du} H_{x',x}^*(u) \Big/ \frac{d}{du} H_{x',x}(u)$$

is increasing in u for all choices of $x, x' \in \mathbb{R}$. These authors showed, among others, that Gaussian distributions are ordered in $\prec_3$ by their correlation coefficient. The following result extends their finding to meta-elliptical distributions under mild conditions on the scale function g.

PROPOSITION 1.5 *Let (Z_1, Z_2), (Z_1^*, Z_2^*) be observations from two elliptically contoured distributions with the same scale function g but different parameters r and r^*, respectively. Further assume that g is twice differentiable, decreasing and log-concave. Then $(Z_1, Z_2) \prec_3 (Z_1^*, Z_2^*) \Leftrightarrow r \le r^*$.*

Proof. It follows at once from the definitions of $H_{x',x}$ and $H_{x',x}^*$ that

$$J(u) = \left(x' - x\right) \frac{g\left[(x')^2 + \left\{(x - x')\,q(r^*) + L_x^{-1}(u)\right\}^2\right]}{g\left[(x')^2 + \left\{(x - x')\,q(r) + L_x^{-1}(u)\right\}^2\right]}.$$

Thus if $\Delta = x' - x$, $s = x'$, $t = L_x^{-1}(u) - \Delta q(r^*)$ and $q = q(r^*) - q(r) \geq 0$, what needs to be shown is that

$$\Delta \, \frac{g\left(s^2 + t^2\right)}{g\left\{s^2 + (t + \Delta q)^2\right\}}$$

is increasing in t for every Δ and s. Equivalently, one must check that

$$\Delta(t + \Delta q) \, \frac{g'\{s^2 + (t + \Delta q)^2\}}{g\{s^2 + (t + \Delta q)^2\}} \leq \Delta t \, \frac{g'(s^2 + t^2)}{g(s^2 + t^2)}$$

for fixed $q \geq 0$ and arbitrary s, t, Δ. Since $(t + \Delta q) - t$ is of the same sign as Δ, the conclusion clearly obtains if

$$t \, \frac{g'(s^2 + t^2)}{g(s^2 + t^2)}$$

is decreasing in t for arbitrary s. As this is guaranteed by the log-concavity and decreasingness of g, the argument is complete.   □

The conditions of Proposition 1.5 seem close to minimal. It is easy to check, for example, that the bivariate Cauchy distributions, which are generated by the log-convex function $g(t) \propto (1 + t)^{-3/2}$, are not ordered by their values of r in the $\prec_3$ relation.

Naturally, the assumptions that g is twice differentiable, decreasing and log-concave also imply that as r increases, an observation from (Z_1, Z_2) from a meta-elliptical distribution becomes more and more left-tail decreasing and right-tail increasing, in the sense given to those orderings by Avérous and Dortet–Bernadet (2000). This is because their orders, like those denoted $\prec_{2-}$ and $\prec_{2+}$ by Capéraà and Genest (1990), are intermediate between $\prec_1$ and $\prec_3$.

Recently, Genest and Verret (2002) showed that bivariate Gaussian distributions are ordered by an even stronger relation than $\prec_3$ due to Kimeldorf and Sampson (1987). It would be interesting to know whether this property is shared by other meta-elliptical families of distributions.

5.   Discussion

In years past, elliptically contoured distributions have proved a useful alternative to the multivariate Gaussian paradigm, not only in statistics, but in several areas of applications such as actuarial science, economics and finance. They have played a prominent role, notably in robustness studies and in modelling multidimensional populations with heavy tails and dependent extreme values.

It is only natural that similar applications should jump to mind for the class of meta-elliptical distributions introduced by Fang, Fang and

Kotz (2002). Among their advantages are the facts that for fixed scale function g: (i) they can have arbitrary marginals; (ii) they cover all possible degrees of association (as measured by Kendall's tau, say); and (iii) variations in the parameter r are consistent with the monotone regression dependence relation $\prec_1$ and (subject to appropriate conditions on g) with the stronger ordering $\prec_3$.

There are, however, two serious limitations to modelling association with meta-elliptical copulas. First, no value of r corresponds to independence, unless the copula is actually that of the normal. Second, except in that special meta-Gaussian case or in the conditions of Proposition 1.2, it is not entirely clear under which circumstances elliptically contoured structures of association meet the concept of positive quadrant dependence. Yet, the latter represents a bare minimum in many applications.

To illustrate this point, consider a vector $X = (X_1, \ldots, X_p)$ of insurance claim amounts and their total $S = X_1 + \cdots + X_p$. One common measure of the portfolio's riskiness is given by the stop-loss premium

$$\pi(S, d) = \mathrm{E}\{\max(0, S - d)\}, \quad d \geq 0.$$

Given marginal distributions $K_1, \ldots, K_p$ and two possible dependence structures C and C^* for the vector X, Müller (1997) showed that the stop-loss premiums may be ordered for all retention amounts $d \geq 0$, provided that the two copulas are ordered in the supermodular ordering $\prec_{\mathrm{SM}}$. Specifically, one has $C \prec_{\mathrm{SM}} C^*$ if and only if

$$\mathrm{E}_C\{\varphi(X)\} \leq \mathrm{E}_{C^*}\{\varphi(X)\}$$

holds true for all supermodular functions φ for which both expectations exist (for twice differentiable functions φ, supermodularity is equivalent to the condition that $\partial^2\varphi(x_1, \ldots, x_p)/\partial x_i \partial x_j \geq 0$ for all $i \neq j$). However if C stands for the independence copula and $p = 2$, $C \prec_{\mathrm{SM}} C^*$ could not possibly hold true unless C^* is at least positive quadrant dependent. Thus if actuaries chose to model the dependence between insurance contracts using a meta-elliptical distribution, they could not tell offhand whether the total loss associated with this portfolio is smaller or larger than under mutual independence of the risks.

As a second example, suppose that amounts $\alpha_1, \ldots, \alpha_p$ have been invested in $p \geq 2$ dependent assets. Let $X_1, \ldots, X_p$ and $X_1^*, \ldots, X_p^*$ represent their returns under two stochastic models with possibly different marginals but the same underlying copula structure C. Müller and Scarsini (2001) show that if C is conditionally increasing and $\pi(X_i, d) \leq \pi(X_i^*, d)$ for every $d \geq 0$ and $i \in \{1, \ldots, p\}$, then

$$\pi\left(\sum_{i=1}^{p}\alpha_i X_i, d\right) \leq \pi\left(\sum_{i=1}^{p}\alpha_i X_i^*, d\right)$$

uniformly in $d \geq 0$. Equivalently, if $\mathrm{E}\{\varphi(X_i)\} \leq \mathrm{E}\{\varphi(X_i^*)\}$ for every $i \in \{1, \ldots, p\}$ and every convex function φ for which these expectations exist, then also

$$\mathrm{E}\left\{\varphi\left(\sum_{i=1}^{p}\alpha_i X_i\right)\right\} \leq \mathrm{E}\left\{\varphi\left(\sum_{i=1}^{p}\alpha_i X_i^*\right)\right\}$$

with φ any convex utility function.

In view of the work of Karlin and Rinott (1980), conditional increasingness of a $p-$variate copula C is verified as soon as it is absolutely continuous with density c such that

$$c(x)c(y) \leq c(x \wedge y)c(x \vee y)$$

for all $x, y \in \mathbb{R}^p$. Here, $\wedge$ and $\vee$ refer to the componentwise minimum and maximum operators. The latter concept, termed multivariate total positivity of order two, reduces to (1.3) in dimension $p = 2$. As mentioned before, it holds true for the Gaussian distribution but *contra* Theorem 3.3 of Fang, Fang and Kotz (2002), it is not generally verified for other meta-elliptical distributions. Proposition 1.2 delineates conditions under which it is.

Another attractive feature of the class of meta-elliptical distributions is the fact that some of its members exhibit tail dependence, in the sense given to that term in Chapter 2 of the book by Joe (1997). It is this property of the multivariate Student and generalized hyperbolic distributions that motivated Frey, McNeil and Nyfeler (2001) to use them in modelling credit portfolio losses.

In dimension $p = 2$, a pair (X_1, X_2) with marginals K_1 and K_2 is said to exhibit (upper) tail dependence whenever the index

$$\lambda = \lim_{u \to 1} \mathrm{P}\left\{X_2 > K_2^{-1}(u) | X_1 > K_1^{-1}(u)\right\}$$

is well defined and strictly positive. For meta-elliptical vectors, this copula-based property is equivalent to the condition

$$\lambda = \lim_{z \to \infty} \mathrm{P}\left(Z_2 > z | Z_1 > z\right) > 0$$

where as before, $Z_i = F^{-1}\{K_i(X_i)\}$, $i = 1, 2$. Schmidt (2002) recently showed that this behavior is induced by a property of regular variation

(at infinity) of the scale function g. Namely if there exists $\beta > 0$ such that

$$\lim_{t \to \infty} \frac{g(xt)}{g(t)} = x^{-1-\beta/2}$$

for all $x > 0$, then

$$\lambda = \int_0^{\sqrt{(1+r)/2}} \frac{t^\beta}{\sqrt{1-t^2}} \, dt \Big/ \int_0^1 \frac{t^\beta}{\sqrt{1-t^2}} \, dt.$$

See Schmidt (2002) for a formulation and proof of this result in arbitrary dimension p. Note that a typographical error in his final expression (he writes $t^2 - 1$ instead of $1 - t^2$ under the two square roots) is repeated by Frahm, Junker and Szimayer (2003), who give alternative expressions and illustrations in special cases. Refer also to Abdous, Fougères and Ghoudi (2005) for a more general study of the asymptotic behavior of the conditional distribution of one component on the other in a bivariate meta-elliptical distribution.

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Chapter 2

THE STATISTICAL SIGNIFICANCE OF PALM BEACH COUNTY

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Abstract   This paper emphasizes certain issues and problems that arise when a
statistical analysis must be undertaken on complex and evolving data,
under tight constraints of time. In such circumstances, it typically is
not possible to develop extensive or problem-specific methodology, yet
an answer may be required almost immediately, and must be correct,
defensible, understandable, and carry impact. It must also be able to
withstand the test of comparison with analyses yet to come.

   We illustrate these points by presenting the background to, and an
analysis of, the State of Florida results in the 7 November, 2000 U.S
Presidential elections with emphasis on Palm Beach County. The anal-
ysis we discuss was carried out in the days immediately following that
election. The statistical evidence strongly suggested that the use of
the 'butterfly' ballot in Palm Beach County had resulted in a signifi-
cant number of votes having been counted for presidential candidate Pat
Buchanan which had not so been intended. The design of the 'butterfly'
ballot suggests that many of these votes had likely been intended for the
Democratic candidate Al Gore This confusion was sufficient to affect
the overall outcome of the 2000 U S Presidential election, conferring
the office to George W. Bush, and this result is statistically significant.

1.   Mise en scène

On the evening of Tuesday November 7, 2000, the United States of
America, along with much of the world, found itself in a state of sus-
pended animation as a consequence of an inconclusive outcome to the
U.S. federal election. While history will record the remarkable circum-
stances of that day, and its subsequent consequences, it should be borne
in mind that at the core of these events and ensuing controversies, no
discipline played a more substantive role than Statistics.

By now, some three years later, and almost on the eve of the November 2004 elections, many articles have begun to appear in statistical journals providing substantive analyses of data related to the November 2000 elections. In some of these articles, their authors develop new methodologies and explore their value for the analysis of such data. However, important as such work is, these articles do not (and, of course, do not claim) to capture the situation as it was "on the ground" among statisticians who became involved in the analysis of this evolving data set within its actual context of (punitively severe) "real time". In fact, to have been of any value at all in that election's context, and its legal battles in particular, it is hardly any exaggeration to say that such analyses had necessarily to be completed within a mere matter of days if not hours, and using less than the most comprehensive or most appropriate data possible. In addition, these statistical controversies arose, literally, without any prior warning whatever, and fell upon statisticians who, in many cases, already held previous commitments and could thus make only a portion of their time available for carrying out the required analyses. In short, this was a perfectly typical problem, under entirely typical circumstances, in the real-world arena of statistical practice.

The authors of this article have been involved in forecasting elections, and particularly election night forecasting for Canadian television networks where primary tasks have included 'declaring' candidates of ridings to be 'elected' using statistical algorithms designed to allow such 'calls' to be made as quickly and accurately as possible after the counting of ballots commences, as well as 'declaring' the winning party as quickly as possible, both under appropriately stringent accuracy requirements. It was therefore natural for us to become involved in statistical analysis of the November 2000 elections. In particular, within what were the very real constraints of time (and of our schedules), we analyzed the results of the vote counts in the State of Florida with particular reference to Palm Beach County

It is widely accepted now, and it was clear enough even then, that more than any other among the many peculiarities of that election, it was the use of the 'butterfly ballot' in Palm Beach County that cost Al Gore and the Democratic Party the Presidency of the United States, and it was for that reason that we had focused all our statistical energies on Palm Beach County As is well known, the butterfly ballot used (designed by Palm Beach's subsequently much beleaguered supervisor of elections, Theresa LePore) was found to be confusing by many voters, and it is claimed that this confusion led some voters intending to vote for Al Gore to cast their vote instead for the Reform Party candidate, Pat Buchanan, whose name appeared interveningly and adjacent to

Gore's on the ballot; see Figure 2.1. It is perhaps an understatement to say that the demographics of Palm Beach County were not favourable to a candidate such as Pat Buchanan (even by his own admission); and indeed every published statistical analysis to date has reaffirmed that the total of 3407 votes that were counted for Buchanan in Palm Beach is out of all proportion to what is predicted when reasonable statistical models are applied to patterns occurring in the remaining 66 (out of the total of 67) Florida counties. Furthermore, such models generally indicate that the extent to which the Buchanan vote exceeded the numbers predicted by such models is significantly greater than the final number of 537 votes (out of a total of some 6 million votes) by which the Republicans ultimately carried the State of Florida, thus gaining its 25 electoral seats, and hence — by way of a resulting 4 vote margin of 271 to 267 in the Electoral College — the Presidency of the United States. Thus it seems very highly probable, though of course not conclusively provable, that had a different voting mechanism been used in Palm Beach County, the outcome of the 2000 election would have been different. To resort to linguistic coincidence, what happened in Palm Beach County exemplifies the 'butterfly effect', a term coined by chaos theorists concerned about such matters as the unforecastability of climate over long time horizons due to the chaotic instabilities of the governing physical dynamics and associated equations.
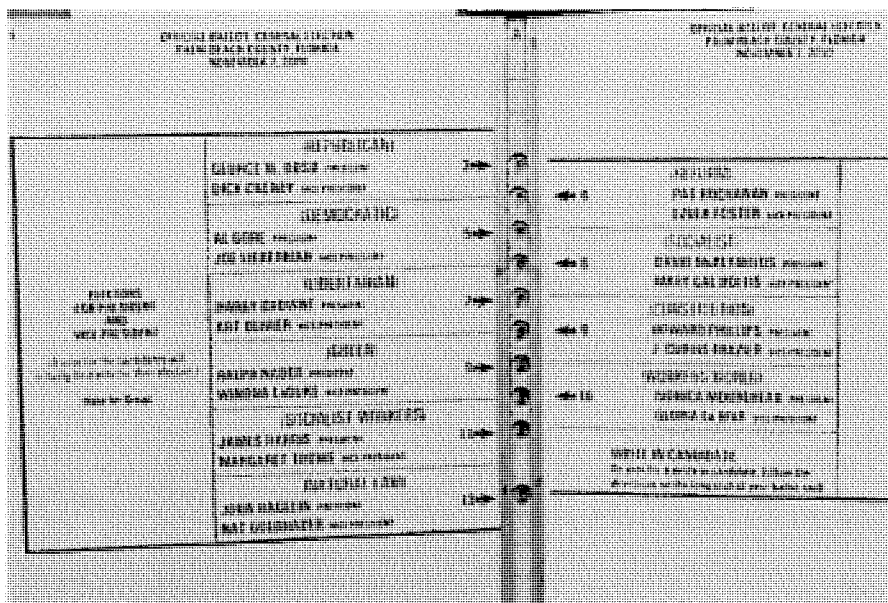
Figure 2.1 The Butterfly Ballot of Palm Beach County.

Of course, what is self-evident to statisticians does not always accord with U.S. constitutional law. Thus it came as a surprise to us, as to many others in the statistical community, although less so to specialists in law, that David Boies and others of the legal team representing Gore and the Democratic Party chose not to pursue Palm Beach's butterfly ballot in the courts. Instead, they pursued the matter of 'overcounts' and 'undercounts' (also known as the issue of 'completely unattached' versus 'hanging' or 'dimpled' chads) and fought to have hand recounts conducted in several counties — a legal battle which pitted statisticians Nicolas Hengartner for Gore against Laurentius Marias for Bush in the Leon County Circuit Court of Judge N. Sanders Sauls. Statistical analyses of state-wide counting issues lead to results which are less categorical and less dramatic; depending upon the exact standards set for counting, they mostly support Gore's position, but in certain instances they support the position of Bush. To quote from the Supreme Court's ultimate decision, "only in very close elections do such matters make a difference. ... upon due consideration ... it is obvious that the recount cannot be conducted in compliance with the requirement of equal protection and due process without substantial additional work"; see Supreme Court (2000). At the end, this matter travelled expeditiously from the Florida Eleventh Circuit Court to the Florida Supreme Court, and finally to the Supreme Court of the United States which -- accepting what it called an "unsought responsibility" — rendered a controversial and deeply divided (five justices in favour, four against) verdict on December 12, 2000, bringing "this agonizingly long election process to a definitive conclusion". The mind-numbing ambiguity which gripped the world for more than a month was thus finally settled under strict protocols of American constitutional law, and George W. Bush was declared elected — the 43rd President of the United States.

Our purpose in writing this article is to emphasize certain issues that arise when a statistical analysis must be undertaken on a set of complex (and rapidly evolving) data under tight constraints of time. No political motive is intended by the authors, and we take no such positions here, other perhaps than supporting notions of reasonable democracy. Of course, it is well known that the *popular* vote went to Al Gore over George Bush by a margin exceeding 500,000 votes nation-wide, but that due to vagaries of the Electoral College system, Bush was the winning candidate. Such discrepancies from 'true' democracy are by no means uncommon. For example, in Canada, there have been many instances (both federally and provincially) in which the party which took leadership by virtue of winning the most ridings was not the party that obtained the highest popular vote. In fact, the allocation of campaign

resources, as well as campaigning strategy, are typically decided by candidates after taking explicit account of election regulations. When viewed in the framework of the Electoral College system, the year 2000 U.S. elections were, in essence, a 'statistical tie' and, however one might define that term, such ties are not unduly rare. Even *exact* ties can occur in many types of elections and must then be broken using one of an imaginative variety of prescribed devices — such as tossing a coin, playing out a hand of poker by tying candidates, or by casting a tie-breaking vote by a prescribed official, to name three. In fact, in 'evenly contested' elections, the occurrence of ties is disproportionately high relative to the inverse of the number of voters. For if n is even and a fair coin is tossed n times, the probability of an exact tie is $2^{-n} \binom{n}{n/2} \approx \sqrt{2/\pi n}$ which scales as $1/\sqrt{n}$.

Returning to our purpose in writing this article, the first point we wish to make is that in typical problems of statistical consultation involving non-trivial data there frequently is not time to develop new and/or problem-specific methodology. An answer may be required immediately, and this generally necessitates using off-the-shelf solutions — more specifically, trusted and familiar statistical routines in familiar software packages. This is not to say there is no role for developing novel methods, but when time is the enemy, they cannot generally be relied upon. (Perhaps there is a modest role to play -- in graduate courses on 'statistical consulting' -- by the statistical equivalent of 'speed-chess'!)

Our second point is that while time may be of essence, and implementation of a 'demonstrably optimal' statistical procedure becomes an unattainable goal, it is nevertheless important for the resulting analysis to be essentially correct. By this we do not mean that statisticians (who after all are human) never make errors. In fact, even the term 'correct' here is ambiguous. The data here were not collected under controlled randomized conditions which lend precise structure to inference. There is no 'true model' underlying data of this type. The most that can be hoped for is to find models having a satisfactory degree of explanatory validity. In this process, experience, some understanding of the phenomena being investigated, as well as availability of an adequate number of experimental units are all invaluable commodities. Here being correct also entails not focusing categorically on only one plausible model, but in fact pursuing all, or as many reasonable models as is feasible. It also entails that a full account be rendered of the true uncertainties of conclusions which stem from uncertainties about the (non-existent) correct model. In this respect, selection of a 'best' model via an 'information' criterion does not provide full information to 'consumers' of the analysis. We posit that it is better, in such circumstances, to present as wide a

variety of reasonably conceived analyses as possible, and allow variations among their results to speak for the true uncertainties inherent in the problem overall.

Indeed, such a collection of analyses contributes to the court of public knowledge and opinion without trivializing or simplifying to the point of what, strictly speaking, becomes untruth. They represent an admission of the real uncertainty which underlies the problem — an admission that there is no single right answer. Such an approach also recognizes that additional analyses will later be carried out by others, using ever more extensive data and more sophisticated models. Hence the analysis will be subject to the scrutiny of future light; there will be a sequence of tests to pass, and any conclusions of the analysis will be subjected to consistency checks against all analyses yet to come.

Our third point is that statistical analyses must sometimes be as straightforward and easy to understand as possible. Statistics is not easy for non-statisticians, and except in instances all too rare, lawyers and judges are not statisticians. Nevertheless they are amongst the decision-making professionals to whom the statistical ideas, analyses, and results need to be explained; and it is often they who, on the basis of their understanding, must make substantive decisions. That some level of complexity is necessarily inherent in an analysis of this type cannot be avoided, but one can avoid going farther than what is required for capturing the essential conclusions, at least insofar as materials 'presented' to such professionals is concerned. In this respect, understandable graphical displays that carry impact are of utmost importance.

This paper contains three additional sections. Section 2 discusses the data set whose analysis is present here. The actual analysis is carried out in Section 3. It is a matter of principle that the analysis we present in Section 3 is exactly as carried out by us in the days immediately after November 7, 2000. We have meticulously avoided embellishing or improving upon our original results or adding any follow-up to that work. It thus appears here 'warts and all' in its entirety. The only exceptions are that the explanatory text has been edited for clarity and context, and that fewer displays are included here in order to keep the length of this paper reasonable and avoid the repetitive display of graphs all having very similar appearance. A significant aspect of the work reported in Section 3 revolved around designing effective, convincing, and statistically accurate graphical displays. Finally, in Section 4, we cite some references to later work that others have done using more substantive data and more complex statistical models. We compare our result to theirs and thereby apply the 'test of time' to the work we had done. Some concluding remarks are also given there.

2.   Description of the data

Immediately following recognition of the crucial importance of the vote in Florida to the outcome of the U.S. federal elections of 7th November, 2000, the ABC Television Network began posting, on its website, a county by county current tabulation of the votes for many of the candidates in that state. Although, in developing our analyses, we first worked with earlier posted versions of these counts, our final analyses were ultimately 'frozen' and based on the data set as posted on the ABC website at 9 am on Sunday, November 12th. This data reflects the votes as tabulated (after the first "recount") of the Florida State ballots. Of course, the nature of the statistical methods we used are such that our results were not expected to vary in any important way under the small subsequent changes to this data that were anticipated to occur under the repetitive recounting of the votes.

The downloaded file was processed to make it suitable for reading into the statistical analysis package S-Plus which was used for our analyses. (See Becker, Chambers and Wilks, 1988.) This processed version of the data file is exhibited as Table 2.1. That table gives a breakdown by county, for all 67 Florida counties, of the number of votes counted (after first "recount") for the four presidential candidates George W. Bush, Al Gore, (Reform Party candidate) Pat Buchanan, and (Green Party candidate) Ralph Nader. The file also gives the number of votes cast for three Senatorial candidates, Bill Nelson, Bill McCollum, and Willie Logan. These Senatorial candidates are respectively Democrat, Republican, and an Independent with central leanings. Several other candidates also ran in both the presidential and the senatorial races but received extremely small vote counts; these were not reported on the ABC website and were not included in our analysis.

3.   The statistical analysis

The analysis we present was based on the seven data variables appearing in Table 2.1, namely the raw vote counts for seven candidates — four presidential, and three senatorial. In addition to these seven variables, two variables can be constructed which are each proxies for 'county size', namely the total number of votes counted for these four presidential candidates in each county, and the total number of votes counted for the three senatorial candidates. Of course, these two county size proxy variables are in nearly perfect correlation. In our analyses, we used the first of these as our actual proxy for 'county size'. We also defined additional variables representing the proportions of votes cast for each of the seven candidates. Presidential candidate proportions were

Table 2.1. Florida Election Results, Raw Data, by County, First Recount

This Data From ABC Website as at 9am Sunday November 12, 2000

COUNTY	PRESIDENT				SENATE		
	GORE	BUSH	BUCHANAN	NADER	NELSON	MCCOLLUM	LOGAN
ALACHUA	47365	34124	262	3215	49005	31003	1733
BAKER	2392	5610	73	53	3104	4578	50
BAY	18850	38637	248	828	22914	33901	358
BRADFORD	3075	5414	65	84	4118	4697	92
BREVARD	97318	115185	570	4470	112255	98813	2304
BROWARD	386561	177323	789	7099	377081	174980	5974
CALHOUN	2155	2873	90	39	2809	2055	31
CHARLOTTE	29645	35426	182	1462	28947	37026	746
CITRUS	25525	29766	270	1379	27566	27025	947
CLAY	14632	41736	186	562	16094	39054	561
COLLIER	29918	60433	122	1400	28207	60508	822
COLUMBIA	7047	10964	89	258	8942	9031	255
DADE	328764	289492	560	5352	304878	264801	11796
DE.SOTO	3320	4256	36	157	3593	3736	127
DIXIE	1826	2697	29	75	2450	2007	36
DUVAL	107864	152098	652	2757	121805	145930	3214
ESCAMBIA	40943	73017	502	1727	45907	67607	771
FLAGLER	13897	12613	83	435	13980	11988	293
FRANKLIN	2046	2454	33	85	2498	2018	31
GADSDEN	9735	4767	39	139	10838	4306	553
GILCHRIST	1910	3300	29	97	2558	2561	46
GLADES	1442	1841	9	56	1649	1620	67
GULF	2397	3550	71	86	3393	2739	42
HAMILTON	1722	2146	23	37	2172	1722	44
HARDEE	2339	3765	30	75	2972	3051	88
HENDRY	3240	4747	22	103	3760	4513	116
HERNANDO	32644	30646	242	1501	32916	29099	1106
HIGHLANDS	14167	20206	127	545	11630	1434	296
HILLSBOROUGH	169557	180760	847	7490	176667	15919	5928
HOLMES	2177	5011	76	91	3201	3252	31
INDIAN.RIVER	19768	28635	105	950	21050	27223	545
JACKSON	6868	9138	102	138	8648	7529	168
JEFFERSON	3041	2478	29	76	3513	2101	139
LAFAYETTE	789	1670	10	26	1299	1175	28
LAKE	36571	50010	289	1459	40726	47333	800
LEE	73560	106141	305	3587	69308	107824	2610
LEON	61425	39053	282	1932	61728	35468	2914
LEVY	5398	6858	67	284	6654	5796	142
LIBERTY	1017	1317	39	19	1375	948	33
MADISON	3014	3038	29	54	3528	2492	69
MANATEE	49177	57952	272	2489	51400	54104	1608
MARION	44665	55141	563	1809	48947	50896	962
MARTIN	26620	33970	108	1075	21826	28065	456
MONROE	16483	16059	47	1090	16588	14778	455
NASSAU	6879	16280	90	253	8489	14413	198
OKALOOSA	16948	52093	267	985	18667	48897	421
OKEECHOBEE	4588	5057	43	131	5320	4410	244
ORANGE	140220	134517	446	3881	140897	119652	3014
OSCEOLA	28181	26212	145	732	29722	23856	624
PALM.BEACH	269696	152954	3407	5564	269835	154528	4385
PASCO	69564	68582	570	3392	73338	63081	2172
PINELLAS	200629	184823	1010	9986	207974	168508	7333

Table 2.1. (cont.) Florida Election Results, Raw Data, by County; First Recount.

This Data From ABC Website as at 9am Sunday November 12, 2000

COUNTY	GORE	PRESIDENT			SENATE		
		BUSH	BUCHANAN	NADER	NELSON	MCCOLLUM	LOGAN
POLK	75197	90196	538	2060	81159	79837	2990
PUTNAM	12102	13447	148	377	13124	11876	304
SANTA.ROSA	12802	36274	311	724	14504	33650	222
SARASOTA	72853	83100	305	4069	71434	80641	2094
SEMINOLE	59174	75677	194	1940	63037	69865	1377
ST.JOHNS	19502	39546	229	1217	20558	37275	930
ST.LUCIE	41559	34705	124	1368	41082	33050	1065
SUMTER	9637	12127	114	306	10271	11384	231
SUWANNEE	4075	8006	108	180	5544	6797	130
TAYLOR	2649	4056	27	59	3431	3386	105
UNION	1407	2332	29	32	1560	11	23
VOLUSIA	97063	82214	396	2436	99135	76033	2554
WAKULLA	3838	4512	46	149	4496	3778	131
WALTON	5642	12182	120	265	6842	10295	115
WASHINGTON	2798	4994	88	93	4065	3661	60

obtained by dividing their vote counts by the first of the vote totals mentioned, while senatorial candidate proportions were obtained by dividing their vote counts by the second of the totals. Finally, we also considered logarithmic transformations in each of these variables in order to obtain variables that more nearly satisfy the assumptions and requirements of the statistical methods we used. Such requirements typically include approximate linearity, constancy of variance, and normality (or at least approximate symmetry, together with tails that are not too heavy) of the model-generated error terms. For example, the logarithms of proportions (especially when small) often have more uniform variability over their range of values than do raw proportions; likewise, logarithms of raw vote counts often give more normally distributed residuals than untransformed values. Some might argue for logits of proportions, but here these are almost identical to logarithms which are more widely understood. Furthermore, positive variables are often described by additive models based on their logarithms. Others might argue for square roots of proportions because this tends to stabilize variance. However, on balance, we felt that linearity was more important here. Discussions on such matters may be found, for example, in Belsley (1980), Cook and Weisberg (1999), Draper and Smith (1998), Mosteller and Tukey (1977), or Myers (1990).

Our choice for dependent variable was governed by the purpose of the analysis, namely, to determine the number of votes for Buchanan attributable to the nature of the ballot in Palm Beach. This is equivalent

to estimating the proportion of such votes. However the number of votes for any candidate in a county is roughly proportional to the number of electors in the county. Because counties vary considerably in the number of electors, the variation in votes is considerably higher than the variation in proportions. Following the general principle of removing known sources of variation, it is more effective for estimating the overvote to use proportions rather than votes.

Voter preferences are determined by many personal factors associated with age, education, income, party affiliation, etc., and by many community factors associated with employment, density, and so on. While data on these were not readily available to us, we do have the effect of voter preferences as shown by votes cast for the other candidates. The proportions of votes for these other candidates act as surrogates for underlying determining variables. For this reason explanatory models were constructed from the proportions of votes for the other candidates. In addition, community size may be associated with other important factors. (Small communities may be more closely knit, and may inspire greater voter participation, for example.) To voter proportions, we added total vote as a surrogate for such variables. Using these variables, we found that the proportion of votes for Buchanan in a county could be reliably predicted from the pattern of votes for other candidates in the counties.

On the basis of these variables, we analyzed a large number of regression models fitted to this data. Our rationale for examining many models was based firstly on our expectation that such data would be subjected to widespread analysis by many others. We therefore chose to report the results of many reasonably selected analyses in the hope of assisting those who would seek to form their own conclusions. Secondly, fitting explanatory variables explains variation leaving less variation in the estimation of error. Hence methods of variable selection can result in error estimates that are biased downward and may thus affect the validity of prediction intervals. (Indeed, this leads to questions of research caliber.) Partly for this reason, we considered instead sets of possible explanatory variables, fitting a sequence of increasingly complex models. We contend that the resulting collection of error estimates provides more information than would the results from variable selection.

In our reporting, all regression analyses were based on a single 'dependent' variable, namely the logarithm of the proportion of votes (county by county) cast for Pat Buchanan. Regression models were fitted for this dependent variable against many plausible combinations of predictor variables. Given a regression model which fits such data in a statistically appropriate way, an estimated vote count for Buchanan can be

obtained from a model-based estimate of the logarithm of the Buchanan proportion, by just exponentiating (to obtain the estimated proportion) and then multiplying by the county vote total (to obtain the estimated Buchanan vote count). Our regression analyses were all based on first removing Palm Beach County from the statistical fitting. Since Florida has 67 counties, our regression fits are all based on 66 (multivariate) observations. For each model we fitted in this way, we obtained the model-based prediction of the number of votes for Buchanan in Palm Beach County. This estimate was then compared to the actual number of 3407 votes counted for Buchanan in Palm Beach. It is the difference between these two numbers that is of essence and the focus of our analysis. To assess the statistical significance of this difference, we obtained (for each model) a prediction interval for the log Buchanan proportion, and transformed this (in the manner indicated above) into a prediction interval for the Buchanan vote count in Palm Beach. These regressions were all based on unweighted, ordinary least squares, and classical statistical prediction intervals having confidence levels of 95%. Appropriate checks were conducted, during the course of this work, to assure that the key requirements for regression analysis were being adequately met.

Three series of regression analyses were carried out. The 'series A' regressions were each based on a single predictor variable, while the 'series B' and 'series C' regressions were each based on two and three predictor variables, respectively. There are a total of 7, 6, and 3 regressions in the 'A', 'B', and 'C' series and they are summarized in Tables 2.2, 2.3, and 2.4 (discussed further below.) The key findings from these analyses were then transformed into a carefully crafted series of figures which we correspondingly labelled as Graphs A1–A7, B1–B6, and C1–C3; these figures are all very similar in overall impact and appearance, and to save space only some of them are reproduced here. However it should be borne in mind that the repetitively similar nature of all 16 figures in itself carries useful information. A substantial amount of our efforts was spent on the design of these displays since we had anticipated that they might be used by non-statisticians, and thus knew that they had to accurately, effectively, and unbiasedly carry the statistically substantive information. The particular displays reproduced here include Graphs A2, A6, B2, B4, C2 and C3. See Figures 2.2–2.4. (The criteria for their inclusion here is explained further below.)

Each of these displays plots the actual Buchanan vote counts on the vertical axis, against the predicted number (i.e. the model-based 'fitted' values) for the Buchanan vote counts on the horizontal axis, for all 67 counties. (The regression fits themselves, of course, excluded Palm Beach.) Note, however, that a logarithmic scale was used for the

horizontal axis. The 67 bullet points on each graph give the actual versus predicted Buchanan vote counts in the counties, and the smooth solid curve represents the regression fit to the data, i.e. the model-based predicted values; it is just the identity line. (Except for the effect of the logarithmic horizontal scale, this curve would be a straight line with height equal to the horizontal axis coordinate at each point.) The 67 vertical line segments represent the model-based *prediction* intervals, each having confidence level 95%, for the Buchanan vote count for each of the counties. As may be discerned, the tops and bottoms of these intervals do not lie along any particular patterns; this reflects the effects of the predictor variables in the models which are not otherwise visible in these graphs. Nevertheless the lengths of the prediction intervals do increase in a reasonably smooth manner with the fitted vote counts for Buchanan. Note that a high proportion of the actual votes for Buchanan (other, of course, than Palm Beach county) fall inside their respective prediction bands. Other indications of the quality of these fits may be obtained by examining typical residual plots; as a general rule, the quality of these fits are all very good. We also experimented with weighted regressions using weights related to the county vote totals (e.g., inverse total votes, or inverse square root of total votes). These results all corroborate the findings presented, but are not included here.

On each of these plots, two arrows are used to help identify the bullet point for Palm Beach county. As is evident from examining the plots, the data point for Palm Beach County is a statistically highly significant outlier in every one of these models. It is possible to determine an approximate two-sided p-value for the Palm Beach County outlier through the following simple device: the prediction interval for Palm Beach County can be enlarged by increasing its significance level until the upper end of the interval just touches the Palm Beach County bullet. The difference between unity and the confidence level of that interval gives the two-sided p-value. (If one were to adopt the viewpoint that the nature of the butterfly ballot could not lead to an *undercount* for the Buchanan vote, then a one-sided p-value could be obtained by taking one half of the two-sided p-value.) Significance levels so computed do not account for any selection effect that might have led to the study of Palm Beach County. However, allowing for such selection bias at most multiplies the significance levels by a factor of 67, and this would still leave our results statistically significant. In this respect, it is also worth noting that Florida had been selected by others for focus because its results were so close, while the selection of counties as the natural unit of aggregation was also made by others.

Table 2 2 Series "A" Regression Results — One Predictor Variable.

Regression Model	Predicted Buchanan	Estimated Overcount	95% Pred. Interval	Minimum Overcount
A1: $\mathcal{L}$Tot	760	2647	(250, 1680)	1727
A2: $\mathcal{L}$Gore	686	2721	(229, 1640)	1767
A3: $\mathcal{L}$Bush	867	2540	(282, 2182)	1225
A4: $\mathcal{L}$Nader	852	2555	(290, 2064)	1343
A5: $\mathcal{L}$Nelson	690	2717	(221, 1695)	1712
A6: $\mathcal{L}$McColl	935	2472	(296, 2423)	984
A7: $\mathcal{L}$Logan	797	2610	(292, 1812)	1595

The regression series A1–A7, B1–B6, and C1–C3 are also summarized in Tables 2.2, 2.3 and 2.4. Table 2.2 gives the results of seven regressions for the dependent variable '$\mathcal{L}$ Buchanan$\mathcal{P}$' (i.e. the logarithm of the proportion of votes cast for Buchanan — see below) each against a single predictor variable, with an intercept term included. In model A1, the predictor variable is the logarithm of the total number of votes cast for all presidential candidates, while models A2–A7 are based on the same 'independent' variable, but modelled, respectively, against the logarithm of the total number of votes for each of the six other candidates (presidential as well as senatorial) appearing in the Table 2.2 (and in the order given in that table): Gore, Bush, Nader, Nelson, McCollum, and Logan. In Table 2.2 (as in Tables 2.3 and 2.4), the first column lists the predictor variables defining the regression. The notations 'Tot', 'Gore', 'Bush', 'Buchanan', 'Nader', 'Nelson', 'McColl', and 'Logan' represent the total (presidential) vote count, and the 7 individual candidate vote counts. When a vote proportion instead of a vote total is used, we indicate this by a suffix $\mathcal{P}$, and when a logarithm is taken we indicate this by a prefix $\mathcal{L}$. Tables 2.3 and 2.4 give the results, respectively, of our regression analyses each using two and three predictor variables, but always the same dependent variable, namely, $\mathcal{L}$ buchanan$\mathcal{P}$. Thus, for example, the row labelled as 'C2' in Table 2.4 gives the results for the regression of $\mathcal{L}$ buchanan$\mathcal{P}$ against the predictor variables $\mathcal{L}$ Tot, Gore$\mathcal{P}$, and Nader$\mathcal{P}$, i.e., against the logarithm of the total vote counts, and the vote proportions for Gore and for Nader. The remaining columns in Tables 2.2, 2.3, and 2.4 respectively give the model-based vote projections for Buchanan in Palm Beach County, the estimated overcount of the vote for Buchanan (obtained by taking the difference between the projection in column 2 and Buchanan's actual count of 3407 votes), 95% prediction intervals for the Buchanan vote, and in the last column, the minimum overcount for Buchanan consistent with these prediction intervals. It may be seen that none of our point predictions for Buchanan's vote

exceeds 1000, with most lying well below this value, and correspondingly, the estimated overcounts all exceed 2400. Further, our *minimum* overcounts are all well above 1000, except for one instance which occurs in one of the single-predictor regressions. At final tally, the official plurality by which the State of Florida was won by Bush amounted to 537 votes. As may be seen, the minimum overcount exceeds this value by a substantial (and significant) margin in every one of these regression models.

Table 2.3. Series "B" Regression Results — Two Predictor Variables.

Regression Model	Predicted Buchanan	Estimated Overcount	95% Pred. Interval	Minimum Overcount
B1: $\mathcal{L}$Gore+$\mathcal{L}$Bush	622	2785	(195, 1503)	1904
B2: $\mathcal{L}$Tot+$\mathcal{L}$Logan$\mathcal{P}$	850	2557	(303, 1939)	1468
B3: $\mathcal{L}$Tot+$\mathcal{L}$Logan	839	2568	(298, 1920)	1487
B4: $\mathcal{L}$Tot+Bush$\mathcal{P}$	616	2791	(192, 1496)	1911
B5: $\mathcal{L}$Nelson+$\mathcal{L}$McColl	697	2710	(215, 1738)	1669
B6: $\mathcal{L}$Logan+$\mathcal{L}$Nader	798	2609	(291, 1824)	1583

Table 2.4. Series "C" Regression Results — Three Predictor Variables.

Regression Model	Predicted Buchanan	Estimated Overcount	95% Pred. Interval	Minimum Overcount
C1: $\mathcal{L}$Tot+$\mathcal{L}$Gore$\mathcal{P}$+$\mathcal{L}$Nader$\mathcal{P}$	663	2744	(201, 1621)	1786
C2: $\mathcal{L}$Tot+Gore$\mathcal{P}$+Nader$\mathcal{P}$	631	2776	(185, 1555)	1852
C3: $\mathcal{L}$Tot+Logan$\mathcal{P}$+Nader$\mathcal{P}$	860	2547	(285, 2036)	1371

Finally, we indicate the criteria by which the Graphs A2, A6, B2, B4, C2 and C3 were selected for inclusion here. The extent to which a figure is visually and statistically 'persuasive' is governed by the distance of the Palm Beach County bullet point from its model predicted value, as measured in units of the width of its prediction band. Thus, within each of the series A, B and C graphs, we selected their most and least persuasive representatives for inclusion here. (Note that the same graphs would have been selected had the criterion been based instead on the minimum overcount values.)

To check that the use of linear models had not hidden important information, tree regressions were fitted to both vote counts and vote proportions. In both cases, the known dependence of variance on size was approximated by weighting these tree regressions by the inverse of the total vote counts. Tree regression fits step functions based on explanatory variables and is not restricted to any assumed linearity. In effect, it groups counties with the same fitted values. See Breiman et al. (1984) for details concerning this procedure.

Graph A2 Palm Beach County Vote Is Out of Line

Graph A6: Palm Beach County Vote is Out of Line

Figure 2.2 Two results of regression analysis (with Palm Beach omitted) for log Buchanan vote percentages, each against a single predictor variable (see text). Intervals shown are level 95% prediction bands for Buchanan's vote in all 67 counties

Graph B2   Palm Beach County Vote is Out of Line

Graph B4· Palm Beach County Vote is Out of Line

Figure 2 3.   Two results of regression analysis (with Palm Beach omitted) for log Buchanan vote percentages, each against two predictor variables (see text). Intervals shown are level 95% prediction bands for Buchanan's vote in all 67 counties.

Graph C2 Palm Beach County Vote is Out of Line
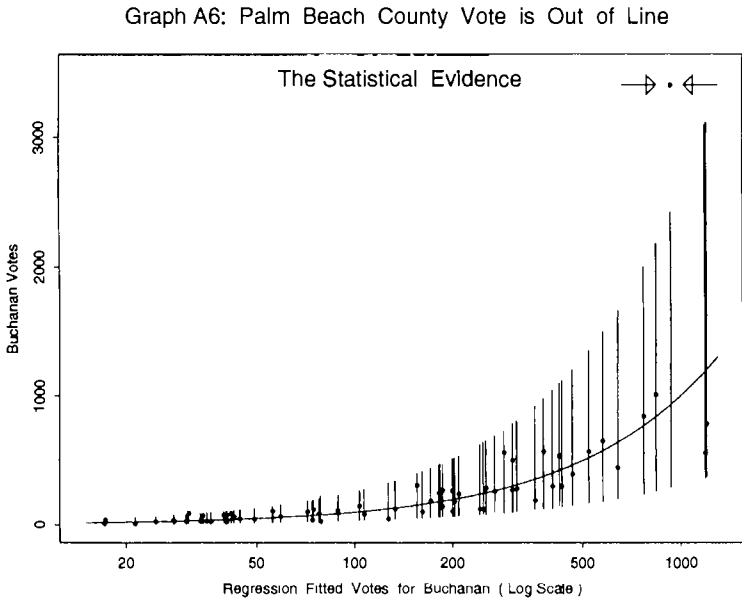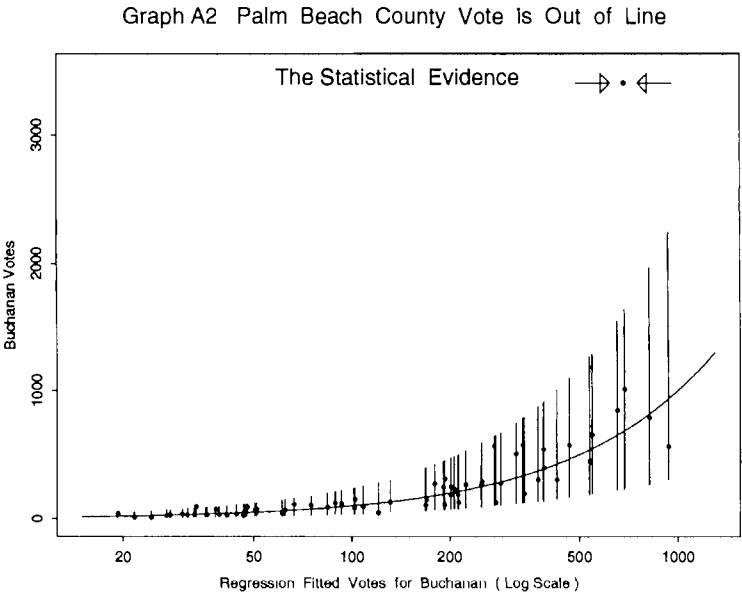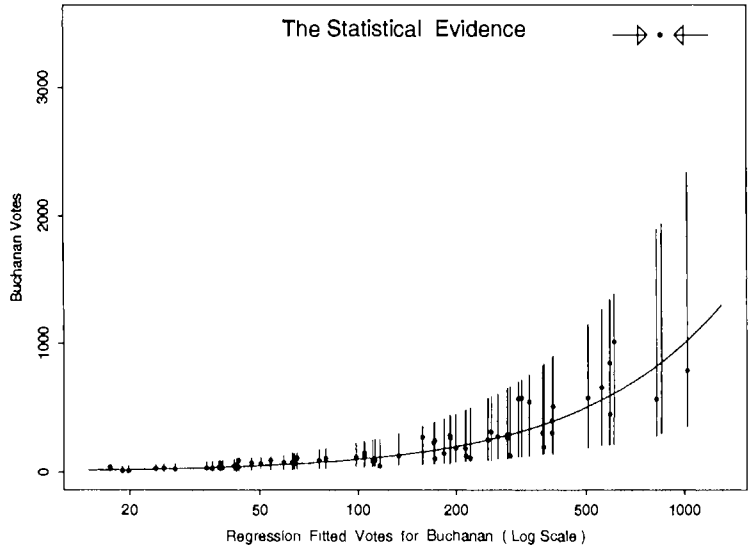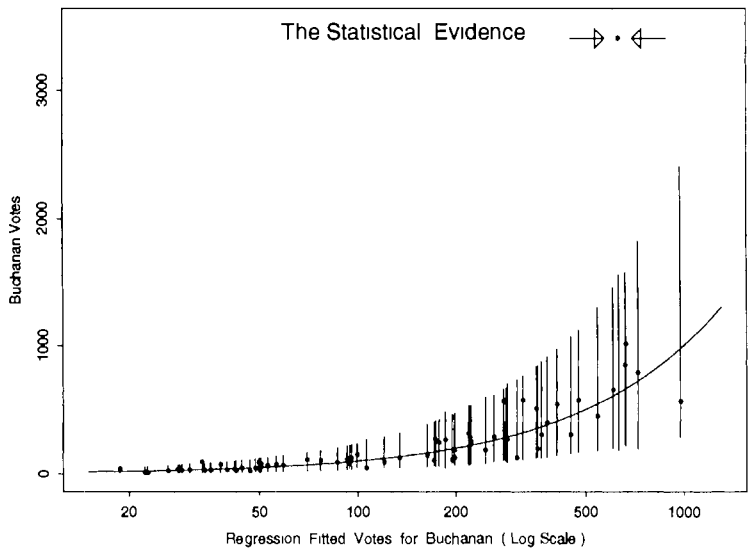

Graph C3 Palm Beach County Vote is Out of Line
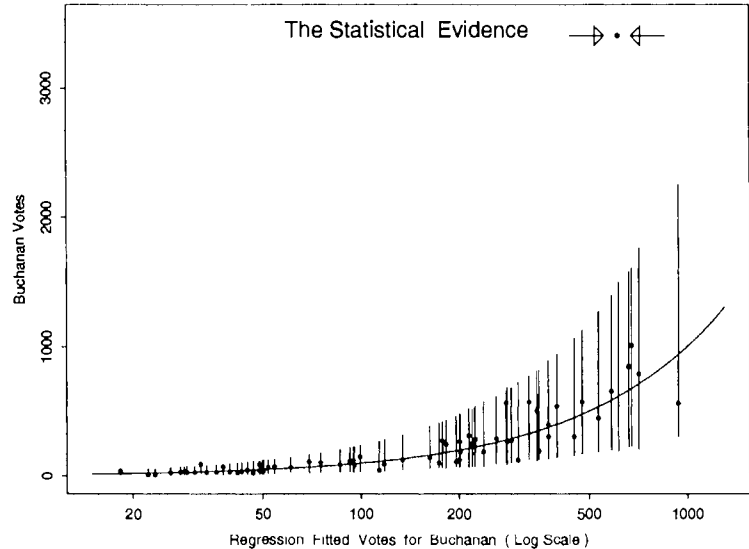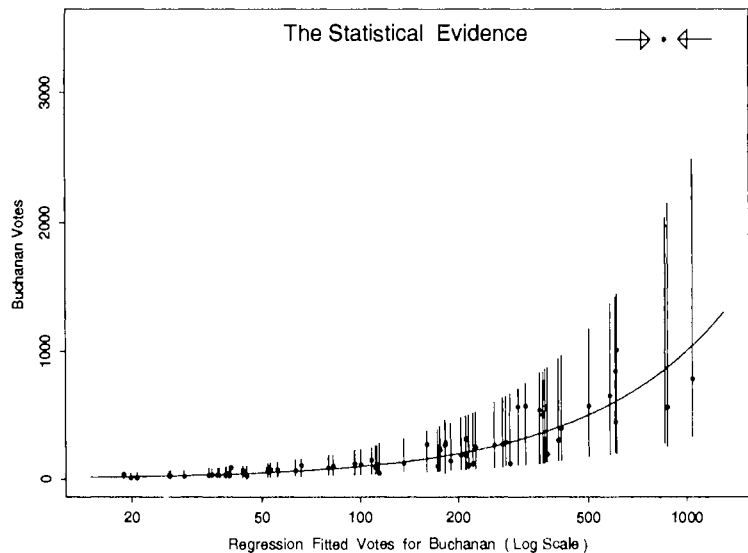

Figure 2 4 Two results of regression analysis (with Palm Beach omitted) for log Buchanan vote percentages, each against three predictor variables (see text) Intervals shown are level 95% prediction bands for Buchanan's vote in all 67 counties

Graphs D1–D6 in Figures 2.5–2.7 show tree regressions using the data from all 67 counties, and predictor variables as indicated in the graph headings. Each plot gives either the average votes or the average proportions for Buchanan for the counties within the identified groups. The trees are displayed together with the splitting values of the explanatory variables. The groups of counties are positioned in the display so that average votes per county increases as one goes from left to right. Examination of the groups to which Palm Beach is assigned shows that even after extensive fitting, Palm Beach stands out with far higher values than other counties in those groups. For example, the plot in Graph D1 identifies one group at the right. This group is formed by those counties with total vote exceeding 97030, and Nader vote exceeding 5458. There are, in fact, 4 such counties. One is Palm Beach which 'gave' 3407 votes to Buchanan, and 3 others whose average Buchanan vote is less than a third of this value. The Buchanan vote in Palm Beach is thus seen to be extreme relative to the 3 other counties having similar voting patters. This unusual behaviour occurs in all of the 6 tree models fitted. The tree regressions show that the apparent unusual nature of Palm Beach County is not an artifact of the nature of a linear model.

While we knew then that further analysis on this (and expanded) data sets should (and no doubt would) be carried out, it was clear — even at that early stage for such analyses — that the votes as counted in Palm Beach County, with very high likelihood, did not reflect the intended votes of those voters. Every reasonable statistical model we had examined indicated a statistically significant overcount for Buchanan in Palm Beach County. It was our conclusion at the time, based on these analyses, that the explanation of this singular 'outlier' cannot rest on factors to which all counties are subject to a greater or lesser degree, but rather must rest on some aspect of the voting peculiar to Palm Beach County. It is widely believed, and we would now concur, that many of the overcounted Buchanan votes were in fact intended for Gore, and were likely misdirected owing to voter confusion with the butterfly ballot that was used in Palm Beach County.

4.   Concluding remarks

As indicated in the introduction, the analyses as presented in the previous section were carried out in the days immediately following the November 2000 elections. Since that time, many other analyses have, as expected, appeared. As examples, we refer the reader to Agresti and Presnell (2001, 2002), Hansen (2003), Smith (2002), Wand et al. (2001), and the references therein.

Graph D1: Classification and Regression Tree of Buchanan Vote Fitted to Total Vote and Votes for Gore, Bush and Nader Weighted by Inverse Total Votes (in 1000's).

End nodes give average Buchanan votes for counties

Graph D2: Classification and Regression Tree of Buchanan Percentage Fitted to Total Vote and Vote Percentages for Gore, Bush, and Nader Weighted by Inverse Total Votes (in 1000's).

End nodes give average Buchanan percentage for counties

Figure 2 5 Classification and regression trees

**Graph D3: Classification and Regression Tree of Buchanan Vote
Fitted to Votes for Gore, Bush, and Nader
Weighted by Inverse Total Votes (in 1000's)**

End nodes give average Buchanan votes for counties

**Graph D4: Classification and Regression Tree of Buchanan Percentage
Fitted to Vote Percentages for Gore, Bush and Nader
Weighted by Inverse Total Votes.**

End nodes give average Buchanan percentage for counties

Figure 2 6   Classification and regression trees

Graph D5: Classification and Regression Tree of Buchanan Vote Fitted to Total Vote and Votes for Gore, Bush, Nader, Nelson, McCollum and Logan Weighted by Inverse Total Votes (in 1000's).

Total< 97 03

McCollum< 6 296   Nader< 5 458

Gore< 2 1   Bush< 29 2   Nelson< 72 39

                                                    1 5

0 025   Logan>=0 0645   0 11   0 22   0 36   0 53

0 037   0 08
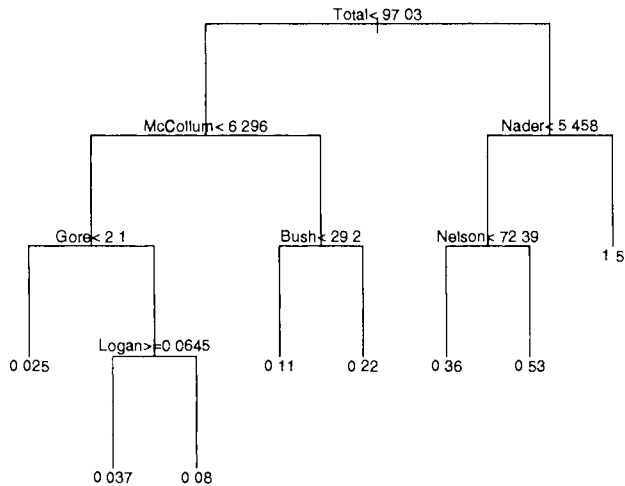
End nodes give average Buchanan votes for counties

Graph D6: Classification and Regression Tree of Buchanan Percentage Fitted to Total Vote and Vote Percentages for Gore, Bush, Nader, Nelson, McCollum and Logan Weighted by Inverse Total Votes (in 1000's).

NaderP>=0 8182

LoganP>=0 7859

                                    1 5

NaderP>=0 8631

                        0 91

LoganP>=1 118

            0 73

NelsonP< 52 5   Total>=22 84

LoganP>=1 72   Total>=13 64   0 3   0 63

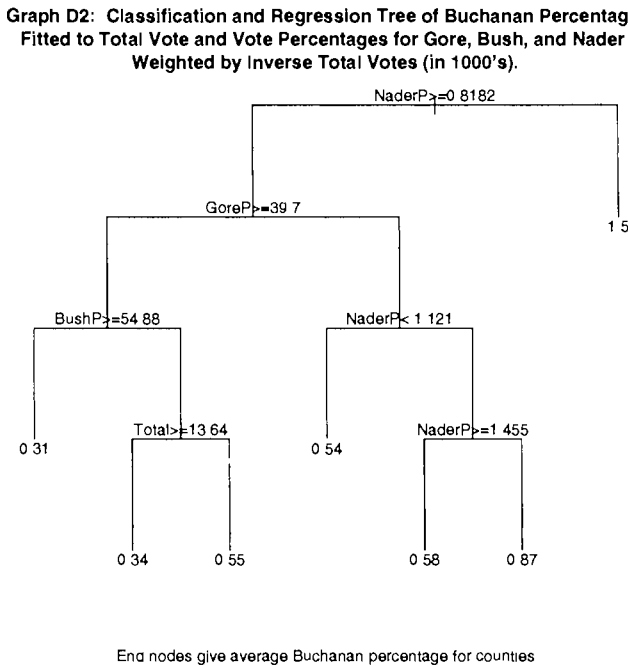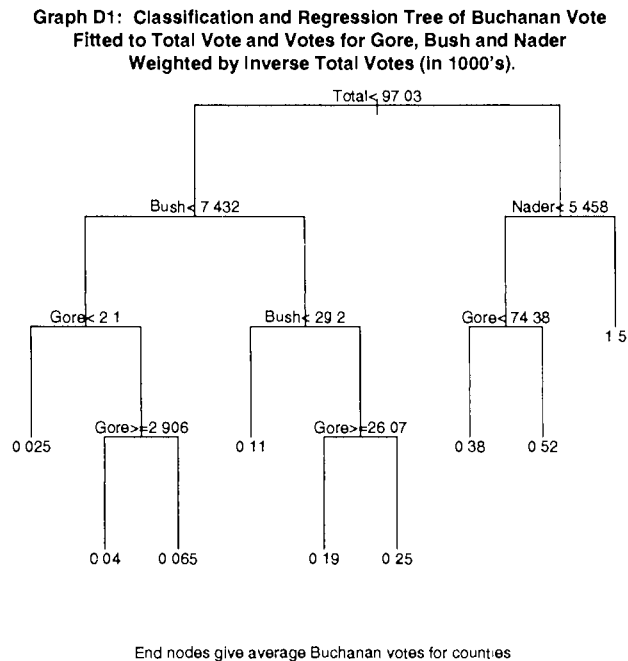0 27   0 4   0 26   0 5
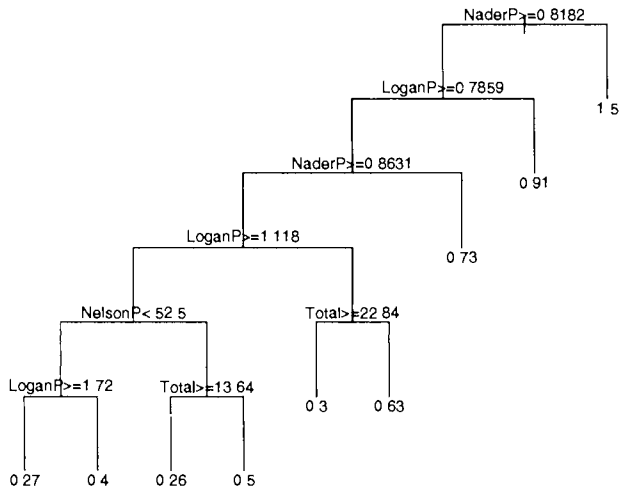
End nodes give average Buchanan percentage for counties

Figure 2.7.   Classification and regression trees.

In particular, Smith (2002) carries out a carefully thought through series of regression analyses based on data which also include the vote counts for Libertarian presidential candidate Browne, but not the votes for 5 other fringe presidential candidates who each received less than 0.1% of the vote (although some of these latter may perhaps carry some degree of explanatory power for the Buchanan vote). Smith does not use data from any of the senatorial races, but he obtains and uses demographic data related to ethnicity, age, education and income for the counties. The predictor variables in his models were selected using either Mallow's C_p or backward selection. After detailed analysis, Smith selects three linear regression models for in depth consideration. In these models, the three resulting 95% prediction intervals range from a lower end value of 180 votes, to an upper end value of 758 votes for the Buchanan vote in Palm Beach. Further analyses, based on 3 logistic regressions, ranged similarly from 237 at the low end, to 606 votes at the high end.

Smith's prediction intervals and our own are consistent, and hence confirmatory for us. Of course, Smith's intervals are narrower, as one would expect, based as they are on a more comprehensive set of explanatory variables. In fact, Smith's intervals are remarkably tight, especially at the high end, and benefit heavily from inclusion of the demographic variables (although in his article Smith maintains that his analyses are not meant to be definitive but only a positive example of regression methods). The higher right endpoints for our own prediction intervals also suggest that the analyses which we carried out at the time were, in fact, fairly conservative.

By way of concluding remarks, it seems fair to say that statistical methodology is characterized by the development of increasingly sophisticated models. While developing theory leads to increasingly accurate assessment of significance, this significance is grounded in the correctness of the assumed model. While such models are generally accepted in designed experiments, this is not the case for observational studies where confounding covariates potentially lead to controversy. In fact there is, in such cases, no single correct answer, and even the term 'correct' as used here is ambiguous. In place of Herculean efforts to identify a single correct model, it is sometimes best to pursue and present many reasonable models. Within legal courts, it has been considered a useful practice to bring before jurors more than one case — typically the strongest case for, and the strongest case against. But in the court of public opinion there are many cases to be presented and it is the public who must then determine where the preponderance of evidence lies. The role of the statistician can be to present this full range of evidence using arguments and displays that must be as clear and as understandable as

possible to be effective. Here we have illustrated this approach in the context of the singular events at Palm Beach County. Of course, there is no one 'right' answer. But by now, the court of public opinion has rendered a verdict: Bush would not have won this election with a clearer ballot in Palm Beach.

As an aside, we allow ourselves here to remark that in elections, it is not uncommon for a party to garner a majority of 'seats' while another party holds a larger share of the popular vote. Here the issues are not statistical, of course, but rather lie at the core of arguments for proportional representation. Such arguments sometimes confuse party support with local representation. The voting schemes of the U.S., Canada, and the U.K., for instance, are based on a principle that communities, and not parties, should be represented in the legislative bodies. So far, this has led to comparatively stable governments in those countries. There is no compelling evidence of which we are aware that proportional representation leads to better or more effective government.

Another point we have tried to illustrate here is that many statistical challenges can be usefully addressed via methodologies that have been carefully developed in the past and the problem considered here is a case in point. What is then new in any analysis is the application of the methodologies; this is the art of the statistician. Here the challenge is typical. It is not to test a hypothesis or to make inferential statements about a parameter. It is to measure something on the basis of available data, namely, the number of votes intended for Gore that went to Buchanan. Like all measures this one has bias and error and the challenge is to develop the measure and to estimate its bias and error. Furthermore, sometimes the effectiveness of an analysis depends critically on whether the statistician can deliver, in timely fashion, credible, understandable, and defensible results, under circumstances in which simplicity and presentation are highly influential.

Finally we might remark here that within statistics, outliers are always of essence and occur for many reasons. Some are no more than 'secretarial' errors, some are influential but nevertheless valid observations, some are symptomatic of model deficiencies, an occasional few are worth patenting, and a very few — like the one in Palm Beach County (for which clear and convincing explanations exist as to how it occurred) — change the course of history.

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Chapter 3

BAYESIAN FUNCTIONAL ESTIMATION OF HAZARD RATES FOR RANDOMLY RIGHT CENSORED DATA USING FOURIER SERIES METHODS

Jean-François Angers
Brenda MacGibbon

Abstract   This paper discusses a Bayesian functional estimation method, based on Fourier series, for the estimation of the hazard rate from randomly right-censored data A nonparametric approach, assuming that the hazard rate has no specific and prespecified parametric form, is used. A simulation study is also done to compare the proposed methodology with the estimators introduced in Antoniadis et al. (1999) The method is illustrated with a real data set consisting of survival data from bone marrow transplant patients

1.   Introduction

In medical research, it is useful to have clear summaries of the data for clinicians and, as advocated by Efron (1988), this can often be achieved by a graphical presentation of the hazard function. Various authors have used splines for estimating the survival function and the hazard rate in the random right censoship model. We cite, in particular, Bloxom (1985), Klotz (1986), Whittemore and Keller (1986), Efron (1988), O'Sullivan (1988), Jarjoura (1988), Kooperberg and Stone (1992), Kooperberg et al. (1995). Senthilselvan (1987) proposed penalized likelihood methods and Loader (1999) used local likelihood methods for hazard rate estimation with censored data. Kernel estimation of the hazard rate has also proved to be a useful method (see Ramlau-Hansen (1983), Roussas (1989, 1990), Izenman and Tran (1990)). Parametric empirical Bayes methods have been previously used for hazard rate estimation in the uncensored case by Arjas and Liu (1995).

Some authors have previously used orthogonal series methods; in particular Patil (1997) used orthogonal wavelet methods for hazard rate estimation in the uncensored case and Antoniadis et al. (1999)) in the random right censorship model. In fact, the procedure described by Antoniadis et al. (1999) is a very promising one. Their method is based on dividing the time axis into a dyadic number of intervals of equal length and then counting the number of events falling into each interval. The set of uncensored events and the set of all the observations are considered separately, each one being modelled separately and smoothed over time using linear wavelets smoothers. Then the hazard rate function estimators are obtained by taking the appropriate ratio as explained in Section 1.1. It performs extremely well on the simulations presented. However, it is a complex method and may be slightly difficult to implement not because it involves wavelets but because of the preliminary manipulations of the data required in order to satisfy the constraints imposed by the use of wavelets. Furthermore, the choice of the length of the interval and the resolution level (which control the smoothness of the estimator) depend on the number of observations and the smoothness (number of continuous derivatives) of the unknown function. These choices can have an important impact on the resulting estimator.

It is our purpose here to develop a Bayesian adaptation of the Antoniadis et al. (1999) method to estimate the hazard function with randomly right censored data. We employ Bayesian nonparametric estimation techniques in order to obtain a procedure that is easier to implement. Our method does not perform as well as the method of Antoniadis et al. (1999) for the estimation of the sub-density but in simulations, it is shown to be as good or superior to their method for the estimation of the hazard rate. It should also be noted that our method can be used with any orthogonal series, although here we develop it using Fourier series. This use of Fourier series also has the advantage that it may be more accessible to applied statisticians who are unfamiliar with wavelets. Of course, it can also be easily implemented with wavelet packages.

We proceed as in Antoniadis et al. (1999) to estimate the number of events and the survival functions separately. In order to describe our method here, we follow the description as given by Antoniadis et al. (1999) in Section 1.1. For ease of presentation, Section 1.2 is devoted to recalling the Bayesian approach to linear models. In Section 2 we develop our method of Bayesian functional estimation for the hazard rate problem with right censored data. Section 3 contains a simulation study and the comparison of our results with those of Antoniadis et al. (1999). Section 4 presents an application of our method to a bone marrow transplant data set. Section 5 consists of some concluding remarks.

1.1   The random right censorship model

Survival analysis is usually based on the study of a group of individuals of size n for which we assume their failure times, the non-negative random variables $T_1, \cdots, T_n$, are independent and identically distributed with distribution function $F(t)$, survival function $S(t) = 1 - F(t)$ and density $f(t)$. However, one of the features that distinguishes the analysis of survival data from classical statistical analysis is the possibility that the data may be incomplete; that is, some individuals may not be observed until failure. For example, some patients will survive to the end of a clinical trial and thus their failure times cannot be observed. If this happens in a random fashion then this type of incompleteness is modelled by assuming that there exist $C_1, \cdots, C_n$ independent and identically distributed random variables with distribution function G and density g representing the censoring mechanism. Instead of observing the complete data $T_1, \cdots, T_n$, we observe $X_i = \min(T_i, C_i)$, $i = 1, \cdots, n$ and an indicator function $\delta_i = 1$ if $T_i \leq C_i$ and $= 0$ if not.

Since the density function of T exists, the hazard rate function can also be defined as

$$\lambda(t) = \frac{f(t)}{1 - F(t)} \qquad F(t) < 1.$$

With T_j, C_j, δ_j defined as above, the observed random variables are then X_j and δ_j. Henceforth we assume that

(a) $T_1, T_2, \cdots, T_n$ are non-negative, independent and identically distributed with distribution function F and density f,

(b) $C_1, C_2, \cdots, C_n$ are non-negative, independent and identically distributed with distribution function G and density g, and

(c) the T's and C's are independent.

In the censored case, if $G(t) < 1$, we have

$$\lambda(t) = \frac{f(t)\{1 - G(t)\}}{\{1 - F(t)\}\{1 - G(t)\}}, \qquad F(t) < 1.$$

If we let $L(t) = P(X_i \leq t)$, then

$$1 - L(t) = \{1 - F(t)\}\{1 - G(t)\}.$$

Letting

$$f^*(t) = f(t)\{1 - G(t)\},$$

be the sub-density of those observations that are still to fail, then clearly

$$\lambda(t) = \frac{f^*(t)}{1 - L(t)}, \qquad L(t) < 1.$$

1.2   The Bayesian model

The estimator for the hazard rate proposed in the next section is obtained by writing the estimation problem using a Bayesian linear model. Hence, for ease of presentation, we first recall the Bayesian linear model as found in Lindley and Smith (1972) and Robert (2001). Let

$$Y = X\theta + \varepsilon,$$

where

Y is a $n \times 1$ vector of observations,

X is a $n \times p$ known matrix,

θ is a $p \times 1$ vector of regression coefficients,

$\varepsilon \sim N_n(0, \sigma^2 I_n)$.

Note that X is assumed to be of full rank but even if X is singular the theory holds. Furthermore, σ^2 might be known or unknown. If σ^2 is unknown, it will also be considered as a random variable.

Given this model, the likelihood function is given by

$$\ell(\theta, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left\{ -\frac{1}{2\sigma^2}(Y - X\theta)'(Y - X\theta) \right\}.$$

The loss function typically used is:

$$L(\theta, \hat{\theta}) = (\theta - \hat{\theta})'Q(\theta - \hat{\theta}), \tag{3.1}$$

where Q is a positive definite matrix.

Let

$$\theta_{LS} = (X'X)^{-1}X'Y,$$
$$S = (Y - X\theta_{LS})'(Y - X\theta_{LS}),$$

then the likelihood function can be rewritten as:

$$
\begin{aligned}
\ell(\theta, \sigma^2) &\propto \frac{1}{(\sigma^2)^{n/2}} \exp\left\{ -\frac{1}{2\sigma^2} \left[(\theta - \theta_{LS})X'X(\theta - \theta_{LS}) + S \right] \right\} \\
&= \left(\frac{1}{(\sigma^2)^{p/2}} \exp\left\{ -\frac{1}{2\sigma^2}(\theta - \theta_{LS})X'X(\theta - \theta_{LS}) \right\} \right) \\
&\qquad \times \left(\frac{1}{(\sigma^2)^{(n-p)/2}} \exp\left\{ -\frac{S}{2\sigma^2} \right\} \right) \\
&= \left[\theta \mid \sigma^2, Y \sim N_p(\theta_{LS}, \sigma^2(X'X)^{-1}) \right] \\
&\qquad \times \left[\sigma^2 \mid Y \sim I\Gamma((n - p - 2)/2, S/2) \right]
\end{aligned}
\tag{3.2}
$$

where $N_p(\mu, \Sigma)$ denotes the multivariate normal density with mean μ and covariance matrix Σ while $I\Gamma(a, b)$ represents the inverse gamma density with shape parameter a and scale parameter b. (Note that if $\lambda \sim I\Gamma(a, b)$

$$\pi(\lambda) = \left\{ \begin{array}{ll} \frac{b^a}{\Gamma(a)\lambda^{a+1}} \, e^{-b/\lambda} & \text{if } \lambda > 0, \\ 0 & \text{otherwise.} \end{array} \right\}$$

Now a conjugate prior for (θ, σ^2) is given by:

$$\theta \mid \sigma^2 \sim N_p(\eta, \sigma^2 C), \tag{3.3}$$

$$\sigma^2 \sim I\Gamma(\alpha/2, \gamma/2), \tag{3.4}$$

where η, C, α and γ are assumed to be known.

With the prior model given in equations (3.3) and (3.4) and the likelihood function given in equation (3.2), the posterior density on (θ, σ^2) and the marginal of the least squares estimator θ_{LS} are:

$$\theta \mid \sigma^2, Y \sim N_p(\theta_*, \sigma^2 C_*), \tag{3.5}$$

$$\sigma^2 \mid Y \sim I\Gamma\left(\frac{n+\alpha}{2}, \frac{\gamma_*}{2}\right), \tag{3.6}$$

$$\theta_{LS} \sim T_p\left(n + \alpha - p, \theta_0, \frac{S+\gamma}{n+\alpha-p} A_*\right), \tag{3.7}$$

where

$$\theta_* = \theta_{LS} - C_* C^{-1}(\theta_{LS} - \eta),$$
$$C_* = (X'X + C^{-1})^{-1} = C - C(C + (X'X)^{-1})^{-1}C,$$
$$\gamma_* = S + \gamma + (\theta_{LS} - \eta)' A_*^{-1}(\theta_{LS} - \eta),$$
$$A_* = (X'X)^{-1} + C.$$

Then, under the loss function given in equation (3.1), the Bayes estimator of θ is given by:

$$\hat{\theta} = \mathbb{E}(\theta \mid Y) = \theta_{LS} - C_* C^{-1}(\theta_{LS} - \eta).$$

2. Fourier series Bayesian functional model

Now, we can develop the Fourier series Bayesian functional estimation model using the Bayesian linear model described in the previous section as a basis. Let $y_{(1)t}$ represent the "empirical" density of the failure times evaluated at X_t, that is

$$y_{(1)t} = \frac{\#\{X_i \le X_t\}}{n+1} \tag{3.8}$$

for $t = 1, 2, \ldots, n$. (We divide by $n + 1$ in order to have $0 \leq y_{(1)t} < 1 \, \forall t$.) As it is well known, the Fourier analysis is simpler for estimating symmetric functions. In order to take advantage of this property, we use a doubling procedure in order to obtain symmetric observations, which does not affect the performance of the estimators but which will reduce the number of parameters to estimate. More explicitly, let

$$
y_t = \begin{cases} y_{(1)t} & \text{if } t = 1, 2, \ldots n, \\ y_{(1)2n+1-t} & \text{if } t = n + 1, n + 2, \ldots, 2n. \end{cases}
$$

Then, using a Fourier series for symmetric function, we have

$$
y_t = \theta_0 + \sum_{\ell=1}^{\infty} \theta_\ell \cos\left(\frac{\ell \pi t}{T}\right) + \varepsilon_t, \tag{3.9}
$$

where

$$
\varepsilon_t \sim N(0, \sigma^2)
$$
$$
\theta_\ell \sim N(\eta_\ell, c_\ell \sigma^2), \qquad \ell = 0, 1, \cdots
$$

Let us rewrite equation (3.9) as

$$
y_t = \theta_0 + \sum_{\ell=1}^{m} \theta_\ell \cos\left(\frac{\ell \pi t}{T}\right) + \sum_{\ell=m+1}^{\infty} \theta_\ell \cos\left(\frac{\ell \pi t}{T}\right) + \varepsilon_t. \tag{3.10}
$$

Now the second sum, denoted by z_t, will be considered as a nuisance parameter and using known results about Bayesian estimation in linear models, we have

$$
\mathbb{E}(z_t) = \sum_{\ell=m+1}^{\infty} E(\theta_\ell) \cos\left(\frac{\ell \pi t}{T}\right)
$$
$$
= \sum_{\ell=m+1}^{\infty} \eta_\ell \cos\left(\frac{\ell \pi t}{T}\right)
$$
$$
= 0 \text{ as long as } \eta_\ell = 0, \ell = m + 1, \cdots
$$

and

$$
\mathrm{Cov}(z_t, z_s)
$$
$$
= \mathrm{Cov}\left(\sum_{\ell=m+1}^{\infty} \theta_\ell \cos\left(\frac{\ell \pi t}{T}\right), \sum_{j=m+1}^{\infty} \theta_j \cos\left(\frac{j \pi s}{T}\right)\right)
$$

$$= \sum_{\ell=m+1}^{\infty} \sum_{j=m+1}^{\infty} \mathrm{Cov}(\theta_\ell, \theta_j) \cos\left(\frac{\ell\pi t}{T}\right) \cos\left(\frac{j\pi s}{T}\right)$$

where $\mathrm{Cov}(\theta_\ell, \theta_j) = c_\ell$ if $\ell = T$ and 0 elsewhere

$$= \sum_{\ell=m+1}^{\infty} c_\ell \sigma^2 \cos\left(\frac{\ell\pi t}{T}\right) \cos\left(\frac{\ell\pi s}{T}\right)$$

$$= \frac{\sigma^2}{2} \left[c_m(t+s) + c_m(t-s) \right]$$

where

$$c_m(z) = \left[\sum_{\ell=1}^{\infty} - \sum_{\ell=1}^{m} \right] c_\ell \cos\left(\frac{\ell\pi z}{T}\right).$$

Now if we let $c_\ell = 1/\ell^2$ then

$$c_m(z) = \frac{\pi^2}{6} - \frac{\pi}{2}\left[\frac{\pi|z|}{T}\right] + \frac{1}{4}\left[\frac{\pi z}{T}\right]^2 - \sum_{\ell=1}^{m} \frac{1}{\ell^2} \cos\left(\frac{\ell\pi z}{T}\right)$$

$$= \frac{\pi^2}{2}\left(\frac{1}{3} - \frac{|z|}{T} + \frac{1}{2}\frac{z^2}{T^2}\right) - \sum_{\ell=1}^{m} \frac{1}{\ell^2} \cos\left(\frac{\ell\pi z}{T}\right)$$

and $\mathrm{Var}(z_t) = \frac{\sigma^2}{2}\left[c_m(2t) + c_m(0)\right]$,

$$c_m(0) = \frac{\pi^2}{2}\left(\frac{1}{3} - 0 + 0\right) - \sum_{\ell=1}^{m} \frac{1}{\ell^2} \cos(0)$$

$$= \frac{\pi^2}{6} - \sum_{\ell=1}^{m} \frac{1}{\ell^2},$$

$$c_m(2t) = \frac{\pi^2}{2}\left(\frac{1}{3} - \frac{2t}{T} + \frac{2t^2}{T^2}\right) - \sum_{\ell=1}^{m} \frac{1}{\ell^2} \cos\left(\frac{2\ell\pi t}{T}\right).$$

$D_{i,j} = \left(\mathrm{Cov}(z_{t_i}, z_{t_j})\right)$ for $i, j = 1, \cdots, 2n$ then

$$y_t = \theta_0 + \sum_{\ell=1}^{m} \theta_\ell \cos\left(\frac{\ell\pi t}{T}\right) + \varepsilon_t^*, \tag{3.11}$$

where $\varepsilon_t^* = (z_t + \varepsilon_t)$ and $\varepsilon^* = \left(\varepsilon_{t_1}^*, \cdots, \varepsilon_{t_{2n}}^*\right) \sim N_{2n}(0, \Sigma)$, and $\Sigma = \sigma^2\left(I_{2n} + D\right)$, or

$$\Sigma_{i,j} = \begin{cases} \frac{\sigma^2}{2}\left[c_m(t_i + t_j) + c_m(t_i - t_j)\right] & \text{if } i \neq j; \\ \sigma^2 + \frac{\sigma^2}{2}\left[c_m(2t_i) + c_m(0)\right] & \text{if } i = j. \end{cases}$$

This implies that
$$Y \mid \theta, \sigma^2 \sim N_{2n}(X\theta, \Sigma),$$
where $\theta = (\theta_0, \theta_1, \cdots, \theta_m) \sim N_{m+1}(\eta, \sigma^2 C)$,

$$X = \begin{pmatrix} 1 & \cos(\pi x_1/T) & \ldots & \cos(m\pi x_1/T) \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \cos(\pi x_n/T) & \ldots & \cos(m\pi x_n/T) \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \cos(\pi x_{2n}/T) & \ldots & \cos(m\pi x_{2n}/T) \end{pmatrix},$$

$x_i = \min(T_i, C_i)$, $x_{2n+1-i} = x_n + \delta - x_i$ for $i = 1, 2, \ldots, n$, δ is an arbitrary nonnegative number and

$$C = \begin{pmatrix} 1 & & & & & 0 \\ & 1 & & & & \\ & & \frac{1}{2^2} & & & \\ & & & \frac{1}{3^2} & & \\ & & & & \ddots & \\ 0 & & & & & \frac{1}{m^2} \end{pmatrix}.$$

Let θ_{WLS} denote the weighted least squares estimator given by

$$\theta_{WLS} = \left(X'\Sigma^{-1}X\right)^{-1} X'\Sigma^{-1}Y.$$

It is well-known that $\theta_{WLS}|\theta \sim N_{m+1}\left(\theta, \left(X'\Sigma^{-1}X\right)^{-1}\right)$. Consequently, under the loss function (3.1) and the posterior densities given in equations (3.5) and (3.6), the Bayes estimator is given by

$$\widehat{\theta}_* = \mathbb{E}(\theta \mid Y) = \hat{\theta}_{WLS} - C_* C^{-1} \left(\hat{\theta}_{WLS} - \eta\right), \qquad (3.12)$$

where

$$C_* = C - C \left(C + \left(X'\Sigma^{-1}X\right)^{-1}\right)^{-1} C$$
$$= \left(C + X'\Sigma^{-1}X\right)^{-1},$$

and

$$\sigma^2|Y \sim I\Gamma\left(\frac{n+\alpha}{2}, \frac{\gamma_*}{2}\right),$$

where

$$\gamma_* = S + \gamma + (\theta_{WLS} - \eta)' A_*^{-1} (\theta_{WLS} - \eta)$$
$$A_* = \left(X'\Sigma^{-1}X\right)^{-1} + C.$$

2.1   Choice of m

In order to use the model proposed in the previous subsection, the appropriate value for m has to be selected. One way to do this is to perform Bayesian testing using Bayes factors (*cf.* Angers and Delampady, 2001). Hence, let consider the hypotheses:

$$H_i : m = i,$$

for $i = 0, 1, \ldots$, where m denotes the truncation point in equation (3.10). Let $f_m(Y)$ denotes the marginal of Y (or equivalently of θ_{WLS}) if m is the selected truncated point. Using equation (3.7), it can be shown that

$$\theta_{WLS} \sim T_{m+1} \left(n + \alpha - m - 1, \eta, \frac{S + \gamma}{n + \alpha - m - 1} A_* \right).$$

The best value of m should be the one corresponding to the hypothesis with the largest posterior probabilities. An alternative would be to use the Bayes factor. In order to test the hypotheses

$$H_0 : m = 0 \text{ against } H_1 : m = l,$$

we can compute the ratio of the posterior odds to the prior odds,

$$\mathrm{BF}_l = \frac{\mathbb{P}(m = l \mid Y)/\mathbb{P}(m = 0 \mid Y)}{\mathbb{P}(m = l)/\mathbb{P}(m = 0)} = \frac{f_l(Y)}{f_0(Y)}.$$

The Bayes factor BF_l can also be thought of as a Bayesian likelihood ratio test where the likelihood functions are replaced by the marginals under both hypotheses (*cf.* Robert, 2001). For multiple hypotheses testing, we select the hypothesis which satisfies

$$m = \mathrm{argmax}_{l \geq 0} \mathrm{BF}_l,$$

where the Bayes factor in our problem is given by

$$\mathrm{BF}_l = \frac{f_l(Y)}{f_0(Y)}$$

$$= \sqrt{\frac{|d_0 A_{*0}|}{|d_l A_{*l}|}} \left(\frac{\sqrt{n + \alpha - 1}}{(n + \alpha - l - 1)^{(l+1)/2} \pi^{l/2}} \right) \left(\frac{\Gamma([n + \alpha - 1]/2)}{\Gamma([n + \alpha - l - 1]/2)} \right)$$

$$\left(\frac{1 + (\theta_{WLS,0} - \eta_0)' A_{*0}^{-1} (\theta_{WLS,0} - \eta_0)/(S_0 + \gamma)}{1 + (\theta_{WLS,l} - \eta_l)' A_{*l}^{-1} (\theta_{WLS,l} - \eta_l)/(S_l + \gamma)} \right)^{(n+\alpha)/2},$$

$$d_l = \frac{S_l + \gamma}{n + \alpha - l - 1}.$$

The quantities S_l, A_{*l}, $\theta_{WLS,l}$ are the same as defined earlier but a subscript l has been added to explicitly indicate their dependency on l. (Note that it is assumed that $\mathrm{BF}_0 = 1$.)

2.2   Estimator

To obtain the estimator of $f^*(t)$, we start by estimating the cumulative distribution function (cdf) F^* using equation (3.12) based only on the uncensored observations (values of i such that $\delta_i = 1$). The vector Y, described at the beginning of Section 2, will then be based on the empirical cdf of the uncensored observations; that is,

$$Y = \frac{1}{n_o + 1}(1, 2, \ldots, n_o - 1, n_o, n_o, n_o - 1, \ldots, 1)',$$

where n_o represent the number of uncensored observations. Referring to equations (3.8) and (3.11), it is clear that the estimator of y_t (*cf.* equation (3.11)) is also an estimator of the sub-distribution which we denote as $\widehat{F}^*(t)$ given by

$$\widehat{F}^*(t) = \widehat{\theta}_{*0} + \sum_{l=1}^{m} \widehat{\theta}_{*l} \cos\left(\frac{l\pi t}{T}\right),$$

where $\widehat{\theta}_{*l}$ is defined by equation (3.12). To obtain the estimator of $f^*(t)$, we proceed as follows:

$$\widehat{f}^*(t) = \frac{\partial}{\partial t}\widehat{F}^*(t)$$

$$= -\frac{\pi}{T}\sum_{l=1}^{m} l\widehat{\theta}_{*l} \sin\left(\frac{l\pi t}{T}\right).$$

To estimate $L(t) = P(X_i \leq t)$, we proceed as for $F^*(t)$ in order to obtain $\widehat{L}(t)$, but this time all the observations (censored and uncensored) are used. The estimator of the hazard function is then given by

$$\widehat{\lambda}(t) = \frac{\widehat{f}^*(t)}{1 - \widehat{L}(t)}.$$

3.   Simulations

As in Antoniadis et al. (1999), two different models for the simulation studies have been considered. First, a sample of size n $T_i, 1 \leq i \leq n$, from the gamma distribution with shape parameter 5 and scale parameter 1, denoted by f_1 and an independent sample $C_i, 1 \leq i \leq n$, from the exponential distribution with mean 6 (the mean was chosen to yield about 50% censoring). In the second set-up, the T_i's are generated from a bimodal density (*cf.* Kooperberg and Stone, 1992), denoted f_2, given by

$$f_2 = 0.8g + 0.2h,$$

where g is the density of $\exp\{Z/2\}$, with Z having the standard normal distribution, and h is the normal density with mean 2 and standard

deviation 0.17. The C_i's are generated from the exponential distribution with mean 2.5. The performance measure used to compare different values of m with the Antoniadis et al. (1999) method is the average mean-squared error obtained by averaging the mean-squared errors given by:

$$\text{ASE}(f^*) = n_*^{-1} \sum_{i=1}^{n_*} [\widehat{f}^*(t_i) - f^*(t_i)]^2,$$

$$\text{ASE}(\lambda) = n_*^{-1} \sum_{i=1}^{n_*} [\widehat{\lambda}(t_i) - \lambda(t_i)]^2,$$

where n_* represents the number of observations with $t_i \leq 6$ for the first simulation and ≤ 2.5 for the second. Two values of n are considered, that is $n = 200$ and $n = 500$.

The simulation results are given in Table 3.1 for the first simulation set-up and in Table 3.2 for the second one.

Table 3.1. Average mean-squared errors ($\times 10^{-5}$ for the sub-density and $\times 10^{-3}$ for the hazard function) in the first simulation set-up for Antoniadis et al. (1999) based on 200 repetitions. For the wavelet based estimator of Antoniadis et al. (1999), the ASE for f_1^* varies between 14.6 and 20.5 for $n = 200$ and between 5.2 and 13.6 for $n = 500$ and for λ_1 between 2.5 and 5.8 for $n = 200$ and between 1.6 and 5.9 $n = 500$ respectively.

	f_1^*				λ_1			
m	$n = 200$		$n = 500$		$n = 200$		$n = 500$	
	OLS	Bayes	OLS	Bayes	OLS	Bayes	OLS	Bayes
4	29.2	53.3	27.6	25.8	6.3	0.5	7.0	0.3
5	24.6	55.6	24.3	25.2	6.5	0.6	7.3	0.3
6	32.5	79.9	27.4	46.4	6.1	0.8	4.4	0.5
7	26.9	84.3	22.3	45.9	4.9	0.8	3.6	0.5

For both simulation studies, it can be seen from Tables 3.1 and 3.2 that in the estimation of the sub-densities, the Fourier series method does not perform as well as the wavelet estimator proposed in Antoniadis et al. (1999). It should be noted that the ordinary least squared estimator of f^* is slightly better than the Bayes estimator which is based on the weighted least squared estimator. For the hazard function, the opposite situation occurs. The Bayes estimator is much better than the ordinary least squared estimator and it is clearly superior (for λ_1) and as least as good or superior (for λ_2) to the estimator proposed by Antoniadis et al. (1999). As our main objective is to estimate the hazard function rather than the sub-density, the simulations indicate that the Bayesian method presented here is at least as good as (and in some cases superior

Table 3.2. Average mean-squared errors ($\times 10^{-3}$ for the sub-density and $\times 10^{-1}$ for the hazard function) in the second simulation set-up for Antoniadis et al. (1999) based on 200 repetitions. For the wavelet based estimator of Antoniadis et al. (1999), the ASE for f_2^* varies between 3.0 and 5.5 for $n = 200$ and 2.1 and 4.6 for $n = 500$ and for λ_2 between 0.3 and 3.0 for $n = 200$ and between 0.5 and 1.8 for $n = 500$ respectively.

	f_2^*				λ_2			
	$n = 200$		$n = 500$		$n = 200$		$n = 500$	
m	OLS	Bayes	OLS	Bayes	OLS	Bayes	OLS	Bayes
12	19.5	34.5	12.2	38.7	84.5	0.3	6701.8	0.4
13	21.7	80.9	210.7	266.9	83.3	0.8	14255.1	2 7
14	54.2	38.6	137.6	47.9	2979 9	0.5	7211 9	0.5
15	27.0	79.8	382.8	175.9	4593.0	0 8	4229.3	0.2

to) the wavelet method proposed by Antoniadis et al. (1999) for the estimation of hazard rate with right-censored observations.

4.   Example

In this section, a real data set is considered and its sub-density along with its hazard function are estimated using a Fourier based estimator.

We have chosen to illustrate our method on a data set consisting of a follow-up study of acute leukaemia patients after allogenic bone marrow transplantation. The survival times are given in months. For a more complete description of this data, see Brochstein et al. (1987). In the original article by Brochstein et al. (1987), Kaplan-Meier estimates of disease-free survival at five years were compared for second, third and fourth remission patients on a data base of 97 children with acute lymphoblastic leukemia (ALL) or acute myelogenous leukemia (AML) and who received HLA-identical bone marrow transplants (BMT) from sibling donors followed by total-body irradiation and high dose cyclophosphamide. Subsequently new patients were added to the study and followed and a data base of 162 patients (including 63 deaths) has been make available to us by Dr R.J. O'Reilly of the Sloan Kettering Memorial Cancer Center and Dr. Susan Groshen of the Keek School of Medicine at the University of Southern California.

Various subsets of this data have been previously used by Mueller and Wang (1990) and Antoniadis et al. (2000) to illustrate different methods of location of change points in the hazard rate with right censored observations. Here as a preliminary step in a more complete data analysis to be pursued elsewhere we have chosen to use the complete data set with death due to any cause as the end point and leukaemic release or end of study as the censoring mechanism. This seems an ideal choice since

clinical findings would indicate that the hazard rate would be increasing. As the Bayesian method proposed here does not take into account monotonicity, this choice should provide a good testing ground for our method.

We optimize our choice of the number of terms in the Fourier series by using Bayes factors (see Figure 3.1); while Figure 3.2 illustrates our estimate of the sub-density along with the estimator proposed in Antioniadis et al. (1999). (This estimator has been computed using Rice Wavelet Toolbox, version 2.4.) From Figure 3.1, it can be seen that the best value of m is equal to 4. Figure 3.3 gives our estimate of the actual hazard rate for this example and the one using wavelets proposed by Antioniadis et al. (1999). Note that the estimators based on the Fourier series, although they are not as smooth as the one based on wavelets, they have no sharp change of behavior between 70 and 80 months as indicated by the wavelet estimator. This means our model would fit better with clinical expectations since there does not seem to be any *a priori* reason for these changes shown in the wavelet estimator during that time period. It should be noted that except for the largest time values, the hazard function using Fourier series is essentially increasing while the one using wavelets is always increasing except for the sharp change between 70 and 80 months. This corresponds with clinical findings also.
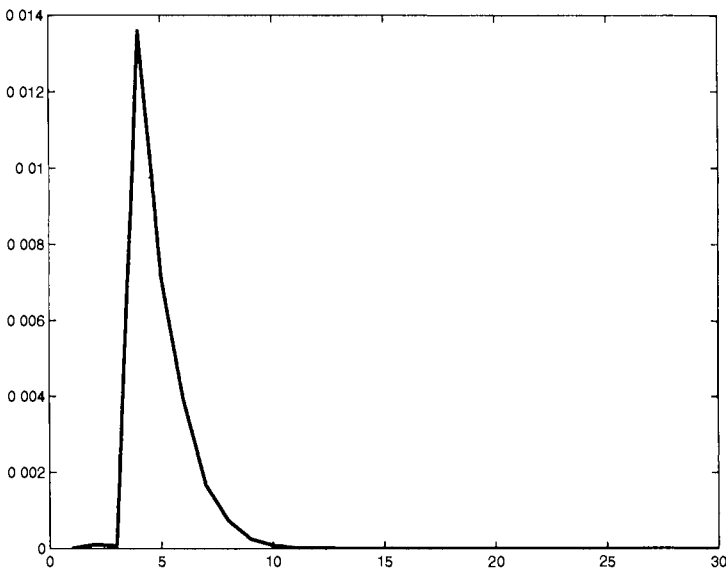
Figure 3 1. Choice of number of terms (m) using Bayes factor.
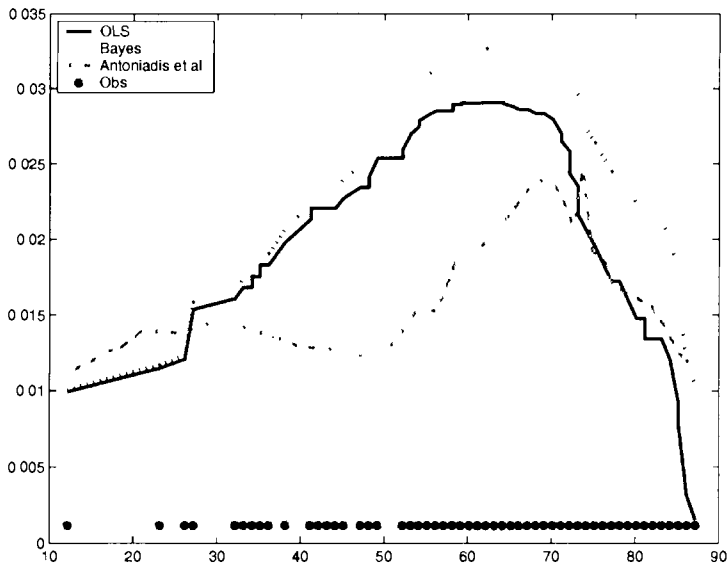
Figure 3.2. Estimate of the sub-density $\widehat{f}^*$.
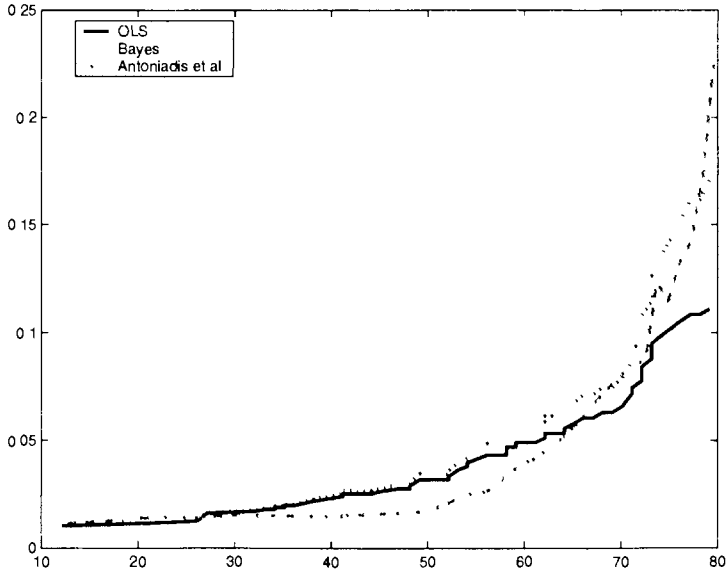
Figure 3.3. Estimate of the hazard rate function $\widehat{\lambda}$.

5.   Concluding remarks

The objective of this research was to use Bayesian functional estimation techniques combined with Bayes factors for optimal choice of model parameters and Fourier series to estimate the hazard rate with randomly right censored data by a relatively easy method to implement. The technique can be viewed as a Bayesian adaptation of the method proposed by Antoniadis et al. (1999). The simulation studies indicate that our method is not quite as good as that of Antoniadis et al. (1999) for estimation of the sub-density; however it as good as or even superior to their method for hazard rate estimation, our main objective here. Again in the real data example which we used for illustrative purposes, our hazard rate estimator performs as well as that of Antoniadis et al. (1999). Our method is also extremely flexible. An advantage of Bayesian methods is that, by the use of Bayes factors, an optimal choice of the model parameters can be made. The statistician also can choose to use a preferred orthogonal basis such as the Fourier one, which would be useful for applied statisticians who are less familiar with wavelets, or any one of the orthogonal wavelet bases.

In future research, we will be pursuing the use of different orthogonal bases such as wavelets which can incorporate inhomogeneous smoothness in order to improve the performance of our hierarchical Bayesian functional estimator of the hazard rate.

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Chapter 4

CONDITIONS FOR THE VALIDITY OF *F*-RATIO TESTS FOR TREATMENT AND CARRYOVER EFFECTS IN CROSSOVER DESIGNS

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Abstract Continuous data from crossover trials are often analysed using ordinary least squares with the assumption of independent errors. Because each experimental unit receives a sequence of treatment and repeated measurements are collected, it is more realistic to assume that the errors within an experimental unit are correlated. In this paper, we extend to crossover designs the conditions on the covariance structure of the errors, found by Huynh and Feldt (1970) for randomized block and split-plot designs, that will not invalidate the *F*-ratio tests for treatment and carryover effects. We also show that results on optimal crossover designs remain valid under this more general structure of the covariance matrix

1.   Introduction

In crossover designs, experimental units are used repeatedly by exposing them to a sequence of different treatments. Let t treatments be compared in p periods via n experimental units. Altogether np observations are taken. An allocation of the t treatments into the np observations is called a repeated measurements design, crossover design or change-over design. The main advantage of repeated measurements designs is in the production of treatment comparisons of sufficient precision with a reduce number of experimental units. This is due to the elimination of between-subject variation, each experimental unit providing a direct comparison of treatment effects. The comparisons are then made using within-subject variability which is in general much less than

between-subject variability. The advantage of crossover designs over parallel group designs are not however without some statistical modelling complications. There might be a period effect, that is an effect on the response due to being observed in that period. A learning or fatigue effect over a sequence of psychological tests or of products tasting in an experimental session are examples of a period effect. Another complication is the possibility of the persistence of the effect of a treatment administered in previous treatment periods which is added to the effect of the treatment in the current period. This effect is called a carryover effect. To take into account those additional effects, most papers in the literature on crossover designs assume the following model for the continuous response of subject j in period k:

$$Y_{jk} = \mu + \alpha_j + \pi_k + \tau_{d(j,k)} + \lambda_{d(j,k-1)} + \varepsilon_{jk} \qquad (4.1)$$

where $j = 1, \ldots, n$, $k = 1, \ldots, p$, and where the unknown constants μ, α_j, π_k, $\tau_{d(j,k)}$ and $\lambda_{d(j,k-1)}$ are respectively called the overall mean, the effect of the jth experimental unit, the effect of the kth period, the direct effect of treatment $d(j,k)$ i.e. of the treatment assigned by the crossover design d to the jth experimental unit in the kth period, and the first order carryover effect of treatment $d(j, k - 1)$ i.e. of the treatment subject j received in the previous period. The ε_{jk} are random errors, and $\lambda_{d(j,0)} = 0$ for all j because there is no carryover of preceding treatment in the first period.

The hypotheses of interest are those of no treatment and no carryover effects. The errors ε_{jk} are usually assumed to be independent, identically distributed normal random variables with mean zero and variance σ^2, and the analysis is performed through ordinary least squares procedure (Jones and Kenward, 1989). If we refer to the works of Hedayat and Afsarinejad (1978), Cheng and Wu (1980), Kunert (1984) or Kushner (1998), the same assumptions are also made to find optimal crossover designs. Since the experimental units are used repeatedly over p periods, it is usually inappropriate to assume independence between measurements within the same unit. Suggestions have been made to include error structures in the analysis; see for instance, Kunert (1985,1987), Matthews(1987, 1989, 1990), Jones and Kenward (1989), Bellavance, Tardif and Stephens (1996), Goad and Johnson (2000) and Jones and Wang (2000).

The purpose of this paper is to extend to crossover designs the conditions on the covariance structure of the errors found by Huynh and Feldt (1970) for randomized block and split-plot designs that will not invalidate the usual F-ratio tests. Chen, Zhao and Zhang (2002) claim without proof that the type H structure, as defined in Huynh and Feldt

(1970), is a sufficient and also a necessary condition to validate the F-ratio tests for treatment and carryover effects. We actually prove in Section 3 that the type H structure is a necessary and sufficient condition for the validity of the F-ratio tests for testing jointly the absence of treatment and carryover effects and a sufficient condition for testing separately the absence of treatment effects adjusted to the presence of carryover effects and the absence of carryover effects adjusted to the presence of treatment effects.

We consider in this paper an extension of model (4.1) in which we include a group effect. Typically in practice, the group effect represents centers in multicenter clinical trials, or physician's practice when several physicians are recruiting patients in the trial, or geographical areas in agricultural experiments. In sensory experiments the group effect represents replicates of the design in different sessions with different subjects to increase sample size. Therefore, the n experimental units are divided into g groups with n_i subjects in group i, $i = 1, \ldots, g$ and $n = \sum_{i=1}^{g} n_i$. Let $d(i, j, k)$ denotes the treatment assigned by design d in the kth period to the jth experimental unit in the ith group. Let Y_{ijk} be the response under $d(i, j, k)$ and consider the following model:

$$Y_{ijk} = \mu + \gamma_i + \alpha_{ij} + \pi_{ik} + \tau_{d(i,j,k)} + \lambda_{d(i,j,k-1)} + \varepsilon_{ijk} \qquad (4.2)$$

where $i = 1, \ldots, g$, $j = 1, \ldots, n_i$, $k = 1, \ldots, p$, and $\lambda_{d(i,j,0)} = 0$ for all i, j, and where, as in model (4.1), the unknown constants μ, γ_i, α_{ij}, π_{ik}, $\tau_{d(i,j,k)}$ and $\lambda_{d(i,j,k-1)}$ are respectively the overall mean, the effect of the ith group, the effect of the jth experimental unit within the ith group, the effect of the kth period within the ith group, the direct effect of treatment $d(i, j, k)$, and the first order carryover effect of treatment $d(i, j, k-1)$. The ε_{ijk} are random errors. The next section presents linear models in matrix notation, the general form of the sum of squares and of the F-ratio tests in the ANOVA table. In the third section we provide the conditions under which the F-ratio tests for treatment and carryover effects are valid. In the fourth section we investigate the impact of those conditions on crossover designs that have optimal properties under the assumption of uncorrelated errors.

Other related work is Monga and Tardif (1992) who showed that the F-ratio test for treatment effects in replicated latin square designs is valid under relaxed conditions in a model similar to model (4.2) but without carryover effects.

2.   Preliminaries

In matrix notation, any linear model, like those in (4.1) and (4.2), can be written in the form

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

$$= (\mathbf{X}_1 \ldots \mathbf{X}_l \ldots \mathbf{X}_m) \begin{pmatrix} \boldsymbol{\beta}_1 \\ \vdots \\ \boldsymbol{\beta}_l \\ \vdots \\ \boldsymbol{\beta}_m \end{pmatrix} + \boldsymbol{\varepsilon}$$

if $\mathbf{X}$ and $\boldsymbol{\beta}$ are respectively partitioned into m sub-matrices and sub-vectors where $\mathbf{X}_l$ is the sub-matrix associated with the sub-vector $\boldsymbol{\beta}_l$, $l = 1, \ldots, m$. For $1 \leq l \leq m$, let

$$\mathbf{M}_l = (\mathbf{X}_1 \ldots \mathbf{X}_{l-1}\ \mathbf{X}_{l+1} \ldots \mathbf{X}_m),$$

$$\mathbf{B}_l = \left(\boldsymbol{\beta}_1^{'} \ldots \boldsymbol{\beta}_{l-1}^{'}\ \boldsymbol{\beta}_{l+1}^{'} \ldots \boldsymbol{\beta}_m^{'} \right)^{'},$$

$$R(\boldsymbol{\beta}) = \mathbf{Y}^{'}\mathbf{X}(\mathbf{X}^{'}\mathbf{X})^{-}\mathbf{X}^{'}\mathbf{Y},$$

$$R(\mathbf{B}_l) = \mathbf{Y}^{'}\mathbf{M}_l(\mathbf{M}_l^{'}\mathbf{M}_l)^{-}\mathbf{M}_l^{'}\mathbf{Y}.$$

Then,

$$R(\boldsymbol{\beta}_l | \mathbf{B}_l) = R(\boldsymbol{\beta}) - R(\mathbf{B}_l)$$

is the sum of squares due to $\boldsymbol{\beta}_l$ adjusted to $\mathbf{B}_l$. (Searle 1987, Chapter 8, Section 8.5). Without lost of generality, general linear models can be rewritten under the form

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

$$= (\mathbf{X}_l\ \mathbf{M}_l) \begin{pmatrix} \boldsymbol{\beta}_l \\ \mathbf{B}_l \end{pmatrix} + \boldsymbol{\varepsilon}$$

and, if we let $\mathbf{C}_l = \mathbf{X}_l^{'}[\mathbf{I} - \mathbf{M}_l(\mathbf{M}_l^{'}\mathbf{M}_l)^{-}\mathbf{M}_l^{'}]\mathbf{X}_l$ denotes the information matrix associated with $\boldsymbol{\beta}_l$, then $(\mathbf{X}^{'}\mathbf{X})^{-}$ can be written as the following partitioned matrix

$$\begin{pmatrix} \mathbf{C}_l^{-} & -\mathbf{C}_l^{-}\mathbf{X}_l^{'}\mathbf{M}_l(\mathbf{M}_l^{'}\mathbf{M}_l)^{-} \\ -(\mathbf{M}_l^{'}\mathbf{M}_l)^{-}\mathbf{M}_l^{'}\mathbf{X}_l\mathbf{C}_l^{-} & (\mathbf{M}_l^{'}\mathbf{M}_l)^{-} + (\mathbf{M}_l^{'}\mathbf{M}_l)^{-}\mathbf{M}_l^{'}\mathbf{X}_l\mathbf{C}_l^{-}\mathbf{X}_l^{'}\mathbf{M}_l(\mathbf{M}_l^{'}\mathbf{M}_l)^{-} \end{pmatrix}$$

from which we get

$$\hat{\boldsymbol{\beta}}_l = \mathbf{C}_l^{-}\mathbf{X}_l^{'}[\mathbf{I} - \mathbf{M}_l(\mathbf{M}_l^{'}\mathbf{M}_l)^{-}\mathbf{M}_l^{'}]\mathbf{Y}$$

and

$$R(\boldsymbol{\beta}_l | \mathbf{B}_l) = \mathbf{Y}^{'}[\mathbf{I} - \mathbf{M}_l(\mathbf{M}_l^{'}\mathbf{M}_l)^{-}\mathbf{M}_l^{'}]\mathbf{X}_l\mathbf{C}_l^{-}\mathbf{X}_l^{'}[\mathbf{I} - \mathbf{M}_l(\mathbf{M}_l^{'}\mathbf{M}_l)^{-}\mathbf{M}_l^{'}]\mathbf{Y},$$

$$= \mathbf{Y}'\mathbf{A}_l\mathbf{Y}, \text{ say.}$$

The error sum of squares is given by

$$SS_{error} = \mathbf{Y}'[\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^-\mathbf{X}']\mathbf{Y}$$
$$= \mathbf{Y}'\mathbf{E}\mathbf{Y}, \text{ say.}$$

The matrices $\mathbf{A}_l$ and $\mathbf{E}$ are symmetric and idempotent. Furthermore $\mathbf{A}_l\mathbf{E} = \mathbf{E}\mathbf{A}_l = \mathbf{O}$, where $\mathbf{O}$ is a matrix with all entries equal to zero.

If we now assume that the vector $\mathbf{Y}$ has a multinormal distribution $\mathcal{N}(\mathbf{X}\beta, \Sigma)$, where Σ is positive definite, then a necessary and sufficient condition for the quadratic form $\mathbf{Y}'\mathbf{A}_l\mathbf{Y}$ to be distributed as $\theta\chi^2(r(\mathbf{A}_l), \beta'\mathbf{X}'\mathbf{A}_l\mathbf{X}\beta)$ is that $\mathbf{A}_l\Sigma\mathbf{A}_l = \theta\mathbf{A}_l$, where θ is a positive constant and $r(\mathbf{A}_l)$ is the rank of $\mathbf{A}_l$ (Theorem 3.5 of Serfling, 1980). Under the null hypothesis $H_0 : \beta_l = \mathbf{0}$, the noncentrality parameter $\beta'\mathbf{X}'\mathbf{A}_l\mathbf{X}\beta$ is equal to zero. Also, the quadratic form $\mathbf{Y}'\mathbf{E}\mathbf{Y}$ is distributed as $\theta\chi^2(r(\mathbf{E}))$ if and only if $\mathbf{E}\Sigma\mathbf{E} = \theta\mathbf{E}$. Furthermore, the two quadratic forms $\mathbf{Y}'\mathbf{A}_l\mathbf{Y}$ and $\mathbf{Y}'\mathbf{E}\mathbf{Y}$ are independent if and only if $\mathbf{A}_l\Sigma\mathbf{E} = \mathbf{O}$. Consequently, $\mathbf{Y}'\mathbf{A}_l\mathbf{Y}/\mathbf{Y}'\mathbf{E}\mathbf{Y}$ is a ratio of two independent chi-squared variables if and only if, for some positive constant θ,

$$\mathbf{A}_l\Sigma\mathbf{A}_l = \theta\mathbf{A}_l, \quad \mathbf{E}\Sigma\mathbf{E} = \theta\mathbf{E} \quad \text{and} \quad \mathbf{A}_l\Sigma\mathbf{E} = \mathbf{O}. \quad (4.3)$$

This will entail that the F-ratio $[r(\mathbf{E})/r(\mathbf{A}_l)]\mathbf{Y}'\mathbf{A}_l\mathbf{Y}/\mathbf{Y}'\mathbf{E}\mathbf{Y}$ follows a noncentral Fisher distribution $\mathcal{F}(r(\mathbf{A}_l), r(\mathbf{E}), \beta'\mathbf{X}'\mathbf{A}_l\mathbf{X}\beta)$. A word of caution is in order here: (4.3) does not provide a necessary and sufficient condition for the F-ratio to admit a Fisher distribution since a random variable having a Fisher distribution is not necessarily a ratio of two independent chi-squared variables. Kotlarski (1964) has characterized the set of distributions of bivariate random variables where the quotient of their coordinates follows a Fisher distribution.

3.   Validity conditions for the F-ratio tests

Consider now model (4.2). In matrix notation, let

$$\mathbf{Y}_{(ij)} = (Y_{ij1}, \ldots, Y_{ijp})'$$

be the vector of observations from the jth experimental unit within the ith group,

$$\mathbf{Y}_{(i)} = (\mathbf{Y}'_{(i1)}, \ldots, \mathbf{Y}'_{(in_i)})'$$

be the vector of n_ip observations from the ith group and

$$\mathbf{Y} = (\mathbf{Y}'_{(1)}, \ldots, \mathbf{Y}'_{(g)})'$$

be the vector of all np observations. Then, model (4.2) can be written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

where $\mathbf{X} = (\mathbf{1}_{np}\ \ \mathbf{J}_n \otimes \mathbf{1}_p\ \ \mathbf{I}_n \otimes \mathbf{1}_p\ \ \mathbf{J}_n \otimes \mathbf{I}_p\ \ \mathbf{X}_{\boldsymbol{\tau}}\ \ \mathbf{X}_{\boldsymbol{\lambda}})$, with $\otimes$ denoting the Kronecker product, $\mathbf{1}_m$ being a $m \times 1$ vector with all entries equal to 1, $\mathbf{J}_n$ being the block-diagonal matrix $\text{diag}(\mathbf{1}_{n_1}, \ldots, \mathbf{1}_{n_g})$ and $\mathbf{X}_{\boldsymbol{\tau}}$ and $\mathbf{X}_{\boldsymbol{\lambda}}$ representing the design matrices associated with the treatment and carryover components, respectively. Moreover, $\boldsymbol{\beta} = (\mu\ \ \boldsymbol{\gamma}'\ \ \boldsymbol{\alpha}'\ \ \boldsymbol{\pi}'\ \ \boldsymbol{\tau}'\ \ \boldsymbol{\lambda}')'$, where $\boldsymbol{\gamma}' = (\gamma_1, \ldots, \gamma_g)$, $\boldsymbol{\alpha}' = (\alpha_{11}, \ldots, \alpha_{1n_1}, \ldots, \alpha_{g1}, \ldots, \alpha_{gn_g})$. $\boldsymbol{\pi}' = (\pi_{11}, \ldots, \pi_{1p}, \ldots, \pi_{g1}, \ldots, \pi_{gp})$, $\boldsymbol{\tau}' = (\tau_1, \ldots, \tau_t)$, $\boldsymbol{\lambda}' = (\lambda_1, \ldots, \lambda_t)$, and $\boldsymbol{\varepsilon}' = (\varepsilon_{111}, \ldots, \varepsilon_{gn_gp})$.

Based on the ordinary least squares analysis, the sum of squares due to both direct and carryover effects together is given by $R(\boldsymbol{\tau}, \boldsymbol{\lambda}|\mu, \boldsymbol{\gamma}, \boldsymbol{\alpha}, \boldsymbol{\pi})$

$$= \mathbf{Y}'[\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^-\mathbf{X}_1']\mathbf{X}_{\boldsymbol{\tau}\boldsymbol{\lambda}}\mathbf{C}_{\boldsymbol{\tau}\boldsymbol{\lambda}}^-\mathbf{X}_{\boldsymbol{\tau}\boldsymbol{\lambda}}'[\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^-\mathbf{X}_1']\mathbf{Y}$$
$$= \mathbf{Y}'\mathbf{A}_{\boldsymbol{\tau}\boldsymbol{\lambda}}\mathbf{Y}, \text{ say},$$

where $\mathbf{X}_1 = (\mathbf{1}_{np}\ \ \mathbf{J}_n \otimes \mathbf{1}_p\ \ \mathbf{I}_n \otimes \mathbf{1}_p\ \ \mathbf{J}_n \otimes \mathbf{I}_p)$, $\mathbf{X}_{\boldsymbol{\tau}\boldsymbol{\lambda}} = (\mathbf{X}_{\boldsymbol{\tau}}\ \ \mathbf{X}_{\boldsymbol{\lambda}})$, and $\mathbf{C}_{\boldsymbol{\tau}\boldsymbol{\lambda}} = \mathbf{X}_1'[\mathbf{I} - \mathbf{X}_{\boldsymbol{\tau}\boldsymbol{\lambda}}(\mathbf{X}_{\boldsymbol{\tau}\boldsymbol{\lambda}}'\mathbf{X}_{\boldsymbol{\tau}\boldsymbol{\lambda}})^-\mathbf{X}_{\boldsymbol{\tau}\boldsymbol{\lambda}}']\mathbf{X}_1$. If the combined effect of the treatment and carryover components is significantly different from zero, we are then interested in the effect of each component separately. For that purpose, the sum of squares for direct treatment effects adjusted to all other effects in the model is given by $R(\boldsymbol{\tau}|\mu, \boldsymbol{\gamma}, \boldsymbol{\alpha}, \boldsymbol{\pi}, \boldsymbol{\lambda})$

$$= \mathbf{Y}'[\mathbf{I} - \mathbf{M}_{\boldsymbol{\tau}}(\mathbf{M}_{\boldsymbol{\tau}}'\mathbf{M}_{\boldsymbol{\tau}})^-\mathbf{M}_{\boldsymbol{\tau}}']\mathbf{X}_{\boldsymbol{\tau}}\mathbf{C}_{\boldsymbol{\tau}}^-\mathbf{X}_{\boldsymbol{\tau}}'[\mathbf{I} - \mathbf{M}_{\boldsymbol{\tau}}(\mathbf{M}_{\boldsymbol{\tau}}'\mathbf{M}_{\boldsymbol{\tau}})^-\mathbf{M}_{\boldsymbol{\tau}}']\mathbf{Y}$$
$$= \mathbf{Y}'\mathbf{A}_{\boldsymbol{\tau}}\mathbf{Y}, \text{ say},$$

where $\mathbf{M}_{\boldsymbol{\tau}} = (\mathbf{X}_1\ \ \mathbf{X}_{\boldsymbol{\lambda}})$ and $\mathbf{C}_{\boldsymbol{\tau}} = \mathbf{X}_{\boldsymbol{\tau}}'[\mathbf{I} - \mathbf{M}_{\boldsymbol{\tau}}(\mathbf{M}_{\boldsymbol{\tau}}'\mathbf{M}_{\boldsymbol{\tau}})^-\mathbf{M}_{\boldsymbol{\tau}}']\mathbf{X}_{\boldsymbol{\tau}}$, and the sum of square for carryover effects adjusted to all other effects in the model is given by $R(\boldsymbol{\lambda}|\mu, \boldsymbol{\gamma}, \boldsymbol{\alpha}, \boldsymbol{\pi}, \boldsymbol{\tau})$

$$= \mathbf{Y}'[\mathbf{I} - \mathbf{M}_{\boldsymbol{\lambda}}(\mathbf{M}_{\boldsymbol{\lambda}}'\mathbf{M}_{\boldsymbol{\lambda}})^-\mathbf{M}_{\boldsymbol{\lambda}}']\mathbf{X}_{\boldsymbol{\lambda}}\mathbf{C}_{\boldsymbol{\lambda}}^-\mathbf{X}_{\boldsymbol{\lambda}}'[\mathbf{I} - \mathbf{M}_{\boldsymbol{\lambda}}(\mathbf{M}_{\boldsymbol{\lambda}}'\mathbf{M}_{\boldsymbol{\lambda}})^-\mathbf{M}_{\boldsymbol{\lambda}}']\mathbf{Y}$$
$$= \mathbf{Y}'\mathbf{A}_{\boldsymbol{\lambda}}\mathbf{Y}, \text{ say},$$

where $\mathbf{M}_{\boldsymbol{\lambda}} = (\mathbf{X}_1\ \ \mathbf{X}_{\boldsymbol{\tau}})$ and $\mathbf{C}_{\boldsymbol{\lambda}} = \mathbf{X}_{\boldsymbol{\lambda}}'[\mathbf{I} - \mathbf{M}_{\boldsymbol{\lambda}}(\mathbf{M}_{\boldsymbol{\lambda}}'\mathbf{M}_{\boldsymbol{\lambda}})^-\mathbf{M}_{\boldsymbol{\lambda}}']\mathbf{X}_{\boldsymbol{\lambda}}$.

Let us now assume that the vector $\mathbf{Y}$ has a multivariate normal distribution with $E(\mathbf{Y}) = \mathbf{X}\boldsymbol{\beta}$ and the following covariance structure:

$$\text{Cov}(\mathbf{Y}_{(i)}, \mathbf{Y}_{(i')}) = \begin{cases} \boldsymbol{\Sigma}_i & \text{if } i = i' \\ \mathbf{O} & \text{if } i \neq i' \end{cases}.$$

In other words, observations from different groups are independent and observations within groups are possibly correlated. Recall that in clinical trials, the group factor typically represents different centres or physicians' practices where the treatments are investigated. This can possibly introduce some correlation between subject measurements within the groups. It is however reasonable to assume independence between experimental units from different groups and completely inappropriate to assume independence between observations within the same experimental unit.

The F-ratios, based on the ordinary least squares procedure, for testing the hypotheses of no direct treatment and carryover effects, either jointly or separately, are

$$\mathcal{F}_{\boldsymbol{\tau}\boldsymbol{\lambda}} = \frac{[(n-g)(p-1)-2(t-1)]R(\boldsymbol{\tau},\boldsymbol{\lambda}|\mu,\boldsymbol{\gamma},\boldsymbol{\alpha},\boldsymbol{\pi})}{2(t-1)SS_{error}},$$

$$\mathcal{F}_{\boldsymbol{\tau}} = \frac{[(n-g)(p-1)-2(t-1)]R(\boldsymbol{\tau}|\mu,\boldsymbol{\gamma},\boldsymbol{\alpha},\boldsymbol{\pi},\boldsymbol{\lambda})}{(t-1)SS_{error}},$$

and

$$\mathcal{F}_{\boldsymbol{\lambda}} = \frac{[(n-g)(p-1)-2(t-1)]R(\boldsymbol{\lambda}|\mu,\boldsymbol{\gamma},\boldsymbol{\alpha},\boldsymbol{\pi},\boldsymbol{\tau})}{(t-1)SS_{error}}.$$

According to Section 2, $[r(\mathbf{A}_{\boldsymbol{\tau}\boldsymbol{\lambda}})/r(\mathbf{E})]\mathcal{F}_{\boldsymbol{\tau}\boldsymbol{\lambda}}$ is a ratio of two independent chi-squared variables if and only if, for some $\theta > 0$,

$$\mathbf{A}_{\boldsymbol{\tau}\boldsymbol{\lambda}}\boldsymbol{\Sigma}\mathbf{A}_{\boldsymbol{\tau}\boldsymbol{\lambda}} = \theta\mathbf{A}_{\boldsymbol{\tau}\boldsymbol{\lambda}}, \quad \mathbf{E}\boldsymbol{\Sigma}\mathbf{E} = \theta\mathbf{E} \quad \text{and} \quad \mathbf{A}_{\boldsymbol{\tau}\boldsymbol{\lambda}}\boldsymbol{\Sigma}\mathbf{E} = \mathbf{O}, \quad (4.4)$$

whence $\mathcal{F}_{\boldsymbol{\tau}\boldsymbol{\lambda}}$ will follow a Fisher distribution. This means that all the elements of $\boldsymbol{\Sigma}$ can be expressed as linear combinations of at most $1 + np^2 + p\sum_{i=1}^{g} n_i^2$ constants, as the following theorem will show.

THEOREM 4.1 *The quantity* $[r(\mathbf{A}_{\boldsymbol{\tau}\boldsymbol{\lambda}})/r(\mathbf{E})]\mathcal{F}_{\boldsymbol{\tau}\boldsymbol{\lambda}}$ *is a ratio of two independent chi-squared variables if and only if each covariance matrix* $\boldsymbol{\Sigma}_i = ((\sigma_{ijj'kk'}))$, $1 \le i \le g$, *have elements of the form:*

$$\left. \begin{array}{l} \sigma_{ijj'kk'} = v_{ijj'k} + v_{ij'jk'} + w_{ijkk'} + w_{ij'k'k} + \theta\delta_{jj'}\delta_{kk'}, \\ j, j' = 1, \ldots, n_i \text{ and } k, k' = 1, \ldots, p, \end{array} \right\} \quad (4.5)$$

where $\theta > 0$, $v_{ijj'k}$ *and* $w_{ijkk'}$ *are arbitrary constants,* $\delta_{ll'}$ *is the Kronecker symbol and* $\sigma_{ijj'kk'} = \mathrm{Cov}(Y_{ijk}, Y_{ij'k'})$.

Proof. *Sufficiency.* First, define for each i, $1 \le i \le g$, the $p \times 1$ vectors $\mathbf{v}_{ijj'} = (v_{ijj'1}, \ldots, v_{ijj'p})'$ and $\mathbf{w}_{ijk'} = (w_{ij1k'}, \ldots, w_{ijpk'})'$ along with the $n_i p \times n_i$ matrix $\mathcal{V}_i$ and the $n_i p \times p$ matrix $\mathcal{W}_i$, where

$$\mathcal{V}_i = \begin{pmatrix} \mathbf{v}_{i11} & \cdots & \mathbf{v}_{i1n_i} \\ \vdots & \ddots & \vdots \\ \mathbf{v}_{in_i1} & \cdots & \mathbf{v}_{in_in_i} \end{pmatrix} \text{ and } \mathcal{W}_i = \begin{pmatrix} \mathbf{w}_{i11} & \cdots & \mathbf{w}_{i1p} \\ \vdots & \ddots & \vdots \\ \mathbf{w}_{in_i1} & \cdots & \mathbf{w}_{in_ip} \end{pmatrix}.$$

Thus, under assumption (4.5), the covariance matrix $\boldsymbol{\Sigma}_i$ can be written as $\mathbf{V}_i + \mathbf{V}'_i + \mathbf{W}_i + \mathbf{W}'_i + \theta\mathbf{I}$, where $\mathbf{V}_i = \mathcal{V}_i \otimes \mathbf{1}'_p = \mathcal{V}_i(\mathbf{I}_{n_i} \otimes \mathbf{1}'_p)$ and $\mathbf{W}_i = \mathbf{1}'_{n_i} \otimes \mathcal{W}_i = \mathcal{W}_i(\mathbf{1}'_{n_i} \otimes \mathbf{I}_p)$, $1 \le i \le g$, and it follows that $\boldsymbol{\Sigma} = \mathbf{V} + \mathbf{V}' + \mathbf{W} + \mathbf{W}' + \theta\mathbf{I}$, where

$$\mathbf{V} = \mathrm{diag}(\mathbf{V}_1, \dots, \mathbf{V}_g) = \mathrm{diag}(\mathcal{V}_1, \dots, \mathcal{V}_g)(\mathbf{I}_n \otimes \mathbf{1}'_p)$$

and

$$\mathbf{W} = \mathrm{diag}(\mathbf{W}_1, \dots, \mathbf{W}_g) = \mathrm{diag}(\mathcal{W}_1, \dots, \mathcal{W}_g)(\mathbf{J}'_n \otimes \mathbf{I}_p).$$

But, because $[\mathbf{I} - \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^-\boldsymbol{X}']\boldsymbol{X} = \mathbf{O}$

$$\Rightarrow [\mathbf{I} - \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^-\boldsymbol{X}'](\mathbf{I}_n \otimes \mathbf{1}_p) = \mathbf{O}$$
$$\text{and } [\mathbf{I} - \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^-\boldsymbol{X}'](\mathbf{J}_n \otimes \mathbf{I}_p) = \mathbf{O}$$
$$\Rightarrow [\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^-\mathbf{X}']\mathbf{V}' = \mathbf{O} \quad \text{and} \quad [\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^-\mathbf{X}']\mathbf{W}' = \mathbf{O}$$
$$\Rightarrow \mathbf{V}[\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^-\mathbf{X}'] = \mathbf{O} \quad \text{and} \quad \mathbf{W}[\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^-\mathbf{X}'] = \mathbf{O}.$$

Replacing $\mathbf{X}$ by $\mathbf{X}_1$, it can be shown in a similar fashion that, for $\mathbf{Z}=\mathbf{V}$ or $\mathbf{W}$:

$$[\mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1]\mathbf{Z}' = \mathbf{Z}[\mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1] = \mathbf{O}.$$

These, along with the fact that the matrices $\mathbf{A}_{\tau\lambda}$ and $\mathbf{E}$ are idempotent and $\mathbf{A}_{\tau\lambda}\mathbf{E} = \mathbf{O}$ (Section 2), imply easily (4.4).

Necessity. First, according to Section 2, the matrix $(\mathbf{X}'\mathbf{X})^-$ can be written as

$$\begin{pmatrix} \mathbf{C}^-_{\tau\lambda} & -\mathbf{C}^-_{\tau\lambda}\mathbf{X}'_{\tau\lambda}\mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^- \\ -(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1\mathbf{X}_{\tau\lambda}\mathbf{C}^-_{\tau\lambda} & (\mathbf{X}'_1\mathbf{X}_1)^- + (\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1\mathbf{X}_{\tau\lambda}\mathbf{C}^-_{\tau\lambda}\mathbf{X}'_{\tau\lambda}\mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^- \end{pmatrix}$$

where $\mathbf{X} = (\mathbf{X}_{\tau\lambda} \quad \mathbf{X}_1)$ and $\mathbf{C}_{\tau\lambda} = \mathbf{X}'_{\tau\lambda}[\mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1]\mathbf{X}_{\tau\lambda}$. Hence,

$$\begin{aligned} \mathbf{X}(\mathbf{X}'\mathbf{X})^-\mathbf{X}' = {}& \mathbf{X}_{\tau\lambda}\mathbf{C}^-_{\tau\lambda}\mathbf{X}'_{\tau\lambda} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1\mathbf{X}_{\tau\lambda}\mathbf{C}^-_{\tau\lambda}\mathbf{X}'_{\tau\lambda} \\ & - \mathbf{X}_{\tau\lambda}\mathbf{C}^-_{\tau\lambda}\mathbf{X}'_{\tau\lambda}\mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1 + \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1 \\ & + \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1\mathbf{X}_{\tau\lambda}\mathbf{C}^-_{\tau\lambda}\mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1 \\ = {}& \mathbf{A}_{\tau\lambda} + \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1 \end{aligned}$$

and the matrix $\mathbf{E}$ can be expressed as $\mathbf{E} = \mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1 - \mathbf{A}_{\tau\lambda}$. Now, assume that (4.4) is satisfied. Then, we have in particular the relation

$$\mathbf{E}\boldsymbol{\Sigma}\mathbf{E} = \theta\mathbf{E}$$
$$\Leftrightarrow [\mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1 - \mathbf{A}_{\tau\lambda}]\boldsymbol{\Sigma}\mathbf{E} = \theta\mathbf{E}$$
$$\Leftrightarrow [\mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1]\boldsymbol{\Sigma}\mathbf{E} = \theta\mathbf{E}$$
$$\Leftrightarrow [\mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1]\boldsymbol{\Sigma}[\mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1]$$
$$\quad -[\mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1]\boldsymbol{\Sigma}\mathbf{A}_{\tau\lambda} = \theta[\mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^-\mathbf{X}'_1] - \theta\mathbf{A}_{\tau\lambda}.$$

However,

$$\mathbf{A}_{\tau\lambda}\mathbf{\Sigma E} = \mathbf{O} \Rightarrow \mathbf{E\Sigma A}_{\tau\lambda} = \mathbf{O}$$
$$\Rightarrow [\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^-\mathbf{X}_1']\mathbf{\Sigma A}_{\tau\lambda} = \mathbf{A}_{\tau\lambda}\mathbf{\Sigma A}_{\tau\lambda} = \theta\mathbf{A}_{\tau\lambda}.$$

Hence, $\mathbf{E\Sigma E} = \theta\mathbf{E}$ if and only if

$$[\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^-\mathbf{X}_1']\mathbf{\Sigma}[\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^-\mathbf{X}_1'] = \theta[\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^-\mathbf{X}_1'].$$

Recall that $\mathbf{X}_1 = (\mathbf{1}_{np}\ \ \mathbf{J}_n \otimes \mathbf{1}_p\ \ \mathbf{I}_n \otimes \mathbf{1}_p\ \ \mathbf{J}_n \otimes \mathbf{I}_p)$. After some tedious algebra, we get

$$[\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^-\mathbf{X}_1'] = [\mathbf{I}_n - \mathbf{J}_n(\mathbf{J}_n'\mathbf{J}_n)^{-1}\mathbf{J}_n'] \otimes (\mathbf{I}_p - \tfrac{1}{p}\mathbf{1}_p\mathbf{1}_p'),$$

where $\mathbf{J}_n(\mathbf{J}_n'\mathbf{J}_n)^{-1}\mathbf{J}_n' = \mathrm{diag}(\tfrac{1}{n_1}\mathbf{1}_{n_1}\mathbf{1}_{n_1}', \ldots, \tfrac{1}{n_g}\mathbf{1}_{n_g}\mathbf{1}_{n_g}')$. Consequently,

$$[\mathbf{I}_n - \mathbf{J}_n(\mathbf{J}_n'\mathbf{J}_n)^{-1}\mathbf{J}_n'] \otimes (\mathbf{I}_p - \tfrac{1}{p}\mathbf{1}_p\mathbf{1}_p')\mathbf{\Sigma}[\mathbf{I}_n - \mathbf{J}_n(\mathbf{J}_n'\mathbf{J}_n)^{-1}\mathbf{J}_n'] \otimes (\mathbf{I}_p - \tfrac{1}{p}\mathbf{1}_p\mathbf{1}_p') =$$
$$\theta[\mathbf{I}_n - \mathbf{J}_n(\mathbf{J}_n'\mathbf{J}_n)^{-1}\mathbf{J}_n'] \otimes (\mathbf{I}_p - \tfrac{1}{p}\mathbf{1}_p\mathbf{1}_p')$$

if and only if, for each i, $1 \le i \le g$,

$$[(\mathbf{I}_{n_i} - \tfrac{1}{n_i}\mathbf{1}_{n_i}\mathbf{1}_{n_i}') \otimes (\mathbf{I}_p - \tfrac{1}{p}\mathbf{1}_p\mathbf{1}_p')]\mathbf{\Sigma}_i[(\mathbf{I}_{n_i} - \tfrac{1}{n_i}\mathbf{1}_{n_i}\mathbf{1}_{n_i}') \otimes (\mathbf{I}_p - \tfrac{1}{p}\mathbf{1}_p\mathbf{1}_p')] =$$
$$\theta[(\mathbf{I}_{n_i} - \tfrac{1}{n_i}\mathbf{1}_{n_i}\mathbf{1}_{n_i}') \otimes (\mathbf{I}_p - \tfrac{1}{p}\mathbf{1}_p\mathbf{1}_p')],$$

that is, if and only if, for each i, j, j', k and k', $1 \le i \le g$, $1 \le j$ and $j' \le n_i$, $1 \le k$ and $k' \le p$,

$$\left\{ \begin{array}{l} \sigma_{ijj'kk'} - \sigma_{ijj'k} - \sigma_{ijj'\,k'} + \sigma_{ijj'.} \\ -\sigma_{ij.kk'} + \sigma_{ij.k} + \sigma_{ij..k'} - \sigma_{ij.} \\ -\sigma_{i.j'kk'} + \sigma_{i.j'k} + \sigma_{i.j'\,k'} - \sigma_{i.j'.} \\ +\sigma_{i..kk'} - \sigma_{i..k} - \sigma_{i...k'} + \sigma_{i...} \end{array} \right\} = \theta(\delta_{jj'} - \frac{1}{n_i})(\delta_{kk'} - \frac{1}{p}), \quad (4.6)$$

where a dot stands for an average taken over the corresponding subscript.

Let us fix the index i, where $1 \le i \le g$. If we define $c_{ijj'kk'} = \sigma_{ijj'kk'} - \sigma_{ijj'k} - \sigma_{ijj'\,k'} + \sigma_{ijj'}$ and $d_{ijj'kk'} = c_{ijj'kk'} - c_{ij.kk'} - c_{i.j'kk'} + c_{i..kk'}$, we notice that identity (4.6) simply boils down to

$$d_{ijj'kk'} = \theta(\delta_{jj'} - \frac{1}{n_i})(\delta_{kk'} - \frac{1}{p}), \quad \text{for all } j, j', k \text{ and } k'. \quad (4.7)$$

Now, $\mathbf{\Sigma}_i$ being symmetric, it holds that $\sigma_{ijj'kk'} = \sigma_{ij'jk'k}$, for all j, j', k and k'. On the one hand, this entails $\sigma_{ijj'k} = \sigma_{ij'j.k}$, for all j, j' and k, and $\sigma_{ijj'.} = \sigma_{ij'j..}$ for all j and j'; on the other hand, this implies $c_{ijj'kk'} = c_{ij'jk'k}$, for all j, j', k and k', from which $c_{ij.kk'} = c_{i.jk'k}$, for all j, k and k', and $c_{i..kk'} = c_{i..k'k}$, for all k and k', follow. Moreover, if we define $a_{ijj'k} = \sigma_{ijj'k} - \frac{1}{2}\sigma_{ijj'}$, we may always rewrite $\sigma_{ijj'kk'}$ as

$$\sigma_{ijj'kk'} = (\sigma_{ijj'k} - \frac{1}{2}\sigma_{ijj'.}) + (\sigma_{ijj'.k'} - \frac{1}{2}\sigma_{ijj'.})$$

$$+ (\sigma_{ijj'kk'} - \sigma_{ijj'k} - \sigma_{ijj'.k'} + \sigma_{ijj'}.)$$
$$= a_{ijj'k} + a_{ij'jk'} + c_{ijj'kk'}. \tag{4.8}$$

Similarly, if we put $b_{ijkk'} = c_{ij\,kk'} - \frac{1}{2}c_{i\,.kk'}$, $c_{ijj'kk'}$ may always be rewritten as

$$c_{ijj'kk'} = (c_{ij\,kk'} - \frac{1}{2}c_{i.\,kk'}) + (c_{i\,j'kk'} - \frac{1}{2}c_{i\,kk'})$$
$$+ (c_{ijj'kk'} - c_{ij\,kk'} - c_{i.j'kk'} + c_{i\,.kk'})$$
$$= b_{ijkk'} + b_{ij'k'k} + d_{ijj'kk'}$$
$$= b_{ijkk'} + b_{ij'k'k} + \theta(\delta_{jj'} - \frac{1}{n_i})(\delta_{kk'} - \frac{1}{p}),$$

in view of (4.7). By inserting the latter identity into (4.8), we finally get (4.5) where $v_{ijj'k} = a_{ijj'k} - \frac{1}{2p}\theta\delta_{jj'}$ and $w_{ijkk'} = b_{ijkk'} - \frac{1}{2n_i}\theta(\delta_{kk'} - \frac{1}{p})$. $\square$

Any matrix whose elements satisfy the covariance structure (4.5) will be referred to as a matrix of type F.

THEOREM 4.2 *If each covariance matrix* Σ_i, $1 \le i \le g$, *has a type F structure, then both* $\mathcal{F}_\tau$ *and* $\mathcal{F}_\lambda$ *follow a Fisher distribution.*

Proof. Proceeding as in the first part of the proof of Theorem 4.1, it can be shown that, for $\mathbf{Z}=\mathbf{V}$ or $\mathbf{W}$ and for $l=\tau$ or λ, we have

$$[\mathbf{I} - \mathbf{M}_l(\mathbf{M}_l'\mathbf{M}_l)^-\mathbf{M}_l']\mathbf{Z}' = \mathbf{Z}[\mathbf{I} - \mathbf{M}_l(\mathbf{M}_l'\mathbf{M}_l)^-\mathbf{M}_l'] = \mathbf{O}.$$

These, along with the fact that the matrices $\mathbf{A}_l$ and $\mathbf{E}$ are idempotent and $\mathbf{A}_l\mathbf{E} = \mathbf{O}$ (Section 2), imply $\mathbf{A}_l\Sigma\mathbf{A}_l = \theta\mathbf{A}_l$ and $\mathbf{A}_l\Sigma\mathbf{E} = \mathbf{O}$. $\square$

The covariance structure (4.5) seems complicated, but using the same transformation Huynh and Feldt (1970) employed in their paper, we can express it in a simpler form, and thus a test of the satisfaction of the covariance assumption leading to exact F-tests could be performed using Mauchly's sphericity criterion (Anderson 1984, Chen et al. 2002). To show that the sphericity test applies, consider the $(m - 1) \times m$ matrix $\mathbf{B}$ such that the $m \times m$ matrix noted below is orthonormal:

$$\begin{pmatrix} m^{-1/2} & \cdots & m^{-1/2} \\ & \mathbf{B} & \end{pmatrix}.$$

The matrix $\mathbf{B}$ will be referred to as an Helmert matrix of size m and has the following properties:

1. $\mathbf{B}\mathbf{B}' = \mathbf{I}_{(m-1)}$,
2. $\mathbf{B}'\mathbf{B} = \mathbf{I}_m - \frac{1}{m}\mathbf{1}_m\mathbf{1}_m'.$

We can now state the following theorem.

THEOREM 4.3 *Let* $\mathbf{C}$ *be an arbitrary Helmert matrix of size* p *and* $\mathbf{D}_i$ *be an arbitrary Helmert matrix of size* n_i, $1 \leq i \leq g$. *Then, for* $1 \leq i \leq g$, *the covariance matrix* $\boldsymbol{\Sigma}_i$ *has a type F structure if and only if the covariance matrix of* $\mathbf{Y}_{(i)}^* = (\mathbf{D}_i \otimes \mathbf{C})\mathbf{Y}_{(i)}$ *is* $\boldsymbol{\Sigma}_i^* = \theta \mathbf{I}_{(n_i-1)(p-1)}$.

Proof. Let $\boldsymbol{\Sigma}_i$, $1 \leq i \leq g$, be of type F with same constant $\theta > 0$. Then, it can be written as

$$\boldsymbol{\Sigma}_i = \mathbf{V}_i + \mathbf{V}_i' + \mathbf{W}_i + \mathbf{W}_i' + \theta \mathbf{I}.$$

It is easy to show that $\mathbf{V}_i(\mathbf{D}_i' \otimes \mathbf{C}') = \mathbf{W}_i(\mathbf{D}_i' \otimes \mathbf{C}') = \mathbf{O}$ and $(\mathbf{D}_i \otimes \mathbf{C})\mathbf{V}_i' = (\mathbf{D}_i \otimes \mathbf{C})\mathbf{W}_i' = \mathbf{O}'$. Thus,

$$\boldsymbol{\Sigma}_i^* = (\mathbf{D}_i \otimes \mathbf{C})\boldsymbol{\Sigma}_i(\mathbf{D}_i' \otimes \mathbf{C}') = \theta \mathbf{I}_{(n_i-1)(p-1)}.$$

To complete the proof, let $\boldsymbol{\Sigma}_i^* = \theta \mathbf{I}_{(n_i-1)(p-1)}$, $1 \leq i \leq g$. Then,

$$(\mathbf{D}_i \otimes \mathbf{C})\boldsymbol{\Sigma}_i(\mathbf{D}_i' \otimes \mathbf{C}') = \theta \mathbf{I}_{(n_i-1)(p-1)}$$

$$\Leftrightarrow (\mathbf{D}_i' \otimes \mathbf{C}')(\mathbf{D}_i \otimes \mathbf{C})\boldsymbol{\Sigma}_i(\mathbf{D}_i' \otimes \mathbf{C}')(\mathbf{D}_i \otimes \mathbf{C}) = \theta(\mathbf{D}_i' \otimes \mathbf{C}')(\mathbf{D}_i \otimes \mathbf{C})$$

$$\Leftrightarrow [(\mathbf{I}_{n_i} - \frac{1}{n_i}\mathbf{1}_{n_i}\mathbf{1}_{n_i}') \otimes (\mathbf{I}_p - \frac{1}{p}\mathbf{1}_p\mathbf{1}_p')]\boldsymbol{\Sigma}_i[(\mathbf{I}_{n_i} - \frac{1}{n_i}\mathbf{1}_{n_i}\mathbf{1}_{n_i}') \otimes (\mathbf{I}_p - \frac{1}{p}\mathbf{1}_p\mathbf{1}_p')] =$$

$$\theta[(\mathbf{I}_{n_i} - \frac{1}{n_i}\mathbf{1}_{n_i}\mathbf{1}_{n_i}') \otimes (\mathbf{I}_p - \frac{1}{p}\mathbf{1}_p\mathbf{1}_p')].$$

Hence $\boldsymbol{\Sigma}_i$ is of type F by the same reasoning employed in the proof of Theorem 4.1. $\qquad\square$

Some particular cases ensuing from Theorem 4.1 are worthy of mention. For instance, if we set $v_{ijj'k} = \delta_{jj'}v_{i1} + (1 - \delta_{jj'})v_{i2}$ and $w_{ijkk'} = \delta_{kk'}w_{i1} + (1 - \delta_{kk'})w_{i2}$, for all i, j, j', k and k', we are in a situation where random errors associated with experimental units are exchangeable within groups and where random errors associated with the responses of an experimental unit within periods are exchangeable. Even more particularly, if we put $n_1 = \ldots = n_g = p = t$, $v_{i1} = \frac{1}{2}\sigma^2(\rho_1 - \frac{1}{2}\rho_3)$, $w_{i1} = \frac{1}{2}\sigma^2(\rho_2 - \frac{1}{2}\rho_3)$, $v_{i2} = w_{i2} = \frac{1}{4}\sigma^2\rho_3$ and $\theta = \sigma^2(1 - \rho_1 - \rho_2 + \rho_3)$, we get the conditions under which Monga and Tardif (1992) established the validity of the F-ratio test for treatment effects in replicated latin square designs. On the other hand, if we set $v_{ijj'k} = \delta_{jj'}v_{ijk}$ and $w_{ijkk'} = 0$, for all i, j, k and k', we have the situation where all experimental units are independent and the conditions for the validity of the F-ratio tests are then that the covariance matrices of $\mathbf{Y}_{(ij)}$ $1 \leq i \leq g$ and $1 \leq j \leq n_i$,

possess the type H structure introduced by Huynh and Feldt (1970) for randomized block and split-plot designs.

It is also worthy of mention that Theorems 4.1 and 4.2 immediately generalize to models including more parameters such as treatment by period interaction and higher order carryover effects (see for example Bose and Mukherjee 2003). Finally, it is also important to stress that the type F structure is only a sufficient condition for the validity of the tests for direct treatment effects adjusted to carryover effects and the other parameters in the model and for carryover effects adjusted to the direct treatment effects and the other parameters. Therefore, $\mathcal{F}_\tau$ and $\mathcal{F}_\lambda$ can be valid under other covariance structures. These other structures will however depend on the the specific experimental design $\mathbf{X}_\tau$ considered and necessary conditions for the validity of $\mathcal{F}_\tau$ will in general not be the same as those for the validity of $\mathcal{F}_\lambda$.

4.   Optimality results under type F structure

In the general design case, optimality criteria are usually defined in terms of functions of the information matrix of the design or the covariance matrix $\mathbf{\Sigma}^*$ of $(t-1)$ orthogonal and normalized contrasts between the t treatments. A good design is one which makes $\mathbf{\Sigma}^*$ 'small' in some sense. Different ways of defining 'small' have led to different optimality criteria:

1. the D-optimal design minimizes the determinant of $\mathbf{\Sigma}^*$;
2. the A-optimal design minimizes the trace of $\mathbf{\Sigma}^*$; and
3. the E-optimal design minimizes the maximum eigenvalue of $\mathbf{\Sigma}^*$.

Kiefer (1975) subsumed these criteria and others into his criterion of universal optimality: the universal (U-)optimal design is also D-, A- and E-optimal. Since most of the optimality results for crossover designs were developed under the assumption of uncorrelated errors and common variance (Cheng and Wu 1980, Hedayat and Afsarinejad 1978, Kunert 1984, Kushner 1998), it is worth examining how the assumption of a type F structure for the covariance matrix affects these results.

Let $\mathbf{D}$ be a $(t-1) \times t$ matrix such that its rows form a set of $(t-1)$ orthonormal contrasts. Then, for $l = \tau$ or λ,

$$\mathbf{\Sigma}^* = \mathrm{Var}(\mathbf{D}\hat{\boldsymbol{\beta}}_l)$$
$$= \mathbf{D}\mathbf{C}_l^- \mathbf{X}_l'[\mathbf{I} - \mathbf{M}_l(\mathbf{M}_l'\mathbf{M}_l)^- \mathbf{M}_l']\mathbf{\Sigma}[\mathbf{I} - \mathbf{M}_l(\mathbf{M}_l'\mathbf{M}_l)^- \mathbf{M}_l']\mathbf{X}_l\mathbf{C}_l^- \mathbf{D}'.$$

Under the assumption of uncorrelated errors with common variance θ, $\mathbf{\Sigma} = \theta\mathbf{I}$ and we get $\mathbf{\Sigma}^* = \theta\mathbf{D}\mathbf{C}_l^- \mathbf{D}'$. However, under the assumption of a type F matrix, we have

$$\Sigma^* = \theta \mathbf{D} \mathbf{C}_l^- \mathbf{D}' +$$
$$\mathbf{D} \mathbf{C}_l^- \mathbf{X}_l' [\mathbf{I} - \mathbf{M}_l (\mathbf{M}_l' \mathbf{M}_l)^- \mathbf{M}_l'] (\mathbf{V} + \mathbf{V}' + \mathbf{W} + \mathbf{W}')$$
$$[\mathbf{I} - \mathbf{M}_l (\mathbf{M}_l' \mathbf{M}_l)^- \mathbf{M}_l'] \mathbf{X}_l \mathbf{C}_l^- \mathbf{D}'$$
$$= \theta \mathbf{D} \mathbf{C}_l^- \mathbf{D}'.$$

Hence, the optimality results for crossover designs remain valid under the wider assumption of a type F structure for all covariance matrices Σ_i, $1 \leq i \leq g$, with common positive constant θ. Note that this result simply generalizes Corollary 2.2 in Kushner (1997) for the type H structure and model (4.1) to the type F structure and model (4.2).

5. Conclusion

Standard practice in analysing continuous data from crossover trials ignores the fact that the observations from different periods constitute a sequence of repeated measurements which are probably correlated. This paper has shown that the covariance matrix may exhibit a more general structure than is usually assumed to be essential for the validity of the ordinary least squares analysis. Hence, the practitioner might feel more comfortable using that technique. However, if the covariance structure is very different than a type F, the usual F-ratio tests for treatment and carryover effects can lead to serious errors in inference, as was shown by Bellavance, Tardif and Stephens (1996) in there simulations results. In this situation, it is preferable to use the modified F-test approximation they have proposed. In their simulations, this latter approximation test gave adequate control over the Type I error.

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Chapter 5

BIAS IN ESTIMATING THE VARIANCE OF K-FOLD CROSS-VALIDATION

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Yves Grandvalet

Abstract   Most machine learning researchers perform quantitative experiments to estimate generalization error and compare the performance of different algorithms (in particular, their proposed algorithm). In order to be able to draw statistically convincing conclusions, it is important to estimate the uncertainty of such estimates. This paper studies the very commonly used K-fold cross-validation estimator of generalization performance. The main theorem shows that there exists no universal (valid under all distributions) unbiased estimator of the variance of K-fold cross-validation, based on a single computation of the K-fold cross-validation estimator. The analysis that accompanies this result is based on the eigen-decomposition of the covariance matrix of errors, which has only three different eigenvalues corresponding to three degrees of freedom of the matrix and three components of the total variance. This analysis helps to better understand the nature of the problem and how it can make naive estimators (that don't take into account the error correlations due to the overlap between training and test sets) grossly underestimate variance. This is confirmed by numerical experiments in which the three components of the variance are compared when the difficulty of the learning problem and the number of folds are varied.

1.   Introduction

In machine learning, the standard measure of accuracy for trained models is the prediction error (PE), i.e. the expected loss on future examples. Learning algorithms themselves are often compared according to their average performance, which is formally defined as the expected value of prediction error (EPE) over training sets.

When the data distribution is unknown, PE and EPE cannot be computed. If the amount of data is large enough, PE can be estimated by the mean error over a hold-out test set. The usual variance estimates for means of independent samples can then be computed to derive error bars on the estimated prediction error, and to assess the statistical significance of differences between models.

The hold-out technique does not account for the variance with respect to the training set, and may thus be considered inappropriate for the purpose of algorithm comparison (Dietterich (1999)). Moreover, it makes an inefficient use of data which forbids its application to small sample sizes. In this situation, one rather uses computer intensive resampling methods such as cross-validation or bootstrap to estimate PE or EPE.

We focus here on K-fold cross-validation. While it is known that cross-validation provides an unbiased estimate of EPE, it is also known that its variance may be very large (Breiman (1996)). This variance should be estimated to provide faithful confidence intervals on PE or EPE, and to test the significance of observed differences between algorithms. This paper provides theoretical arguments showing the difficulty of this estimation.

The difficulties of the variance estimation have already been addressed (Dietterich (1999); Kohavi (1995); Nadeau and Bengio (2003)). Some distribution-free bounds on the deviations of cross-validation are available, but they are specific to some locally defined decision rules, such as nearest neighbors (Devroye et al. (1996)). This paper builds upon the work of Nadeau and Bengio (2003), which investigated in detail the theoretical and practical merits of several estimators of the variance of cross-validation. Our analysis departs from this work in the sampling procedure defining the cross-validation estimate. While Nadeau and Bengio (2003) consider K independent training and test splits, we focus on the standard K-fold cross-validation procedure, where there is no overlap between test sets: each example of the original data set is used once and only once as a test example.

This paper is organized as follows. Section 2 defines the measures of performance for algorithms, their estimation by K-fold cross-validation and similar procedures such as delete-m jackknife. Our theoretical findings are summarized in Sections 3–6. They are followed in Section 7 by experiments illustrating the effect of experimental conditions on the total variance and its decomposition in three components, and confirming the underestimation of variance obtained by the naive estimator commonly used by researchers.

2. General framework

2.1 Measures of performance

In machine learning, the performance measure differs according to the experimenter's viewpoint. In applications, we are interested in finding the best algorithm for solving the particular task at hand, specified by one particular training set and some information about the data generating process. In algorithm evaluation, we want to compare several learning algorithms for different learning tasks, and we care about the sensitivity of the learning algorithm to the choice of training examples.

Let $\mathcal{Z}$ be the vector space in which examples are represented. We have a training set $D = \{z_1, \ldots, z_n\}$, $z_i \in \mathcal{Z}$, which is obtained by independent draws from an unknown distribution P. We also have a learning algorithm A, which maps a data set of (almost) arbitrary size to a function F, that is $A : \mathcal{Z}^* \to \mathcal{F}$. Throughout this paper, we consider symmetric algorithms, i.e. A is insensitive to the ordering of examples in the training set D. The discrepancy between the prediction and the observation z is measured by a loss functional $L : \mathcal{F} \times \mathcal{Z} \to \mathbb{R}$. Typically, L is the quadratic loss in regression $(L(f, (x, y)) = (f(x) - y)^2)$ and the misclassification $\{0, 1\}$-loss in classification $((L(f, (x, y)) = 1_{f(x) \neq y})$.

Let $f = A(D)$ be the function returned by algorithm A on the training set D. In application based evaluation, the goal of learning is usually stated as the minimization of the prediction error, i.e. the expected loss on future test examples

$$\text{PE}(D) = E[L(f, z)], \tag{5.1}$$

where the expectation is taken with respect to z sampled from P.[1]

In algorithm based evaluation, we are not really interested in performances on a specific training set; we would like comparisons on a more general basis. In this context, the lowest level of generality can be stated as "training sets of size n sampled from P^n", and the performance of learning algorithm A can be measured by the expected performance of the functions returned in this situation

$$\text{EPE}(n) = E[L(A(D), z)], \tag{5.2}$$

where the expectation is taken with respect to D sampled from P^n and z independently sampled from P.

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[1]Note that we are using the same notation for random variables and their realization. The intended meaning will be specified when not clear from the context

Note that other types of performances measure can be proposed, based for example on parameters, or defined by the predictability in other frameworks, such as the prequential analysis (Dawid (1997)).

When the data distribution is unknown, PE and EPE cannot be computed. They have to be estimated, and it is often crucial to assess the uncertainty attached to this estimation:

- in application-oriented experiments, to give a confidence interval on PE;

- in algorithm-oriented experiments, to take into account the stability of a given algorithm. For comparisons between algorithms, it is essential to assess the statistical significance of observed differences in the estimate $\widehat{EPE}$.

Although this point is often overlooked, estimating the variance of the estimates $\widehat{PE}$ and $\widehat{EPE}$ requires caution.

2.2   Hold-out estimates of performance

If the amount of data is large enough, PE can be estimated by the mean error over a hold-out test set, and the usual variance estimate for means of independent variables can then be computed. However, even in the ideal situation where several independent training and test sets would be available, this estimate should not be applied to compute the variance of $\widehat{EPE}$.

As the performance measure EPE integrates over the training set, the latter is now considered as a random variable. Hence, even though training and test examples are independent, the test errors computed from a given training set are correlated due to the training set effect: a "bad" training set will cause large test errors while a "good" training set will cause small test errors. The consequences of neglecting the correlations of test errors are illustrated in the simple experimental setup described below.

EXPERIMENT 5.1 *Ideal hold-out estimate of* EPE.

We have $K = 10$ *independent training sets* $D_1, \ldots, D_K$ *of* n *independent examples* $\mathbf{z}_i = (\mathbf{x}_i, y_i)$, *where* $\mathbf{x}_i = (x_{i1}, \ldots, x_{id})'$ *is a* d-*dimensional centered Gaussian vector* ($d = 30$) *with covariance matrix identity,* $y_i = \sqrt{3/d} \sum_{k=1}^{d} x_{ik} + \varepsilon_i$ *with* ε_i *being independent, centered, unit variance Gaussian variables.*[2] *We also have* K *independent test sets* $T_1, \ldots, T_K$ *of size* n *sampled from the same distribution.*

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[2]The $\sqrt{3/d}$ factor provides an R^2 of approximately 3/4

The learning algorithm consists in fitting a line by ordinary least squares, and the estimate of EPE is the average quadratic loss on test examples $\widehat{\mathrm{EPE}} = \bar{L} = \frac{1}{K}\sum_{k=1}^{K}\frac{1}{n}\sum_{\mathbf{z}_i \in T_k} L_{ki}$, *where* $L_{ki} = L(A(D_k), \mathbf{z}_i)$.

The first estimate of variance of $\widehat{\mathrm{EPE}}$ *is* $\widehat{\theta}_1 = \frac{1}{Kn(Kn-1)}\sum_{k=1}^{K}\sum_i (L_{ki} - \bar{L})^2$, *which is unbiased provided there is no correlation between test errors. The second estimate is* $\widehat{\theta}_2 = \frac{1}{K(K-1)n^2}\sum_{k=1}^{K}\sum_{i,j}(L_{ki} - \bar{L})(L_{kj} - \bar{L})$, *which takes into account correlations between test errors.*

Figure 5.1 displays the mean of the two variance estimators $\widehat{\theta}_1$ and $\widehat{\theta}_1$ vs. the empirical variance of the hold-out estimate, in an ideal situation where 10 independent training and test sets are available. The variance of $\widehat{\mathrm{EPE}}(n)$ (estimated on 100 000 independent experiments) is displayed for reference by the dotted line. The average of $\widehat{\theta}_1$, the variance estimator ignoring correlations, shows that this estimate is highly biased, even for large sample sizes, whereas the variance estimator $\widehat{\theta}_2$, taking into account correlations, is unbiased.
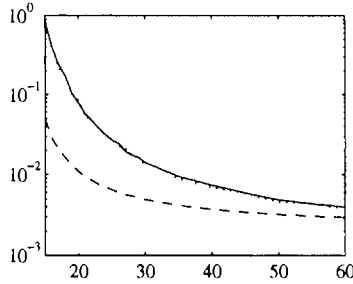
Figure 5 1. Estimates of the variance of $\widehat{\mathrm{EPE}}(n)$ vs empirical variance of $\widehat{\mathrm{EPE}}(n)$ (shown by bold curve) on 100 000 experiments. The average of the variance estimators $\widehat{\theta}_1$ (ignoring correlations, dashed curve) and $\widehat{\theta}_2$ (taking into account correlations, dotted curve) are displayed for different training sample size n

Looking at Figure 5.1 suggests that asymptotically the naive estimator of variance converges to the true variance. This can be shown formally by taking advantage of the results in this paper, as long as the learning algorithm converges as the amount of training data goes to infinity (i.e. as $n \to \infty$ the function $A(D)$ obtained does not depend on the particular training set D). In that limit, the correlations between test errors converge to 0. The rate of convergence will depend on the stability of the learning algorithm as well as on the nature of the data distribution (e.g., the presence of thick tails and outliers will slow down convergence).

The hold-out technique makes an inefficient use of data which forbids its application in most real-life applications with small samples. Then, K-fold cross-validation can provide estimates of PE or EPE.

2.3 K-fold cross-validation estimates of performance

Cross-validation is a computer intensive technique, using all available examples as training and test examples. It mimics the use of training and test sets by repeatedly training the algorithm K times with a fraction $1/K$ of training examples left out for testing purposes. This kind of hold-out estimate of performance lacks computational efficiency due to the repeated training, but the latter are meant to lower the variance of the estimate (Stone (1974)).

In practice, the data set D is first chunked into K disjoint subsets (or *blocks*) of the same size[3] $m \overset{\triangle}{=} n/K$. Let us write T_k for the k-th such block, and D_k the training set obtained by removing the elements in T_k from D. The cross-validation estimator is defined as the average of the errors on test block T_k obtained when the training set is deprived from T_k:

$$\text{CV}(D) = \frac{1}{K} \sum_{k=1}^{K} \frac{1}{m} \sum_{\mathbf{z}_i \in T_k} L(A(D_k), \mathbf{z}_i). \tag{5.3}$$

Does CV estimate PE or EPE? Such a question may seem pointless considering that PE(D) is an estimate of EPE(n), but it becomes relevant when considering the variance of CV: does it inform us of the uncertainty about PE or EPE?

On the one hand, only one training set, D, enters the definition of CV, which can be, up to an approximation, an unbiased estimate of PE(D) (Hastie and Tibshirani (1990)).[4] Some distribution-free bounds on the expected deviations of $|\text{CV}(D) - PE(D)|$ are available for leave-one-out cross-validation applied to specific algorithms A such as nearest neighbors (Devroye et al. (1996)). In a more general context, it has also been proved that, under suitable stability assumptions on the algorithm A, CV(D) estimates PE(D) at least as accurately as the training error (Kearns and Ron (1996): Anthony and Holden (1998)). A more appealing result states that CV is a more accurate estimate of PE than

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[3]To simplify the analysis below we assume that n is a multiple of K

[4]More precisely, following (Hastie and Tibshirani (1990)), when L is the quadratic loss, and writing $f = A(D)$, $f^{-k} = A(D_k)$, assuming that for $(\mathbf{x}_i, y_i) = \mathbf{z}_i \in T_k$, $\frac{1}{K} \sum_{k=1}^{K} f^{-k}(\mathbf{x}_i) \approx f(\mathbf{x}_i)$ (which is weaker than $f^{-k} \approx f$) yields $E(\text{CV}) \approx E[\frac{1}{n} \sum_{i=1}^{n} (f(\mathbf{x}_i) - y_i)^2]$, where the expectation is taken with respect to $y_1, \quad , y_n$

hold-out testing (Blum et al. (1999)). However, this statement does not apply to PE(D), but to the prediction error of a randomized algorithm picking solutions uniformly within $\{A(D_k)\}_{k=1}^{K}$.

On the other hand, CV is explicitly defined from the learning algorithm A, and not from the function $f = A(D)$. The inner average in the definition of CV (5.3) is an average test loss for $A(D_k)$ which thus estimates unbiasedly PE(D_k). The training sets $D_1, \ldots, D_K$ are clearly not independent, but they are sampled from P^{n-m}. Hence, the outer average of (5.3) estimates unbiasedly EPE($n-m$).[5] Here, following Dietterich (1999); Nadeau and Bengio (2003), we will adopt this latter point of view.

The variance estimate of $\widehat{\text{EPE}}$ provided by the hold-out estimate has to account for test error dependencies due to the choice of training set, which cannot be estimated using a single training/test experiment. Here, the situation is more complex, since there are additional dependencies due to the overlapping training sets $D_1, \ldots, D_K$. Before describing this situation in detail and summarizing the results of our theoretical analysis in Sections 3-6, we detail some procedures similar to K-fold cross-validation, for which the forthcoming analysis will also hold.

2.4 Other estimates of the K-fold cross-validation type

One of the main use of variance estimates of $\widehat{\text{EPE}}$ is to compare learning algorithms. The analysis presented in this paper also applies to the version of cross-validation dedicated to this purpose: if we want to compare the performances of algorithms A_1 and A_2, cross-validation with matched pairs should be the method of choice

$$\Delta\text{CV}(D) = \frac{1}{K} \sum_{k=1}^{K} \frac{1}{m} \sum_{\mathbf{z}_i \in T_k} L(A_1(D_k), \mathbf{z}_i) - L(A_2(D_k), \mathbf{z}_i). \quad (5.4)$$

Compared to the difference of two independent cross-validation estimates, ΔCV avoids the additional variability due to train/test splits.

In application oriented experiments, we would like to estimate PE(D), the expected error when training with the given D. We have seen in Section 2.3 that under stability assumptions, CV can be used to estimate PE. Alternatively, we may resort to the jackknife or the delete-m jack-

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[5]Note that leave-one-out cross-validation is known to fail to estimate EPE for unsmooth statistics (e.g. Breiman (1996); Efron and Tibshirani (1993)). This failure is due to the similarity of the training sets $D_1, \ldots, D_K$ which are far from being representative samples drawn from P^{n-m}

knife (see e.g. Efron and Tibshirani (1993)) to estimate the optimism (i.e. the bias of the mean error on training examples, when the latter is used to estimate PE(D)). Ideally, the estimate of optimism should be an average over all subsets of size $n - m$, but a less computationally intensive alternative is

$$(K - 1) \left(\frac{1}{K(n - m)} \sum_{k=1}^{K} \sum_{\mathbf{z}_i \in D_k} L(A(D_k), \mathbf{z}_i) - \frac{1}{n} \sum_{i=1}^{n} L(A(D), \mathbf{z}_i) \right).$$
(5.5)

The link with cross-validation is exhibited more clearly by the following expression of the (debiased) jackknife estimate of PE

$$\mathrm{JK} = \mathrm{CV} + \frac{1}{n} \sum_{k=1}^{K} \sum_{i=1}^{n} \left(L(A(D), \mathbf{z}_i) - L(A(D_k), \mathbf{z}_i) \right).$$
(5.6)

For additional information about jackknife estimates and clues on the derivation of (5.5) and (5.6), the reader is referred to Efron and Tibshirani (1993).

2.5   Generic notations

This paper studies the variance of statistics such as CV, ΔCV or JK. In what follows, these statistics will be denoted by $\hat{\mu}$, a generic notation for means of observations e_i split in K groups.

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} e_i$$

$$= \frac{1}{K} \sum_{k=1}^{K} \frac{1}{m} \sum_{i \in T_k} e_i,$$

where, slightly abusing notation, $i \in T_k$ means $\mathbf{z}_i \in T_k$ and

$$\forall i \in T_k, \ e_i = \begin{cases} L(A(D_k), \mathbf{z}_i) & \text{for } \hat{\mu} = \mathrm{CV}, \\ L(A_1(D_k), \mathbf{z}_i) - L(A_2(D_k), \mathbf{z}_i) & \text{for } \hat{\mu} = \Delta\mathrm{CV}, \\ K L(A(D), \mathbf{z}_i) - \sum_{\ell \neq k} L(A(D_\ell), \mathbf{z}_i) & \text{for } \hat{\mu} = \mathrm{JK}. \end{cases}$$

Note that $\hat{\mu}$ is the average of identically distributed (dependent) variables. Thus, it asymptotically converges to a normally distributed variable, which is completely characterized by its expectation $E(\hat{\mu})$ and its variance $\mathrm{Var}(\hat{\mu}) = E(\hat{\mu}^2) - E(\hat{\mu})^2$.

3.   Structure of the covariance matrix

The variance of $\hat{\mu}$ is defined as follows

$$\theta = \frac{1}{n^2} \sum_{i,j} \mathrm{Cov}(e_i, e_j),$$

where $\mathrm{Cov}(e_i, e_j) = E(e_i e_j) - E(e_i)E(e_j)$ is the covariance between variables e_i and e_j.

By using symmetry arguments over permutations of the examples in D, we show that many distributions on e_i and pairwise joint distributions on (e_i, e_j) are identical. As a result, the covariance matrix Σ has a very particular block structure, with only three possible values for $\Sigma_{ij} = \mathrm{Cov}(e_i, e_j)$, and the expression of θ is thus a linear combination of these three values.

LEMMA 5.1 *Using the notation introduced in section 2.5,*

1 *all e_i are identically distributed:*

   there exists f such that, $\forall i$, $P(e_i = u) = f(u)$.

2 *all pairs (e_i, e_j) belonging to the same test block are jointly identically distributed:*

   there exists g such that, $\forall (i,j) \in T_k^2 : j \neq i$, $P(e_i = u, e_j = v) = g(u,v)$.

3 *all pairs (e_i, e_j) belonging to different test blocks are jointly identically distributed:*

   there exists h such that, $\forall i \in T_k$, $\forall j \in T_\ell : \ell \neq k$, $P(e_i = u, e_j = v) = h(u,v)$.

Proof.   These results are derived immediately from the permutation-invariance of $P(D)$ and the symmetry of A.

- invariance with respect to permutations within test blocks:

   1 $\forall (i,i') \in T_k^2$, $P(e_i = u) = P(e_{i'} = u) = f_k(u)$;
   $\forall (i,i') \in T_k^2$, $\forall j \in T_\ell$:
   $P(e_i = u, e_j = v) = P(e_{i'} = u, e_j = v)$
   hence:
   2 $\forall (i,j) \in T_k^2 : j \neq i$, $P(e_i = u, e_j = v) = g_k(u,v)$.
   3 $\forall i \in T_k$, $\forall j \in T_\ell : \ell \neq k$, $P(e_i = u, e_j = v) = h_{k\ell}(u,v)$.

■ invariance with respect to permutations between test blocks.

1 $\forall (k, k'),\ f_k(u) = f_{k'}(u) = f(u);$

2 $\forall (k, k'),\ g_k(u, v) = g_{k'}(u, v) = g(u, v);$

3 $\forall (k, k'),\ \forall (\ell, \ell') : \ell \neq k, \ell \neq k', \ell' \neq k, \ell' \neq k',\ h_{k\ell}(u, v) = h_{k\ell'}(u, v) = h_{k'\ell'}(u, v) = h_{k'\ell}(u, v) = h(u, v).$

$\square$

COROLLARY 5.1 *The covariance matrix* $\mathbf{\Sigma}$ *of cross-validation errors* $\mathbf{e} = (e_1, \ldots, e_n)'$ *has the simple block structure depicted in Figure 5.2:*

1 *all diagonal elements are identical*

$\forall i,\ \mathrm{Cov}(e_i, e_i) = \mathrm{Var}(e_i) = \sigma^2;$

2 *all the off-diagonal entries of the* K $m \times m$ *diagonal blocks are identical*

$\forall (i, j) \in T_k^2 : j \neq i.\ \mathrm{Cov}(e_i, e_j) = \omega;$

3 *all the remaining entries are identical*

$\forall i \in T_k,\ \forall j \in T_\ell : \ell \neq k,\ \mathrm{Cov}(e_i, e_j) = \gamma.$
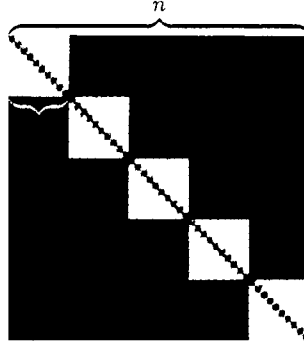
Figure 5.2. Structure of the covariance matrix

COROLLARY 5.2 *The variance of the cross-validation estimator is a linear combination of three moments:*

$$\theta = \frac{1}{n^2} \sum_{i,j} \mathrm{Cov}(e_i, e_j)$$

$$= \frac{1}{n}\sigma^2 + \frac{m-1}{n}\omega + \frac{n-m}{n}\gamma \tag{5.7}$$

Hence, the problem of estimating θ does not involve estimating $n(n + 1)/2$ covariances, but it cannot be reduced to that of estimating a single variance parameter. Three components intervene, which may be interpreted as follows when $\hat{\mu}$ is the K-fold cross-validation estimate of EPE:

1. the variance σ^2 is the average (taken over training sets) variance of errors for "true" test examples when algorithm A is fed with training sets of size $m(K - 1)$;

2. the within-block covariance ω would also apply to "true" test examples; it arises from the dependence of test errors stemming from the common training set.

3. the between-blocks covariance γ is due to the dependence of training sets (which share $n(K - 2)/K$ examples) and the fact that test block T_k appears in all the training sets D_ℓ for $\ell \neq k$.

The forthcoming section makes use of this structure to show that there is no universal unbiased estimator of θ.

4. No unbiased estimator of $\mathrm{Var}(\hat{\mu})$ exists

Consider a generic estimator $\hat{\theta}$ that depends on the sequence of cross-validation errors $\mathbf{e} = (e_1, e_2, \ldots, e_n)'$. Let us assume that $\hat{\theta}$ is an analytic function of the errors, so that we can write its Taylor expansion:

$$\hat{\theta} = \alpha_0 + \sum_i \alpha_1(i)e_i + \sum_{i,j} \alpha_2(i,j)e_ie_j + \sum_{i,j,k} \alpha_3(i,j,k)e_ie_je_k + \ldots \quad (5.8)$$

We first show that for unbiased variance estimates (i.e. $E(\hat{\theta}) = \mathrm{Var}(\hat{\mu})$), all the α_i coefficients must vanish except for the second order coefficients $\alpha_{2,i,j}$.

LEMMA 5.2 *There is no universal unbiased estimator of* $\mathrm{Var}(\hat{\mu})$ *that involves the* e_i *in a non-quadratic way.*

Proof. Take the expected value of $\hat{\theta}$ expressed as in (5.8), and equate it with $\mathrm{Var}(\hat{\mu})$ (5.7):

$$\begin{cases} E(\hat{\theta}) = \alpha_0 + \sum_i \alpha_1(i)E(e_i) + \sum_{i,j} \alpha_2(i,j)E(e_ie_j) \\ \qquad + \sum_{i,j,k} \alpha_3(i,j,k)E(e_ie_je_k) + \ldots \\ \theta = \frac{1}{n}\sigma^2 + \frac{m-1}{n}\omega + \frac{n-m}{n}\gamma. \end{cases}$$

For having $E(\hat{\theta}) = \theta$ for all possible values of the moments of **e**, one must have $\alpha_0 = 0$ because θ has no such constant term, not depending on any of the moments of **e**. Similarly, $\alpha_1(\cdot)$ must be zero because θ has no term in $E(e_i) = \mu$. Finally, the third and higher order coefficients $\alpha_\ell(\ldots)$, $\ell > 2$ must also be zero because θ has only quantities depending on the second order moments σ^2, ω and γ.   □

Since estimators that include moments other than the second moments in their expectation are biased, we now focus on the class of estimators which are quadratic forms of the errors, i.e.

$$\hat{\theta} = \mathbf{e}'\mathbf{W}\mathbf{e} = \sum_{i,j} W_{ij} e_i e_j. \tag{5.9}$$

LEMMA 5.3 *The expectation of quadratic estimators $\hat{\theta}$ defined as in (5.9) is a linear combination of only three terms*

$$E(\hat{\theta}) = a(\sigma^2 + \mu^2) + b(\omega + \mu^2) + c(\gamma + \mu^2), \tag{5.10}$$

where (a, b, c) are defined as follows:

$$\begin{cases} a & \triangleq \sum_{i=1}^{n} W_{ii}, \\ b & \triangleq \sum_{k=1}^{K} \sum_{i \in T_k} \sum_{j \in T_k : j \neq i} W_{ij}, \\ c & \triangleq \sum_{k=1}^{K} \sum_{\ell \neq k} \sum_{i \in T_k} \sum_{j \in T_\ell} W_{ij}. \end{cases}$$

A "trivial" representer of estimators with this expected value is

$$\hat{\theta} = as_1 + bs_2 + cs_3, \tag{5.11}$$

*where (s_1, s_2, s_3) are the only quadratic statistics of **e** that are invariants to the within blocks and between blocks permutations described in Lemma 5.1:*

$$\begin{cases} s_1 & \triangleq \dfrac{1}{n} \sum_{i=1}^{n} e_i^2, \\ s_2 & \triangleq \dfrac{1}{n(m-1)} \sum_{k=1}^{K} \sum_{i \in T_k} \sum_{j \in T_k : j \neq i} e_i e_j, \\ s_3 & \triangleq \dfrac{1}{n(n-m)} \sum_{k=1}^{K} \sum_{\ell \neq k} \sum_{i \in T_k} \sum_{j \in T_\ell} e_i e_j. \end{cases} \tag{5.12}$$

Proof. This result is obtained exploiting Corollary 5.1 and grouping the terms of $\hat{\theta}$ in Equation (5.9) that have the same expected values.

$$E[\hat{\theta}] = \sum_{k=1}^{K} \sum_{i \in T_k} \left(W_{ii} E(e_i^2) + \sum_{j \in T_k : j \neq i} W_{ij} E(e_i e_j) + \sum_{\ell \neq k} \sum_{j \in T_\ell} W_{ij} E(e_i e_j) \right)$$

$$= (\sigma^2 + \mu^2) \sum_{i=1}^{n} W_{ii} + (\omega + \mu^2) \sum_{k=1}^{K} \sum_{i \in T_k} \sum_{j \in T_k : j \neq i} W_{ij} +$$

$$(\gamma + \mu^2) \sum_{k=1}^{K} \sum_{\ell \neq k} \sum_{i \in T_k} \sum_{j \in T_\ell} W_{ij}$$

$$= a(\sigma^2 + \mu^2) + b(\omega + \mu^2) + c(\gamma + \mu^2)$$

$$= aE(s_1) + bE(s_2) + cE(s_3),$$

which is recognized as the expectation of the estimator defined in Equation (5.11). $\qquad\square$

We now use Lemma 5.3 to prove that there is no *universally* unbiased estimator of $\mathrm{Var}(\hat{\mu})$, i.e. there is no estimator $\hat{\theta}$ such that $E(\hat{\theta}) = \mathrm{Var}(\hat{\mu})$ for all possible distributions of $\mathbf{e}$.

THEOREM 5.1 *There exists no universally unbiased estimator of* $\mathrm{Var}(\hat{\mu})$.

Proof. Because of Lemma 5.2 and 5.3, it is enough to prove the result for estimators that are quadratic forms expressed as in Equation (5.11). To obtain unbiasedness, the expected value of that estimator must be equated with $\mathrm{Var}(\hat{\mu})$ (5.7):

$$a(\sigma^2 + \mu^2) + b(\omega + \mu^2) + c(\gamma + \mu^2) = \frac{1}{n}\sigma^2 + \frac{m-1}{n}\omega + \frac{n-m}{n}\gamma. \quad (5.13)$$

For this equality to be satisfied for all distributions of cross-validation errors, it must be satisfied for all admissible values of μ, σ^2, ω, and γ. This imposes the following unsatisfiable constraints on (a, b, c):

$$\begin{cases} a & = & \frac{1}{n}, \\ b & = & \frac{m-1}{n}, \\ c & = & \frac{n-m}{n}, \\ a+b+c & = & 0. \end{cases} \quad (5.14)$$

$\qquad\square$

5.   Eigenanalysis of the covariance matrix

One way to gain insight on the origin of the negative statement of Theorem 5.1 is via the eigenanalysis of $\boldsymbol{\Sigma}$, the covariance of $\mathbf{e}$. This decomposition can be performed analytically thanks to the very particular block structure displayed in Figure 5.2.

LEMMA 5.4 *Let* $\mathbf{v}_k$ *be the binary vector indicating the membership of each example to test block k. The eigensystem of $\boldsymbol{\Sigma}$ is as follows:*

- $\lambda_1 = \sigma^2 - \omega$ *with multiplicity* $n - K$ *and eigenspace defined by the orthogonal of basis* $\{\mathbf{v}_k\}_{k=1}^{K}$;

- $\lambda_2 = \sigma^2 + (m-1)\omega - m\gamma$ *with multiplicity* $K - 1$ *and eigenspace defined in the orthogonal of* $\mathbf{1}$ *by the basis* $\{\mathbf{v}_k\}_{k=1}^{K}$;

- $\lambda_3 = \sigma^2 + (m-1)\omega + (n-m)\gamma$ *with eigenvector* $\mathbf{1}$.

Proof. From Corollary 5.1, the covariance matrix $\boldsymbol{\Sigma} = E(\mathbf{ee}') - E(\mathbf{e}) E(\mathbf{e})'$ can be decomposed as

$$\boldsymbol{\Sigma} = (\sigma^2 - \omega)\boldsymbol{\Sigma}_1 + m(\omega - \gamma)\boldsymbol{\Sigma}_2 + n\gamma\boldsymbol{\Sigma}_3,$$

where $\boldsymbol{\Sigma}_1 = \mathbf{I}$, $\boldsymbol{\Sigma}_2 = \frac{1}{m}(\mathbf{v}_1 \dots \mathbf{v}_K)(\mathbf{v}_1 \dots \mathbf{v}_K)'$ and $\boldsymbol{\Sigma}_3 = \frac{1}{n}\mathbf{1}\mathbf{1}'$.

$\boldsymbol{\Sigma}_1$, $\boldsymbol{\Sigma}_2$ and $\boldsymbol{\Sigma}_3$ share the same eigenvectors, with eigenvalues being equal either to zero or one:

- the eigenvector $\mathbf{1}$ has eigenvalue 1 for $\boldsymbol{\Sigma}_1$, $\boldsymbol{\Sigma}_2$ and $\boldsymbol{\Sigma}_3$;

- the eigenspace defined in the orthogonal of $\mathbf{1}$ by the basis $\{\mathbf{v}_k\}_{k=1}^{K}$ defines $K - 1$ eigenvectors with eigenvalues 1 for $\boldsymbol{\Sigma}_1$ and $\boldsymbol{\Sigma}_2$ and 0 for $\boldsymbol{\Sigma}_3$;

- all remaining eigenvectors have eigenvalues 1 for $\boldsymbol{\Sigma}_1$ and 0 for $\boldsymbol{\Sigma}_2$ and $\boldsymbol{\Sigma}_3$.

$\square$

Lemma 5.4 states that the vector $\mathbf{e}$ can be decomposed into three uncorrelated parts: $n - K$ projections to the subspace orthogonal to $\{\mathbf{v}_k\}_{k=1}^{K}$, $K - 1$ projections to the subspace spanned by $\{\mathbf{v}_k\}_{k=1}^{K}$ in the orthogonal of $\mathbf{1}$, and one projection on $\mathbf{1}$. A single vector example with n independent elements can be seen as n independent examples. Similarly, these projections of $\mathbf{e}$ can be equivalently represented by respectively $n - K$, $K - 1$ and one uncorrelated one-dimensional examples, corresponding to the coordinates of $\mathbf{e}$ in these subspaces.

In particular, for the projection on $\mathbf{1}$, with only a single one-dimensional point, the sample variance is null, resulting in the absence of an unbiased variance estimator of λ_3. The projection of $\mathbf{e}$ on the eigenvector $\frac{1}{n}\mathbf{1}$ is precisely $\hat{\mu}$. Hence there is no unbiased estimate of $\mathrm{Var}(\hat{\mu}) = \frac{\lambda_3}{n}$ when we have only one realization of the vector $\mathbf{e}$. For the same reason, even with simple parametric assumptions on $\mathbf{e}$ (such as $\mathbf{e}$ Gaussian), the maximum likelihood estimate of θ is not defined. Only λ_1 and λ_2 can be estimated unbiasedly. Note that this problem cannot be addressed by performing multiple K-fold splits of the data set. Such a procedure would not provide independent realizations of $\mathbf{e}$.

6.   Possible values for ω and γ

Theorem 5.1 states that no estimator is unbiased, and in its demonstration, it is shown that the bias of any quadratic estimator is a linear combination of μ^2, σ^2, ω and γ. Regarding estimation, it is thus interesting to see what constraints restrict the possible range of these quantities.

LEMMA 5.5 *For $\hat{\mu} = \mathrm{CV}$ and $\hat{\mu} = \Delta\mathrm{CV}$, the following inequalities hold:*

$$\left\{ \begin{array}{ccccc} 0 & \leq & \omega & \leq & \sigma^2 \\ -\frac{1}{n-m}(\sigma^2 + (m-1)\omega) & \leq & \gamma & \leq & \frac{1}{m}(\sigma^2 + (m-1)\omega) \end{array} \right.$$
$$\Rightarrow \left\{ \begin{array}{ccccc} 0 & \leq & \omega & \leq & \sigma^2 \\ -\frac{m}{n-m}\sigma^2 & \leq & \gamma & \leq & \sigma^2. \end{array} \right.$$

The shape of the admissible (ω, γ) region corresponding to the first set of (tighter) inequalities is displayed in Figure 5.3.
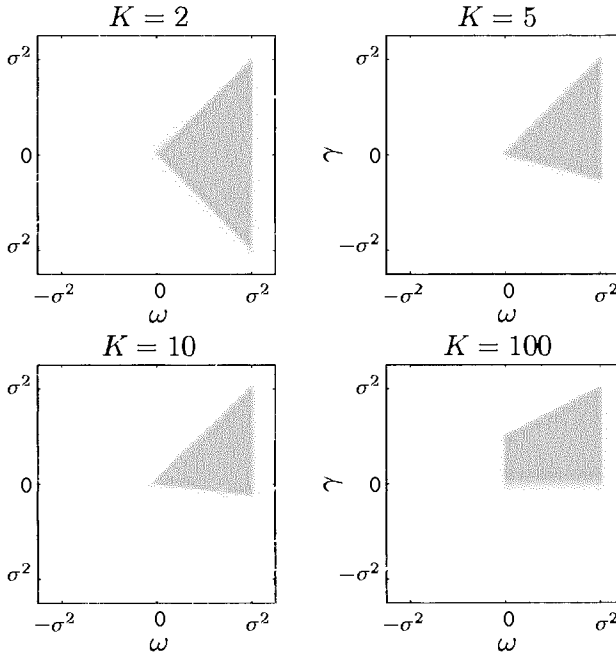
Figure 5.3. Possible values of (ω, γ) according to σ^2 for $n = 200$ and $K = \{2, 5, 10, 100\}$.

Proof. The constraints on ω result from the Cauchy-Schwartz inequality which provides $\mathrm{Cov}^2(u, v) \leq \mathrm{Var}(u)\mathrm{Var}(v)$, hence

$$-\sigma^2 \leq \omega \leq \sigma^2.$$

Moreover, the following reasoning shows that, for $\hat{\mu} = \text{CV}$ and $\hat{\mu} = \Delta\text{CV}$, ω is non-negative: ω is the covariance of (differences in) test errors for training sets of size $n - m$ and test sets of size $\ell = m$. The variance of the average test error is given by the mean of covariances $\frac{1}{\ell}(\sigma^2 + (\ell - 1)\omega)$. The variance σ^2 and covariance ω of test errors are not affected by ℓ, and the variance of the average test error should be non-negative for any test set size ℓ. Hence ω is bound to be non-negative. When this type of reasoning cannot be used, as for $\hat{\mu} = \text{JK}$, ω can only be proved to be greater than $-\sigma^2/(m - 1)$.

The constraints on γ simply rephrase that the eigenvalues λ_2 and λ_3 of the covariance matrix $\boldsymbol{\Sigma}$ should be non-negative. The simpler (and looser) form is obtained by using $\omega \leq \sigma^2$. $\qquad\square$

The admissible (ω, γ) region obtained in Lemma 5.5 is very large. Furthermore, there is no constraint linking μ and σ^2, the mean and variance of e_i. Hence we cannot propose a variance estimate with universally small bias.

7. Experiments

We already mentioned that the bias of any quadratic estimator is a linear combination of μ^2, σ^2, ω and γ. The admissible values provided in the preceding section suggest that ω and γ cannot be proved to be negligible compared to σ^2. This section illustrates that in practice, the contribution to the variance of $\hat{\mu}$ due to ω and γ (see Equation (5.7)) can be of same order than the one due σ^2. It therefore suggests that the estimators of θ should indeed take into account the correlations of e_i.

EXPERIMENT 5.2 *True variance of K-fold cross-validation.*

We repeat the experimental setup of Experiment 5.1, except that now, we are in the more realistic situation where only one sample of size n is available. Since cross-validation is known to be sensitive to the instability of algorithms, in addition to this standard setup, we also consider another one with outliers:

The input $\mathbf{x_i} = (x_{i1}, \ldots, x_{id})'$ is still 30-dimensional, but it is now a mixture of two centered Gaussian variables: let t_i be a binary variable, with $P(t_i = 1) = p = 0.95$; when $t_i = 1$, $x_i \sim \mathcal{N}(0, \mathbf{I})$; when $t_i = 0$, $x_i \sim \mathcal{N}(0, 100\mathbf{I})$; $y_i = \sqrt{3/(d(p + 100(1 - p)))} \sum_{k=1}^{d} x_{ik} + \varepsilon_i$ with $\varepsilon_i \sim \mathcal{N}(0, 1/(p + 100(1 - p)))$ when $t_i = 1$ and $\varepsilon_i \sim \mathcal{N}(0, 100/(p + 100(1 - p)))$ when $t_i = 0$.

We now look at the variance of K-fold cross-validation ($K = 10$), and decompose in the three orthogonal components σ^2, ω and γ. The results are shown in Figure 5.4. (In this figure, σ^2, ω and γ are estimated by

the usual estimate of covariance on $10\,000$ independent experiments for each sample size, i.e. respectively by the empirical means of $(s_1 - \hat{mu}^2)$, $(s_2 - \hat{mu}^2)$ and $(s_3 - \hat{mu}^2)$.)

no outliers   outliers
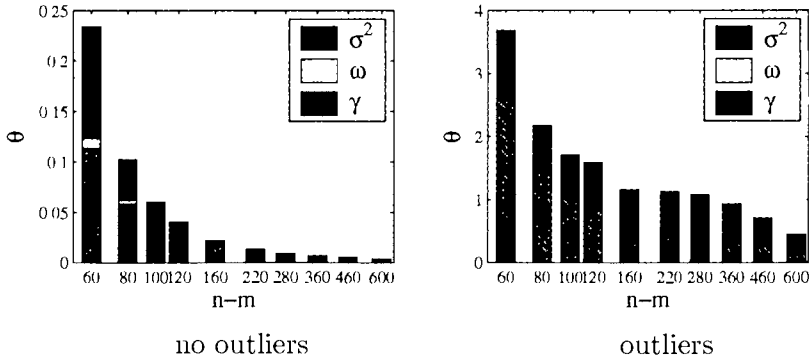
Figure 5 4. Bar plots of the contributions to total variance Var(CV) due to σ^2, ω and γ *vs* the number of training examples $n - m$ for Experiment 5 2

When there are no outliers, the contribution of γ is very important for small sample sizes. For large sample sizes, the overall variance is considerably reduced and is mainly caused by σ^2. In these situations, the learning algorithm returns very similar answers for all training sets. When there are outliers, ω has little effect, but the contribution of γ is of same order as the one of σ^2, even when the ratio of examples to free parameters is large (here up to 20). Thus, in difficult situations, where $A(D)$ varies according to the realization of D, neglecting the effect of ω and γ can be expected to introduce a bias of the order of the true variance.

It is also interesting to see how these quantities are affected by the number of folds K. The decomposition of θ in σ^2, ω and γ (5.7) does not imply that K should be set either to n or to 2 (according to the sign of $\omega - \gamma$) in order to minimize the variance of $\hat{\mu}$. Modifying K affects σ^2, ω and γ through the size and overlaps of the training sets $D_1, \ldots, D_K$, as illustrated in Figure 5.5. For a fixed sample size, the variance of $\hat{\mu}$ and the contribution of σ^2, ω and γ effects varies smoothly with K.[6] The experiments with and without outliers illustrate that there is no general trend either in variance or decomposition of the variance in its σ^2, ω and γ components. The minimum variance can be reached for $K = n$ or for an intermediate value of K.

---

[6] Of course, the mean of $\hat{\mu}$ is also affected in the process

no outliers   outliers
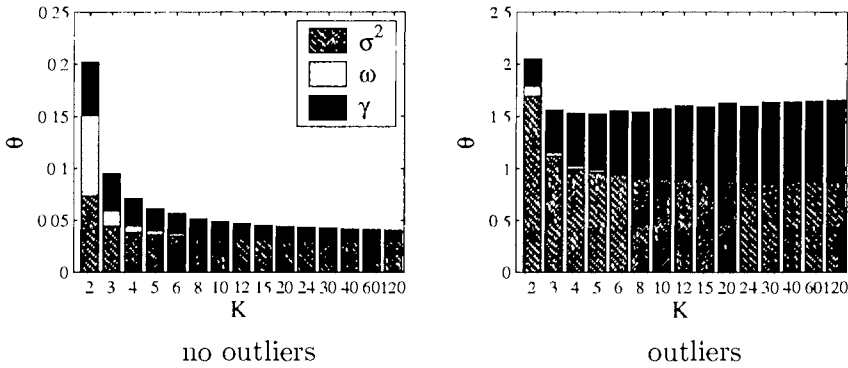
Figure 5.5. Bar plots of contributions of σ^2, ω and γ to θ vs. K for $n = 120$ for Experiment 5.2.
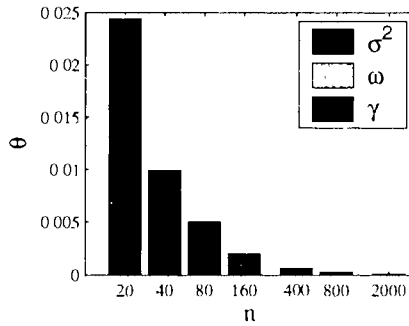
Figure 5.6. Bar plots of the contributions to total variance Var(CV) due to σ^2, ω and γ vs. the number of training examples n for Experiment 5.3.

We also report an experiment illustrating that the previous observations also apply to classification on real data. The variance of K-fold cross-validation ($K = 10$), decomposed in the three orthogonal components σ^2, ω and γ is displayed in Figure 5.6.

EXPERIMENT 5.3 *Classification with trees on the Letter dataset.*

The Letter dataset comprises 20 000 examples described by 16 numeric features. The original setup considers 26 categories reprensenting the letters of the roman alphabet. Here, we used a simplified setup with 2 classes (A to M) vs. (N to Z) in order to obtain sensible results for small sample sizes.

Accurate estimates of σ^2, ω and γ require many independent training samples. This was achieved by considering the set of 20 000 examples to

be the population, from which 10 000 independent training samples were drawn by uniform sampling with replacement.

Here again, the variance of CV is mainly due to σ^2 and γ. According to the number of training examples, σ^2 is only responsible for 50 to 70 % of the total variance, so that a variance estimate based solely on σ^2 has a negative bias of the order of magnitude of the variance itself.

8. Special cases

8.1 Hold-out estimate of EPE

When having K *independent training and test sets*, the structure of hold-out errors resemble the one of cross-validation errors, except that we know (from the independence of training and test sets) that $\gamma = 0$. This knowledge allows to build the unbiased variance estimate $\widehat{\theta_2}$ described in 2.2. This can be seen directly in the proof of Theorem 5.1: knowing that $\gamma = 0$ removes the third equation in the linear system (5.14). In practice, one is often restricted to $K = 1$ (ordinary hold-out test), which allows to estimate the variance due to the finite test set but not due to the particular choice of training set.

8.2 Two-fold cross validation

Two-fold cross-validation has been advocated to perform hypothesis testing (Dietterich (1999); Alpaydin (1999)). It is a special case of K-fold cross-validation since the training blocks are mutually independent since they do not overlap. However, this independence does not modify the structure of **e** in the sense that γ is not null. The between-block correlation stems from the fact that the training block D_1 is the test block T_2 and vice-versa.

8.3 Leave-one-out cross validation

Leave-one-out cross validation is a particular case of K-fold cross-validation, where $K = n$. The structure of the covariance matrix is simplified, without diagonal blocks: $\Sigma = (\sigma^2 - \gamma)\Sigma_1 + n\gamma\Sigma_3$. The estimation difficulties however remain: even in this particular case, there is no unbiased estimate of variance. From the definition of b (Lemma 5.3), we have $b = 0$, and with $m = 1$ the linear system (5.14) reads

$$\begin{cases} a & = & \frac{1}{n}, \\ c & = & \frac{n-1}{n}, \\ a+c & = & 0. \end{cases}$$

which still admits no solution.

9.   Conclusions

It is known that K-fold cross-validation may suffer from high variability, which can be responsible for bad choices in model selection and erratic behavior in the estimated expected prediction error.

In this paper, we show that estimating the variance of K-fold cross-validation is difficult. Estimating a variance can be done from independent realizations or from dependent realizations whose correlation is known. K-fold cross-validation produces dependent test errors. Our analysis shows that although the correlations are structured in a very simple manner, their values cannot be estimated unbiasedly. Consequently, there is no unbiased estimator of the variance of K-fold cross-validation.

Our experimental section shows that in very simple cases, the bias incurred by ignoring the dependencies between test errors will be of the order of the variance itself. These experiments illustrate thus that the assessment of the significance of observed differences in cross-validation scores should be treated with much caution. The problem being unveiled, the next step of this study consists in building and comparing variance estimators dedicated to the very specific structure of the test error dependencies.

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Chapter 6

EFFECTIVE CONSTRUCTION OF MODIFIED HISTOGRAMS IN HIGHER DIMENSIONS

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Abstract   Density estimation raises delicate problems in higher dimensions especially when strong convergence is required and data marginals can be highly correlated. Modified histograms have been introduced to circumvent the problem of low bin counts when convergence is considered in the sense of information divergence. These estimates are defined from some reference probability density and an associated partition which is defined in the univariate case from the quantiles of the reference density. Therefore, in the multivariate case, the definition of the partition causes an additional problem related to the lack of total order. In this paper, we present a method for constructing modified multivariate histograms such that the corresponding partition is well adapted to the observed data. The approach is based on a data-driven coordinate system selected by cross-validation. We discuss the performance of our estimate with the help of a finite sample simulation study.

1.   Introduction

We consider the problem of estimating an unknown probability density f defined on $\mathbb{R}^d$ based on independent, identically distributed observations $X_1, \ldots, X_n$ from f. Here the quality of estimation will be evaluated by a nonnegative divergence $F(f, f_n)$. Of interest are estimators f_n consistent in the sense

$$\lim_{n \to \infty} F(f, f_n) = 0 \ a.s. \quad \text{or} \quad \lim_{n \to \infty} \mathbf{E} F(f, f_n) = 0$$

where $\mathbf{E}$ denotes the expectation with respect to the random vector $(X_1, \ldots, X_n)$ figuring in the estimate f_n. The two most important divergences in mathematical statistics and information theory are the

total variation V and the information divergence D. They are defined by

$$V(f,g) = \frac{1}{2} \int_{\mathbb{R}^d} |f(x) - g(x)| \lambda(dx) = \frac{1}{2} \|f - g\|_{L_1}$$

$$D(f,g) = \begin{cases} \int_{\mathbb{R}^d} f(x) \log \frac{f(x)}{g(x)} \lambda(dx) & \text{if } f \ll g \\ \infty & \text{otherwise,} \end{cases}$$

where $\ll$ denotes absolute continuity. It is well known (cf. Csizár (1967), Kemperman (1969), and Kullback (1967)) that for all densities f and g, $V(f,g)$ and $D(f,g)$ are linked by the following inequality, called Kullback-Csiszár-Kemperman inequality:

$$2V^2(f,g) \leq D(f,g),$$

which entails that the information divergence is topologically stronger than the total variation. In numerous application fields of statistics (data compression, telecommunication networks, classification, pattern recognition, neural networks...), the consistency defined by total variation may prove inadequate. This is the case when precise estimation of tail probabilities or convergence of integrals of various functionals are required (see Berlinet, Vajda and van der Meulen (1998) for discussion). Another concern with convergence in total variation is that, given any sequence of density estimates, the rate of convergence of the expected L_1 error can be arbitrary slow (Devroye, 1983). Therefore stronger topologies such as information divergence are often preferred.

Classical nonparametric density estimates such as kernel estimates and histograms are not universally consistent in information divergence (see Hall (1987)). The modified histograms introduced by Barron (1988) and Barron, Györfi and van der Meulen (1992) circumvent this problem. They are defined as follows.

Suppose that we observe independent $\mathbb{R}^d$-valued random variables X_1, $\ldots, X_n$ with common unknown density f.

- Denote by g a known density on $\mathbb{R}^d$ and by ν the associated probability measure;

- Define a sequence of integers $\{m_n\}_{n \geq 1}$ such that $1 \leq m_n \leq n$ and let $h_n = 1/m_n$;

- Introduce a sequence of partitions $\mathcal{P}_n = \{A_{n,1}, A_{n,2}, \ldots, A_{n,m_n}\}$, $n \geq 1$, such that $\nu(A_{n,i}) = h_n$, $i = 1, \ldots, m_n$;

- Finally consider, for $a_n = 1/(nh_n + 1)$ the following estimator f_n

$$f_n(x) = \left[(1 - a_n)\frac{\mu_n\big(A_n(x)\big)}{h_n} + a_n\right]g(x) = \frac{n\mu_n\big(A_n(x)\big) + 1}{nh_n + 1}g(x).$$
(6.1)

where μ_n stands for the empirical measure associated with the sample $X_1, \ldots, X_n$ and $A_n(x)$ stands for $A_{n,i}$ if $x \in A_{n,i}$.

The estimate (6.1) is a mixture of a histogram-type density estimate and the known density g. It can also be regarded as a piecewise transformation of g itself, which is thus often called in this context the *reference density*.

Under the conditions

$$D(f, g) < \infty, \qquad \lim_{n \to \infty} h_n = 0 \text{ and } \lim_{n \to \infty} nh_n = \infty,$$

almost sure consistency in information divergence and consistency in expected information divergence have been proved by Barron, Györfi and van der Meulen (1992).

For further results on modified histograms we refer the reader to Berlinet and Brunel (2004), Berlinet, Györfi and van der Meulen (1997), Berlinet and Biau (2004) and Györfi et al. (1998).

When $d = 1$, the quantiles of the reference density are used to partition $\mathbb{R}$. Formally, denoting by G the distribution function associated with the probability density g (g is defined on $(a; b)$, a and b may be infinite), we set

$$A_{n,i} = \left(G^{-1}\Big(\frac{i-1}{m_n}\Big), G^{-1}\Big(\frac{i}{m_n}\Big)\right], \ i = 1, \ldots, m_n,$$

where the interval $(.,.]$ is understood as open on the left and closed on the right only when its upper bound is finite and where G^{-1} is the quantile function defined by

$$\begin{cases} G^{-1}(\alpha) = \inf\{x : G(x) \geq u\} & \text{if } 0 < \alpha < 1 \\ G^{-1}(\alpha) = a & \text{if } \alpha = 0 \\ G^{-1}(\alpha) = b & \text{if } \alpha = 1. \end{cases}$$
(6.2)

Thus, univariate modified histograms result from the comparison of the quantiles of g with the empirical quantiles. Under mild conditions the choice of g does not affect dramatically the asymptotics. Practically, however, g should not be "too far" from f, so that the comparison between the empirical measure and the reference density over the partition makes sense.

For $d \geq 2$, the choice of such a partition is much more delicate because the lack of total order does not allow to define multivariate quantiles having the same properties as univariate ones. The aim of this paper is to propose a method for constructing multivariate modified histograms. In Section 2, we give two algorithms to construct this estimate. The first one uses rectangles to partition $\mathbb{R}^d$ (as for the standard multivariate regular histogram estimate). However, the performance of this estimate becomes poor in the presence of high correlation among components of the data vector. This leads us to a more effective method which results from a transformation of these rectangles. We use the data-driven coordinate system introduced by Chaudhuri and Sengupta (1993). In Section 3, we select this coordinate system by cross-validation and we end with some simulations showing the very good performance of the second estimate.

2.   Construction of the estimator

Not any sequence of partitions of $\mathbb{R}^d$ has good properties to build consistent estimates. The following concept, introduced by Csizár (1973) has a great importance in the definition of suitable partitions.

DEFINITION 6.1 *A sequence of partitions $\{\mathcal{P}_n\}$ of $\mathbb{R}^d$ is said to be ν-approximating for a given probability measure ν if, for every measurable set A and for every $\epsilon > 0$, there is for all n sufficiently large a set A_n equal to a union of sets in $\{\mathcal{P}_n\}$ such that*

$$\nu(A_n \bigtriangleup A) < \epsilon,$$

where $A_n \bigtriangleup A$ denotes the symmetric difference of A_n and A.

As proved by Barron, Györfi and van der Meulen (1992) this notion is basic in the proof of consistency of modified histograms.
The partition of a univariate modified histogram is computed from the quantiles of the reference density. Several authors have proposed extensions of quantiles to multidimensional spaces. Chaudhuri (1996) proposed the notion of geometric quantile which generalizes the spatial median studied earlier (see Brown (1983), Kemperman (1987)). Chakraborty (2001) transformed these geometric quantiles in order to obtain affine equivariant multivariate quantiles. Liu, Parelius and Singh (1999) proposed to define affine equivariant multivariate quantiles using depth analysis. They generalized half-space depth quantiles introduced by Tukey (1975). Given a measure ν, using *quantile contour plots* of Chakraborty (2001) or *center outward quantiles surfaces* of Liu, Parelius and Singh (1999), one can construct a sequence of partitions

$\mathcal{P}_n = \{A_{n,1}, \ldots, A_{n,m_n}\}$ such that $\nu(A_{n,i}) = h_n$ $(i = 1, \ldots, m_n)$. These sequences are nested in the sense that for all n there exists a sequence

$$B_{n,1} \subset B_{n,2} \subset \ldots \subset B_{n,m_n}$$

such that

$$\forall i = 1, \ldots, m_n, \ A_{n,i} = B_{n,i} - \bigcup_{j=1}^{i-1} B_{n,j} . \tag{6.3}$$

Such a sequence of partitions is not ν-approximating for any measure ν.
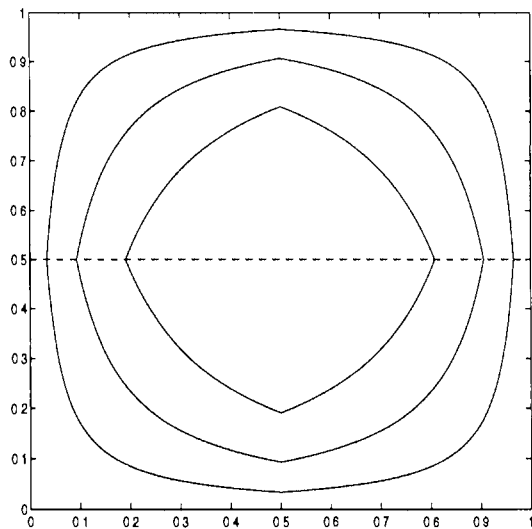
Figure 6.1. Half-space depth center-outward quantile surface of order 0.25, 0.5 and 0.75 for the uniform distribution on the square $[0, 1]^2$.

For example, let ν be the uniform distribution on the square $[0, 1]^2$ and consider a sequence of partitions built from halfspace depth quantiles (see Liu, Parelius and Singh (1999)). Formally, for $i = 1, \ldots, m_n$, $B_{n,i}$ is *a half-space depth center-outward quantile surface* of order i/m_n and $A_{n,i}$ is defined by (6.3) (see Figure 6.1). Consider the vertical line which passes through the center of the square (dashed line in Figure 6.1). This line splits the square into two rectangles. If A denotes one of these rectangles, it is easily seen that for all sets A_n equal to a union of sets in $\mathcal{P}_n$, we have

$$\nu(A_n \bigtriangleup A) = 0.5 \,,$$

which entails that $\mathcal{P}_n$ is not ν-approximating.

Other authors have defined quantiles in multidimensional spaces (see Brown and Hettmansperger (1987), Eddy (1983, 1985)), but as far as

we know none permits the construction of modified histograms for any reference density. This leads us to restrict our attention to a certain class of reference densities.

2.1   Regular modified histograms

The standard regular (unmodified) histogram is defined by a partition of $\mathbb{R}^d$ into rectangular cells of widths $h_1, \ldots, h_d$. The goal of this paragraph is the adaptation of this partition to modified histograms. In this regard we only consider reference densities g such that

$$g(x_1, \ldots, x_d) = g_1(x_1) \ldots g_d(x_d), \qquad (6.4)$$

where $g_1, \ldots, g_d$ are univariate densities. For $j = 1, \ldots, d$, we denote by G_j the distribution function associated with the probability density g_j and by G_j^{-1} the quantile function as in (6.2).

Given i.i.d. observations $X_1, \ldots, X_n$ from a density f on $\mathbb{R}^d$ and given a reference density g such as (6.4), modified multivariate histograms are built as follows.

- Set $m = m_1 \ldots m_d$ with $m_1, \ldots, m_d$ positive integers and let $h_j = 1/m_j$ for $j = 1, \ldots, d$;

- For $j = 1, \ldots, d$ and $i_j = 1, \ldots, m_j - 1$, compute univariate quantiles of order $i_j h_j$ of g_j. Denote by q_{j,i_j} these quantiles *i.e.*

$$q_{j,i_j} = G_j^{-1}(i_j h_j)$$

  with the convention $q_{j,0} = -\infty$ and $q_{j,m_j} = \infty$;

- Consider the grid defined by the above family $\{q_{j,i_j}\}$; this grid leads to a partition of $\mathbb{R}^d$ into m hyperrectangles (see Figure 6.2), say

$$A_{i_1, \ldots, i_d} = \prod_{j=1}^{d} (q_{j,i_j-1}, q_{j,i_j}]; \qquad (6.5)$$

- For each of these cells, compute the empirical measure:

$$\mu_n(A_{i_1, \ldots, i_d}) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}_{\{X_i \in A_{i_1, \ldots, i_d}\}};$$

- The *regular modified multivariate histogram density estimate* f_n is defined by:

$$f_n(x) = \frac{n\mu_n(A(x)) + 1}{nh + 1} g(x) \qquad (6.6)$$
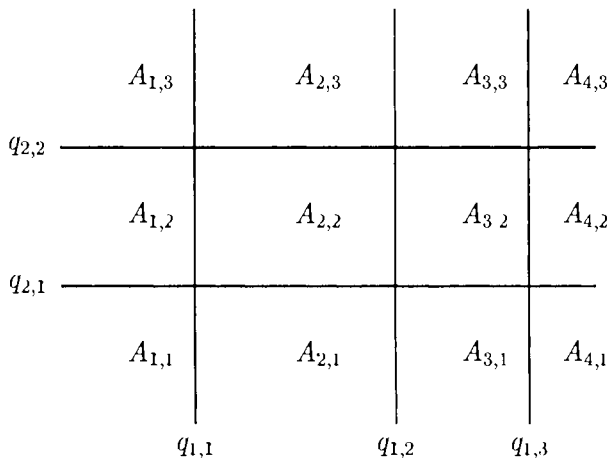
Figure 6.2. Example of partition in $\mathbb{R}^2$: $m_1 = 4$, $m_2 = 3$.

where $h = h_1 \ldots h_d$ and $A(x)$ stands for $A_{i_1, \ldots, i_d}$ if $x \in A_{i_1, \ldots, i_d}$. Denote by ν the probability measure associated with the reference density g. It is easily seen that, for any set $A_{i_1, \ldots, i_d}$,

$$\nu(A_{i_1, \ldots, i_d}) = h \, .$$

Consistency in information divergence and expected information divergence is established in our next theorem.

THEOREM 6.1 *Let f_n be the regular modified histogram defined in (6.6). Assume that $D(f, g) < \infty$.*

(i) *If $h_j = h_{j,n}$ $(j = 1, \ldots, d)$ and $\lim\limits_{n \to \infty} \max\limits_{1 \le j \le d} h_{j,n} = 0$ then the sequence of partition*

$$\{\mathcal{P}_n\} = \{A_{n, i_1, \ldots, i_d}\}_{\substack{1 \le j \le d \\ 1 \le i_j \le m_{j,n}}}$$

defined in (6.5) is ν-approximating.

(ii) *Moreover assume that $\lim\limits_{n \to \infty} n h_n = \infty$ $(h_n = h_{1,n} \ldots h_{d,n})$, then*

$$\lim_{n \to \infty} \mathbf{E} D(f, f_n) = 0 \text{ and } \lim_{n \to \infty} D(f, f_n) = 0 \text{ a.s.}$$

Proof. We first prove (i). Let S denote the support of ν and $\overline{S}$ its complement in $\mathbb{R}^d$. With a slight abuse of notation, we denote

$$\{\mathcal{P}_n\} = \{A_{n,1}, \ldots, A_{n,m_n}\} \, .$$

For $j = 1, \ldots, d$, let $a_j = \inf\{x \in \mathbb{R} : g_j(x) \neq 0\}$ and $b_j = \sup\{x \in \mathbb{R} : g_j(x) \neq 0\}$ (a_j and b_j may be infinite). Let S_j (resp. $\overline{S}_j$) be the projection of S (resp. $\overline{S}$) on (a_j, b_j). $\overline{S}_j$ is the union of k_j distinct intervals of length $l(i)$ ($i = 1, \ldots, k_j$). For $x = (x_1, \ldots, x_d) \in S$, let $p_j(x_j)$ denote the number of intervals of $\overline{S}_j$ before x_j and consider for $j = 1, \ldots, d$

$$T_j : \quad S_j \quad \longrightarrow \mathbb{R}$$

$$x_j \quad \longrightarrow x_j - \sum_{i=1}^{p_j(x_j)} l(i)$$

and

$$T : \quad S \quad \longrightarrow \mathbb{R}^d$$

$$(x_1, \ldots, x_d) \quad \longrightarrow (T_1(x_1), \ldots, T_d(x_d)).$$

The application T allows to remove the hyperrectangles R of $\mathbb{R}^d$ such that $\nu(R) = 0$.

Fix a measurable set A. If A_n is equal to a union of sets in $\mathcal{P}_n$ then

$$\nu(A_n \triangle A) = \nu(T(A_n) \triangle T(A)).$$

Therefore, it suffices to prove that the partition

$$\{\mathcal{P}_n^T\} = \{T(A_{n,1}), \ldots, T(A_{n,m_n})\}$$

is ν-approximating. Note that $T(A_{n,i})$ ($i = 1, \ldots, m_n$) are hyperrectangles of $\mathbb{R}^d$ such that $\nu(T(A_{n,i})) = h_{1,n} \ldots h_{d,n}$. Since $\lim_{n \to \infty} h_{j,n} = 0$, $j = 1, \ldots, d$, we have for each ball B centered at some point x_0

$$\lim_{n \to \infty} \max_{\{i\, :\, T(A_{n,i}) \cap B \neq \emptyset\}} \operatorname{diam}(T(A_{n,i})) = 0$$

where $\operatorname{diam}(E) = \sup_{x,y \in E} d(x,y)$ and $d(x,y)$ denotes the distance in $\mathbb{R}^d$. It follows from Csiszár (1973, p. 168) that the partition $\{\mathcal{P}_n^T\}$ is ν-approximating.

Combining (i) with Theorem 2 in Barron, Györfi and van der Meulen (1992) gives (ii). $\square$

2.2   Influence of correlation

Through an example, we study the influence of the shape of the data vector on the performance of the density estimate defined in (6.6). Table 6.1 gives the information divergence $D(f, f_n)$ and the total variation

Table 6.1. Information divergence and total variation according to the correlation.

ρ	0	0.25	0.5	0.75	0.95
$D(f, f_n)$	0.32	0.33	0.35	0.43	0.74
$V(f, f_n)$	0.19	0.19	0.21	0.22	0.34

$V(f, f_n)$ between binormals and their standard modified histogram esti-
mates. Simulated binormals have 0 mean, unit standard deviation and
varying correlation (from 0 to 0.95), the size of the samples is $n = 250$.
To construct the estimate, we take $m_1 = m_2 = 5$ and the reference
density g is a product of Gumbel densities:

$$g(x, y) = \exp\left(-x - \exp(-x)\right) \exp\left(-y - \exp(-y)\right). \qquad (6.7)$$

Results are clearly better in the presence of weak correlation. One can
explain it as follows. On Figure 6.3, we have represented a sample of
size $n = 250$ from a binormal with 0 mean and identity variance ma-
trix (LEFT) and the image of this sample by the affine transformation
(RIGHT):

$$T(x) = \Sigma^{1/2} x + a$$

where

$$\Sigma = \begin{pmatrix} 1 & 0.95 \\ 0.95 & 1 \end{pmatrix} \text{ and } a = \begin{pmatrix} -1 \\ 0 \end{pmatrix}.$$

Note that the transformed sample can be seen as a sample simulated
from a binormal $\mathcal{N}(a, \Sigma)$. We represent on these graphics the partition
used to construct regular modified histograms with a reference density
of Gumbel (see (6.7)) and $m_1 = m_2 = 5$. For the transformed sample,
only few classes possesses observations, the partition is not well adapted
to the data cloud. Therefore the comparison between the empirical mea-
sure and the reference density over the partition does not make much
sense.
To correct this, we will construct data dependent modified histograms
for which keeping the parameters g and m_j $(j = 1, \ldots, d)$ fixed, the cor-
responding partition is equivariant under affine transformation of data
vectors. Our method is inspired by the affine equivariant *quantile con-
tour plots* defined by Chakraborty (2001).

2.3 Data-driven modified histograms

Statistical practice suggests that histograms based on data-dependent
partitions will provide better performance than those based on a fixed
sequence of partitions. Theoretical evidence for this superiority was put
forward by Stone (1985). In this paragraph, we construct a modified
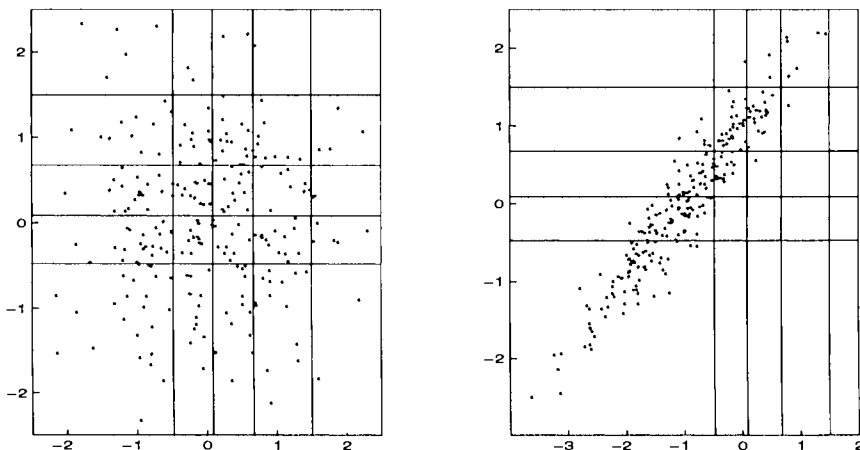
Figure 6.3. See text in Subsection 2.2.

histogram based on a data-dependent partition equivariant under affine transformation of the data vector (for g and m_j, $j = 1, \ldots, d$ fixed). The approach is based on a "data-driven coordinate system" introduced by Chaudhuri and Sengupta (1993). Formally, fix n_0 such that $n_0 > d + 1$ and consider $n_0 + n$ data points $X_1, \ldots, X_{n_0+n}$ i.i.d. from a density f on $\mathbb{R}^d$. Split the data into a set $X_1, \ldots, X_{n_0}$ used for choosing the "data-driven coordinate system" and a set $X_{n_0+1}, \ldots, X_{n_0+n}$ used for constructing the density estimate. To lighten the notation we will write $X_1^\star, \ldots, X_n^\star$ for $X_{n_0+1}, \ldots, X_{n_0+n}$.

■ Set $m = m_1 \ldots m_d$ with $m_1, \ldots, m_d$ positive integers, and let $h_j = 1/m_j$ for $j = 1, \ldots, d$;

■ Let $\alpha = \{k_0, k_1, \ldots, k_d\}$ denote a subset of $\{1, 2, \ldots, n_0\}$ of size $(d+1)$. Consider the points $X_{k_0}, \ldots, X_{k_d}$ which will form a "data-driven coordinate system", where X_{k_0} will determine the origin and the lines joining that origin to the remaining d data points $X_{k_1}, \ldots, X_{k_d}$ will form various coordinate axis. Consider the $d \times d$ matrix

$$X(\alpha) = \{X_{k_1} - X_{k_0}, \ldots, X_{k_d} - X_{k_0}\}.$$

If f is absolutely continuous on $\mathbb{R}^d$, $X(\alpha)$ is an invertible matrix with probability one for any choice of α (see Chaudhuri and Sengupta (1993)). Next, transform all the observations in terms of the

new coordinate system as

$$
\begin{cases}
\dot{X}_i = \{X(\alpha)\}^{-1} X_i, & i = 1, \ldots, n_0, \\[2mm]
\dot{X}_i^\star = \{X(\alpha)\}^{-1} X_i^\star, & i = 1, \ldots, n.
\end{cases}
$$

■ Let $\tilde{g}$ be a density on $\mathbb{R}^d$ such that

$$
\tilde{g}(x_1, \ldots, x_d) = \tilde{g}_1(x_1) \ldots \tilde{g}_d(x_d), \tag{6.8}
$$

where $\tilde{g}_1(x_1), \ldots, \tilde{g}_d(x_d)$ are univariate densities.
Define $p = (p_1, \ldots, p_d)$ the coordinatewise median associated with the density $\tilde{g}$, *i.e.*

$$
p_j = \tilde{G}_j^{-1}(0.5), \quad j = 1, \ldots, d,
$$

and let $\dot{X}_{([n_0/2])}$ be the empirical coordinatewise median from the sample $\dot{X}_1, \ldots, X_{n_0}$ *i.e.*

$$
\dot{X}_{([n_0/2])} = (\dot{X}^{(1)}_{([n_0/2])}, \ldots, \dot{X}^{(d)}_{([n_0/2])}).
$$

where [ ] stands for the integer part and $\dot{X}^{(j)}_{(1)}, \ldots, \dot{X}^{(j)}_{(n_0)}$ denotes the order statistics of the j-th components of the data vector $\dot{X}_1, \ldots, \dot{X}_{n_0}$. Consider the vector $b_X^\alpha = p - \dot{X}_{([n_0/2])}$ and let $\tilde{X}_i^\star$ be the image of $\dot{X}_i^\star$ by the translation of vector b_X^α, *i.e.*

$$
\tilde{X}_i^\star = \dot{X}_i^\star + b_X^\alpha, \quad i = 1, \ldots, n.
$$

As for the regular modified histograms presented above, for $j = 1, \ldots, d$ and $i_j = 1, \ldots, m_j - 1$, denote $\tilde{q}_{j,i_j}$ the quantile of order $i_j h_j$ of $\tilde{g}_j$. These quantiles lead to a partition of $\mathbb{R}^d$ into m hyperrectangles say

$$
\tilde{A}_{i_1, \ldots, i_d} = \prod_{j=1}^d (\tilde{q}_{j, i_j - 1}, \tilde{q}_{j, i_j}].
$$

Let μ_n (resp. $\tilde{\mu}_n$) be the empirical measure associated with the sample $X_1^\star, \ldots, X_n^\star$ (resp. $\tilde{X}_1^\star, \ldots, \tilde{X}_n^\star$);

■ Express the $\tilde{A}_{i_1, \ldots, i_d}$'s in terms of the original coordinate system, *i.e.*

$$
A_{i_1, \ldots, i_d} = X(\alpha) (\tilde{A}_{i_1, \ldots, i_d} - b_X^\alpha).
$$

$\tilde{A}_{i_1,\ldots,i_d}$ is the image of the hyperrectangle $A_{i_1,\ldots,i_d}$ by an affine transformation therefore $\tilde{A}_{i_1,\ldots,i_d}$ is an hyperparallelogram (see Figure 6.4). Moreover, it is easily seen that

$$\mu_n(A_{i_1,\ldots,i_d}) = \tilde{\mu}_n(\tilde{A}_{i_1,\ldots,i_d});$$

- Finally, fix

$$g_\alpha(x) = \frac{1}{\left|\det\left(X(\alpha)\right)\right|}\, \tilde{g}\left(\{X(\alpha)\}^{-1}x + b_X^\alpha\right), \qquad (6.9)$$

then the *data-driven modified histogram density estimate* is defined by

$$f_n(x) = \frac{n\mu_n\big(A(x)\big) + 1}{nh + 1}\, g_\alpha(x), \qquad (6.10)$$

where $h = h_1 \ldots h_d$ and $A(x)$ stands for $A_{i_1,\ldots,i_d}$ if $x \in A_{i_1,\ldots,i_d}$.

LEMMA 6.1 *The estimate $f_n(x)$ defined in (6.10) is a modified histogram in the sense of (6.1).*

Proof. It suffices to prove the following assertions:

- g_α is a density (we will denote by ν the measure associated with this density);

- for $j = 1, \ldots, d$ and $i_j = 1, \ldots, m_j$, $\nu(A_{i_1,\ldots,i_d}) = h$.

These assertions are direct consequences of the change of variables theorem. $\qquad\square$
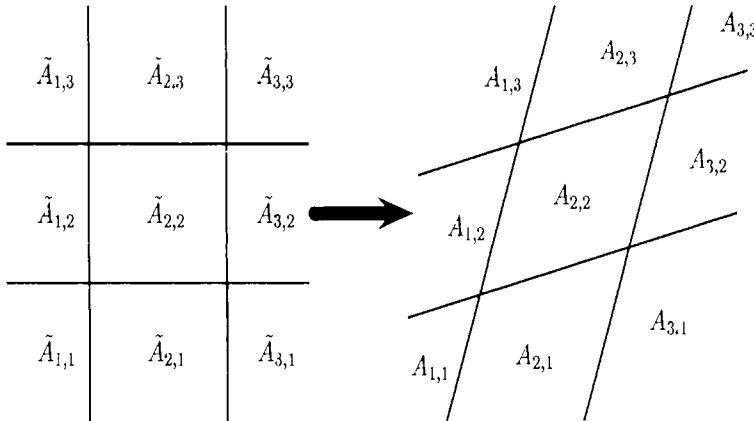
Figure 6.4. Transformation of the partition.

REMARK 6.1 One can use other translations, however our choice of b_X^α seems to be well adapted to our estimate. Indeed, modified histograms result from the comparison between the reference density and the empirical measure. Thus, our translation is chosen so that the image of $\dot{X}_1, \ldots, \dot{X}_{n_0}$ has the same median as the density $\tilde{g}$. This translation can be seen as a "bias correction". We choose the median because of its robustness.

From now on, given a sample $T_1, \ldots, T_{n_0+n}$, we write $T_1^\star, \ldots, T_n^\star$ for $T_{n_0+1}, \ldots, T_{n_0+n}$ and $\mu_n(A; T_1^\star, \ldots, T_n^\star)$ for the empirical measure associated with $T_1^\star, \ldots, T_n^\star$. Moreover, with a slight abuse of notation, we will denote by $\{A_{i_1,\ldots,i_d}\}$ the partition

$$\{A_{i_1,\ldots,i_d}\}_{\substack{1 \leq j \leq d \\ 1 \leq i_j \leq m_j}} .$$

We now prove the equivariance of the partition under arbitrary affine transformations of data vectors.

THEOREM 6.2 *The partition $\{A_{i_1,\ldots,i_d}\}$ is equivariant under arbitrary affine transformations of data vectors. We can formulate it as follows. Let the d-dimensional vectors $X_1, \ldots, X_{n_0+n}$ be transformed into $Z_1, \ldots, Z_{n_0+n}$ with $Z_i = M X_i + c$ where M is a $d \times d$ nonsingular matrix and c is a vector in $\mathbb{R}^d$. Suppose that we use the same density $\tilde{g}$ and the same integers m_j $(j = 1, \ldots, d)$ to construct the data-driven modified histogram from $X_1, \ldots, X_{n_0+n}$ and $Z_1, \ldots, Z_{n_0+n}$. If $\{A_{i_1,\ldots,i_d}\}$ (resp. $\{B_{i_1,\ldots,i_d}\}$) denotes the partition computed from the sample $X_1, \ldots, X_{n_0+n}$ (resp. $Z_1, \ldots, Z_{n_0+n}$), then for all integers $i_1, \ldots, i_d$ such that $1 \leq i_j \leq m_j$ and $1 \leq j \leq d$ we have*

(i) $B_{i_1,\ldots,i_d} = M A_{i_1,\ldots,i_d} + c$.

(ii) $\mu_n(A_{i_1,\ldots,i_d}; X_1^\star, \ldots, X_n^\star) = \mu_n(B_{i_1,\ldots,i_d}; Z_1^\star, \ldots, Z_n^\star)$.

Proof. Let $\alpha = \{k_0, k_1, \ldots, k_d\}$ be a subset of $\{1, \ldots, n_0\}$ of size $d + 1$. Consider

$$X(\alpha) = \{X_{k_1} - X_{k_0}, \ldots, X_{k_d} - X_{k_0}\}$$

and

$$Z(\alpha) = \{Z_{k_1} - Z_{k_0}, \ldots, Z_{k_d} - Z_{k_0}\}$$

so that we have $Z(\alpha) = M X(\alpha)$.
Note that for $i = 1, \ldots, n_0$

$$\dot{Z}_i = Z(\alpha)^{-1} Z_i$$

$$= X(\alpha)^{-1} X_i + \left(M X(\alpha) \right)^{-1} c$$
$$= \dot{X}_i + \left(M X(\alpha) \right)^{-1} c \,.$$

Therefore $\dot{Z}_{[n_0/2]} = \dot{X}_{[n_0/2]} + (M X(\alpha))^{-1} c$ and $b_Z^\alpha = b_X^\alpha - \left(M X(\alpha) \right)^{-1} c$. As we use the same density $\tilde{g}$ and the same integers m_j $(j = 1, \ldots, d)$, the partitions computed for transformed observations will be the same for the samples $X_1, \ldots, X_{n_0+n}$ and $Z_1, \ldots, Z_{n_0+n}$. We denote $\{ \tilde{A}_{i_1, ., i_d} \}$ this partition. To obtain $\{ A_{i_1, ., i_d} \}$ and $\{ B_{i_1, ., i_d} \}$ we only have to re-transform $\{ \tilde{A}_{i_1, ., i_d} \}$. For all integers $i_1, \ldots, i_d$ such that $1 \leq i_j \leq m_j$ and $1 \leq j \leq d$, it follows that

$$
\begin{aligned}
B_{i_1, ., i_d} &= Z(\alpha)(\tilde{A}_{i_1, ., i_d} - b_Z^\alpha) \\
&= M X(\alpha) \left(\tilde{A}_{i_1, ., i_d} - \left(b_X^\alpha - (M X(\alpha))^{-1} c \, \textdot{i} g \right) \right) \\
&= M \left(X(\alpha) \left(\tilde{A}_{i_1, ., i_d} - b_X^\alpha \right) \right) + c \\
&= M A_{i_1, ., i_d} + c \,,
\end{aligned}
$$

which gives *(i)*.
Since $\tilde{X}_i^\star = X(\alpha)^{-1} X_i^\star + b_X^\alpha$ and $\tilde{Z}_i^\star = Z(\alpha)^{-1} Z_i^\star + b_Z^\alpha$ $(i = 1, \ldots, n)$, it easily follows that

$$\forall i = 1, \ldots, n, \ \tilde{X}_i^\star = \tilde{Z}_i^\star \,.$$

Therefore

$$\mu_n(\tilde{A}_{i_1, \ldots, i_d}; \tilde{X}_1^\star, \ldots, \tilde{X}_n^\star) = \mu_n(\tilde{A}_{i_1, \ldots, i_d}; \tilde{Z}_1^\star, \ldots, \tilde{Z}_n^\star)$$

and *(ii)* is proved.   □

REMARK 6.2 It is worth pointing out that the actual reference density (in the sense of (6.1)) is g_α which implies that the reference density depends on the data. However, one can have some a priori idea on the density to estimate and thus want to construct modified histogram for a given reference density g. It is possible to use this algorithm provided that g may be written in the form

$$g(x) = \frac{1}{|\det(M)|} \tilde{g}(M^{-1} x + a) \qquad (6.11)$$

where $x = (x_1, \ldots, x_d)$, M is an invertible matrix $d \times d$, a is a vector of $\mathbb{R}^d$ and $\tilde{g}$ is a product of univariate densities *i.e.*

$$\tilde{g}(x) = \tilde{g}_1(x_1) \ldots \tilde{g}_d(x_d) \,.$$

In that case we no longer split the data (all the observations are used to construct the modified histogram) and we replace $X(\alpha)$ by M and b_X^α by a. Note that multinormal densities $g_{\mu,\Sigma}$ are in the form of (6.11). Nevertheless Theorem 6.2 does not hold for such modified histograms.

Summarizing, we have found a partition equivariant under arbitrary affine transformation. Consistency in information divergence of this new estimate is a straightforward consequence of the next lemma (whom proof is straightforward).

LEMMA 6.2 *The information divergence is invariant under invertible transformation of the data sample.*

COROLLARY 6.1 *Let f_n be the data-driven modified histogram defined in (6.10). Assume that $D(f, g_\alpha) < \infty a.s.$ Moreover, assume that for $i = 1, \ldots, d$, $h_i = h_{i,n}$ (therefore $h = h_n$),*

$$\lim_{n \to \infty} \max_{1 \le i \le d} h_{i,n} = 0 \text{ and } \lim_{n \to \infty} n h_n = \infty,$$

then

$$\lim_{n \to \infty} \mathbf{E}^{(n_0)} D(f, f_n) = 0 a.s. \text{ and } \lim_{n \to \infty} D(f, f_n) = 0 \text{ a.s.}$$

where $\mathbf{E}^{(n_0)}$ denotes the conditional expectation given the X_i's for which $1 \le i \le n_0$.

Proof. Fix $X_1, \ldots, X_{n_0}$ such that $D(f, g_\alpha) < \infty$. Let $\tilde{f}$ (resp. $\tilde{f}_n$) be the density to estimate f (resp. the density estimator f_n) in the transformed coordinate system *i.e.*

$$\begin{cases} \tilde{f}(x) = & \left| \det \left(X(\alpha) \right) \right| f \left(X(\alpha)(x - b_X^\alpha) \right) \\[2mm] \tilde{f}_n(x) = & \left| \det \left(X(\alpha) \right) \right| f_n \left(X(\alpha)(x - b_X^\alpha) \right). \end{cases}$$

$\tilde{f}_n$ is the regular modified histogram density estimate of $\tilde{f}$ (see page 102) with $\tilde{g}$ as reference density. From Theorem 6.1, it follows that

$$\begin{cases} \lim_{n \to \infty} D(\tilde{f}, \tilde{f}_n) = 0 \text{ a.s.} \\[3mm] \lim_{n \to \infty} \mathbf{E} D(\tilde{f}, \tilde{f}_n) = 0. \end{cases}$$

The conclusion follows from Lemma 6.2.

3.   Selection of α

The performance of the data-driven modified histogram clearly depends upon the choice of m_j $(j = 1, \ldots, d)$, $\tilde{g}$ and α. Here we will restrict our attention to the choice of α. Recent univariate results obtained by Berlinet and Brunel (2004) show that the Kullback-Leibler cross-validation technique works well for selecting m_1 from the data. We will apply the same method to find the best α.

Let $X_1, \ldots, X_{n_0+n}$ be i.i.d. observations from a density f and let S_{n_0} denote the collection of all subsets of size $d + 1$ of $\{1, \ldots, n_0\}$. Fix m_j $(j = 1, \ldots, d)$ and $\tilde{g}$ (such as (6.8)). For $\alpha \in S_{n_0}$, let us denote by f_n^α the data-driven modified multivariate histogram defined in (6.10). Expanding the actual information divergence error yields

$$D(f, f_n^\alpha) = \int_{\mathbb{R}^d} f(x) \log f(x) \, dx - \int_{\mathbb{R}^d} f(x) \log f_n^\alpha(x) \, dx. \qquad (6.12)$$

The second integral could be written as $\mathbf{E}(\log f_n^\alpha(X))$, where the expectation is taken with respect to the evaluating point and not over the sample. The cross-validation device consists in removing one data point among $X_1^\star, \ldots, X_n^\star$ and using the remaining $(n-1)$ points to construct an estimator of $\mathbf{E}(\log f_n^\alpha(X))$. This step is repeated for each $X_i^\star$ $(i = 1, \ldots, n)$. Let $f_n^{\alpha,i}$ be the modified histogram density estimate defined after deleting the i-th observation *i.e.*

$$f_n^{\alpha,i}(x) = \frac{n\mu_n^i\big(A(x)\big) + 1}{nh + 1} g_\alpha(x)$$

where g_α is defined by (6.9) and

$$\mu_n^i\big(A(x)\big) = \frac{1}{n-1} \sum_{j \neq i} 1_{\{X_j^\star \in A(x)\}}.$$

With this notation, an estimate of $\mathbf{E}(\log f_n^\alpha(X))$ is given by

$$\frac{1}{n} \sum_{i=1}^{n} \log f_n^{\alpha,i}(X_i^\star)$$

and since the first integral in (6.12) does not depend on α, we deduce a cross validation criterion for the choice of α:

choose $\hat{\alpha} \in S_{n_0}$ which minimizes $CV(\alpha) = -\dfrac{1}{n} \sum_{i=1}^{n} \log f_n^{\alpha,i}(X_i^\star)$.

Note that if $D(f, g_{\hat{\alpha}}) < \infty$ a.s., consistency of the selected estimate $f_n^{\hat{\alpha}}$ follows from Corollary 6.1.

For fixed α, we have seen that the partition is affine equivariant. The next theorem states the analogue with α selected by cross-validation.

THEOREM 6.3 *The choice of α by cross-validation is invariant under arbitrary affine transformations of data vectors. We can formulate it as follows.*
Let the d-dimensional vectors $X_1, \ldots, X_{n_0+n}$ be transformed into $Z_1, \ldots, Z_{n_0+n}$ with $Z_i = MX_i + c$ where M is a $d \times d$ nonsingular matrix and c is a vector in $\mathbb{R}^d$. Suppose that we use the same density $\tilde{g}$ and the same integers m_j $(j = 1, \ldots, d)$ to construct the data-driven modified histograms $f_{n,X}^\alpha$ (with $X_1, \ldots, X_{n_0+n}$) and $f_{n,Z}^\alpha$ (with $Z_1, \ldots, Z_{n_0+n}$). Then

$$\hat{\alpha} \text{ minimizes } -\frac{1}{n} \sum_{i=1}^n \log f_{n,X}^{\alpha,i}(X_i^\star) \Leftrightarrow \hat{\alpha} \text{ minimizes } -\frac{1}{n} \sum_{i=1}^n \log f_{n,Z}^{\alpha,i}(Z_i^\star).$$

Proof. We will denote by $\{A_{i_1,\ldots,i_d}\}$ (resp. $\{B_{i_1,\ldots,i_d}\}$) the partition used to construct the modified histogram from the sample $X_1, \ldots, X_{n_0+n}$ (resp. $Z_1, \ldots, Z_{n_0+n}$).
We have

$$\frac{1}{n} \sum_{i=1}^n \log f_{n,Z}^{\alpha,i}(Z_i^\star) = \frac{1}{n} \sum_{i=1}^n \log \frac{n\mu_n^i(B(Z_i^\star)) + 1}{nh + 1} g_\alpha(Z_i^\star)$$

where

$$g_\alpha(Z_i^\star) = \frac{1}{|\det(Z(\alpha))|} \tilde{g}(Z(\alpha)^{-1} Z_i^\star + b_Z^\alpha).$$

Theorem 6.2 and its proof give

$$\begin{cases} Z(\alpha) & = MX(\alpha) \\ b_Z^\alpha & = b_X^\alpha - (MX(\alpha))^{-1} c \\ B_{i_1,\ldots,i_d} & = MA_{i_1,\ldots,i_d} + c. \end{cases}$$

Moreover, it is easily seen that $\mu_n^i(B(Z_i^\star)) = \mu_n^i(A(X_i^\star))$. Putting all pieces together, we obtain

$$-\frac{1}{n} \sum_{i=1}^n \log f_{n,Z}^{\alpha,i}(Z_i^\star) = -\frac{1}{n} \sum_{i=1}^n \log f_{n,X}^{\alpha,i}(X_i^\star) + \log(|\det(M)|).$$

Since M does not depend on α, the proof is complete. $\qquad\square$

4.   Simulations

In this paragraph we are presenting some finite sample simulation results on the efficiency of the data-driven modified histogram f_n^α defined by (6.10) compared with the regular modified histogram f_n defined by (6.6). We use two data sets.

We first simulated 50 samples of size $n_0 + n$ ($n_0 + n = 150, 300, 550$) from bivariate normal populations with zero means, unit standard deviations and varying correlation coefficients $\rho = 0, 0.25, 0.5, 0.75$ and 0.95. For each sample, we have computed modified histograms f_n and f_n^α (α is selected by cross-validation). These estimates are built with

$$\begin{cases} \tilde{g}(x, y) = \exp\big(-x - \exp(-x)\big) \exp\big(-y - \exp(-y)\big) \\ n_0 = 50 \\ m_1 = m_2 = 4 \text{ for } n = 100 \\ m_1 = m_2 = 5 \text{ for } n = 250 \\ m_1 = m_2 = 6 \text{ for } n = 500 \, . \end{cases}$$

We display in Table 6.2 the average of $D(f, f_n)$ and $D(f, f_n^\alpha)$ and the gain Ga in information divergence

$$Ga = \frac{D(f, f_n) - D(f, f_n^\alpha)}{D(f, f_n)} \, .$$

Table 6.2. Comparison of performance between regular and data-driven modified histograms.

n	ρ	$D(f, f_n)$	$D(f, f_n^\alpha)$	Ga
100	0	0.36	0.23	0.36
250		0.32	0.15	0.53
500		0.29	0.11	0.62
100	0.25	0.36	0.24	0.33
250		0.32	0.15	0.53
500		0.30	0.11	0.63
100	0.5	0.39	0.23	0.41
250		0.35	0.15	0.57
500		0.31	0.11	0.65
100	0.75	0.50	0.23	0.54
250		0.41	0.15	0.63
500		0.36	0.10	0.72
100	0.95	0.85	0.24	0.72
250		0.73	0.14	0.81
500		0.64	0.11	0.83
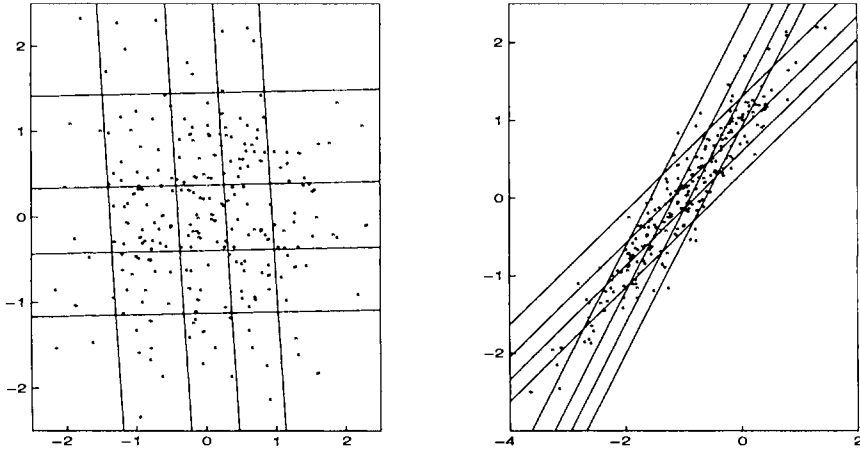
Figure 6.5. Partition of data-driven modified histogram. Simulated samples are the same as in Figure 6.3. $\tilde{g}$ is a product of Gumbel densities and $m_1 = m_2 = 5$.

For the second set of data, points are generated from multivariate symmetric Laplace distributions (see Anderson (1992)) with density

$$f(x) = \frac{2}{(2\pi)^{d/2}|\Sigma|^{1/2}}(x^t\Sigma^{-1}x/2)^{v/2}K_v\left(\sqrt{2x^t\Sigma^{-1}x}\right),$$

where $v = (2-d)/2$, Σ is a $d \times d$ non-negative definite symmetric matrix and $K_v(u)$ is the modified Bessel function of the third kind given by

$$K_v(u) = \frac{1}{2}\left(\frac{u}{2}\right)^v \int_0^\infty t^{-v-1}\exp\left(-t - \frac{u^2}{4t}\right)dt, \ u > 0.$$

We set $d = 2, 4, 8, 10$ and several sample sizes $n_0 + n$. For each $(d, n_0 + n)$, we simulated 50 samples from a symmetric Laplace distribution with

$$\Sigma = \begin{pmatrix} 1 & \rho & \cdots & \rho \\ \rho & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \rho \\ \rho & \cdots & \rho & 1 \end{pmatrix} \qquad \rho = 0; 0.5; 0.95.$$

The density $\tilde{g}$ is a multivariate standard normal distribution and we take $m_j = 3$ $(j = 1, \ldots, d)$. For $d = 2$ and 4 we again take $n_0 = 50$ to select α by cross-validation. However, for higher dimension the optimization problem is very heavy and takes too much time to reach an adequate solution. Thus, for $d = 8$ and 10, we propose the following alternative. We choose the transformation matrix $X(\alpha)$ in such a way that the image

of $X_1, \ldots, X_{n_0}$ has the same variance-covariance matrix as the density $\tilde{g}$ (identity in our example). In other words, we replace $X(\alpha)$ with $\hat{\Sigma}^{1/2}$ where $\hat{\Sigma}$ is an affine equivariant estimate of the variance-covariance matrix of the distribution (computed from $X_1, \ldots, X_{n_0}$). The rest of the construction does not change. Note that the corresponding estimate no longer depends on α but on $\hat{\Sigma}$. In this regard it will be denoted by $f_n^{\hat{\Sigma}}$ and for the sake of clarity the associated reference density g_α and vector b_X^α will be denoted by $g_{\hat{\Sigma}}$ and $b_X^{\hat{\Sigma}}$. Consistency Corollary 6.1 is still true for $f_n^{\hat{\Sigma}}$. We take $n_0 = 1000$ for $d = 8$ and 10. $D(f, f_n)$ and $D(f, f_n^\alpha)$ are computed from Monte-Carlo method. The results are displayed in Table 6.3.

Table 6.3. Comparison of performance between regular and data-driven modified histograms.

$d; n$	ρ	$D(f, f_n)$	$D(f, f_n^\alpha)$ or $D(f, f_n^{\hat{\Sigma}})$	Ga
2;250	0	0.12	0.12	0
	0.5	0.18	0.13	0.28
	0.95	0.73	0.12	0.84
4;1000	0	0 34	0.36	-0.06
	0.5	0.55	0.37	0.33
	0.95	2.32	0.37	0.84
8;10000	0	0.90	0.90	0
	0.5	1.58	0.93	0.41
	0.95	6.10	0.93	0.85
10;500000	0	1.08	1.12	-0.04
	0.5	1.90	1.14	0.40
	0.95	7.52	1.12	0.85

5.   Concluding remarks

1) Our examples demonstrate rather strikingly that f_n^α is on the whole better than f_n. The difference increases with the correlation and the dimension. Moreover, keeping n and d fixed, $D(f, f_n^\alpha)$ is stable whatever the correlation. It is worth pointing out that the partition is well adapted to the data cloud even with high correlation (see Figure 6.5).

2) Unlike with the first set of data, f_n^α is not better than f_n when $\rho = 0$ for the second set. It is due to the fact that the symmetric Laplace distribution and the standard gaussian distribution have the same median. Therefore the translation vector is close to zero and the reference density and the density to estimate are close enough without the transformation.

On the other hand, for the first data set the two distributions do not have the same coordinatewise median. The translation can be seen as a "bias corrector" between the two densities.

3) For the second data set, the partition is not equivariant by affine transformation of the data sample when $d = 8$ or $d = 10$. All the same, the estimate is performant and the computation is quick even in large dimension. We emphasize that the transformation-retransformation procedure just allows to select a reference density which is not "too far" from the density to estimate. In other words our choice of the transformation matrix is motivated by the fact that the reference density should be as close as possible to the density f to estimate. Since f is unknown in practice, we select the affine transformation such that the image of $X_1, \ldots, X_{n_0}$ and the random variable with density $\tilde{g}$ have the same variance-covariance matrix (with the help of the linear transformation $\hat{\Sigma}^{-1/2}$) and the same median (by the vector translation $b_{\hat{X}}^{\hat{\Sigma}}$). Note that when f is elliptically symmetric, similar conditions on the choice of the transformation matrix are discussed by Chakraborty (2001) in the asymptotic study of the affine equivariant multivariate quantiles.

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Chapter 7

ON ROBUST DIAGNOSTICS AT INDIVIDUAL LAGS USING RA-ARX ESTIMATORS

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Abstract   The aim of this paper is to present robust individual tests in autoregressive models with exogenous variables. We derive the asymptotic distribution of the RA-ARX estimators introduced in Duchesne (2004a), following an approach similar to Bustos and Yohai (1986). In particular, we give the asymptotic covariance structure of the RA-ARX estimators. Using this result, we establish the asymptotic distribution of the robustified residual autocorrelations under the null hypothesis of adequacy, which is normal. Some simulation results are reported.

1.   Introduction

Let $\{Y_t, t \in \mathbb{Z}\}$ and $\{X_t, t \in \mathbb{Z}\}$ be two mean zero second order stationary stochastic processes. We consider the following linear dynamic autoregressive model with exogenous variables (ARX):

$$\phi(B)Y_t = \nu(B)X_t + u_t, \tag{7.1}$$

where the backshift operator B is such that $BY_t = Y_{t-1}$, $\phi(z) = 1 - \phi_1 z - \ldots - \phi_p z^p$ denotes the autoregressive polynomial of order p and $\nu(z) = \sum_{l=0}^{s} \nu_l z^l$ is a polynomial of order s. It is assumed that all roots of $\phi(z)$ are outside the unit circle. Let $\phi^{-1}(z) = \sum_{h=0}^{\infty} s_h z^h$, $s_0 = 1$. Throughout the paper, $s_h = 0$ for $h < 0$. The variable Y_t represents the dependent variable and is called the output, while the exogenous variable X_t corresponds to the input. Let $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_p)^\top$ and $\boldsymbol{\nu} = (\nu_0, \nu_1, \ldots, \nu_s)^\top$. The vector of unknown parameters of the model (7.1) is given by $\boldsymbol{\lambda} = (\boldsymbol{\phi}^\top, \boldsymbol{\nu}^\top)^\top$. The variance of X_t is noted σ_X^2 and the autocovariance function of the process $\{X_t\}$ is $\Gamma_X(\cdot)$. The

following assumption is a natural condition to impose on the innovation process $\{u_t, t \in \mathbb{Z}\}$.

ASSUMPTION A. The process $\{u_t, t \in \mathbb{Z}\}$ is independently and identically distributed (iid for short) such that $E(u_t) = 0$ and $E(u_t^2) = \sigma_u^2 < \infty$. Furthermore, we assume that u_t admits a symmetric distribution.

Under Assumption A, the law of the process $\{Y_t\}$ with exogenous process $\{X_t\}$, as given by (7.1), is denoted by ARX(p,s). Strict exogeneity is assumed for $\{X_t\}$, as stated in the following assumption.

ASSUMPTION B. The exogenous process $\{X_t\}$ is strictly exogenous, that is $\{X_t, t \in \mathbb{Z}\}$ and $\{u_t, t \in \mathbb{Z}\}$ are independent stochastic processes.

Additive outliers occur in the model (7.1) when this is not the true process $\{Y_t\}$ which is observed, but for example the process $\{Y_t + W_t\}$, where $\{Y_t\}$ and $\{W_t\}$ are independent, with $\{W_t\}$ being an iid sequence that generates the outliers, typically with a small probability. The problem of outliers in time series is introduced in Hampel et al. (1986).

When additive outliers are suspected in the output Y_t, $t = 1, \ldots, n$, we can estimate the parameters of the ARX model with the RA-ARX estimators introduced in Duchesne (2004a). These estimators are expected to be much less biased than the non robust least squares (LS) estimators. The basic idea of the RA-ARX estimators consists in modifying the equation of the system leading to the conditional LS estimators. Let $r_t(\boldsymbol{\lambda}) = \phi(B)Y_t - \nu(B)X_t$ be the residuals based on the vector $\boldsymbol{\lambda}$. We will write simply r_t for the residuals when no confusion is possible. The RA-ARX estimators for $\boldsymbol{\lambda}$ are defined by solving the following system of nonlinear equations:

$$
\sum_{i=0}^{s} \nu_i \sum_{h=0}^{n-j-i-1} s_h \gamma_{rx}(h + i + j; \psi)
$$
$$
+ \sigma_u \sum_{h=0}^{n-p-j-1} s_h \gamma_{rr}(h + j; \eta) = 0, \quad j = 1, \ldots, p, \qquad (7.2)
$$
$$
\gamma_{rx}(j; \psi) = 0, \quad j = 0, 1, \ldots, s,
$$

where γ_{rx} and γ_{rr} are defined by

$$
\gamma_{rx}(i; \psi) = n^{-1} \sum_{t=i+1 \vee p+1}^{n} \psi(r_t/\sigma_u) X_{t-i}, \qquad (7.3)
$$

$$\gamma_{rr}(i;\eta) \;=\; n^{-1} \sum_{t=p+i+1}^{n} \eta(r_t/\sigma_u, r_{t-i}/\sigma_u). \tag{7.4}$$

Several choices for functions η and ψ are possible, but we assume that ψ is odd and continuous. For example, if $\eta(u,v) = uv$ and $\psi(u) = u$, we retrieve the usual LS estimators and (7.3) and (7.4) denote the lag-i cross-covariance between $\{X_t\}$ and $\{r_t/\sigma_u\}$, and the lag-i autocorrelation of $\{r_t\}$. These important special cases are denoted $R_{rx}(i)$ and $R_{rr}(i)$, respectively. However, these correlation measures are not robust to additive outliers. In order to obtain robustified estimators and robust measures, we can adopt η functions in the Mallows or Hampel families:

$$\eta_M(u,v) \;=\; \psi(u)\psi(v), \quad \text{Mallows,}$$
$$\eta_H(u,v) \;=\; \psi(uv), \qquad \text{Hampel.}$$

Note that at the estimation stage, another example of interest is $\eta(u,v) = \psi(u)v$, and the resulting estimators correspond essentially to M estimators, obtained by solving $\min \sum \rho(u_t/\sigma_u)$, where the derivative of $\rho(\cdot)$ is such that $\rho' = \psi$.

A first example of a bounded ψ function is given by the Huber family:

$$\psi_H(u;c) = \text{sign}(u)\min(|u|,c).$$

Another possibility is the bisquare family and a member is given by:

$$\psi_B(u;c) = \begin{cases} u(1-u^2/c^2)^2 & \text{if } 0 \le |u| \le c, \\ 0 & \text{elsewhere.} \end{cases}$$

The constant c in $\psi_H(u;c)$ and $\psi_B(u;c)$ is called the tuning parameter. Efficiency considerations, with respect to LS estimators, under perfectly observed ARX models, lead to some choice of c. When η is of the Mallows type, Duchesne (2004a) provides an iterative least squares scheme, which is particularly easy to implement. Under a general η function, Newton-Raphson algorithms can be used to obtain the RA-ARX estimators.

Note that in the system (7.2), simultaneous estimation of λ and σ_u using general Newton-Raphson algorithms is possible and desirable. In Duchesne (2004a), an additional equation is necessary for the estimation of σ_u, based on a certain π function (see also Martin and Yohai (1985), pp. 131-132 and p. 137). In practice, if one uses Mallows type η function and the iterative least-square scheme, then at each iteration a robust scale estimator for σ_u can be estimated with the observations, using for example

$$\hat{\sigma}_u = \text{med}\{|r_{p+1}|,\ldots,|r_n|\}/.6745.$$

Furthermore, a constant term can be included in the model (7.1) and if this is the case, the model becomes $\phi(B)(Y_t - \mu) = \nu(B)X_t + u_t$. In this situation, an additional equation for μ is also necessary in the previous system defining the RA-ARX estimators, and all parameters of the model can be estimated simultaneously. For simplicity, the processes $\{Y_t\}$ and $\{X_t\}$ are assumed to have zero mean in this paper.

Duchesne (2004a) introduced RA-ARX estimators to develop robust and powerful serial correlation tests in the error term of an adjusted ARX model, using a spectral approach. These kernel-based spectral tests provide generalized robust versions of the robust portmanteau test statistics of Li (1988) and are described in the recent monograph of Li (2004). They depend of a robust kernel-based spectral density estimator. The spectral tests admit an asymptotic standard normal distribution under the null hypothesis of model adequacy. More precisely, an appealing property of the kernel-based tests concerns their model-free asymptotic distribution. By comparison, the robust portmanteau test statistics introduced by Li (1988) admit a χ^2 distribution, with degrees of freedom that depend on the autoregressive and moving average orders. Furthermore, the flexible weighting of the spectral test statistics of Duchesne (2004a) gives the possibility to attribute more weight to lower orders lags, and less weight to higher orders lags. Since many autocorrelation functions decay quickly to zero as the lag orders increase, such weighting scheme should provide more powerful test statistics than Li's test statistic for many time series of practical interest.

The test statistics of Li (1988) and of Duchesne (2004a) are of the portmanteau type, in the sense that they take into account several lags. However, from the practitioner point of view, more insight is gained by considering test statistics based on individual residual autocorrelations, giving test statistics at each lag Such approach necessitates the asymptotic distribution of the robust residual autocorrelation function. That is exactly what we provide in this paper.

The primary goal of this paper is to complement the results of Duchesne (2004a). The paper is organized in the following way. In Section 2, asymptotic properties of the RA-ARX estimators are investigated. We establish the asymptotic normality of the RA-ARX estimators, following an approach similar to Bustos and Yohai (1986). In particular, we state explicitly the asymptotic covariance structure of the RA-ARX estimators. In Section 3, the asymptotic distribution of the residual autocorrelations is established. Based on this result, robust test statistics at individual lags are introduced and their asymptotic distributions are derived as a corollary of our main theorem. The new one-lag tests admit χ^2 distributions with one degree of freedom, under the null

hypothesis of model adequacy. In Section 4, some empirical experiments are reported. We investigate empirically the biases of the estimators and also the efficiencies of the RA-ARX estimators with respect to the LS estimators, when additive outliers are both present and absent in the time series. The RA-ARX estimators are studied when the η functions are of the Mallows and Hampel types, and for ψ functions that belong to Huber and bisquare families. We compute RA-ARX estimators using Newton-Raphson algorithms for an η function of the Hampel type. Next, the levels and powers of the new individual test statistics are investigated. Finally, we complete the paper with some concluding remarks in Section 5.

2. Asymptotic normality of RA-ARX estimators

In Duchesne (2004a), the consistency of the RA-ARX estimators was investigated. In this section, we establish the asymptotic distribution of the RA-ARX estimators, following an approach similar to Bustos and Yohai (1986).

Set

$$L_j^*(\boldsymbol{\lambda}) = \sum_{i=0}^{s} \nu_i \sum_{t=i+j+1}^{n} \delta_{rx,(i+j)t}^* + \sigma_u \sum_{t=p+j+1}^{n} \delta_{rr,jt}^* = 0, \ j = 1, \ldots, p,$$

$$L_j^*(\boldsymbol{\lambda}) = \sum_{t=j-p}^{n} \delta_{jt}^* = 0, \ j = p+1, \ . \ ,p+s+1,$$

and

$$\delta_{rx,kt}^* = \sum_{h=0}^{t-k-1} s_h \psi(r_t/\sigma_u) X_{t-k-h},$$

$$\delta_{rr,jt}^* = \sum_{h=0}^{t-p-j-1} s_h \eta(r_t/\sigma_u, r_{t-j-h}/\sigma_u), \ j = 1, \ . \ ,p,$$

$$\delta_{jt}^* = \psi(r_t/\sigma_u) X_{t-j+p+1}, \ j = p+1, \ . ,p+s+1.$$

We can then write system (7.2) as

$$\mathbf{L}^*(\boldsymbol{\lambda}) = \left(L_1^*(\boldsymbol{\lambda}), L_2^*(\boldsymbol{\lambda}), \ldots L_{p+s+1}^*(\boldsymbol{\lambda})\right)^\top = \mathbf{0}.$$

Under smoothness conditions on η and ψ, and using a Taylor series expansion, we obtain that

$$n^{1/2}(\hat{\boldsymbol{\lambda}} - \boldsymbol{\lambda}_0) = -[n^{-1}D\mathbf{L}^*(\boldsymbol{\lambda}_0)]^{-1}[n^{-1/2}\mathbf{L}^*(\boldsymbol{\lambda}_0)] + o_p(1), \qquad (7.5)$$

where $D\mathbf{L}^*(\boldsymbol{\lambda}_0)$ represents the derivative of the vector $\mathbf{L}^*$ with respect to $\boldsymbol{\lambda}$, evaluated at $\boldsymbol{\lambda}_0$. Let $\xrightarrow{D}$ and $\xrightarrow{P}$ stand for convergence in distribution and convergence in probability. First note that since ψ is odd and by Assumption A, $\mathbf{L}^*(\boldsymbol{\lambda}_0)$ has null expectation. We will show, adopting arguments similar to those of Bustos and Yohai (1986), that

$$n^{-1/2}\mathbf{L}^*(\boldsymbol{\lambda}_0) \quad \xrightarrow{D} \quad N(\mathbf{0}, \mathbf{A}), \tag{7.6}$$

$$n^{-1}D\mathbf{L}^*(\boldsymbol{\lambda}_0) \quad \xrightarrow{P} \quad \mathbf{B}, \tag{7.7}$$

where $\mathbf{A}$ and $\mathbf{B}$ are $(p + s + 1) \times (p + s + 1)$ matrices. It is assumed that $\mathbf{B}$ is a nonsingular matrix. Consequently, the matrix $n^{-1}D\mathbf{L}^*(\boldsymbol{\lambda}_0)$ in (7.5) is invertible for large n. The proofs of (7.6) and (7.7) involve the central limit theorem for stationary sequences and the ergodic theorem (see Durrett 1995). Explicit expressions for $\mathbf{A}$ and $\mathbf{B}$ are given below. Using (7.5)–(7.7) yield

$$n^{1/2}(\hat{\boldsymbol{\lambda}} - \boldsymbol{\lambda}_0) \xrightarrow{D} N\left(\mathbf{0}, \mathbf{B}^{-1}\mathbf{A}\mathbf{B}^{-1\top}\right)$$

By hypotheses, s_h decays exponentially as $h \to \infty$, and asymptotically

$$L_j^*(\boldsymbol{\lambda}) = L_j(\boldsymbol{\lambda}) + o_p(1), \; j = 1, \ldots, p + s + 1, \tag{7.8}$$

where

$$L_j(\boldsymbol{\lambda}) = \sum_{t=1}^{n} \delta_{jt}(\boldsymbol{\lambda}), \; j = 1, \ldots, p + s + 1, \tag{7.9}$$

and

$$\delta_{jt}(\boldsymbol{\lambda}) = \sum_{i=0}^{s} \nu_i \delta_{rx,(i+j)t} + \sigma_u \delta_{rr,jt}, \; j = 1, \ldots, p,$$

$$\delta_{jt}(\boldsymbol{\lambda}) = \psi(r_t/\sigma_u)X_{t-j+p+1}, \; j = p + 1, \ldots, p + s + 1,$$

$$\delta_{rx,(i+j)t} = \sum_{h=0}^{\infty} s_h \psi(r_t/\sigma_u)X_{t-i-j-h},$$

$$\delta_{rr,jt} = \sum_{h=0}^{\infty} s_h \eta(r_t/\sigma_u, r_{t-j-h}/\sigma_u).$$

Consider the multivariate process

$$\boldsymbol{\delta}_t(\boldsymbol{\lambda}_0) = \left(\delta_{1t}(\boldsymbol{\lambda}_0), \delta_{2t}(\boldsymbol{\lambda}_0), \ldots, \delta_{(p+s+1)t}(\boldsymbol{\lambda}_0)\right)^\top$$

By Assumption A and strict exogeneity of $\{X_t\}$, the $\boldsymbol{\delta}_t(\boldsymbol{\lambda}_0)$'s are martingale differences and they also form a stationary and ergodic stochastic

process. Then relation (7.8) and the central limit theorem together give (7.6). The asymptotic covariance matrix $\mathbf{A}$ is given by $A_{ij} = \sum_{m=-\infty}^{\infty} v_{ij}(m)$, $v_{ij}(m) = E[\delta_{it}(\boldsymbol{\lambda}_0)\delta_{j(t-m)}(\boldsymbol{\lambda}_0)]$, which reduces to

$$A_{ij} = E[\delta_{it}(\boldsymbol{\lambda}_0)\delta_{jt}(\boldsymbol{\lambda}_0)].$$

Applying the ergodic theorem yields

$$n^{-1}D\mathbf{L}^*(\boldsymbol{\lambda}_0) \xrightarrow{P} E[D\delta_t(\boldsymbol{\lambda}_0)] = \mathbf{B}.$$

Consistent estimators of the matrices $\mathbf{A}$ and $\mathbf{B}$ may be obtained by substituting $\hat{v}_{ij}(m) = n^{-1}\sum \delta_{it}^*(\hat{\boldsymbol{\lambda}})\delta_{j,(t-m)}^*(\hat{\boldsymbol{\lambda}})$ to $v_{ij}(m)$ and by setting $\hat{\mathbf{B}} = n^{-1}\sum_{t=1}^{n}D\delta_t(\hat{\boldsymbol{\lambda}})$.

We now give explicit expressions for $\mathbf{A}$ and $\mathbf{B}$. If $\boldsymbol{\lambda} = \boldsymbol{\lambda}_0$, note that $r_t = u_t$. Let

$$
\begin{aligned}
a &= E[\eta^2(u_t/\sigma_u, u_{t-1}/\sigma_u)], & (7.10)\\
b &= E[\eta_1(u_t/\sigma_u, u_{t-1}/\sigma_u)u_{t-1}],\\
a^* &= E[\psi^2(u_t/\sigma_u)],\\
b^* &= E[\psi'(u_t/\sigma_u)],
\end{aligned}
$$

where $\eta_1(u,v) = \partial\eta(u,v)/\partial u$ and $\psi'(u) = d\psi(u)/dx$ Since the u_t's are iid with symmetric distributions, $\eta(\cdot,\cdot)$ is odd in each variable, the matrix $\mathbf{A}$ is given by

$$
\begin{aligned}
A_{ij} &= a^* \sum_{k_1,k_2=0}^{s} \sum_{h_1,h_2=0}^{\infty} \nu_{k_1}\nu_{k_2}s_{h_1}s_{h_2}\Gamma_x(k_2 - k_1 + h_2 - h_1 + j - i)\\
&\quad + a\sigma_u^2 \sum_{h=0}^{\infty} s_h s_{h+i-j}, \quad i,j \in \{1,\ldots,p\},\\
A_{ij} &= a^* \sum_{k=0}^{s} \nu_k \sum_{h=0}^{\infty} s_h \Gamma_x(j - i - k - h - p - 1), \quad i \in \{1,\ldots,p\},\\
&\quad j \in \{p+1,\ldots,p+s+1\},\\
A_{ij} &= a^* \sum_{k=0}^{s} \nu_k \sum_{h=0}^{\infty} s_h \Gamma_x(i - j - k - h - p - 1), \quad j \in \{1,\ldots,p\},\\
&\quad i \in \{p+1,\ldots,p+s+1\},\\
A_{ij} &= a^*\Gamma_x(j - i), \quad i,j \in \{p+1,\ldots,p+s+1\},
\end{aligned}
$$

and the elements of the matrix $\mathbf{B}$ are

$$
B_{ij} = -b^*\sigma_u^{-1} \sum_{k_1,k_2=0}^{s} \sum_{h_1,h_2=0}^{\infty} s_{h_1}s_{h_2}\nu_{k_1}\nu_{k_2}\Gamma_x(k_1 - k_2 + h_1 - h_2 + i - j)
$$

$$-b\sum_{h=0}^{\infty} s_h s_{h+i-j}, \quad i,j \in \{1,\dots,p\},$$

$$B_{ij} = -b^* \sigma_u^{-1} \sum_{k=0}^{s} \nu_k \sum_{h=0}^{\infty} s_h \Gamma_x(j-i-k-h-p-1), \quad i \in \{1,\dots,p\},$$

$$j \in \{p+1,\dots,p+s+1\},$$

$$B_{ij} = -b^* \sigma_u^{-1} \sum_{h=0}^{\infty} \sum_{k=0}^{s} \nu_k s_h \Gamma_x(i-j-k-h-p-1), \quad j \in \{1,\dots,p\},$$

$$i \in \{p+1,\dots,p+s+1\},$$

$$B_{ij} = -b^* \sigma_u^{-1} \Gamma_x(j-i), \quad i,j \in \{p+1,\dots,p+s+1\}.$$

In the situation of M estimators, that is $\eta(u,v) = \psi(u)v$, we have that $\mathbf{A} = a^* \mathbf{A}_1$, $\mathbf{B} = b^* \sigma_u^{-1} \mathbf{B}_1$, and $\mathbf{B}^{-1}\mathbf{A}\mathbf{B}^{-1^{\top}} = a^* b^{*-2} \sigma_u^2 \mathbf{B}_1^{-1} \mathbf{A}_1 \mathbf{B}_1^{-1^{\top}}$, where the elements of $\mathbf{A}_1$ and $\mathbf{B}_1$ are the autocovariances $\mathrm{Cov}(Y_i, Y_j)$ and the cross-covariances $\mathrm{Cov}(Y_t, X_{t-k})$. In this particular case, the efficiency of the RA-ARX estimators with respect to LS estimators is then given by ν^{-1}, where $\nu = a^*/b^{*2}$.

3. Asymptotic distribution of the robust residual autocovariances and applications

Let $\hat{r}_t = r_t(\hat{\boldsymbol{\lambda}})$ be the residuals based on the RA-ARX estimators $\hat{\boldsymbol{\lambda}}$ and $\gamma_{\hat{r}\hat{r}}(j)$ be defined as $\gamma_{r\,r}(j)$, but based on the $\hat{r}_t$'s and on $\hat{\sigma}_u$. In this section, we establish the asymptotic distribution of the robust residual autocorrelations $\boldsymbol{\gamma}_{\hat{r}\hat{r}} = (\gamma_{\hat{r}\hat{r}}(1),\dots,\gamma_{\hat{r}\hat{r}}(M))^{\top}$, under the null hypothesis of adequacy of an ARX model, where $1 \le M < n$ is a fixed number relative to the sample size n. In particular, we give explicitly the asymptotic covariance structure of $n^{1/2}\boldsymbol{\gamma}_{\hat{r}\hat{r}}$. Based on this result, we will propose one-lag test statistics.

3.1 Asymptotic distribution of $n^{1/2}\boldsymbol{\gamma}_{\hat{r}\hat{r}}$

To derive the asymptotic distribution of $n^{1/2}\boldsymbol{\gamma}_{\hat{r}\hat{r}}$, we first note that, using the fact that $\{\eta(u_t/\sigma_u, u_{t-i}/\sigma_u)\}$ are martingale differences, $i = 1,\dots,M$, it can be shown that

$$n^{1/2}\boldsymbol{\gamma}_{rr} \xrightarrow{D} N(0, a\mathbf{I}_M),$$

that is $n^{1/2}\boldsymbol{\gamma}_{rr}$ converges in distribution to a normal with mean $\mathbf{0}$ and covariance matrix $a\mathbf{I}_M$, where a is given by (7.10) and $\mathbf{I}_M$ denotes the identity matrix of dimension $M \times M$. Furthermore, $n^{1/2}((\hat{\boldsymbol{\lambda}} - \boldsymbol{\lambda})^{\top}, \boldsymbol{\gamma}_{rr}^{\top})^{\top}$ converges jointly in distribution to a normal. Using (7.5), the asymptotic

covariance structure between $n^{1/2}(\hat{\boldsymbol\lambda} - \boldsymbol\lambda)$ and $n^{1/2}\boldsymbol\gamma_{rr}$ is given by

$$\lim_n n\mathrm{Cov}(\hat{\boldsymbol\lambda} - \boldsymbol\lambda, \boldsymbol\gamma_{rr}) = -\mathbf{B}^{-1}\lim_n E[\mathbf{L}(\boldsymbol\lambda_0)\boldsymbol\gamma_{rr}^{\top}],$$

where $\mathbf{L}(\boldsymbol\lambda_0) = (L_1(\boldsymbol\lambda_0), \ldots, L_{p+s+1}(\boldsymbol\lambda_0))^{\top}$ is given by (7.8) with $\boldsymbol\lambda = \boldsymbol\lambda_0$. We now give an explicit expression for $E[\mathbf{L}(\boldsymbol\lambda_0)\boldsymbol\gamma_{rr}^{\top}]$. Let $\mathbf{Z} = (z_{ij})$ be a $M \times (p + s + 1)$ matrix, where $z_{ij} = \lim_n E[L_j(\boldsymbol\lambda_0)\gamma_{rr}(i)]$. Using the relation

$$E[\eta(u_{t_1}/\sigma_u, u_{t_1 - j}/\sigma_u)\eta(u_{t_2}/\sigma_u, u_{t_2 - k}/\sigma_u)] = 0,$$

if $t_1 \neq t_2$ or $j \neq k$, and since $\{X_t\}$ and $\{u_t\}$ are independent, it follows that

$$\begin{aligned} z_{ij} = \lim_n E[L_j(\boldsymbol\lambda_0)\gamma_{rr}(i)] &= a\sigma_u s_{i-j}, \quad j = 1, \ldots, p, \\ &= 0, \quad j = p+1, \ldots, p+s+1, \end{aligned}$$

where $i = 1, \ldots, M$. Consequently,

$$\lim_n n\mathrm{Cov}(\hat{\boldsymbol\lambda} - \boldsymbol\lambda, \boldsymbol\gamma_{rr}) = -\mathbf{B}^{-1}\mathbf{Z}^{\top}.$$

By expanding $\boldsymbol\gamma_{\hat{r}\hat{r}}$ in a Taylor's series expansion, we obtain

$$\boldsymbol\gamma_{\hat{r}\hat{r}} = \boldsymbol\gamma_{rr} + D\boldsymbol\gamma(\boldsymbol\lambda)(\hat{\boldsymbol\lambda} - \boldsymbol\lambda) + o_p(n^{-1/2}),$$

where $D\boldsymbol\gamma(\boldsymbol\lambda)$ denotes the $M \times (p + s + 1)$ matrix of derivatives satisfying $D\boldsymbol\gamma_{rr}(\boldsymbol\lambda)^{\top} = (D\{\gamma_{rr}(1)\}(\boldsymbol\lambda)^{\top}, \ldots, D\{\gamma_{rr}(M)\}(\boldsymbol\lambda)^{\top})$. We write $\mathbf{Z} = a\sigma_u\mathbf{Z}_1$, where $\mathbf{Z}_1 = (\mathbf{Z}_{11}\vdots\mathbf{0})$ and $\mathbf{Z}_{11} = (s_{i-j})_{i=1, ,M;j=1, ,p}$. By adopting arguments similar to those of Li (1988), it can be shown that

$$n^{1/2}\boldsymbol\gamma_{\hat{r}\hat{r}} = n^{1/2}\boldsymbol\gamma_{rr} - \frac{b}{\sigma_u}\mathbf{Z}_1 n^{1/2}(\hat{\boldsymbol\lambda} - \boldsymbol\lambda) + o_p(1).$$

This leads us to the main theorem of this section.

THEOREM 7.1 *Let a time series be generated by equation (7.1). Let $\hat{\boldsymbol\lambda}$ be the RA-ARX estimators of $\boldsymbol\lambda$. Assume Assumptions A and B. Then*

$$n^{1/2}\boldsymbol\gamma_{\hat{r}\hat{r}} \xrightarrow{D} N(\mathbf{0}, \boldsymbol\Omega_\eta),$$

where

$$\boldsymbol\Omega_\eta = a\left\{\mathbf{I}_M + b\mathbf{Z}_1[2\mathbf{B}^{-1} + b/(\sigma_u^2 a)\mathbf{B}^{-1}\mathbf{A}\mathbf{B}^{-1}]\mathbf{Z}_1^{\top}\right\}.$$

The last result is useful for checking robustly the adequacy of an ARX model. In the case of purely autoregressive models, Theorem 7.1

generalizes the main theorem of Li (1988, Section 2). If no exogenous variable is included, then $\mathbf{Z}_1$ reduces to $\mathbf{Z}_{11}$. Furthermore, $\mathbf{A} = a\sigma_u^2 \mathbf{C}$ and $\mathbf{B} = -b\mathbf{C}$, where $\mathbf{C} = (c_{ij})$, $c_{ij} = \sum_{h=0}^{\infty} s_h s_{h+i-j}$. The asymptotic matrix of Theorem 7.1 reduces to $\lim_n n\mathrm{Var}(\boldsymbol{\gamma}_{\hat{r}\hat{r}}) = a\{\mathbf{I}_M - \mathbf{Z}_{11}\mathbf{C}^{-1}\mathbf{Z}_{11}^{\top}\}$, as found by Li (1988).

Duchesne (2004b) derived the asymptotic distribution of matricial autocorrelations in vector ARX models (called VARX models) with linear constraints in the parameters. He shown rigorously that the asymptotic covariance matrix of a vector of matricial autocovariances is nonsingular under certain conditions. To retrieve usual autocorrelations, let $\eta(u, v) = uv$, $\psi(u) = u$ and assuming normality, let $\hat{\boldsymbol{\lambda}}_{MLE}$ be the maximum likelihood estimator (MLE) of $\boldsymbol{\lambda}$. In this case, $a = a^* = b^* = 1$ and $b = \sigma_u$. Furthermore, $\mathbf{B} = -\mathbf{A}/\sigma_u$. Consequently, we obtain the asymptotic covariance structure: $\lim_n n\mathrm{Var}(\boldsymbol{\gamma}_{\hat{r}\hat{r}}) = \mathbf{I}_M - \sigma_u^2 \mathbf{Z}_1 \mathbf{A}^{-1} \mathbf{Z}_1^{\top}$. The results of Duchesne (2004b) are more general in the sense that they are valid in the multivariate case. However, Theorem 7.1 provides a robust version of a part of Theorem 3.1 of Duchesne (2004b), in the special case of univariate ARX models.

3.2   Tests at individual lags

Using Theorem 7.1, we can develop one-lag test statistics, which are useful for checking the adequacy of an ARX model at each lag, when possible additive outliers are observed. Let

$$
\begin{aligned}
\hat{\boldsymbol{\Omega}}_\eta &= \hat{a}\left\{\mathbf{I}_M + \hat{b}\hat{\mathbf{Z}}_1[2\hat{\mathbf{B}}^{-1} + \hat{b}/(\hat{\sigma}_u^2\hat{a})\hat{\mathbf{B}}^{-1}\hat{\mathbf{A}}\hat{\mathbf{B}}^{-1}]\hat{\mathbf{Z}}_1^{\top}\right\}, \\
&= (\hat{\omega}_{ij,\eta}).
\end{aligned}
$$

For any $l \geq 1$, define the one-lag test statistics by the formula

$$
Q_R(l) = n\gamma_{\hat{r}\hat{r}}^2(l)/\hat{\omega}_{ll,\eta}. \tag{7.11}
$$

Under the null hypothesis of adequacy, $Q_R(l) \xrightarrow{D} \chi_1^2$. The modified test statistic

$$
Q_R^*(l) = \frac{n}{n-l}Q_R(l) \tag{7.12}
$$

may have better finite sample properties in practice, specially for larger l. The test statistics $Q_R(l)$ and $Q_R^*(l)$ provide robust versions of the test statistics

$$
\begin{aligned}
Q(l) &= nR_{\hat{r}\hat{r}}^2(l)/\hat{\omega}_{ll}, &\tag{7.13} \\
Q^*(l) &= \frac{n}{n-l}Q(l), &\tag{7.14}
\end{aligned}
$$

where $\hat{\omega}_{ll}$ denotes the asymptotic variance of $n^{1/2}R_{\hat{r}\hat{r}}(l)$. The test statistics $Q(l)$ and $Q^*(l)$ correspond to specialized versions of the test statistics of Duchesne (2004b), in the special case of univariate ARX models. Diagnostic test statistics for VARX models can be found in Duchesne (2004b).

The finite sample properties of $Q(l)$, $Q^*(l)$, $Q_R(l)$ and $Q_R^*(l)$ will be investigated in the next section, under various scenarios for the occurrence of outliers.

4. Simulations

In this section, we report the results of four simulation experiments. In the first and second studies, we compare the LS estimators and the RA-ARX estimators calculated with η functions of the Hampel and Mallows types, when the ψ functions belong to the Huber and bisquare families, using a general Newton-Raphson algorithm. More precisely, in the first experiment, we compare the asymptotic biases of the RA-ARX estimators, with respect to the LS estimators. In the second experiment, we determine the empirical efficiencies of the RA-ARX estimators with respect to the LS estimators. Various η and ψ functions are considered. In the third and forth experiments, we study the finite sample performance of the one-lag tests. The empirical levels and powers of the tests $Q_R(l)$ and $Q_R^*(l)$ are compared to those of the non robust statistics $Q(l)$ and $Q^*(l)$, with RA-ARX estimators based on the η function of the Mallows type and the bisquare ψ function.

4.1 Computation of the asymptotic biases

It seems of interest to investigate the bias of the estimators, with and without additive outliers in the time series. When additive outliers are observed, all the estimators, either robust or non-robust, display a bias (see Denby and Martin (1979, p 142)). However, the bias of a satisfactory robust estimator is expected to be much smaller than the bias of the LS estimators

In order to investigate empirically the bias properties, the following experiment is conducted. The following data generating process (DGP) is considered.

$$(1 - \phi B)Y_t = \nu X_t + u_t, \tag{7.15}$$

where the exogenous variable satisfies $X_t = 0.8X_{t-1} + v_t$, with $\{v_t\}$ a Gaussian white noise with a unit variance. We set $\lambda = (\phi, \nu)^\top = (0.5, 0.5)^\top$. The white noise process $\{u_t\}$ is assumed to be Gaussian and $\sigma_u = 1$ is supposed known.

For the occurrence of outliers, we investigate two strategies: (i) no contamination and (ii) additive outliers. The outliers are obtained by observing $Y_t + W_t$, where $W_t \equiv 0$ with probability 95%, and $W_t = \pm 10$ with probability 5%, the sign being chosen at random. We adopt the sample size $n = 1000$, giving a good idea of the asymptotic values of the estimators. We consider 400 replications of the experiment, due to the intensive calculations of the RA-ARX estimators with a rather large sample size.

The RA-ARX estimators are determined for η function of the Mallows and Hampel types. A Newton-Raphson algorithm is implemented to determine RA-ARX estimators with η function of the Hampel type. With Mallows η function, RA-ARX estimators can be easily computed using the iterative algorithm described in Duchesne (2004a). The ψ functions are chosen in the Huber and bisquare families. For the Huber ψ function, tuning parameter $c = 1.345$ is chosen and for the bisquare ψ function, $c = 4.685$ is adopted. See Bustos and Yohai (1986) and Duchesne (2004a), for a discussion on the choice of the tuning parameter.

Table 7.1 and Table 7.2 report the empirical means, variances, squared bias and relative bias (in absolute value) with no outliers and additive outliers, respectively. From Table 7.1, it appears that the LS estimators are the less variable, as expected. In general, the bias of all the considered estimators are small. From Table 7.2, when additive outliers are observed, the LS estimators are the most biased for both the estimation of ϕ and ν. It appears that the variance of the LS estimators is also more important, particularly for the estimation of ν. The RA-ARX estimators exhibit a much smaller bias. The choice of the ψ function seems important in this experiment: bisquare ψ function displays less biased estimators than Huber ψ function. It seems that the η function of the Hampel type performed well, compared to the Mallows η function, but the difference is rather small.

4.2 Comparison of the efficiencies of the RA-ARX estimators with respect to LS estimators

Another important consideration concerns the efficiency of the robust procedures, both with and without additive outliers in the time series.

In order to investigate empirically the efficiencies, the same model (7.15) is adopted, with the same exogenous variable X_t. However, in this experiment, we consider the sample size $n = 100$ and the Monte Carlo experiment is conducted with 1000 iterations. Again, two scenarios are considered, with and without additive outliers. However, the outliers

Table 7.1. Empirical means, variances, squared biases ($\times 10^{-5}$) and relative biases (in absolute value) for the estimation of ϕ and ν, using RA-ARX estimators based on η functions of the Hampel and Mallows types, for ψ functions in the Huber and bisquare families, compared to the LS estimators, in the case where there is no contamination.

	$\phi = 0.5$			
	Mean	Variance	Sq. Bias	Rel. bias
LS	0 49846	0.00048	0.23510	0.00306
RA-ARX, Mallows, ψ_H	0.49884	0.00051	0 13313	0.00230
RA-ARX, Hampel, ψ_H	0.49874	0.00053	0.15684	0.00250
RA-ARX, Mallows, ψ_B	0.49882	0.00051	0.13892	0 00230
RA-ARX, Hampel, ψ_B	0.49885	0 00058	0.13160	0.00229
	$\nu = 0.5$			
	Mean	Variance	Sq. Bias	Rel. bias
LS	0.50117	0.00056	0.13854	0 00235
RA-ARX, Mallows, ψ_H	0.50086	0.00058	0.07506	0.00173
RA-ARX, Hampel, ψ_H	0.50092	0.00060	0.08570	0.00185
RA-ARX, Mallows, ψ_B	0.50092	0.00058	0.08627	0.00185
RA-ARX, Hampel, ψ_B	0.50089	0.00062	0.08078	0.00179

Table 7.2. Empirical means, variances, squared biases ($\times 10^{-5}$) and relative biases (in absolute value) for the estimation of ϕ and ν, using RA-ARX estimators based on η functions of the Hampel and Mallows types, for ψ functions in the Huber and bisquare families, compared to the LS estimators, in the case where there are additive outliers.

	$\phi = 0.5$			
	Mean	Variance	Sq. Bias	Rel. bias
LS	0.15360	0.00109	11998.7	0.69278
RA-ARX, Mallows, ψ_H	0.43678	0.00080	399.604	0.12642
RA-ARX, Hampel, ψ_H	0.45115	0.00077	238.552	0.09768
RA-ARX, Mallows, ψ_B	0.49835	0.00055	0.26985	0.00328
RA-ARX, Hampel, ψ_B	0.49863	0.00064	0.18596	0.00272
	$\nu = 0.5$			
	Mean	Variance	Sq. Bias	Rel. bias
LS	0.73383	0.00241	5467.78	0.46766
RA-ARX, Mallows, ψ_H	0.54190	0 00080	175.612	0.08381
RA-ARX, Hampel, ψ_H	0.53234	0 00079	104.592	0.06468
RA-ARX, Mallows, ψ_B	0.50048	0.00062	0.02365	0.00097
RA-ARX, Hampel, ψ_B	0 50030	0.00067	0.00938	0 00061

Table 7.3. Empirical means, variances, mean squared errors and efficiencies for the estimation of ϕ and ν, using RA-ARX estimators based on η functions of the Hampel and Mallows types, for ψ functions in the Huber and bisquare families, compared to the LS estimators, in the case where there is no contamination.

	$\phi = 0.5$			
	Mean	Variance	Mean Sq. Err.	Efficiency
LS	0.49241	0.00451	0.00457	1.00000
RA-ARX, Mallows, ψ_H	0.49213	0.00491	0.00497	0.91923
RA-ARX, Hampel, ψ_H	0.49203	0 00515	0.00521	0.87722
RA-ARX, Mallows, ψ_B	0.49225	0.00501	0 00507	0.90117
RA-ARX, Hampel, ψ_B	0.49154	0.00566	0.00573	0.79724
	$\nu = 0.5$			
	Mean	Variance	Mean Sq. Err.	Efficiency
LS	0.50411	0.00617	0 00618	1.00000
RA-ARX, Mallows, ψ_H	0.50398	0.00666	0.00668	0.92580
RA-ARX, Hampel, ψ_H	0.50408	0.00684	0.00686	0.90125
RA-ARX, Mallows, ψ_B	0.50399	0.00668	0.00670	0.92278
RA-ARX, Hampel, ψ_B	0 50445	0.00703	0.00705	0.87738

are obtained by replacing Y_{11}, Y_{33}, Y_{49}, Y_{76} and Y_{90} by 10, -10, 10, -10 and 10, as in Duchesne (2004a).

In Table 7.3 (no contamination) and Table 7.4 (additive outliers), we report the sample means, variances, mean squared errors (MSE) and efficiencies, of the robust estimators, with respect to the LS estimators.

As can be seen from Table 7.3, when no outliers are present, the LS estimators display the highest efficiency, as expected However, the efficiencies of the robust estimators, with respect to the LS estimators, are satisfactory and are in accordance with the results of Duchesne (2004a). It seems that an η function of the Mallows type delivers more efficient estimators than an η function of the Hampel type, at least for this sample size and for the chosen DGP, observed without additive outliers.

Following the results displayed in Table 7.4, the robust estimators clearly outperform the LS estimators, the former being much more efficient than the latter. This is explained by the important component of bias in the MSE of the LS estimators. The variances of the robust and non-robust estimators appear rather comparable concerning the estimation of ϕ. The bisquare ψ function displays the highest efficiency for the estimation of the parameters. However, the differences between the efficiencies are somewhat smaller concerning the estimation of ν. The sample variances of the estimators of ν are smaller for the RA-ARX estimators than the variances of the LS estimators. Both η functions deliver high efficiencies, and neither performs uniformly better than the other.

Table 7.4.   Empirical means, variances, mean squared errors and efficiencies for the estimation of ϕ and ν, using RA-ARX estimators based on η functions of the Hampel and Mallows types, for ψ functions in the Huber and bisquare families, compared to the LS estimators, in the case where there are additive outliers.

	$\phi = 0.5$			
	Mean	Variance	Mean Sq Err	Efficiency
LS	0.13147	0.00610	0.14191	1.00000
RA-ARX, Mallows, ψ_H	0.42021	0.00736	0.01373	10.33220
RA-ARX, Hampel, ψ_H	0.43557	0.00763	0.01178	12.04144
RA-ARX, Mallows, ψ_B	0.48113	0.00686	0.00722	19.64633
RA-ARX, Hampel, ψ_B	0.48108	0.00761	0.00797	17.80034
	$\nu = 0.5$			
	Mean	Variance	Mean Sq. Err.	Efficiency
LS	0.69836	0.02268	0.06203	1.00000
RA-ARX, Mallows, ψ_H	0.54984	0.00873	0.01122	5.52855
RA-ARX, Hampel, ψ_H	0.53983	0.00875	0.01034	5.99954
RA-ARX, Mallows, ψ_B	0.50538	0.00823	0.00825	7.51199
RA-ARX, Hampel, ψ_B	0.50547	0.00853	0.00856	7.24475

4.3   Levels and powers of the one-lag test statistics

We now investigate the finite sample performance of the test statistics $Q(l)$, $Q^*(l)$, $Q_R(l)$ and $Q_R^*(l)$. We still consider the DGP given by (7.15), but the exogenous process $\{X_t\}$ is now iid, such that X_t admits the uniform distribution $U[-2\sqrt{3}, 2\sqrt{3}]$, where $U[a, b]$ denotes the uniform distribution on the interval $[a, b]$. We consider two error terms for u_t: a) $u_t = \epsilon_t$, b) $u_t = 0.6u_{t-1} + \epsilon_t$, where $\{\epsilon_t\}$ is a Gaussian white noise with unit variance. Theses two cases allow us to study the level and power of the test statistics, respectively. We consider the sample size $n = 100$. We examine the same strategies for the occurrence of outliers than in Section (4.2), that is in the first strategy no outliers are observed and in the second strategy additive outliers are created, as in Section (4.2).

We consider the one-lag tests for $l = 1, \ldots, 10$. For the RA-ARX estimators, Mallows type η function and bisquare ψ function with tuning constant $c = 4.685$ are adopted. The iterative algorithm of Duchesne (2004a) was implemented for computing the RA-ARX estimators. In the realization of the algorithm, the scale parameter was simultaneously estimated by the median of the residuals, divided by 0.6745.

Table 7.5 reports the rejection rates (in percentage) under white noise errors at 10% and 5% nominal levels, based on 1000 replications. For a given l, the non robust and robust tests $Q(l)$ and $Q^*(l)$ (and similarly $Q_R(l)$ and $Q_R^*(l)$) exhibit comparable level performance. Under-rejection

is observed for $Q(l)$ and $Q_R(l)$, as expected. For larger l, the factor $n/(n-l)$ improves the level performance and the test statistics $Q^*(l)$ and $Q_R^*(l)$ display reasonable levels at both nominal levels.

Table 7 5   Empirical levels (in percentage) based on 1000 replications of the robust one-lag test statistics $Q_R(l)$ and $Q_R^*(l)$ defined by (7 11) and (7 12), and of the usual test statistics $Q(l)$ and $Q^*(l)$ defined by (7.13) and (7 14), without contamination

	$\alpha = 0.05$				$\alpha = 0.10$			
	$Q(l)$	$Q^*(l)$	$Q_R(l)$	$Q_R^*(l)$	$Q(l)$	$Q^*(l)$	$Q_R(l)$	$Q_R^*(l)$
1	4.3	4 5	4 8	4 8	10 6	10 6	10 5	10 6
2	4 5	4.7	4 8	5.3	10 3	10 8	10 4	10.6
3	4.4	4 9	6.0	6.2	10 4	10.9	11.3	11 4
4	2 7	2 9	3.8	4 5	8.0	8 6	8 2	8 5
5	4.0	4 2	4 2	4 8	7.7	8.6	8 6	9 8
6	3 5	3 7	4 4	5 0	7.6	8.6	8.8	10 5
7	3 4	4.2	3.8	4.8	7 9	9 1	8.6	10 2
8	3 9	5.7	5 1	6 3	9 3	10.6	10.5	12 2
9	2 7	3 5	3.4	4.3	7 1	8 7	8 9	10 5
10	2 8	3 8	3 3	4 6	6 8	9 3	8 7	10.6

Table 7 6   Empirical levels (in percentage) based on 1000 replications of the robust one-lag test statistics $Q_R(l)$ and $Q_R^*(l)$ defined by (7.11) and (7 12), and of the usual test statistics $Q(l)$ and $Q^*(l)$ defined by (7 13) and (7 14), with additive outliers

	$\alpha = 0.05$				$\alpha = 0.10$			
	$Q(l)$	$Q^*(l)$	$Q_R(l)$	$Q_R^*(l)$	$Q(l)$	$Q^*(l)$	$Q_R(l)$	$Q_R^*(l)$
1	29 8	30 4	7 0	7.2	43 9	44.4	12 4	12 7
2	0 1	0.1	6 2	6 7	0 9	0.9	10.9	11.4
3	0 2	0 2	4.6	4.6	0 8	0.8	9 2	9 6
4	0 1	0 2	4.8	5.5	1 0	1 2	9 7	10 3
5	0 2	0 3	4 2	5.1	0 3	0 3	9.6	10 6
6	0 1	0 2	3 6	4 7	0 6	0 6	8 4	9 5
7	0.0	0 0	4.5	4 9	0.0	0 1	8 7	9 8
8	0.1	0.2	3 2	3.8	0.3	0 4	7 7	8.8
9	0 0	0.0	3 3	4.0	0.2	0 3	6 7	8 7
10	0.1	0.2	5 6	7 0	0.3	0.4	10 5	12 0

Table 7.6 reports rejection rates (in percentage) when additive outliers occurred. The robust test statistics exhibit reasonable levels for all the lags considered. In general, the levels are similar to those obtained in Table 7.5, although some over-rejection is observed. However, the non robust test statistics $Q(l)$ and $Q^*(l)$ are severely affected by additive outliers. Severe over-rejection occurred at lag one and serious under-rejection has been observed for all lags $l > 1$. This is in agreement with the level study described in Duchesne (2004a) for the non-robust and robust portmanteau test statistics. In general, Table 7.6 brings

more insight on the outliers problem since the dependence at each lag is presented.

We now examine the empirical powers at the 5% and 10% nominal levels. We computed the power using the asymptotic critical values (ACV) and also based on the empirical (exact) critical values (ECV) obtained from the level study with no outliers. Table 7.7 reports the number of rejection out of 1000 replications under the AR(1) alternative. In general, for small and moderate l, the powers computed with ECV and ACV are very similar. The most powerful one-lag test statistics are obtained when $l = 1$. The test statistics display some power for $l = 2$ and almost no power for $l > 2$. Since the alternative is of the AR(1) type, it was expected that higher power would have been observed for small lags. For lag $l = 1$, the robust test statistics are slightly less powerful than $Q(1)$ and $Q^*(1)$. This represents the price to pay for using robust methods when no additive outliers are recorded. In our experiment, this price does not seem too important.

Finally, Table 7.8 reports the estimated power under the AR(1) alternative when additive outliers occur in the endogenous variables Y_t. A satisfactory test procedure should exhibit a power similar to the one obtained in Table 7.7. However, since the non robust test statistics over-reject at lag one and under-reject for other lags, the power of the non robust tests seems affected. Much lower power than the robust tests has been observed at lag one, and almost no power for lags $l > 1$. By comparison, the new one-lag test statistics display a power similar to the one observed in Table 7.7. Consequently, when additive outliers are suspected, the new robust test statistics provide a much better description of the dependence present in the error term $\{u_t\}$.

5.   Conclusion

The aim of this paper was to present new robust individual tests in autoregressive models with exogenous variables. Such one-lag tests should complete the analysis that can be done with the robust portmanteau test statistics of Duchesne (2004a). We derived the asymptotic distribution of the RA-ARX estimators. In particular, we gave their asymptotic covariance structure. The proof was based on arguments similar to those of Bustos and Yohai (1986), valid in ARMA models. A more complete and rigorous proof could be provided, using probably the results of Bustos et al. (1984). This consideration was beyond the scope of the present paper and is left for future studies.

Using the asymptotic normality result of the RA-ARX estimators, we established the asymptotic distribution of the robustified residual

Table 7 7   Empirical powers (in percentage) based on 1000 replications of the robust one-lag test statistics $Q_R(l)$ and $Q_R^*(l)$ defined by (7 11) and (7 12), and of the usual test statistics $Q(l)$ and $Q^*(l)$ defined by (7.13) and (7 14), without contamination

	$\alpha = 0\ 05$							
	$Q(l)$		$Q^*(l)$		$Q_R(l)$		$Q_R^*(l)$	
l	ACV	ECV	ACV	ECV	ACV	ECV	ACV	ECV
1	97 6	97 7	97 7	97 7	96 7	97 0	96 7	97 0
2	8 1	9.3	8 3	9 3	13 8	14 2	14 8	14 2
3	4 5	4 9	4.7	4 9	4 0	3 2	4 6	3 2
4	8 7	11 5	9 8	11 5	7.3	8 4	8 0	8 4
5	9 4	11 0	9 7	11.0	7 7	9.1	8 5	9 1
6	7 6	10 4	8 7	10 4	7 8	8 6	8.6	8.6
7	6 7	8 2	7 6	8 2	5 4	6 7	6 4	6 7
8	6 4	7 5	7 8	7 5	5 1	5 1	7 0	5 1
9	5 8	8 8	6 8	8 8	5 3	7 1	6 2	7 1
10	5 2	8 6	6 4	8 6	5 6	6 6	6 4	6 6

	$\alpha = 0\ 10$							
	$Q(l)$		$Q^*(l)$		$Q_R(l)$		$Q_R^*(l)$	
l	ACV	ECV	ACV	ECV	ACV	ECV	ACV	ECV
1	98 9	98 8	98 9	98.8	98 5	98 4	98 5	98 4
2	17 4	17 4	17 9	17 4	24 7	23 9	25 2	23 9
3	9 0	8 8	9 3	8 8	8 6	7 9	9 4	7 9
4	13 9	15 8	14 6	15.8	11 9	13 5	12 2	13 5
5	16 0	20.8	17 6	20 8	14.7	16 0	15 5	16 0
6	14 1	17 9	15 7	17 9	13 7	14 6	15 0	14 6
7	12 8	14.7	13 8	14 7	12 1	13 6	13 8	13 6
8	12 4	13 0	14 1	13 0	12 7	12 3	14 5	12 3
9	10 9	14 0	12 4	14 0	11 5	13 0	13 4	13 0
10	9.6	13 0	11 7	13 0	9 3	10 8	11 1	10 8

autocorrelations under the null hypothesis of adequacy, which is normal. Some simulation results were reported. The RA-ARX estimators, based on various η and ψ functions, have been compared, with respect to biases and efficiencies. We provided evidence that the η function of the Mallows type should be adequate in practice; They can be easily implemented with an iterative least squared scheme and they provide much less biased estimators than the LS estimators, when additive outliers are encountered. One-lag test statistics have been studied with respect to levels and powers. While we obtained satisfactory results with robust test statistics, non-robust one-lag test statistics appear unreliable when additive outliers are observed.

Table 7.8.   Empirical powers (in percentage) based on 1000 replications of the robust one-lag test statistics $Q_R(l)$ and $Q_R^*(l)$ defined by (7.11) and (7 12), and of the usual test statistics $Q(l)$ and $Q^*(l)$ defined by (7 13) and (7 14), with additive outliers

	$\alpha = 0.05$							
	$Q(l)$		$Q^*(l)$		$Q_R(l)$		$Q_R^*(l)$	
l	ACV	ECV	ACV	ECV	ACV	ECV	ACV	ECV
1	27 5	29.8	28 0	29 8	95.4	95 8	95.5	95.8
2	2.1	2 6	2 3	2.6	10.8	10 8	11.1	10.8
3	0 7	0 8	0.7	0.8	3.7	2 6	3.8	2.6
4	0.1	0 3	0.1	0 3	4 9	6.1	5 2	6 1
5	0.1	0.1	0 1	0 1	5 3	6 8	6 5	6 8
6	0.0	0 0	0 0	0 0	5 8	6 6	6 6	6 6
7	0 0	0 1	0 0	0 1	5 1	6 1	5.9	6 1
8	0 0	0.0	0.0	0.0	4 8	4.8	5 5	4 8
9	0 2	0 4	0 2	0 4	4 8	7.1	6 4	7 1
10	0.1	0 5	0 2	0 5	4 4	6 5	5 7	6 5

	$\alpha = 0.10$							
	$Q(l)$		$Q^*(l)$		$Q_R(l)$		$Q_R^*(l)$	
l	ACV	ECV	ACV	ECV	ACV	ECV	ACV	ECV
1	43 7	43 2	43.8	43 2	98 3	98 3	98 3	98 3
2	9 7	9 5	10 5	9.5	19 4	18 4	20 1	18 4
3	2.8	2 3	3 4	2 3	8 1	7 3	8 5	7 3
4	1 0	1 5	1 3	1.5	9 2	10 9	9.8	10 9
5	0 8	1 3	1 0	1.3	10.2	11.2	10 9	11 2
6	0.5	1.2	0 8	1 2	11.3	12 0	12.2	12 0
7	0.4	0.7	0 5	0 7	9 6	10 9	11 0	10 9
8	0.0	0 1	0.1	0 1	9.5	8 8	10 7	8 8
9	0.7	1 0	0 8	1 0	9 3	11 0	11.6	11 0
10	0 6	1 2	1.0	1 2	10.2	10.9	11 6	10 9

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Chapter 8

BOOTSTRAP CONFIDENCE INTERVALS FOR PERIODIC PREVENTIVE REPLACEMENT POLICIES

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Abstract This paper presents bootstrap confidence intervals for the optimal time and the minimum cost of a periodic preventive replacement policy. The bootstrap is applied to different parametric and nonparametric estimators of the renewal function and thus of the cost function. A simulation study shows that the bootstrap approach can prove useful in practice for some estimators.

1.   Introduction

In this paper we consider the periodic replacement problem where replacements of a unit occur at failures or at instants T, $2T$, $3T$, ... where T is the parameter of the replacement policy. Much has been written on this problem and the reader is referred to Valdez-Flores and Feldman (1989) for a list of pertinent papers.

Here we consider the following problem. The unit life X is a random variable with continuous and increasing failure rate (IFR) distribution function F with $F(0) = 0$, density function f, finite mean μ and variance σ^2. We wish to replace the unit at failures or at instants T, $2T$, $3T$, ... A cost c_1 is suffered for each replacement at failure and a cost $c_2 < c_1$ is suffered for each nonfailed unit which is exchanged.

It is known from renewal theory (see e.g., Barlow and Proschan (1975), Croteau (2002), and the references therein) that the average cost per unit time, over an infinite time span, associated with the strategy consisting of preventively replacing the equipment at instants T, $2T$, $3T$, ... is given by

$$C(T, F) = \frac{c_1 M(T) + c_2}{T} \tag{8.1}$$

where $M(T)$ is the renewal function given by

$$M(T) = \sum_{n=1}^{\infty} F^{(n)}(T) \tag{8.2}$$

where $F^{(n)}(T)$ is the nth convolution of F with itself, that is

$$F^{(n)}(T) = \int_0^T F^{(n-1)}(T - u)\, dF(u). \tag{8.3}$$

The function $M(T)$ is also the solution of the fundamental renewal equation

$$M(T) = F(T) + \int_0^T M(T - u)\, dF(u). \tag{8.4}$$

The problem is to find $T_0(F)$ which minimizes (8.1). The solution must satisfy $\partial C(T, F)/\partial T = 0$ that is

$$Tm(T) - M(T) = \frac{c_2}{c_1} \tag{8.5}$$

where $m(T) = M'(T)$, the derivative of $M(T)$. If $T_0(F)$ is a solution of (8.5) then $C\big(T_0(F), F\big) = c_1 m\big(T_0(F)\big)$. A typical behavior of $C(T, F)$ is shown in Figure 8.1. In this example, the respective costs are $c_1 = 5$ and $c_2 = 2$ and the life lengths come from a Weibull distribution with density $f_{\alpha,\lambda}(t) = \alpha\lambda t^{\alpha-1} \exp(-\lambda t^{\alpha})$ with $\alpha = 5$ and $\lambda = 1$. For most distribution functions F, no explicit form exists for $M(T)$ or $m(T)$. These functions are obtained numerically and to this effect, the algorithm developed by Cléroux and McConalogue (1976) will be used below.

However, in many practical situations the distribution F is unknown and we face the problem of estimating the cost function (8.1) and the optimal periodic replacement policy $T_0(F)$. And in order to achieve this, one must first estimate $M(T)$.

In this paper we consider four estimators of $M(T)$, one parametric estimator and three nonparametric estimators introduced by Frees (1986 a,b), Schneider et al. (1990), Grenander (1956), Marshall and Proschan (1965). and Rao (1970). For each of these estimators, the bootstrap will be used to obtain confidence intervals for the actual cost of using the estimated policy and confidence intervals for the optimal policy. Two types of bootstrap intervals will be considered in the simulations below: bootstrap pivotal and bootstrap percentile. The reasons for this choice will be explored below. We will see that the quality of
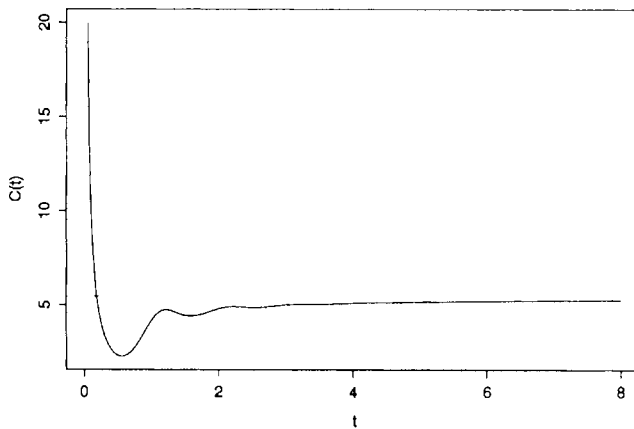
Figure 8 1.   Function $C(T, F)$ when F is Weibull.

the resulting confidence intervals will depend critically on the estimator of $M(T)$.

The problem of confidence intervals for this replacement policy has not been studied previously. Although it is not the objective of this paper, one could in principle use the asymptotic distribution for this purpose. Unfortunately, in many cases, notably for the optimal time, the asymptotic distribution is either not available in the literature or not explicitly known. In other cases, the asymptotic variance is very difficult to estimate so that this approach is not really practical.

The bootstrap methodology introduced by Efron (1979) (see also Efron and Tibshirani (1993)) has also been used in the nonparametric age replacement problem by Léger and Cléroux (1992).

The paper is organized as follows. In Section 2 we present the different estimators of $M(T)$ used in the sequel. In Section 3 some bootstrap confidence intervals are given together with the corresponding numerical algorithms. The results of a simulation study are presented in Section 4 and a conclusion follows in Section 5.

2.   Estimation of $M(t)$

Several estimators of $M(t)$ have been proposed in the scientific literature and four of them will be considered.

2.1   Parametric estimator

In this case, we assume that the class $F_\theta(t)$ of distributions is known (e.g. Weibull, gamma, etc.) but the parameter $\theta = (\theta_1, \theta_2, \ldots, \theta_p)$ is

unknown. Let $\hat{\theta} = (\hat{\theta}_1, \hat{\theta}_2, \ldots, \hat{\theta}_p)$ where for all i, $\hat{\theta}_i$ is a convergent estimator of θ_i. Then $F_\theta(t)$ is estimated by $F_{\hat{\theta}}(t)$ and $F_\theta^{(k)}(t)$ is estimated by $F_{\hat{\theta}}^{(k)}(t)$. Consequently $M(t)$ is estimated by

$$\hat{M}_n^p(t) = \sum_{k=1}^{\infty} F_{\hat{\theta}}^{(k)}(t), \qquad (8.6)$$

where n is the sample size.

It has been shown in Frees (1986b) that if $F_\theta(t)$ is absolutely continuous and if its density function $f_\theta(t)$ is continuous in each θ_i, then $\text{Prob}[\lim_{n\to\infty} \hat{M}_n^p(t) = M(t)] = 1$ for all $t \geq 0$.

In practical applications, there is no need to sum to ∞ in (8.6) since for any t, the function $F_\theta^{(k)}(t)$ flattens quickly as k increases. More details on the practical implementation are provided in Section 4.2. Let us also note in passing that obtaining convergent estimators $\hat{\theta}_i$ for θ_i is not always straightforward and some efficient numerical methods may be needed.

2.2   A nonparametric estimator

This estimator is due to Frees (1986 a,b). Let $N(t)$ be the number of renewals in $[0, t]$. The empirical number of renewals in $[0, t]$ is denoted by $N_n(t)$ and is given by $N_n(t) = \sum_{k=1}^{n} \mathbf{1}(S_k \leq t)$ where $\mathbf{1}(S_k \leq t) = 1$ if $S_k \leq t$ and 0 otherwise, and where S_k is the instant of the kth renewal in the simple renewal process (that is when no replacement policy is used). Here, $S_k = \sum_{i=1}^{k} X_i$ where $X_1, \ldots, X_n$ are the independent and identically distributed (i.i.d.) life lengths of the unit according to the unknown distribution F. It is known from renewal theory that

$$M(t) = E[N(t)] = \sum_{k=1}^{\infty} F^{(k)}(t) = \sum_{k=1}^{\infty} \text{Prob}(S_k \leq t) \qquad (8.7)$$

and we also have

$$E[N_n(t)] = \sum_{k=1}^{n} \text{Prob}(S_k \leq t). \qquad (8.8)$$

One naturally thinks of using $N_n(t)$ as an estimator of $N(t)$ and $\mathbf{1}(S_k \leq t)$ as an estimator of $F^{(k)}(t)$ for $k = 1, 2, \ldots, n$ and 0 as an estimator of $\sum_{k>n} \text{Prob}(S_k \leq t)$. But an unbiased estimator of $F^{(k)}(t)$ with a smaller variance is given by (see Frees (1986a))

$$\widehat{F}_{f,n}^{(k)}(t) = \frac{1}{\binom{n}{k}} \sum_c \mathbf{1}(X_{i_1} + X_{i_2} + \cdots + X_{i_k} \leq t) \qquad (8.9)$$

where c is the set of all $\binom{n}{k}$ combinations of $(i_1, i_2, \ldots, i_k)$. Equation (8.9) defines a U-statistic and the nonparametric estimator of $M(t)$ is given by

$$\hat{M}_n^f(t) = \sum_{k=1}^{n} \widehat{F}_{f,n}^{(k)}(t). \tag{8.10}$$

In practical applications it will not be necessary to sum to n in (8.10) (see Section 4.2). Frees (1986a) shows that under some regularity conditions, $\hat{M}_n^f(t)$ converges almost surely to $M(t)$ for all $t \geq 0$ and is asymptotically normally distributed.

2.3   Modified Frees' estimator

The preceding estimator may be time consuming to obtain, even though the number of terms to be computed in (8.10) turns out to be much smaller than n. A modification has been proposed in Frees (1986 a,b) and developed in Schneider et al. (1990).

Let $\tilde{F}_n^{(1)}(t) = (1/n) \sum_{i=1}^{n} \mathbf{1}(X_i \leq t)$ and define, for $k > 1$,

$$\tilde{F}_n^{(k)}(t) = \int_0^t \tilde{F}_n^{(k-1)}(t - u) \, d\tilde{F}_n^{(1)}(u). \tag{8.11}$$

This is a biased estimator of $F^{(k)}(t)$ for $k \geq 2$ but it is the nonparametric maximum likelihood estimator. It is also a V-statistic. It is easily seen from (8.11) that

$$\tilde{F}_n^{(k)}(t) = \frac{1}{n^k} \sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \cdots \sum_{i_k=1}^{n} \mathbf{1}(X_{i_1} + X_{i_2} + \cdots + X_{i_k} \leq t) \tag{8.12}$$

and if we let $\widehat{M}_n(t) = \sum_{k=1}^{n} \tilde{F}_n^{(k)}(t)$, we can show that $\widehat{M}_n(t)$ converges (under some regularity conditions) almost surely to $M(t)$ and has the same asymptotic distribution as estimator (8.10). But this last estimator of $M(t)$ is much too costly to obtain since it requires $O(n^k)$ numerical operations.

One uses instead the fundamental renewal equation

$$M(t) = F(t) + \int_0^t M(t - x) \, dF(x) \tag{8.13}$$

and partition the interval $[0, t]$ into I subintervals $0 = a_0 < a_1 < a_2 < \cdots < a_I = t$ in order to approximate the second term on the right-hand side of (8.13) in the following way:

$$\int_0^t M(t - x) \, dF(x) \simeq \sum_{i=1}^{l} M(t - \xi_i)[F(a_i) - F(a_{i-1})] \tag{8.14}$$

where $a_{i-1} \leq \xi_i \leq a_i$.

Schneider et al. (1990) suggest using $a_i = i$ and $\xi_i = a_i = i$ for all $i = 0, 1, 2, \ldots, t$. This partition implies that t must be an integer. In order to obtain a good precision in the computations, one proceeds to a change of variable $U_i = 10^r X_i$ where r is chosen to obtain a reasonable number of intervals in the partition. Then each U_i is replaced by its nearest integer. Let $t^* = \lfloor 10^r t \rfloor$.

We now estimate $M(t)$ by

$$\widehat{M_n^*}(t) = \tilde{F}_n^*(t) + \sum_{i=1}^{t^*} \widehat{M_n^*}(t^* - i)[\tilde{F}_n^*(i) - \tilde{F}_n^*(i-1)] \qquad (8.15)$$

and computing $\widehat{M_n^*}(t)$ requires $(t^*)^2$ operations independently of the sample size n. Considering the change of variables, the final form of the estimator is

$$\hat{M}_n^{mf}(t) = \widehat{M_n^*}(10^r t) \qquad (8.16)$$

where $\widehat{M_n^*}(\cdot)$ is given by (8.15).

This estimator has the same convergence properties as estimator (8.10).

2.4   Estimator of $M(t)$ when $F(t)$ is IFR

This is a semi-parametric situation since the form of $F(t)$ is unknown but some information is known about $F(t)$, i.e., it is IFR. We first estimate the failure rate without constraints, modify it if necessary to make it step increasing and from the estimator obtained, estimate $F(t)$ and $M(t)$. Let $X_1, X_2, \ldots, X_n$ be the observed life lengths and $Y_1 \leq Y_2 \leq \cdots \leq Y_n$ be the corresponding order statistics. The estimator of the failure rate $r(t)$ which is step increasing is given by

$$r_n^*(t) = \begin{cases} 0 & \text{if } t < Y_1 \\ \hat{r}_n(Y_i) & \text{if } Y_i \leq t < Y_{i+1}, \quad i = 1, 2, \ldots, n-1 \\ \infty & \text{if } t \geq Y_n \end{cases} \qquad (8.17)$$

where

$$\hat{r}_n(Y_i) = \begin{cases} \min_{v \geq i+1} \max_{u \leq i} \left\{ (v - u) \left[\sum_{j=u}^{v-1} (n-j)(Y_{j+1} - Y_j) \right]^{-1} \right\}, \\ \qquad\qquad\qquad\qquad\qquad\qquad i = 1, 2, \ldots, n-1 \\ \infty \qquad\qquad\qquad\qquad\qquad\qquad i = n \end{cases}$$

$$(8.18)$$

The corresponding estimator of $F(t)$ is given by

$$\widehat{F}_n(t) = 1 - \exp\left\{-\int_0^t \hat{r}_n^*(u)\,du\right\}$$

$$= \begin{cases} 0 & \text{if } t < Y_1 \\ 1 - \exp\left\{-\sum_{j=0}^{i-1} \hat{r}_n(Y_j)[Y_{j+1} - Y_j] - \hat{r}_n(Y_i)[t - Y_i]\right\}, \\ & \text{if } Y_i \leq t < Y_{i+1} \\ 1 & \text{if } t > Y_n \end{cases}$$

$$(8.19)$$

which converges almost surely to $F(t)$ for all t as $n \to \infty$ when $F(t)$ is IFR. Finally the estimator of $M(t)$, when $F(t)$ is assumed to be IFR, is given by

$$\dot{M}_n^{1fr}(t) = \sum_{k=1}^{\infty} \widehat{F}_n^{(k)}(t), \qquad (8.20)$$

where $\widehat{F}_n^{(k)}(t)$ is the kth convolution of $\widehat{F}_n(t)$ with itself. Here again, in actual computations, only a limited number of terms have to be computed in the sum of (8.20) (see Section 4.2). In Mathieu (1999) some empirical computations seem to indicate that this estimator is convergent.

2.5 Estimator of the optimal policy and its cost

Let $\hat{M}(t)$ be an estimator of the renewal function $M(t)$. The associated cost of the policy, based on (8.1), is $\hat{C}(t) = (c_1\hat{M}(t) + c_2)/t$. Then the estimator of the optimal policy $T_0(F)$ is given by

$$\hat{T}_{\text{opt}} = \operatorname*{argmin}_t \hat{C}(t), \qquad (8.21)$$

and its associated cost is $\hat{C}(\hat{T}_{\text{opt}})$. Each of the four estimators of $M(t)$ leads to a different estimator of the optimal policy and its cost and we will now see how to construct bootstrap confidence intervals for these two parameters.

3. Bootstrap confidence intervals

3.1 Nonparametric bootstrap

Let $X_1, X_2, \ldots, X_n$ be a random sample of i.i.d. variables from $F(x)$ and let θ be the parameter to be estimated. Consider the estimator of θ given by $\hat{\theta} = g(X)$, where $X = (X_1, X_2, \ldots, X_n)$. Let

$J_n(x, F)$ be the unknown distribution function of $\hat{\theta}$ centered at θ, i.e., $J_n(x, F) = \text{Prob}_F[n^p(\hat{\theta} - \theta) \le x]$ where p is set so that $J_n(x, F)$ converges weakly. Finally, let $\widehat{F}_n$ be the empirical distribution function of the observations, i.e., the distribution with weight $1/n$ on each observation. The nonparametric bootstrap algorithm to estimate $J_n(x, F)$ is the following:

1. obtain an i.i.d. random sample $X_{1(1)}^*, X_{2(1)}^*, \ldots, X_{n(1)}^*$ from $\hat{F}_n$, i.e., obtain a random sample with replacement from $X_1, \ldots, X_n$;

2. compute $\hat{\theta}_1^* = g(X_{(1)}^*)$ where $X_{(1)}^* = (X_{1(1)}^*, X_{2(1)}^*, \ldots, X_{n(1)}^*)$;

3. repeat 1. and 2. B times to obtain $\hat{\theta}_1^*, \hat{\theta}_2^*, \ldots, \hat{\theta}_B^*$;

4. estimate $J_n(x, F)$ by

$$\widehat{J}_{n,B}(x, \widehat{F}_n) = \frac{1}{B} \sum_{i=1}^{B} 1\left(n^p(\hat{\theta}_i^* - \hat{\theta}) \le x\right).$$

We now consider two particular cases of bootstrap confidence intervals: the basic and the percentile bootstrap intervals which will be used in the computations below.

3.2 Basic and percentile bootstrap confidence intervals

Suppose that F were known and let $J_n^{-1}(\alpha, F)$ be the αth percentile of $J_n(x, F)$. Then we have

$$1 - \alpha = \text{Prob}_F\left[J_n^{-1}\left(\frac{\alpha}{2}, F\right) \le n^p(\hat{\theta} - \theta) \le J_n^{-1}\left(1 - \frac{\alpha}{2}, F\right)\right]$$

$$= \text{Prob}_F\left[\hat{\theta} - n^{-p}J_n^{-1}\left(1 - \frac{\alpha}{2}, F\right) \le \theta \le \hat{\theta} - n^{-p}J_n^{-1}\left(\frac{\alpha}{2}, F\right)\right]$$

and so an exact $1 - \alpha$ confidence interval for θ would be given by

$$\left[\hat{\theta} - n^{-p}J_n^{-1}\left(1 - \frac{\alpha}{2}, F\right), \hat{\theta} - n^{-p}J_n^{-1}\left(\frac{\alpha}{2}, F\right)\right].$$

When F is unknown, one replaces $J_n(x, F)$ by $J_n(x, \widehat{F}_n) = \text{Prob}_{\widehat{F}_n}\left(n^p(\hat{\theta}^* - \hat{\theta}) \le x\right)$ where $\hat{\theta}^*$ is the estimator computed from a bootstrap sample and the $1 - \alpha$ basic bootstrap confidence interval is defined by

$$\left[\hat{\theta} - n^{-p}J_n^{-1}\left(1 - \frac{\alpha}{2}, \widehat{F}_n\right), \hat{\theta} - n^{-p}J_n^{-1}\left(\frac{\alpha}{2}, \widehat{F}_n\right)\right].$$

To define the percentile bootstrap confidence interval in the nonparametric case, we start by defining $G_n(t, \widehat{F}_n) = \text{Prob}_{\widehat{F}_n}(\hat{\theta}^* \leq t)$. Let $G_n^{-1}(\alpha, \widehat{F}_n)$ be the αth centile of this distribution. The $1 - \alpha$ percentile bootstrap interval is given by $[G_n^{-1}(\alpha/2, \widehat{F}_n), G_n^{-1}(1 - \alpha/2, \widehat{F}_n)]$.

The algorithm to obtain these intervals is as follows

1. obtain a random sample $X_{1(1)}^*, X_{2(1)}^*, \ldots, X_{n(1)}^*$ with replacement from the original sample $X_1, X_2, \ldots, X_n$;

2. compute $P_1 = \hat{\theta}_1^* = g(X_{(1)}^*)$ and $Q_1 = \hat{\theta}_1^* - \hat{\theta}$;

3. repeat 1. and 2. B times to obtain $P_1, P_2 \ldots, P_B$ and $Q_1, Q_2 \ldots, Q_B$;

4. order the P_i's and Q_i's to get $P_{(1)} \leq P_{(2)} \leq \cdots \leq P_{(B)}$ and $Q_{(1)} \leq Q_{(2)} \leq \cdots \leq Q_{(B)}$;

5. obtain the bootstrap basic confidence interval $\left[\hat{\theta} - Q_{\left(B(1-\alpha/2)\right)}, \hat{\theta} - Q_{\left(B(\alpha/2)\right)}\right]$ and the bootstrap percentile confidence interval $\left[P_{\left(B(\alpha/2)\right)}, P_{\left(B(1-\alpha/2)\right)}\right]$.

Note that the rate of convergence p is not necessary as the n^{-p} in front of J_n^{-1} cancels the n^p in J_n^{-1}, but it plays an important role in the validity of the method.

3.3 Bootstrap intervals when F is IFR

Generating a random sample $X_{1(1)}^*, X_{2(1)}^*, \ldots, X_{n(1)}^*$ with replacement from the original sample $X_1, X_2 \ldots X_n$ may yield equalities in the $X_{i(1)}^*$ and in this case the estimate of the hazard rate $\hat{r}_n^*$ of (8.18) would be infinite. To avoid this situation, we use the smooth bootstrap, i.e., we smooth the empirical distribution function $\widehat{F}_n$ by convoluting it with a $N(0, \sigma_\epsilon^2)$ distribution with a small variance σ_ϵ^2. Thus, instead of $\widehat{F}_n$, we use $\widehat{F}_n^s = \widehat{F}_n \star N(0, \sigma_\epsilon^2)$ where, here, $\star$ stands for convolution. Consequently the bootstrap algorithm becomes:

1. obtain a random sample $X_{1(1)}^*, X_{2(1)}^*, \ldots, X_{n(1)}^*$ with replacement from $X_1, X_2, \ldots X_n$;

2. transform $X_{i(1)}^*$ into $Y_{i(1)}^* = X_{i(1)}^* + \epsilon_i$, $i \leq 1, 2, \ldots, n$, where the ϵ_i's are i.i.d. $N(0, \sigma_\epsilon^2)$;

3. compute $\hat{\theta}_1^* = g(Y_{(1)}^*)$ where $Y_{(1)}^* = (Y_{1(1)}^*, Y_{2(1)}^*, \ldots, Y_{n(1)}^*)$;

4. repeat 1., 2. and 3. B times to obtain $\hat{\theta}_1^*, \hat{\theta}_2^*, \ldots \hat{\theta}_B^*$;

5. compute the desired confidence interval (basic or percentile).

3.4   Bootstrap intervals and preventive replacements

In order to obtain bootstrap confidence intervals for the minimal cost of a replacement policy and for the optimal policy itself, we work with the following pivots: $n^p(\widehat{T}_{\text{opt}}^* - \widehat{T}_{\text{opt}})$ and $n^q\big(\widehat{C}^*(\widehat{T}_{\text{opt}}^*) - \widehat{C}(\widehat{T}_{\text{opt}}^*)\big)$. We simply adapt the preceding algorithms in the following way:

1. obtain a random sample $X_{1(1)}^*$, $X_{2(1)}^*$, ..., $X_{n(1)}^*$ with replacement from $X_1, X_2, \ldots, X_n$;

2. compute $O_1 = \widehat{T}_{\text{opt}_1}^*$ from (8.21), $P_1 = \widehat{C}^*(\widehat{T}_{\text{opt}_1}^*)$, $Q_1 = \widehat{T}_{\text{opt}_1}^* - \widehat{T}_{\text{opt}}$ and $R_1 = \widehat{C}^*(\widehat{T}_{\text{opt}_1}^*) - \widehat{C}(\widehat{T}_{\text{opt}_1}^*)$;

3. repeat 1. and 2. B times to obtain $O_1, O_2, \ldots, O_B$; $P_1, P_2, \ldots, P_B$; $Q_1, Q_2, \ldots, Q_B$, and $R_1, R_2, \ldots R_B$;

4. compute the basic bootstrap confidence intervals $\big[\widehat{T}_{\text{opt}} - Q_{(B(1-\alpha/2))},$ $\widehat{T}_{\text{opt}} - Q_{(B(\alpha/2))}\big]$ and $\big[\widehat{C}(\widehat{T}_{\text{opt}}) - R_{(B(1-\alpha/2))}, \widehat{C}(\widehat{T}_{\text{opt}}) - R_{(B(\alpha/2))}\big]$;

5. compute the percentile bootstrap confidence intervals $\big[O_{(B(\alpha/2))},$ $O_{(B(1-\alpha/2))}\big]$ and $\big[P_{(B(\alpha/2))}, P_{(B(1-\alpha/2))}\big]$.

3.5   Does the bootstrap procedure always work

The bootstrap is known to work in many situations, i.e., the coverage probability of bootstrap confidence intervals asymptotically converges to the nominal level so that when the sample size is large enough, the actual coverage probability is close to the claimed level. However in some situations, the distribution of $\hat{\theta}^*$ centered at $\hat{\theta}$ (appropriately scaled) will not converge to the distribution of $\hat{\theta}$ centered at θ. This occurs for example when the statistical functional defining the parameter and estimator is not sufficiently smooth. Other examples of situations where the bootstrap does not work are related to the rate of convergence of the estimator, such as when the estimator converges at a rate other than $n^{1/2}$. For other situations where the bootstrap methodology may not work or where the rate of convergence has an influence on resampling methods, the reader is referred to Shao and Tu (1995), Altman and Léger (1997), Léger and Cléroux (1992), and Léger and MacGibbon (2003).

4. A simulation study

We begin by describing the parameters used in the simulation. To compute the estimators introduced earlier, a number of implementation particulars must be specified. We do this in subsection 4.2. Finally, we present the results of the simulation.

4.1 Simulation parameters

For each of the four estimators of $M(t)$ considered in Section 2, each yielding an estimator of the cost function, we obtained the basic and the percentile bootstrap confidence intervals for the optimal time for preventive replacements, $T_{\text{opt}}(F)$, and for the cost of the estimate of the optimal policy, $C(\hat{T}_{\text{opt}})$. Note that the latter "parameter" is random since it is a fixed cost function evaluated at a random estimate. This is the long term cost of using the policy $\hat{T}_{\text{opt}}$ and as such is the relevant parameter, although it is different from the minimum (fixed) cost $C(T_{\text{opt}})$.

The data have been simulated in turn from a Weibull, gamma and truncated normal (truncated at 0) distributions each with mean $\mu = 9080$ and standard deviation $\sigma = 3027$. Each sample is used to obtain all four estimators. The costs of replacement at failure and preventively are $c_1 = 1100$ and $c_2 = 100$, respectively. These distributions and parameters have been used in previous experiments, such as in Léger and Cléroux (1992).

The nominal coverage probabilities have been fixed at 90% (bilateral) and 5% and 95% (unilateral). We used $B = 999$, $n = 50$ and 200, and the parameter $\sigma_\epsilon = 1$ for the smooth bootstrap in the case of the IFR estimator. Recall that the purpose of this parameter is to ensure that all bootstrap observations are distinct; we have not experimented much with this parameter. In each case, we simulated 1000 samples of size n.

4.2 Implementation of the estimators

The computations of the parametric and IFR estimators of $M(T)$ involve a sum of convolutions. The convolutions were computed using the algorithm of Cléroux and McConalogue (1976) which uses spline approximation. Moreover, the infinite sum of convolutions for these two estimators as well as for the Frees' estimator, see e.g. (8.6), has been replaced by the sum of the first five convolutions. The kth convolution of the Frees' estimator, see equation (8.9), involves considering the mean of $\binom{n}{k}$ terms, which is a very large number for $k > 2$. For $3 \leq k \leq 5$ we have replaced the mean over all the corresponding terms by a mean of

1000 randomly selected combinations for each k. For the modified Frees' estimator (8.16) we have used the parameter $r = -1$.

To estimate the optimal policy, we had to minimize the estimated cost function. Two estimators of the cost function are continuous estimators: the parametric and the IFR estimators. The others are discontinuous. In the case of continuous estimators, the cost function has been minimized by evaluating it on a grid of points. The values of the argument t were $2000 + ih$, $i = 0, 1, 2, \ldots, 600$ in order to cover the interval $[2000, 8000]$ with $h = 10$ (for our three distributions, the optimal policy varies between 3859 and 4069). Therefore the minimum obtained is at most h units away from the real minimum. In the case of discontinuous estimators, the cost function has discontinuities at the data points Y_1, $Y_2, \ldots, Y_n$ say and at each point of the form $Y_{i_1} + Y_{i_2} + \cdots + Y_{i_k}$ for all $k = 1, 2 \ldots, n$. It is decreasing between its discontinuity points and has a positive step at each discontinuity. Thus the left limit of each discontinuity point is a local minimum and the global minimum is one of these points. Of course the cost function is not evaluated at all these points as the number of such points is much too large. However it has been noted empirically that the global minimum of the cost function is always among its first few local minimums. Consequently the cost function is evaluated at every data point $Y_1, Y_2, \ldots, Y_n$ and we consider only those yielding the smallest two local minimums, say Y_{k_1} and Y_{k_2}. Then we compute all the sums $Y_i + Y_j$, $l \le i, j \le n$ and keep only those that are at most 50 units away from either Y_{k_1} or Y_{k_2}. The cost function is finally evaluated at each of the points that have been retained and the minimum is obtained in this way.

4.3   Simulation results

Tables 8.1 and 8.2 give the empirical coverage probabilities for the optimal time and the minimum cost respectively in the parametric situation that is using the fact that it is known that F is in turn Weibull, gamma and truncated normal, but the parameters are estimated using maximum likelihood estimation. Tables 8.3 to 8.8 deal with the non-parametric situations where, after generating the data, we behave as if the family of distributions was unknown. Tables 8.3 and 8.4 are obtained using Frees' estimator (Section 2.2), Tables 8.5 and 8.6 using the modified Frees' estimator (Section 2.3) and Tables 8.7 and 8.8 using the IFR estimator (Section 2.4). In each table a result will be declared significantly different from the nominal coverage probability if it does not lie within 2 standard errors of it. For 5%, 95%, and 90% coverage,

the corresponding intervals are [0.036, 0.065], [0.936, 0.964], and [0.881, 0.919].

From Tables 8.1 and 8.2 we can make the following comments. For the optimal time at the 5% unilateral coverage the basic bootstrap always gives good results and the percentile bootstrap improves from $n = 50$ to $n = 200$ but the sample size should be increased in this latter case. At the 95% unilateral coverage, more coverage errors are made. However both types of confidence intervals give good results for the 90% bilateral coverage. The unilateral coverage errors seem to cancel one another. For the minimum cost, both bootstrap methods have some coverage errors in the unilateral intervals, but good coverage probabilities for 90% bilateral confidence intervals.

Table 8.1. Empirical coverage probabilities for the optimal time, with parametric estimator.

Distribution	Sample size	Bootstrap type	5% unilateral coverage	95% unilateral coverage	90% bilateral coverage
gamma	$n = 50$	basic	0.043	0.932	0.889
		percentile	0.100	0.979	0.879
	$n = 200$	basic	0.048	0.925	0.877
		percentile	0.069	0.956	0.887
Weibull	$n = 50$	basic	0.041	0.949	0.908
		percentile	0.096	0.987	0.891
	$n = 200$	basic	0.038	0.948	0.91
		percentile	0.069	0.967	0.898
truncated	$n = 50$	basic	0.038	0.932	0.894
		percentile	0.103	0.975	0.872
normal	$n = 200$	basic	0.056	0.947	0.891
		percentile	0.093	0.976	0.883

From Tables 8.3 to 8.6, when using Frees' or modified Frees' estimators, we see that for the minimum cost, both bilateral bootstrap confidence intervals may give reasonable results even though the empirical coverage probabilities do not necessarily lie in the interval [.881, .919]. A disturbing result, on the other hand, is that the coverage probabilities seem to be decreasing away from 90% as the sample size increases. The decrease is not statistically significant for the basic confidence intervals except for the gamma distribution, but it statistically significant for the percentile intervals for all distributions. As for the optimal time, neither bootstrap confidence interval works well with coverage probabilities far from the target for all sample sizes for the basic interval, and coverage

Table 8.2. Empirical coverage probabilities for the minimum cost, with parametric estimator.

Distribution	Sample size	Bootstrap type	5% unilateral coverage	95% unilateral coverage	90% bilateral coverage
gamma	$n = 50$	basic	0.021	0.921	0.900
		percentile	0.011	0.872	0.861
	$n = 200$	basic	0.040	0.933	0.893
		percentile	0.032	0.924	0.892
Weibull	$n = 50$	basic	0.007	0.901	0.894
		percentile	0.004	0.880	0.876
	$n = 200$	basic	0.029	0.925	0.896
		percentile	0.028	0.923	0.895
truncated	$n = 50$	basic	0.027	0,882	0.855
		percentile	0.026	0.881	0.855
normal	$n = 200$	basic	0.026	0.906	0.880
		percentile	0.030	0.905	0.875

Table 8.3. Empirical coverage probabilities for the optimal time, with Frees' estimator.

Distribution	Sample size	Bootstrap type	5% unilateral coverage	95% unilateral coverage	90% bilateral coverage
gamma	$n = 50$	basic	0.288	0.760	0.472
		percentile	0.488	1.000	0.512
	$n = 200$	basic	0.239	0.765	0 526
		percentile	0.218	0.998	0.780
Weibull	$n = 50$	basic	0.278	0.773	0.495
		percentile	0.344	1.000	0.656
	$n = 200$	basic	0.289	0.747	0.458
		percentile	0.149	0.998	0.849
truncated	$n = 50$	basic	0.283	0.763	0.480
		percentile	0.318	0.996	0.678
normal	$n = 200$	basic	0.224	0.757	0.533
		percentile	0.125	0.986	0.861

probabilities increasing in the case of the percentile interval, but still far from their target.

Finally, from Tables 8.7 and 8.8, it is seen that when using the IFR estimator, all the results for the optimum cost are bad. On the other hand, the percentile coverage probabilities for the optimal time seem reasonable for $n = 200$ (they are bad for $n = 50$), whereas all basic coverage probabilities are bad.

Table 8.4. Empirical coverage probabilities for the minimum cost, with Frees' estimator.

Distribution	Sample size	Bootstrap type	5% unilateral coverage	95% unilateral coverage	90% bilateral coverage
gamma	$n = 50$	basic	0.017	0.918	0.901
		percentile	0.009	0.911	0.902
	$n = 200$	basic	0.034	0.884	0.850
		percentile	0.000	0.792	0.792
Weibull	$n = 50$	basic	.012	0.885	0.873
		percentile	0.003	0.858	0.855
	$n = 200$	basic	0.037	0.882	0.845
		percentile	0.000	0.751	0.751
truncated	$n = 50$	basic	0.021	0.897	0.876
		percentile	0.007	0.866	0.859
normal	$n = 200$	basic	0.030	0.886	0.856
		percentile	0.005	0.782	0.777

Table 8.5 Empirical coverage probabilities for the optimal time, with modified Frees' estimator.

Distribution	Sample size	Bootstrap type	5% unilateral coverage	95% unilateral coverage	90% bilateral coverage
gamma	$n = 50$	basic	0.319	0.789	0.470
		percentile	0.514	1.000	0.486
	$n = 200$	basic	0.250	0.765	0.515
		percentile	0.241	0.999	0.758
Weibull	$n = 50$	basic	0.322	0.819	0.497
		percentile	0.387	1.000	0.613
	$n = 200$	basic	0.298	0.752	0.454
		percentile	0.145	0.997	0.852
truncated	$n = 50$	basic	0.310	0.788	0.478
		percentile	0.340	0.997	0.657
normal	$n = 200$	basic	0.226	0.760	0.534
		percentile	0.129	0.988	0.859

Now are these empirical results supported by the theory? When estimating the minimum cost, we can use the fact that both Frees' and modified Frees' estimators (of $M(T)$) are asymptotically normally distributed with a rate of convergence $n^{1/2}$. Now the cost estimator is just a continuous transformation of that estimator and should converge at the same rate to a normal distribution. Therefore the bootstrap methodology is likely to work for large samples, at least for the basic type. On the other hand, $\hat{r}_n$, appropriately normalized, converges at a rate $n^{1/3}$

Table 8.6. Empirical coverage probabilities for the minimum cost, with modified Frees' estimator.

Distribution	Sample size	Bootstrap type	5% unilateral coverage	95% unilateral coverage	90% bilateral coverage
gamma	$n = 50$	basic	0.024	0.927	0.903
		percentile	0.019	0.903	0.884
	$n = 200$	basic	0.038	0.898	0.860
		percentile	0.002	0.798	0.796
Weibull	$n = 50$	basic	0.024	0.883	0.859
		percentile	0.004	0.848	0.844
	$n = 200$	basic	0.041	0.892	0.851
		percentile	0.000	0.775	0.775
truncated	$n = 50$	basic	0.028	0.904	0.876
		percentile	0.009	0.864	0.855
normal	$n = 200$	basic	0.033	0.892	0.859
		percentile	0.006	0.787	0.781

Table 8.7. Empirical coverage probabilities for the optimal time, with IFR estimator.

Distribution	Sample size	Bootstrap type	5% unilateral coverage	95% unilateral coverage	90% bilateral coverage
gamma	$n = 50$	basic	0.275	0.697	0.422
		percentile	0.407	1.000	0.593
	$n = 200$	basic	0.239	0.741	0.502
		percentile	0.185	0.995	0.810
Weibull	$n = 50$	basic	0.248	0.687	0.439
		percentile	0.249	0.995	0.746
	$n = 200$	basic	0.272	0.734	0.462
		percentile	0.119	0.995	0.876
truncated	$n = 50$	basic	0.246	0.683	0.437
		percentile	0.242	0.991	0.749
normal	$n = 200$	basic	0.218	0.725	0.507
		percentile	0.084	0.977	0.893

(Rao (1970)). Léger and MacGibbon (2003) study the behavior of the bootstrap confidence intervals in the case of cube root asymptotics and show that the bootstrap does not usually work in such cases. It is thus not surprising that Tables 8.7 and 8.8 show bad results.

When estimating the optimal time with nonparametric estimators, Kim and Pollard (1990) show that the estimators defined as the argument which minimizes a function (as in this case) usually converge at a rate $n^{1/3}$. Consequently the bootstrap approach may not work.

Table 8 8. Empirical coverage probabilities for the minimum cost, with IFR estimator.

Distribution	Sample size	Bootstrap type	5% unilateral coverage	95% unilateral coverage	90% bilateral coverage
gamma	$n = 50$	basic	0.036	0.790	0.754
		percentile	0.000	0.159	0.159
	$n = 200$	basic	0.034	0.810	0.776
		percentile	0.000	0.421	0.421
Weibull	$n = 50$	basic	0.029	0.741	0.712
		percentile	0.000	0.303	0.303
	$n = 200$	basic	0.025	0.805	0.780
		percentile	0.000	0.515	0.515
truncated	$n = 50$	basic	0.039	0.740	0.701
		percentile	0.000	0.422	0.422
normal	$n = 200$	basic	0.027	0.809	0.782
		percentile	0.001	0.585	0.584

On the other hand, in the case of the parametric estimator, a heuristic asymptotic argument shows that if the renewal function $M_\theta(T)$ and its derivative are smooth functions of both θ and T, the estimator of the optimal time should converge at the same rate as $\hat{\theta}$. So, with the maximum likelihood estimator, the rate should be $n^{1/2}$ and the asymptotic distribution of the parametric estimator of the optimal time should be normal. Hence it is not surprising that the bootstrap seems to work in this case. In conclusion, for practical situations,

i) in the parametric case, use bootstrap confidence intervals (basic or percentile) for the optimal time and for the minimum cost;

ii) in the nonparametric case, use Frees' or modified Frees' estimators as they converge more rapidly and lead therefore to tighter confidence intervals, and use basic bootstrap confidence intervals for the minimum cost if the sample size is sufficiently large. The bootstrap is not recommended to construct confidence intervals for the optimal time.

5.   Conclusion

In this paper we dealt with the problem of periodic preventive replacements when the underlying life distribution F is unknown. For comparisons purposes we also considered the parametric situation when the form of F is known but not its parameters. Four estimators of the cost function have been obtained starting from different estimators

of the renewal function. Two types of bootstrap confidence intervals have been considered: the basic bootstrap and the percentile bootstrap for the optimal time to perform preventive replacements and for the minimum cost obtained by using the corresponding replacement policy. Simulations have indicated that the bootstrap approach may be useful in practical situations provided the sample size is large enough and certainly larger than $n = 200$. We have limited ourselves to a very simple model. To make the situation more realistic a more complex cost structure should be considered and different actions at failure should be available: minimal repairs, replacements with used equipment, etc. A bootstrap approach, similar to the one proposed in this paper, could also be tried in these more complex models.

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Chapter 9

STATISTICS FOR COMPARISON OF TWO INDEPENDENT cDNA FILTER MICROARRAYS

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Abstract   The great interest in gene expression in microbiology has led to the development of the cDNA array experiment. A very large number of genes can be tested simultaneously for their level of expression through these arrays. This gives rise to data where there are but a few observations for any one gene upon which to base a test of significance, and a very large number of these tests to carry out. Here we consider experiments with two filter microarrays; one from a control and one from a treated preparation. The question of interest is whether or not the k largest observed gene-wise differences are indicative of true differences, or whether the results can be due to background variation. We develop a parametric approach distinct from those based on resampling methods, and obtain an hypothesis test applicable to this experiment that can be easily implemented in standard statistical software. We illustrate the approach on data on herpes-infected cells.

1.   The experiment and a hypothesis test

The human genome project and the development of cDNA microarrays have led to an explosion of experimental activity aimed at discovering how, why and which genes are involved in biological processes. Indeed, nearly every recent issue of *Nature* or *Science* contains an analysis of cDNA data – e.g. see Brown and Botstein (1999) and Lander (1999) for early examples. The experimental data considered here were obtained from a specific type of cDNA experiment where the goal is to discern whether the activity of some genes has been either up-regulated (made more active) or down-regulated (made less active) by the presence of a stress, such as infection by a virus. Knowledge of the effect of a virus on a cell can be used to combat the infection by guiding research towards

key mechanisms of the virus. This paper will not focus on the biological significance of this sample data, but will use it to provide one statistical approach to its analysis. This approach represents an alternative framework for testing for the presence of differentially expressed genes to those based on resampling methods, and can be easily implemented in standard statistical software.

The experiment motivating this paper employs dots of known genetic material (*"probes"*) on glass (or nylon) slides to determine the amount of that material present in a given test preparation. A single slide contains many – from 500 to 15000, or more – distinct dots, generally arranged in an array. Each dot is composed of copies of a single piece of complementary DNA (cDNA) which, for the purposes of this discussion, we will call a *gene*, even though the genetic material in that dot may not correspond exactly to that of a single gene. Each gene may be repeated a small number of times on the slide , but the number of genes remains a relatively large number. Here we take the most typical case where there are 2 dots on the slide for each gene, but other arrangements exist, and the methods below can be adapted to those cases. A key property of cDNA is that it binds (*hybridizes*) to the matching strand of DNA, and not to non-matching strands.

The preparation to be applied to the microarray contains the DNA (or mRNA) from all the genes of the cell or organism under study. These genes are known (e.g. from the Human Genome Project), but the degree to which each gene is expressed (i.e. differentially replicated) in a living cell is not. For example, individual genes may be 'triggered' into activity at different times during the life of a cell, with different roles at different times, or in response to an external stimulus such as heat. Why genes are activated or deactivated is of critical interest. For simplicity one may think of this preparation of cell DNA as a purée of the genetic material of a group of cells from a single cell line. It is generally made up using some marking method, such as radioactive or fluorescent tags so that the future of that sample may be conveniently traced. When this preparation is applied to the slide, if the DNA matches the cDNA on a dot, it will hybridize to that probe to the degree that that gene is expressed in the cell. If it does not, it will be washed away at the end of a fixed time period. Thus at the end of the experiment, we should find that certain dots – those matching the DNA highly expressed in the preparation – on the slide show a strong radioactive (or fluorescent) signature, and that others – those for which no matching DNA is found in the preparation – do not. In this way we can identify (by scanning the magnified image of the slide) which genes are active in the original cell. Of greater interest is the degree to which each gene is expressed,

as measured by the intensity of the signal at the appropriate dot. The degree of expression indicates the degree to which the gene is active, and this can vary with the type of cell, the stress to which it has been subjected, and time.

Unfortunately, this process is subject to a variety of errors. The deposition of cDNA may result in dots of different sizes, there may be flaws in the glass slides, the scanning of the dots to acquire the signal may vary, the image analysis software may not capture the dots correctly, the homogeneity of DNA in the wash may not be perfect and there may be partial binding of DNA to unintended sites, for example. Thus the observed intensity of signal at a single dot can and does exhibit considerable variation – some random and some systematic. A schematic of a highly reduced array is shown in Figure 9.1.
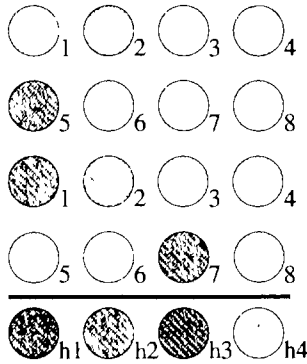

Figure 9.1. A small idealized example of the data obtained from a cDNA array. The intensity of the spot indicates the amount of DNA binding to that dot. There are 8 distinct genes (#1 through #8), each repeated once. There are 4 "housekeeping genes" (h1 through h4) used for calibration purposes.

To complete our description of the experiment considered here, we introduce a second slide containing the same array of gene dots. The first slide is treated with the DNA preparation from a normal cell, and the second (as in the example presented later) with that from the same cell line after infection with a Herpes virus. Of course, we will observe differences in signal intensity for comparable genes from one slide to the other. Indeed we will likely observe many large differences even if there is no differential expression for any gene across treatments because so many – e.g. 10,000 – simultaneous comparisons are being undertaken. The goal of this work is to add another statistical approach to the data in such an experiment, and to establish an hypothesis test that permits the researcher to conclude whether the observed differences in intensity are real, and not due to random fluctuation in the signal. In this manner

we hope to identify which genes are upregulated (made more active) or downregulated (made less active) by the treatment (infection by the herpes virus). Our focus will be on a general method to address the issue of high multiplicity of tests.

There are, as yet, relatively few papers addressing the problem outlined above, although interest is rapidly expanding. Although genomics as a field is still young, there is a large body of work developing algorithms for measuring (evolutionary) distances between DNA sequences (e.g. Thompson (2000)) and a growing collection of papers employing clustering and classification methods on microarray data in an effort to identify functional groupings of genes (e.g. Eisen et al. (1998), but the analysis of comparative experiments such as we address here have an even shorter history. Chen, Dougherty and Bittner (1997), Dudoit et al. (2001), Lee et al. (2000), and Efron et al. (2001) are leading papers in this area, each contributing their own approach to microarray data. Efron et al. (2001) also contrasts several approaches: model-based, Bayesian and bootstrapping methods. Chen et al. (1997) looked at changes in mean response, and Lee et al. (2000) modeled the probability of response rather than the response itself. Recently Newton et al. (2001) established a Bayesian hierarchical model employing gamma densities for signal strength. Kerr, Martin and Churchill (2000) adapt ANOVA methods. Sabatti, Karsten and Geschwind (2002) pursue a data-driven thresholding rule for identifying differentially expressed genes that aims to justify the common practice of declaring as significant all gene expression tests that exceed a given threshold. Much of this work is highly topical, and resides in internet sites – e.g. Nadon et al. (2001). Recent texts that contain some discussion of comparative microarray techniques are those of Ewans and Grant (2001) and of Hastie, Tibshirani and Friedman (2001). A recent issue of *Statistical Science* (volume 18, February 2003) included a Special Section on microarray analysis: Sebastiani et al. (2003), Dudoit, Shaffer and Boldrich (2003), and Tibshirani et al. (2003).

Sebastiani et al. (2003) (and the invited comments) reviews the background for DNA/microarray experimentation, describes the context in terms of determining cell function, and provides an overview of the analytic techniques available to date for the analysis of microarray data. The authors provide pertinent commentary on the open problems and issues related to experimental design, data quality, and the being made in passing from qualitative comparative procedures to quantitative approaches.

The article of Dudoit et al. (2003) pursues an aspect of microarray analysis of great current interest. As indicated above, a single microar-

ray experiment is in fact upwards of 20,000 simultaneous single-gene experiments – e.g. 20,000 simultaneous t-tests – from which we must decide which of the formally statistically significant results are 'real'. Even at very low individual type I error rates, the incidence of false positives in such an experiment will overwhelm the true positives, and render interpretation very difficult. Novel methods are needed to address this volume of data and apparently significant comparisons. Dudoit et al. (2003) provide a review and comparison of several means of controlling various forms of false positive rates: the per-comparison error rate, per-family error rate, family-wise error rate and false discovery rate. The authors also discuss single-step, step-down and step-up adjustment techniques for the collection of p-values generated by the 20,000 simultaneous tests of hypotheses. Many of these methods involve extensive resampling or permutation algorithms.

As in many of these papers, we will assume that the data have been cleaned and normalized to remove slide surface effects, inter-slide scaling effects and other similar problems. See Tseng et al. (2001) for a discussion of these issues, and Kerr et al. (2000) or Ge et al. (2001) and Yang et al. (2001) for suggested approaches. The book of Draghici (2003) provides an excellent discussion of the need for data cleaning and the steps required to achieve reliable data. Although not complete, there is a list of standard effects that should be removed from the data prior to statistical analysis. Once the data has been 'pre-processed' in this way, we may make the essential assumption that the observations in the microarray arise from independent random variables. Most of the cited papers discuss glass microarrays, where two washes (tagged by two different fluorescent dye colours) are hybridized onto each dot, but here we content ourselves with filter microarrays, where only a single wash is applied to each slide. The difference is comparable to that between paired and unpaired experiments.

These kinds of microarray data presents two classical statistical problems. For any single gene, we have but a very few samples upon which to base a test of the hypothesis of equal response – e.g. just two dots per slide. Small sample problems abound in the literature, although relatively infrequently involving only 2 observations. The papers cited above generally approach this issue by employing resampling or pooling techniques to improve the estimation of error. The model-free resampling approach of Dudoit et al. (2001) is very promising, but linking the results of those methods to physically interpretable parameters may be difficult. The work of Newton et al. (2001) employs hierarchical Bayes models to a similar end, but for glass microarrays. Here we will avoid

such questions and assume that an appropriate test of hypothesis has been developed for each gene.

If the single-gene comparison test can be resolved, we are still faced with the fact that a single microarray experiment may require thousands of these single-gene tests. This is a classical multiple-comparison problem, but on a scale not encountered in, for example, analysis of variance. Instead of ten or twenty simultaneous comparisons, a modern microarray experiment may generate 19,000 p-values. Dudoit et al. (2001) apply step-down methods of Westfall and Young (1993) to adjust single-gene p-values to control the family-wise error rate, and the sequential methods of Benjamini and Hochberg (2002) for controlling the false discovery rate may be applied to genetic data (Weller et al. (1998)).

We proceed by developing a simple multiple comparison procedure adapted to testing whether or not at least $k + 1$ genes in the pool of genes exhibit differential expression. This approach to multiple testing can be employed for any single-gene test, not just the one presented in our illustrative example, below. It can also be used in the paired glass slide experiment and other contexts as well. Our approach will be numeric rather than theoretic: Using simulated null distributions and practical simplifications based on empirical evidence will permit us to lay out a plan of action for this problem without waiting for more rigorous theoretical results on the behaviour of distributions. The pace of research in microbiology frequently requires quick and reliable answers, not necessarily theoretically optimal ones. We illustrate our methods on data from Herpes-infected cells.

## 2.		Single-gene comparisons

Here we consider a simple experiment corresponding to the well-known case of two independent samples: a single slide with data from an infected cell, and a slide with data from an uninfected cell. We denote the observed intensity of the ith dot of gene g for the un-infected preparation by X_{gi}. The corresponding value for the infected cell is noted Y_{gi}. We take that $i = 1, 2$ and that g runs over a large number of genes. We assume that the observations are all statistically independent. Further, we assume that the X_{gi} have mean μ_{Xg} and variance σ^2_{Xg}. The Y_{gi} have means μ_{Yg} and variances σ^2_{Yg}, respectively. Note that the means and variances are fixed for a single gene g on a single slide, but may vary from one gene to another and from the control to treatment slides. We require that continuous densities exist in all cases.

For example we could assume normality of the observations. To test the hypothesis that $\mu_{Xg} = \mu_{Yg}$ versus $\mu_{Xg} > \mu_{Yg}$, and since there are

two observations per gene for each of the two slides, one can consider the usual two-sample t-test statistic under the assumption of equality of variances,

$$T_g = \frac{(\overline{X}_g - \overline{Y}_g)}{s_p},$$

where s_p^2 is the pooled estimator of the common variance. Under normality assumptions of the illustrative case, this variable has an t distribution with 2 degrees of freedom, and we reject equality of means for large values of T_g.

REMARK   As shown in Figure 9.1, there are frequently "housekeeping" genes added to each slide in an attempt to compute a normalizing adjustment to the values of the slide. These housekeeping genes should register the same intensity of response for both control and treatment preparations, and so the intensity measurements of the second slide could be adjusted either by the ratio of average values for the housekeeping genes on the treatment to the control slides, or by their difference. This forms part of the pre-processing step.

REMARK   We assume that the p-values p_g obtained across different genes are independent — i.e. that the errors in gene expression measurement are statistically independent. It is well-known that spatially proximate probes or functionally related genes tend to have similar responses, but we will represent this common effect in the values of the mean responses for these probes rather than in through some statistical spatial correlation, and so preserve statistical independence across genes in this model. This is a reasonable idealization so long as the family of curves used to approximate mean response is sufficiently rich.

3.   Multiple comparisons

Now that we have a single-gene test and its sampling distribution, we can address the question of multiple comparisons. The method described here can be applied for any test the reader may decide to use for the single-gene test, and is not limited to the test described in the previous section. For example, if responses were modelled by double exponential distributions instead of normal ones, one could use a test based on the median instead of the sample mean.

Westfall and Young (1993), Benjamini and Hochberg (2002), and Dudoit et al. (2003) provide good introductions to the issues and methods relevant to massively multiple comparisons. The goal of these works is to identify how many of the smallest p-values are indeed significant. Our goal is to present an alternative approach that can be adapted to cases

where either we seek to determine if the kth-smallest p-value is significant, or if a pre-determined group of genes show a cumulative significant effect even if individually no single gene test has a small p-value. The applications of the first case are to experiments where the most important genes are already well-known to have a differential expression, and it is the next in line that is of interest to the biochemist. The second case may arise when the researcher is interested in a possible effect over a group of genes involved in a common biological process - for example whether there is evidence that immune system genes as a whole are influenced by a viral infection.

If $\mu_{Xg} = \mu_{Yg} = \mu$ for a specific gene g, the p-value (noted p_g) of a single-gene test under H_0 is uniformly distributed on $[0, 1]$. On the other hand, if $\mu_{Xg} > \mu_{Yg}$ - i.e. there is a decrease in gene expression - then the sampling distribution of p_g will be more concentrated near zero, i.e. stochastically smaller than the uniform distribution. Of course, we assume that the test statistic has been chosen in a reasonable way and that continuous densities exist. This monotonicity is evident empirically from Figure 9.2 for an illustrative normal case.
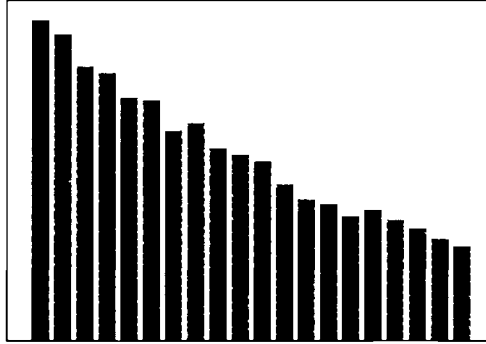

Figure 9.2. A histogram of 20,000 simulations of the p-value of the test of (9.1) using a pooled t-test per gene when the true situation is that the mean is 0.80 for genes on the control slide and 1.20 on the treated slide. One can see the displacement of the density to the left as opposed to the uniform density expected under the null hypothesis.

We now assume that the density (f_1) of p_g when $\mu_{Xg} > \mu_{Yg}$ is monotone decreasing on $[0, 1]$. Denote the uniform density on $[0, 1]$ by f_0. The biochemist will generally already expect to find some number, k, of obviously differentially-expressed genes in the experiment. A practical null hypothesis therefore is that there are at most k differentially-expressed genes known to be present, and the alternative is that the there are such genes beyond these k most obvious ones. For k a fixed positive integer, the likelihood ratio test of

K_0: k p_g are iid f_1 and the rest are iid f_0.

K_1: At least $k + 1$ p_g are iid f_1 and the rest are iid f_0.

rejects if

$$\frac{\max_1 \prod_g h_g(p_g)}{\max_0 \prod_g f_0(p_g)} > c,$$

where h_g is the density of p_g, c is a constant, and where the maxima are over all possible choices of h_g consistent with the alternative and null hypotheses, respectively. Denote the ordered p-values by $\pi_{(1)} < \pi_{(2)} < \ldots < \pi_{(G)}$ and the rank of the p-value for gene g by r_g. Thus $p_{r_g} = \pi_g$. We may rewrite the numerator and denominator of the likelihood expression in the form

$$\max \prod_g h_g(p_g) = \max \prod_g h_{r_g}(\pi_g).$$

Under K_0 there must be exactly k densities h_g that are f_1, and the rest are f_0. By the assumed monotonicity of the densities, the above expression is then maximal if we substitute $f_1(\pi_g)$ for $h_{r_g}(\pi_g)$ for each $r_g \leq k$. Under K_1 there must be at least $k + 1$ densities h_g that are f_1. The product in the numerator continues to increase so long as $f_1(\pi_g) > 1 = f_0(\pi_g)$, i.e. substitute $h_g = f_1$. The remainder of the terms are maximized at $1 = f_0(\pi_g)$. Let the collection of indices g of genes for which the alternative density is larger than the null one and the p-values are not among the k least by $\mathcal{G} = \{g : f_1(\pi_g) > f_0(\pi_g) \text{ and } r_g > k\}$. Then since the first k terms cancel from the numerator and denominator, and since $f_0(x) = 1$, the ratio becomes

$$\prod_{g \in \mathcal{G}} f_1(\pi_g).$$

The evaluation of this product will certainly depend on the choice of f_1. For now we choose a specific alternative,

$$f_1(x) \quad = \quad 2(1 - x)\ 0 < x < 1. \tag{9.1}$$

Now $\mathcal{G} = \{g : \pi_g < 0.5 \text{ and } r_g > k\}$, and the LRT then rejects if

$$\prod_{g \in \mathcal{G}} (1 - \pi_g) > c$$

for some c. Taking logs yields a test that rejects if

$$D \quad := \quad \sum_{g \in \mathcal{G}} \log(1 - \pi_g) > c'. \tag{9.2}$$

In this case, the null distribution of D can be easily simulated since the p_g are uniform on $[0, 1]$. Table 9.1 provide the density of D for several values of k and the number of spots $n = 780$ ($G = 390$). As can be seen from the table and Figure 9.3, the distribution does not vary greatly with k until it becomes moderate in size.

Table 9.1. Critical values for the multiple-gene test when there are $n = 780$ spots ($G = 280$). The table is given for the alternative that at least k observations come from the f_1 of (9.1). Twenty thousand simulations were used for each k.

		Upper quantile				
k	0.01	0.02	0.03	0.04	0.05	0.10
0	-50.42	-51.59	-52.20	-52.75	-53.18	-54.69
1	-50.36	-51.52	-52.22	-52.75	-53.17	-54.59
10	-50.43	-51.45	-52.21	-52.78	-53.11	-54.49
25	-49.77	-50.90	-51.52	-51.98	-52.38	-53.86
50	-47.17	-48.23	-48.93	-49.43	-49.84	-51.26
75	-42.83	-43.84	-44.55	-45.05	-45.43	-46.82
100	-35.75	-37.04	-37.75	-38.34	-38.76	-40.30
125	-26.58	-27.81	-28.56	-29.17	-29.64	-31.33
150	-14.00	-15.49	-16.49	-17.13	-17.75	-19.67
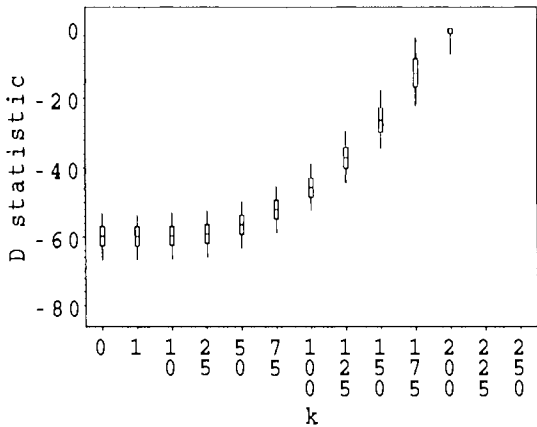
Figure 9.3. Each box plot is computed from 20000 simulations of the loglikelihood of the multiple-gene test of (9.1). The value of k varies from 0 to 225.

REMARK   Note that $-\log(1-\pi_g)$ is exponential of mean 1, and that our statistic is the sum of extremes from an exponential sample. As $n \to \infty$ we can try to obtain the limiting distribution of D through application of extreme value theory, at least in the case where K_0 is that there are exactly k f_1 distributed p-values.

The above development of a multiple-gene test employed f_1 of a mathematically very convenient form. The f_1 that one should use in practice, however, should be the density, f_{1g}, of the p-value for gene g at a specified point its H_1. If that point in the alternative is far from $H_0 : \mu_{Xg} = \mu_{Yg}$, we expect f_{1g} to be strongly concentrated towards 0. We continue to assume a monotone decreasing form. We can obtain an approximate form for f_{1g}, either by assuming a distributional form for the data under H_1 and simulating, or by pooling standardized residuals across genes, and resampling from that collection and adding the required shift in mean. Clearly this will require some homogeneity across genes to implement.

Once f_{1g} is determined, two adjustments must be made to contribution of LR_g to D. First, $\log(f_{1g}(\pi_g))$ replaces $\log(1 - \pi_g)$. Second, the decision whether or not that term even appears in the sum defining D depends on whether or not the p-value at g, π_g, falls below the intersection point of f_1 and f_0 (replacing the cut-off of 0.5 in earlier paragraphs). Denote by c_g the least point where $f_{1g}(c_g) = 1 = f_0(c_g)$, and set $\mathcal{G} = \{g : \pi_g < c_g \text{ and } r_g > k\}$. The test statistic is now

$$D \quad := \quad \sum_{g \in \mathcal{G}} \log(f_{1g}(\pi_g)) \tag{9.3}$$

REMARK   It is not difficult to adjust the above argument to cover $f_1(x) = (\gamma + 1)(1 - x)^\gamma$ for $\gamma \geq 1$ and recover the form given in (9.2). Exchanging $2(1 - x)$ for $\gamma(1 - x) + 1 - \gamma/2$ would lead to a different form for the test statistic and would require new simulations of its null distribution.

REMARK   The fact that microarrays use very few replicates per gene – just 2 per slide in most cases – will mean that f_1 may be expected to be quite close to f_0 even for a point in the alternative fairly removed from H_0.

REMARK   Clearly the above development will depend on the form of the density of the p-value under the alternative, f_1. It is not the intent, however, to pursue such an approach, but rather adopt the simplified linear alternative density as an approximation. Consider the case where the single-gene test statistic, T_g, has a normal distribution with variance 1, and assume that under the null hypothesis the mean $\delta = 0$, and that under the alternative $\delta > 0$. The density of the p-value generated when the mean is δ is

$$f_{pval}(u) = \frac{\exp\{-\frac{1}{2}(\Phi^{-1}(1 - u) - \delta)^2\}}{\exp\{-\frac{1}{2}(\Phi^{-1}(1 - u))^2\}}$$

for $u \in (0, 1)$. Although clearly sigmoidal, the graph of this density can be approximated in practice by a straight line density to which the approach above may be applied.

A second test of interest is whether or not, in the context of so many simultaneous comparisons, there is evidence of general decrease in expression within a *group* or family of genes, instead of just at single probes. One can easily imagine a situation where a large group of genes are all only mildly affected by a treatment, and so that all the corresponding single-gene tests fail to identify a systematic effect. Such a test can be incorporated into the context of this section fairly easily. Suppose $\mathcal{I}$ represents the indices of the probes belonging to the group of genes of interest. The null hypothesis is that there is no change in expression for any member of this family from the treated to the control slide, and the alternative is that there are some genes for which the mean expression has decreased, i.e. the p-value has a density f_1. The likelihood ratio for this group effect is exactly that obtained in the test for $k = 0$ in the above discussion at (9.2), and its null distribution can be simulated as indicated there. This distribution would provide a marginal p-value for this test of group-wise change in gene expression. The p-value for the group test arising from the simulated null distribution of the likelihood ratio can replace the $\#\{\mathcal{I}\}$ individual p-values in the multiple testing procedure described earlier, and so obtain an idea as to the significance of this single test in the presence of the entire collection of p-values generated by all the gene tests. Whether this group test is included in the collection, $\mathcal{G}$, of p-values under the threshold will require the density, $f_{1\mathcal{I}}$ of the group-wise test when at least one $p_g : g \in \mathcal{I}$ has density f_{1g}. The p-value of the group test will count in the calculation of D in (9.3) if it falls below the threshold $c_{\mathcal{I}}$. Note that the previous development did not require that the individual gene tests all have the same form, just that the densities be continuous.

The next section will illustrate these ideas on a real data set.

4.   An example

Dr. Diaz-Mitoma of the Children's Hospital of Eastern Ontario kindly provided a data set to illustrate the use of the methods described above. The data concerned two filter microarray slides, each spotted with 390 pairs of (non-housekeeping) cDNA from immune-response genes. A preparation from a normal nerve cell is applied to the first slide and that from a herpes-infected nerve cell is applied to the second. The goal is to identify which genes are either upregulated or downregulated by the virus. Here we make no claim as to the biological significance of

any analysis. These are intended only as an illustration of the methods described above.

Figure 9.4 provides the histograms of the observed values for the "housekeeping" genes in the control and treatment slides. Ideally, these should all behave as independent and identically distributed observations from a normal distribution with a common mean. The sample sizes are small, but at least there is no strong contra-indication of this assumption of normality.
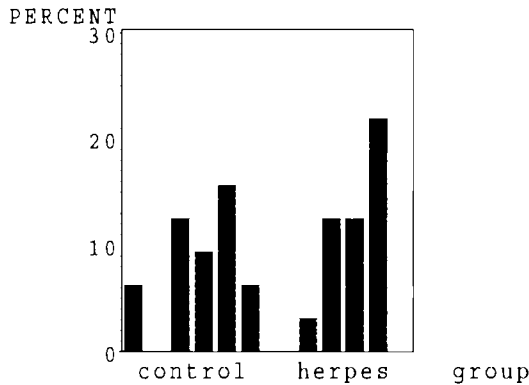

Figure 9.4. Histograms of the values of raw data for the herpes experiment. The left-hand graph shows the distribution of 16 values in the control slide, and the second from the treatment slide. The assumption of normality is not contradicted by these graphs.

Before employing the data, we excluded those genes for which the replicates (for either X or Y) differed by more than 40 percent. This criterion is somewhat arbitrary, but corresponds to a frequently used threshold for deciding whether probes are differentially expressed. A more complete discussion of data preprocessing is found in Yang et al. (2001). The 14 excluded points (out of 390) are illustrated in Figure 9.5. To check for spatial effects in the slide itself, we plotted a contour plot of the average (over the two spots) intensity against location on the control and treated slides. This plot did not exhibit any strong evidence of non-random spatial patterns from one slide to the other, and so we will proceed with the assumption of independence of responses across spots.

Our single-gene test is the standard pooled variance t-test for comparing the means of two independent samples, based on two samples for each group, and the p-value is computed for a right-handed alternative. Table 9.2 provides the results of our test of hypothesis for H_0: 0 observations from f_1 against H_1: there is at least 1 observations from f_1. The
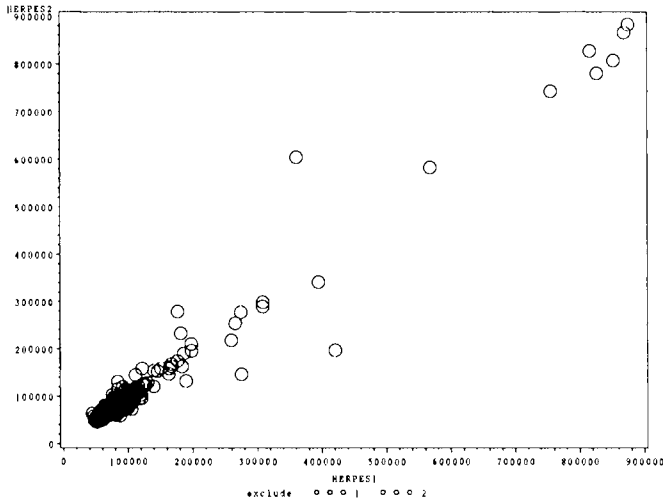
Figure 9.5. The plot of one herpes replicate, Y_{g2}, against the other, Y_{g1}. Fourteen points excluded prior to analysis by the multiple testing procedure are indicated by filled circles. These include those outliers identified in the corresponding plot for the control replicates.

observed value of the D statistic (-19.53) yields an approximate p-value less than 0.01 from Table 9.1. In this case there is strong evidence for the alternative as the D statistic falls well to the right of the estimated 0.01 cut-off point in Table 9.1, and indeed if we had chosen k much larger, we would still see evidence of upregulated genes. The false-discovery-control procedure of Benjamini and HochBerg (2002) (see also Finner and Roters (2002)), when applied to this string of p-values for false discovery rate 0.01, does not conclude that any of the genes is differentially expressed, because the minimum p-value= $0.00016 > 0.000026 \simeq 0.01/390$, and so that method stops without concluding any decrease in expression is present. If we chose a false discovery rate of 0.05, the conclusion remains the same, but for 0.10 the threshold is overcome, and the first 175 p-values are judged significant. In contrast, the value of D, when computed for $k = 100$ or 125 yields values of -18.93 and -18.5, both of which correspond to p-values for D less than 0.01. For $k = 150$, however, $D = -17.83$ and the corresponding p-value is strictly between 0.05 and 0.10. For $k = 175$, the p-value of $D = -16.87$ exceeds 0.10. Consequently, although a plot of p-values versus k does not comprise a rigorous statistical test, this method can be used as an exploratory tool to determine with greater sensitivity the degree of upregulation of genes.

Table 9.2. This is an extract of the first 20 and last 5 of 200 entries in the sum defining D. The final value in the D column (-19.53) is the statistic value used in a test of H_0: no observations from f_1 against H_1: at least 1 observations from f_1. The p-value for this multiple gene test is less than 0.01 (Table 9.1).

single gene pvalue	multi-gene statistic, D	standard gene identifier
0.00016	-0.0002	CCR-5
0.00020	-0.0004	NGFR
0.00030	-0.0007	April
0.00032	-0.0010	CD27L
0.00040	-0.0014	MCAM
0.00055	-0.0019	NCAM
0.00060	-0.0025	GRO-b
0.00074	-0.0033	Integrin-b5
0.00079	-0.0041	MIG
0.00081	-0.0049	CCR-7
0.00091	-0.0058	FGF-10
0.00098	-0.0068	IK
0.00121	-0.0080	M-CSF
0.00123	-0.0092	IGF-II
0.00125	-0.0105	EphB1
0.00150	-0.0120	EphB3
0.00152	-0.0135	Eotaxin-2
0.00167	-0.0151	c-kitLigand
0.00168	-0.0168	Midkine
0.00170	-0.0185	MIP-3
$\vdots$	$\vdots$	$\vdots$
0.37531	-17.1566	pUC19
0.40849	-17.6817	FGFacidic
0.45007	-18.2797	FGFbasic
0.45938	-18.8947	c-met
0.47190	-19.5332	L19

5. Conclusion

This paper presents an alternative framework for testing for the presence of differentially expressed genes to those based on resampling methods, and can be easily implemented in standard statistical software. The single-gene test presented here was an ad-hoc procedure developed under a normality assumption and the working hypothesis that the test should be invariant under scale changes in the data. If these assumptions are not biologically tenable, the multiple comparison test can still be used for any alternative single-gene test that may be suggested as being more appropriate, so long as p-value has a uniform distribution

under the null hypothesis. Practical considerations of this approach will require that a single-gene test be validated for real data sets, and that its behaviour under the alternative, i.e. its appropriate f_1, be ascertained. The single-gene test under the normality assumptions presented here may not be biologically the most accurate model possible, but may still be close enough to the truth to be useful, and the straight-line alternative f_1 may be a good enough approximation to provide insight into the relative importance of the observed upregulations. Rather than a definitive algorithm, this paper provides a template for algorithms that can be developed in particular experiments.

Further, although the multiple comparison procedure here was illustrated on two independent samples, the same approach will work when dealing with several treatments. For example consider 8 filter microarrays in a balanced 2×2 anova design, where factor A is the presence or absence of the virus, and factor B is the presence or absence of a treatment. If, separately by gene probe, normality and constant variance are tenable assumptions, then we can obtain a p-value for each probe from the F-test for interaction between virus and treatment. The method of the previous section could then provide guidance as to which genes are responding to the treatment when the virus is present. Indeed one can now employ all the principles from design of experiments to the single-gene experiment and test for significance across genes. The 3 p-values (factor A, factor B and interaction) obtained for each probe could also subsequently be used in any of a number of clustering algorithms in an effort to discover gene families. Current clustering work has concentrated on using the raw (or transformed) microarray intensity data, but clustering on by-gene p-values should more strongly highlight family groups. Using p-values from tests on contrasts should greatly assist interpretability. Dr. Diaz-Mitoma and the author are currently working on applying this approach to an analysis of the differential effect of AIDS on new and old world monkeys.

The numeric algorithms to simulate null distributions employed here were crude and effective, although long. Work remains to develop faster procedures. Additional work is also required to develop constrained optimization methods when the by-gene means are not completely free, but constrained by spatial proximity or functional groupings of the genes.

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Chapter 10

LARGE DEVIATIONS FOR INTERACTING PROCESSES IN THE STRONG TOPOLOGY

Donald A. Dawson
Pierre Del Moral

Abstract   Strong large deviations principles for a general class of discrete generation and interacting particle systems are developed   The analysis is essentially conducted through an original projective interpretation of the τ-topology, combined with a powerful projective transfer result presented by the first author with J. Gärtner   These large deviations principles simplify and encompass the ones obtained in an earlier joint work of the second author with A Guionnet They are illustrated with simplified versions of McKean-Vlasov diffusions, and Boltzmann type collision models. We also describe the impact of this analysis on a recently developed class of genealogical and interacting particle interpretations of non linear Feynman-Kac-Schrödinger path measures

1.   Introduction

1.1   Description of the models

In this article, we design a natural and general projective technique for proving strong large deviations principles, for a general class of interacting particle systems. This class of interacting measure valued processes arise in various scientific disciplines, including in biology and physics, but also in diverse branches of engineering science. In order that this article is both broad, and has some theoretical and applied basis, we shall briefly review the impact of these deviations on simplified McKean-Vlasov diffusions and Boltzmann type collision models, as well as on a general and abstract class of Feynman-Kac-Schrödinger semigroups. Besides their important physical aspect, these models also arise in the analysis of nonlinear filtering, Bayesian statistics, rare events estimation,

and directed polymers simulations. Readers who are interested in more detailed and precise applications should consult the series of complementary articles Del Moral (1998), Del Moral and Miclo (2000, 2001), as well as the book edited by Doucet and De Freitas and Gordon (2001).

To describe with some precision our models, we need to introduce some notation. We let $\mathbf{P}(E)$ be the set of additive and $[0,1]$-valued set functions on an Hausdorff topological space E, with the Borel σ-field $\mathcal{E}$, and equipped with the τ_1-topology of setwise convergence. Without further mention, we shall assume that $\mathbf{P}(E)$ is furnished with a σ-algebra which contains the Borel σ-field associated to the τ_1-topology on $\mathbf{P}(E)$. As usual, we denote by $\mathcal{B}_b(E)$ the Banach space of all bounded, and $\mathcal{E}$-measurable functions f on E, endowed with the supremum norm $\|f\| = \sup_{x \in E} |f(x)|$. By $\mathcal{P}(E)$ we denote the subset of probability measures on E, equipped with the relative τ-topology.

We consider a collection of Hausdorff topological spaces $(E_n, \mathcal{E}_n)_{n \geq 0}$, and a collection of continuous mappings Φ_n from $\mathbf{P}(E_{n-1})$ into $\mathbf{P}(E_n)$, such that $\Phi_n(\mathcal{P}(E_{n-1})) \subset \mathcal{P}(E_n)$. We also let η_n be the solution of the equation

$$\eta_n = \Phi_n(\eta_{n-1}) \,, \quad \text{with} \quad \eta_0 \in \mathcal{P}(E_0) \tag{10.1}$$

In practice, the above continuity conditions can be easily checked by recalling that $\mathbf{P}(E)$ can be represented as a subset of the algebraic dual of $\mathcal{B}_b(E)$ (see for instance Theorem C3 page 315 in Dembo and Zeitouni (1993)), and the τ_1-topology coincides with the $\mathcal{B}_b(E)$-topology on $\mathbf{P}(E)$.

The interacting particle interpretations of the equations (10.1) can be thought as a stochastic linearization technique. They are defined as a Markov chain $\xi_n^{(N)}$ taking values in the product spaces E_n^N with initial distribution $\eta_0^{\otimes N}$. Its elementary transitions $\xi_{n-1}^{(N)} \rightsquigarrow \xi_n^{(N)}$ are given, for any $n \geq 1$, by the formula

$$\text{Prob}(\xi_n^{(N)} \in d(x_n^1, \ldots, x_n^N) \mid \xi_{n-1}^{(N)}) = \prod_{i=1}^{N} \Phi_n(m_N(\xi_{n-1}^{(N)}))(dx_n^i) \tag{10.2}$$

In the above display, $m_N : x \in E^N \rightarrow m_N(x) \in \mathbf{P}(E)$, is the mapping which associates to each configuration $x = (x^i)_{1 \leq i \leq N} \in E^N$ the empirical measure $m_N(x) = \frac{1}{N} \sum_{i=1} \delta_{x^i}$, with δ_{x^i} denoting the Dirac measure at the site x^i. In other words, the configuration of the system $\xi_n^{(N)} = (\xi_n^{(N,i)})_{1 \leq i \leq N}$ at time n consists in N-conditionally independent random variables, with common distribution $\Phi_n(m_N(\xi_{n-1}^{(N)}))$. We complete this short presentation with an alternative particle interpretation of (10.1). Suppose the one step mapping Φ_n can be rewritten in the following form

$$\Phi_n(\eta_{n-1}) = \eta_{n-1} K_{n,\eta_{n-1}}$$

for some (non unique) collection of Markov kernels $K_{n,\eta_{n-1}}$ from E_{n-1} into E_n. In this situation, it is often more judicious to associate to (10.1) the particle approximating model defined as above, replacing (10.2) by the elementary transitions

$$\text{Prob}(\xi_n^{(N)} \in d(x_n^1, \dots, x_n^N) \mid \xi_{n-1}^{(N)}) = \prod_{i=1}^{N} K_{n, m_N(\xi_{n-1}^{(N)})}(\xi_{n-1}^i, dx_n^i) \quad (10.3)$$

The asymptotic analysis of (10.3) is a little more tricky than the one of the models discussed in the former article. Although the deviations of (10.3) do not fit into our plot, we believe and conjecture that they can be derived using similar arguments. Finally, it is worth mentioning that the rate function which governs the large deviations of (10.3) is often larger than the one associated to (10.2), see for instance Del Moral and Zajic (2003).

1.2 Statement of some results

Before to describe the main results developed in this article, we first present a brief discussion on exponential deviation estimates. We also take this opportunity to fix some classical notation we shall currently use in the further development of this article. We recall that a Markov transition M_n, from a measurable space $(E_{n-1}, \mathcal{E}_{n-1})$ into another $(E_n, \mathcal{E}_n)$, generates two integral operations

$$M_n : \mathcal{B}_b(E_n) \to \mathcal{B}_b(E_{n-1}) \quad \text{and} \quad M_n : \mathcal{P}(E_{n-1}) \to \mathcal{P}(E_n)$$

These two operations are defined, for any $(x_{n-1}, f_n) \in (E_{n-1} \times \mathcal{B}_b(E_n))$, and $(\mu_{n-1}, A_n) \in (\mathcal{P}(E_{n-1}) \times \mathcal{E}_n)$ by the formulae

$$M_n(f_n)(x_{n-1}) = \int_{E_n} M_n(x_{n-1}, dx_n) \, f(x_n)$$

$$\mu_{n-1} M_n(A_n) = \int_{E_{n-1}} \mu_{n-1}(dx_{n-1}) \, M_n(x_{n-1}, A_n)$$

with $M_n(x_{n-1}, A_n) = M_n(1_{A_n})(x_{n-1})$ For any function $f_n \in \mathcal{B}_b(E_n)$, and any distribution $\mu_n \in \mathcal{P}(E_n)$, we often use the notation

$$\mu_n(f_n) = \int \mu_n(dx_n) \, f_n(x_n)$$

Under appropriate regularity conditions, and for both models (10 2) and (10 3), it is known that, in some sense, the particle occupation measures

$$\eta_n^N = m_N(\xi_n^{(N)})$$

converge as N tends to infinity to the desired distribution η_n. For instance, under appropriate Lipschitz-type conditions on Φ_n, we have the sub-Gaussian exponential estimate

$$\mathbb{P}(|\eta_n^N(f_n) - \eta_n(f_n)| > \epsilon) \le c_n \; e^{-N\varepsilon^2/c_n}$$

for any $\varepsilon > 0$, and $f_n \in \mathcal{B}_n(E_n)$ with $\|f_n\| \le 1$, and for some finite constant $c_n < \infty$ (see for instance Del Moral (1998)). As an aside, by the Borel-Cantelli Lemma we have the almost sure convergence

$$\lim_{N \to \infty} \eta_n^N(f_n) = \eta_n(f_n)$$

In addition, if we let $A_{n,\varepsilon}(f_n)$ be the τ-closed subset given by

$$A_{n,\varepsilon}(f_n) = \{\mu_n \in \mathcal{P}(E_n) \; : \; |\mu_n(f_n) - \eta_n(f_n)| > \epsilon\}$$

then we have the asymptotic deviation estimate

$$\limsup_{N \to \infty} \frac{1}{N} \log \mathbb{P}(\eta_n^N \in A_{n,\varepsilon}(f_n)) \le -J_n(A_{n,\varepsilon}(f_n)) \; (\le -\varepsilon^2/c_n)$$

for some constant $J_n(A_{n,\varepsilon}(f_n))$.

The large deviations analysis is concerned with estimating more precisely these exponential deviations rates More generally, they provide sharp exponential estimates of the deviations of the approximating flow $(\eta_p^N)_{p \le n}$ around the solution $(\eta_p)_{p \le n}$ of the limiting measure valued equation (10 1). The study of the deviations of η_n^N around η_n have been started in Del Moral and Guionnet (1998) when the distribution space $\mathcal{P}(E_n)$ is equipped with the weak topology Under appropriate regularity conditions on the mappings Φ_n, these large deviations principles were further extended in Del Moral and Zajic (2003) to path space models. We also mention that in Dawson and Feng (2001) a projective limit approach was also used to obtain the large deviations principles with good rate function on $\mathcal{P}([0,1])$, for the genetic Fleming-Viot process with state-independent mutation in the limit, as the effective population goes to infinity. However, in contrast to the Sanov case, in the Fleming-Viot case there is not a good rate function in the τ_1-topology but only in the weak topology

The objective of the former article is to simplify and further extend these large deviations principles to the particle density profiles $(\eta_p^N)_{0 \le p \le n}$ on the product space $\mathbf{P}^n(E) =_{\text{def}} \prod_{p=0}^n \mathbf{P}(E_p)$ equipped with the τ_1-topology. We also assume that the mappings Φ_n satisfy the following regularity condition(H). For any $n \ge 1$, there exists a

reference measure $\lambda_n \in \mathcal{P}(E_n)$ and some $\rho_n > 0$, such that for any $\mu_{n-1} \in \mathcal{P}(E_{n-1})$ we have

$$\rho_n \, \lambda_n \leq \Phi_n(\mu_{n-1}) \ll \lambda_n$$

For sake of completeness, we recall that a sequence of measures Q^N on an Hausdorff topological space E, equipped with a σ-field $\sigma(E)$ which contains the Borel σ-field $B(E)$, satisfies the large deviations principles with rate function J, if the following conditions are met The function $J \ E \to [0, \infty]$ is lower semi-continuous, and for any pair of closed/open subsets (A, B) we have

$$\limsup_{N \to \infty} \frac{1}{N} \log Q^N(A) \leq -J(A) \quad \text{and} \quad \liminf_{N \to \infty} \frac{1}{N} \log Q^N(B) \geq -J(B)$$

In the above displayed formulae, we have used the notation $J(A) = \inf_A J$ A lower semincontinuous function J with compact level sets $J^{-1}([0, a])$, $a \in [0, \infty)$, is said to be a good rate function

Our main result basically reads

THEOREM 10 1 *For any time horizon $n \geq 0$ the law Q_n^N of the N-particle density profiles $(\eta_p^N)_{0 \leq p \leq n}$ satisfies the large deviations principles on the Cartesian product $\mathbf{P}^n(E)$ equipped with the τ_1-topology with good rate function*

$$J_n((\mu_p)_{0 \leq p \leq n}) \quad = \quad \text{Ent}(\mu_0 | \eta_0) + \sum_{p=1}^{n} \text{Ent}(\mu_p | \Phi_p(\mu_{p-1}))$$

where $\text{Ent}(.|.)$ stands for the traditional Boltzmann or the Shannon-Kullback entropy criterium, with the convention $J_n(\mu) = \infty$ when the flow $\mu = (\mu_p)_{0 \leq p \leq n} \notin \mathcal{P}^n(E) =_{\text{def}} \prod_{p=0}^{n} \mathcal{P}(E_p)$

As we shall see, the above result implies the large deviations principles for the τ-topology (and hence the weak topology) on $\mathcal{P}^n(E)$ with good rate function J_n. Also notice that $J_n(\mu) = 0$ if and only if the flow $\mu = (\mu_p)_{0 \leq p \leq n}$ satisfies the non linear limiting equation (10 1) (with $\mu_0 = \eta_0$)

At first guess, the additive structure of the rate function J_n seems to indicate that the local sampling errors induced at each elementary steps of the particle approximation model propagate with respect to the time parameter. On the other hand we also know from Del Moral and Miclo (2000) that it is possible to control uniformly the propagation of the $\mathbb{L}_p$-errors with respect to the time parameter as soon as the limiting equation (10.1) is sufficiently stable.

To get one step further in our discussion, we need to introduce some additional notation. We let $\|. - .\|_{tv}$ be the total variation distance between probabilities defined by

$$
\begin{aligned}
\|\mu - \nu\|_{tv} &= \sup_{A \in \mathcal{E}} |\mu(A) - \nu(A)| \\
&= 2^{-1} \sup \{|\mu(f) - \nu(f)| \; : \; f \in \mathcal{B}_b(E), \quad \text{with} \quad \|f\| \leq 1\}
\end{aligned}
$$

We also associate to a finite partition $U = (U^i)_{1 \leq i \leq d}$ of the state space E, the Kolmogorov-Smirnov seminorm on $\mathcal{P}(E)$ defined by

$$
d_U(\mu, \nu) = \frac{1}{2} \sum_{i=1} |\mu(U^i) - \nu(U^i)|
$$

Finally, we introduce the following regularity and Lipschitz type condition on the semi-group $\Phi_{p,n}(\eta_p) = \eta_n$ of the limiting model (10.1)

(L) For any $p \leq n$ there exists some positive constants $\beta(\Phi_{p,n})$ such that $\beta(\Phi) =_{def.} \sup_{n \geq 0} \sum_{p \leq n} \beta(\Phi_{p,n}) < \infty$ and for any pair of measures $(\mu_p, \nu_p) \in \mathcal{P}(E_p)$

$$
\|\Phi_{p,n}(\mu_p) - \Phi_{p,n}(\nu_p)\|_{tv} \leq \beta(\Phi_{p,n}) \|\mu_p - \nu_p\|_{tv} \tag{10.4}
$$

COROLLARY 10.1 *Assume that the regularity condition (L) is met for some finite constant $\beta(\Phi) < \infty$. Then, for any $\varepsilon > 0$, and for any finite Borel partitions $U_n = (U_n^i)_{1 \leq i \leq d_n}$ of E_n, we have the uniform asymptotic estimate*

$$
\limsup_{N \to \infty} \frac{1}{N} \log \mathbb{P} \left(\sup_{p \leq n} d_{U_p}(\eta_p^N, \eta_p) \geq \varepsilon \right) \leq -\varepsilon^2 / \beta(\Phi)
$$

The article is organized as follows:

In Section 2, we illustrate the large deviations analysis developed in this article on three different classes of interacting and measure valued processes. The first two models are more related to particle physics and fluid mechanics. They can be interpreted as simplified and discretized versions of traditional McKean-Vlasov diffusions, and Boltzmann collision models. The third and last application is concerned with an abstract class of Feynman-Kac-Schrödinger semigroups and their genealogical and interacting particle interpretation. The initiated reader can skip this section.

In Section 3, we revisit the projective limit approach to large deviations introduced in a joint work of the first author with J. Gärtner, c.f. Dawson and Gärtner (1987), and further developed in a series of three articles de Acosta (1994a,b, 1997).

We provide an original min-max type theorem, and an explicit formula expressing good rate functions in terms of their image measures, with respect to the projection coordinate mappings.

In Section 4, we show that $\mathbf{P}(E)$, furnished with the τ_1-topology, is homeomorphic to a compact projective limit of finite dimensional distribution spaces. We combine this interpretation with the projective contraction results derived in Section 3, to show that the finite space or the strong version of Sanov's Theorem on an Hausdorff topological space are in fact equivalent.

Section 5 is mainly concerned with the proof of Theorem 10.1, and Corollary 10.1. We first extend the projective limit interpretation of the τ_1-topology derived in Section 4 to path-distribution spaces, and by a simple induction we prove that J_n are good rate functions on $\mathbf{P}^n(E)$.

Our approach to Theorem 10.1 is roughly as follows. The proof of the large deviations upper bound is essentially based on the min-max Theorem derived in Section 3, while the proof of the large deviations lower bound is conducted by induction on the time parameter, in the same spirit as in the proof of the strong version of Sanov's Theorem.

2. Motivating examples

2.1 McKean-Vlasov and Boltzmann type models

The McKean-Vlasov and the Boltzmann equations are nonlinear partial and integro-differential equations. Both equations arise in fluid mechanics, and more precisely in the microscopic and macroscopic modeling of gases. For a review on these equations, we refer the reader to the review article of Méléard (1995), and references therein. The central idea behind the particle interpretation of these models is to construct a nonhomogenous Markov process whose distribution laws are (weak) solution of the desired equation in distribution space. The existence and uniqueness of this stochastic model often requires fixed point arguments on path-space distributions, see for instance Theorem 1.1, page 172, in Sznitman (1991). In contrast to the continuous time situation, the discrete time analysis is based on elementary Markov chain techniques.

To give a brief presentation of these models, we recall that the McKean-Vlasov equations correspond to mean-field drift diffusions describing the repulsive or attractive interaction between close gas molecules. The simplified discrete time, and one dimensional version, of this model is given by the following stochastic recursion

$$X_n = a_n(X_{n-1}, \eta_{n-1}) + b_n(X_{n-1}, \eta_{n-1})\, W_n$$

where (a_n, b_n) are bounded functions from $(\mathbb{R} \times \mathcal{P}(\mathbb{R}))$ into $\mathbb{R}$, with $b_n(x, \mu) > 0$ for any $(x, \mu) \in (\mathbb{R} \times \mathcal{P}(\mathbb{R}))$, and $(W_n)_{n \geq 0}$ are independent and identically distributed Gaussian random variables with $\mathbb{E}(W_n) = 0$ and $\mathbb{E}(W_n^2) = 1$. The initial condition is defined by some random variable X_0, with a given distribution $\eta_0 \in \mathcal{P}(\mathbb{R})$.

If we let η_n be the distribution of the random state X_n at time n, then we find that the flow η_n satisfies the following nonlinear measure valued equation

$$\eta_n = \Phi_n(\eta_{n-1}) = \eta_{n-1} K_{n,\eta_{n-1}}$$

with the Markov transition $K_{n,\eta_{n-1}}$ defined by

$$K_{n,\eta_{n-1}}(x_{n-1}, dx_n) = \frac{1}{\sqrt{2\pi}} \exp\left\{ -\frac{1}{2} \left(\frac{x_n - a_n(x_{n-1}, \eta_{n-1})}{b_n(x_{n-1}, \eta_{n-1})} \right)^2 \right\} dx_n$$

Suppose the functions $\mu \to a_n(x, \mu)$ and $\mu \to b_n(x, \mu)$ are uniformly τ-continuous with respect to the parameter x. Also assume that we have $\inf b_n^2 \geq \delta$, for some $\delta > 0$. Under these regularity conditions, we easily prove that the mappings Φ_n are τ-continuous, and they satisfy condition (H) with the constants

$$\rho_n = e^{-\frac{\|a_n\|^2}{\delta}} \, p_n(\mathbb{R})$$

and the reference measures

$$\lambda_n(dx) = p_n(dx)/p_n(\mathbb{R}) \quad \text{with} \quad p_n(dx) = \exp\left(-\delta^{-1} \left[y^2/2 + \|a_n\| \, |y| \right] \right)$$

The N-particle model (10.3) associated to the McKean transitions $K_{n,\eta_{n-1}}$ consists in N-interacting particles $\xi_n^{(N)} = (\xi_n^{(N,i)})_{1 \leq i \leq N}$ evolving according to the simple stochastic recursive equations, defined for any $1 \leq i \leq N$ by

$$\xi_n^{(N,i)} = a_n\left(\xi_{n-1}^{(N,i)}, \frac{1}{N} \sum_{j=1}^{N} \delta_{\xi_{n-1}^{(N,j)}} \right) + b_n\left(\xi_{n-1}^{(N,i)}, \frac{1}{N} \sum_{j=1}^{N} \delta_{\xi_{n-1}^{(N,j)}} \right) W_n^i$$

where $(W_n^i)_{1 \leq i \leq N}$ are N independent copies of the sequence of Gaussian random variables W_n, and $(\xi_0^{(N,i)})_{1 \leq i \leq N}$ are N independent copies of the initial random state X_0. The N-particle model (10.2) is defined in the same way, by introducing at each step an extra level of randomness.

Boltzmann equations represent the macroscopic evolution of rarefied gas models. In contrast to the McKean-Vlasov case, the interaction between gas molecules is now interpreted as a jump/collision mechanism.

The simplified discrete time Boltzmann models described hereafter are rather close to the class of Feynman-Kac-Schrödinger semigroups developed in the next section.

To describe with some generality these equations, it is convenient to introduce some precise topological structure. We let $(E_n, B(E_n))_{n \geq 0}$ be a sequence of Polish spaces. We recall that a Polish space is a complete separable metric space. We denote by $\mathcal{C}_b(E)$, the set of all continuous and bounded functions on some Polish space E.

We let $g_n \in \mathcal{C}_b(E_n^2)$, be a sequence of pair-collision energy positive functions. By $Q_n((x_{n-1}, x'_{n-1}), dx_n)$ we denote a sequence of Markov transitions from E_{n-1}^2 into E_n. The quantity $g_n(x_n, x'_n)$ can be interpreted as the likelihood of interaction between a pair of particles at sites (x_n, x'_n). Given a pair of colliding sites (x_n, x'_n), the distribution $Q_n((x_{n-1}, x'_{n-1}), dx_n)$ represents both, the statistics of the resulting collision, as well as the free evolution of a particle between collisions.

We associate to the pair (g_n, Q_n) the one step mappings Φ_n defined for any $\eta_n \in \mathcal{P}(E_n)$ by

$$
\Phi_{n+1}(\eta_n)(dx_{n+1}) = \int_{E_n^2} \Psi_n(\eta_n \otimes \eta_n)(d(x_n, x'_n)) \; Q_{n+1}((x_n, x'_n), dx_{n+1})
$$

with the Boltzmann-Gibbs measures $\Psi_n(\eta_n \otimes \eta_n) \in \mathcal{P}(E_n^2)$ associated to the collision-energy function g_n, and defined by

$$
\Psi_n(\eta_n \otimes \eta_n)(d(x_n, x'_n)) = \frac{g_n(x_n, x'_n)}{(\eta_n \otimes \eta_n)(g_n)} \; (\eta_n \otimes \eta_n)(d(x_n, x'_n))
$$

As usual, the corresponding N-particle model consists in N-interacting particles. The elementary transition (10.2) is decomposed into two separate mechanisms

$$
\xi_n^{(N)} \in E_n^N \xrightarrow{\text{pair--collisions}} \widehat{\xi}_n^{(N)} \in (E_n^2)^N \xrightarrow{\text{free evolution}} \xi_{n+1}^{(N)} \in E_{n+1}^N
$$

During the pair-collisions transition, we select randomly N pairs of colliding particles $\widehat{\xi}_n^{(N,i)} = (\widehat{\xi}_n^{(N,i,1)}, \widehat{\xi}_n^{(N,i,2)})$ with the discrete distribution

$$
\Psi_n(m_N(\xi_n^{(N)}) \otimes m_N(\xi_n^{(N)}))
$$

$$
= \sum_{1 \leq i,j \leq N} \frac{g_n(\xi_n^{(N,i)}, \xi_n^{(N,j)})}{\sum_{1 \leq k,l \leq N} g_n(\xi_n^{(N,k)}, \xi_n^{(N,l)})} \; \delta_{(\xi_n^{(N,i)}, \xi_n^{(N,j)})}
$$

Notice that a pair of particles $(\xi_n^{(N,i)}, \xi_n^{(N,j)})$ is more likely to collide when its interaction-energy $g_n(\xi_n^{(N,i)}, \xi_n^{(N,j)})$ is high. In practice, close particles

in some local neighborhood are more likely to collide. Given a selected pair, say

$$\widehat{\xi}_n^{(N,k)} = (\xi_n^{(N,i)}, \xi_n^{(N,j)})$$

the particle $\xi_n^{(N,i)}$ collides with $\xi_n^{(N,j)}$, and then evolves according to some free motion. These two mechanisms are performed by sampling a random variable $\xi_{n+1}^{(N,k)}$ with a distribution $Q_{n+1}((\xi_n^{(N,i)}, \xi_n^{(N,j)}), dx_{n+1})$ that depends on the selected colliding pair.

We further assume that $Q_{n+1}(\mathcal{B}_b(E_{n+1})) \subset \mathcal{C}_b(E_n^2)$. In this situation, we can check that the mappings Φ_{n+1} are continuous with respect to the τ-topologies from $\mathcal{P}(E_n)$ into $\mathcal{P}(E_{n+1})$. We finally observe that condition (H) is in fact equivalent to the following one. There exist some positive constants $\rho_n > 0$, and some reference measures $\lambda_n \in \mathcal{P}(E_n)$, such that for any pairs $(x_{n-1}, x'_{n-1}) \in E_{n-1}$, we have

$$\rho_n \, \lambda_n \leq Q_n((x_{n-1}, x'_{n-1}), .) \ll \lambda_n$$

To give a physical sound to these abstract models, we examine the situation where $\eta_n(dx_n)$ represents the distribution of particle

$$x_n = (p_n, v_n) \in E_n = (\mathbb{R}^3 \times \mathbb{R}^3)$$

in position $p_n \in \mathbb{R}^3$, with speed $v_n \in \mathbb{R}^3$. The collision energy function $g_n(x_n, x'_n)$ between two particles $x_n = (p_n, v_n)$ and $x'_n = (p'_n, v'_n)$ is often expressed by a cross-section function that depends on the pair positions (p_n, p'_n), and only on the quantities $|v_n, v'_n|$, and $(v_n - v'_n).u$, where u is a given unit vector. For a more precise description of these cross-sections, we refer the reader to the review article of Méléard (1995), and references therein. The prototype of kernel Q_{n+1} is defined as the composition of a binary collision-speed exchange transition S_n, with a free evolution kernel M_{n+1}

$$Q_{n+1}((x_n, x'_n), dx_{n+1}) = \int \, S_n((x_n, x'_n), d(y_n, y'_n)) \, M_{n+1}(y'_n, dx_{n+1})$$

The form of S_n is dictated by the conservation of kinetic energy, and momentum for binary collisions. It is defined for any $x_n = (p_n, v_n)$ and $x'_n = (p'_n, v'_n)$ by the formula

$$S_n((x_n, x'_n), .) = \delta_{([p_n, v_n + ((v'_n - v_n).u) \, u], [p'_n, v'_n + ((v_n - v'_n).u) \, u])}$$

Notice that this simplified Boltzmann transition Q_{n+1} describes precisely the collision, and the free motion of the first component particle, but it doesn't says anything on the colliding partner. This question can be answered by a traditional state space enlargement. Finally and in this

situation, we observe that the regularity condition (H) is met, as soon as the free motion Markov transitions M_n satisfy this condition. That is, when we have

$$\rho_n\, \lambda_n \leq M_n(x_{n-1}, .) \ll \lambda_n$$

For instance, arguing as in the McKean-Vlasov case, this condition is met for regular Gaussian transitions.

2.2 Feynman-Kac-Schrödinger semigroups

As we mentioned in the introduction, these nonlinear semigroups are at the corner of a variety of application areas. Their probabilistic interpretations depends on the physical, biological, or engineering problem at hand. To capture, both their generality, and their full impact in applications, it is convenient to introduce these models using a rather abstract definition.

We let $(E_n, \mathcal{E}_n)_{n \geq 0}$ be a sequence of Hausdorff topological spaces. We consider a sequence of positive potential functions $G_n \in \mathcal{B}_b(E_n)$, and a collection of Markov transitions $M_n(x_{n-1}, dx_n)$ from E_{n-1} into E_n. We associate to the pair potential/transition (G_n, M_n), the distribution flow η_n defined by the Feynman-Kac measures

$$\eta_n(f_n) = \gamma_n(f_n)/\gamma_n(1) \quad \text{with} \quad \gamma_n(f_n) = \mathbb{E}\left(f_n(X_n) \prod_{0 \leq p < n} G_p(X_p) \right)$$

where X_n is an E_n-valued Markov chain with some initial distribution $\eta_0 \in \mathcal{P}(E_0)$, and elementary transitions M_n. Using the multiplicative structure, and the Markov property, we readily check that the flow η_n satisfies the following equation

$$\eta_n = \Phi_n(\eta_{n-1}) =_{\text{def.}} \Psi_{n-1}(\eta_{n-1}) M_n$$

with the Boltzmann-Gibbs transformation Ψ_n on $\mathcal{P}(E_n)$ defined by

$$\Psi_n(\eta_n) = \frac{1}{\eta_n(G_n)}\, G_n(x_n)\, \eta_n(dx_n)$$

Since for any $f \in \mathcal{B}_b(E_{n+1})$ we have

$$\Phi_{n+1}(\eta_n)(f) = \eta_n(G_n M_{n+1}(f))/\eta_n(G_n)$$

we readily check that Φ_{n+1} is a τ_1-continuous mapping from $\mathbf{P}(E_{n-1})$ into $\mathbf{P}(E_n)$ and $\Phi_n(\mathcal{P}(E_{n-1})) \subset \mathcal{P}(E_n)$. Also notice that condition (H) is equivalent as to have, for any $x_{n-1} \in E_{n-1}$, some positive constants $\rho_n > 0$, and some reference measures $\lambda_n \in \mathcal{P}(E_n)$

$$\rho_n\lambda_n \leq M_n(x_{n-1}, .) \ll \lambda_n$$

For instance, let us suppose that $E_n = \mathbb{R}$ and

$$M_n(x, dy) = \frac{1}{\sqrt{2\pi}}\, e^{-\frac{1}{2}(y - a_n(x))^2}\, dy$$

where a_n is a bounded measurable drift function on $\mathbb{R}$. In this case, condition (H) is clearly met, with the parameters $\rho_n = e^{-\|a_n\|^2/2}\, p_n(\mathbb{R})$, and the reference measures defined by

$$\lambda_n(dx) = p_n(dx)/p_n(\mathbb{R}) \quad \text{with} \quad p_n(dx) = \exp\left(-[y^2/2 + \|a_n\|\, |y|]\right)$$

In connection with Corollary 10.1, we mention the Feynman-Kac semigroup $\Phi_{p,n}$ satisfies condition (L) as soon as the pair potential/kernel (G_n, M_n) are such that for any $(x_n, y_n) \in E_n^2$ and $n \geq 0$

$$G_n(x_n) \geq \varepsilon(G)\, G_n(y_n)$$

and

$$M_{n,n+m}(x_n, .) \geq \varepsilon(M)\, M_{n,n+m}(y_n, .)$$

for some $m \geq 1$ and some pair of constants $(\varepsilon(G), \varepsilon(M)) \in (0, 1]^2$. In the above display, $M_{n,n+m} = (M_{n+1} \dots M_{n+m})$ stands for the composition of the Markov kernels M_p from $p = (n+1)$ to $p = (n+m)$. In this situation, it is known that (10.4) is met with

$$\beta(\Phi_{p,n}) = \frac{2}{\varepsilon(M)\varepsilon(G)^m}\, (1 - \varepsilon(M)^2 \varepsilon(G)^{m-1})^{[(n-p)/m]}$$

We conclude that the estimate stated in Corollary 10.1 holds true with

$$\beta(\Phi) \leq 2m/(\varepsilon(M)^3 \varepsilon(G)^{(2m-1)})$$

For more details we refer the reader to Del Moral and Miclo (2000) and references therein.

Notice that the particle interpretation (10.2) of the Feynman-Kac-Schrödinger flow is a simple selection/mutation genetic algorithm. To be more precise, as in the simplified Boltzmann type model described in the previous section, its elementary transitions (10.2) are decomposed into two separate mechanisms

$$\xi_n^{(N)} \in E_n^N \xrightarrow{\text{selection}} \widehat{\xi}_n^{(N)} \in E_n^N \xrightarrow{\text{mutation}} \xi_{n+1}^{(N)} \in E_{n+1}^N$$

During the first transition, we select randomly N particles $\widehat{\xi}_n^{(N,i)}$ with the discrete distribution

$$\Psi_n(m_N(\xi_n^{(N)})) = \sum_{1 \leq j \leq N} \frac{G_n(\xi_n^{(N,j)})}{\sum_{1 \leq k \leq N} G_n(\xi_n^{(N,k)})}\, \delta_{\xi_n^{(N,j)}}$$

Then, we evolve each selected particle $\widehat{\xi}_n^{(N,i)}$, with an elementary move $\widehat{\xi}_n^{(N,i)} \rightsquigarrow \xi_{n+1}^{(N,i)}$, according to the transition distribution $M_{n+1}(\widehat{\xi}_n^{(N,i)}, .)$.

A final remark is that the random variables X_n may represent the path of an auxiliary Markov chain X'_p, from the origin up to time n, and taking values in some Hausdorff topological spaces E'_p. That is, we have that

$$X_n = (X'_0, \ldots, X'_n) \in E_n = (E'_0 \times \ldots \times E'_n) \qquad (10.5)$$

In this case, the corresponding particle interpretation model forms a genetic algorithm taking values in path space. The mutation mechanism consists in extending each path particle with an elementary transitions. Notice that the selection pressure now depends on the path-potential. Whenever the potential functions only depend on terminal values, this path-particle model can be interpreted as a genealogical tree evolution model (see Del Moral and Miclo (2001) and references therein). In this situation, the Feynman-Kac-Schrödinger model doesn't satisfy anymore the regularity condition (H), and the large deviations analysis developed in this article only provides a large deviation upper bound.

We illustrate this abstract class of semigroups with an elementary filtering problem. We let X_n be an $\mathbb{R}$-valued Markov chain, with initial distribution $\eta_0 = \mathrm{Law}(X_0)$, and elementary Markov transitions M_n. We also let $(Y_n)_{n \geq 0}$, be the random observation sequence defined by

$$Y_n = h_n(X_n) + V_n$$

The sensor function h_n is assumed to be measurable and bounded, and the noise disturbances V_n are independent, and identically distributed, Gaussian random variables with $\mathbb{E}(V_n) = 0$, and $\mathbb{E}(V_n^2) = 1$. To get one step further, we fix a sequence of observations $Y_n = y_n$, $n \geq 0$, and we consider the nonhomogeneous potential functions G_n defined by

$$G_n(x) = \exp\left\{ -\frac{1}{2}\left(y_n - h_n(x)\right)^2 \right\}$$

In this situation, the Feynman-Kac flow η_n associated to the pair potential/transition (G_n, M_n) is a version of the conditional distribution of X_n given $Y_p = y_p$, $p < n$. That is, we have that

$$\eta_n = \mathrm{Law}(X_n |\ Y_0 = y_0, \ldots, Y_{n-1} = y_{n-1})$$

If we consider the path-space model $X_n = (X'_0, \ldots, X'_n)$, then we clearly have that

$$\eta_n = \mathrm{Law}((X'_0, \ldots, X'_n) \mid Y_0 = y_0, \ldots, Y_{n-1} = y_{n-1})$$

In this filtering context, the genetic particle model and its genealogical tree, can be interpreted both, as a natural learning prediction/updating process, but also as a stochastic and adaptive refining grip approximation model. During the mutation/prediction, each individual particle explores the space of possible values of the unobserved transitions of the signal. When the current observation is available, the selection process updates these predictions, and gives more reproductive opportunities to more likely predictions.

This class of Feynman-Kac-Schrödinger models in path-spaces have been extensively studied in the literature (see Del Moral and Miclo (2000, 2001), and references therein). They arise in various scientific disciplines. In signal processing, and Bayesian statistic literature, they represent the conditional path-distribution of a Markov signal given a sequence of partial and noisy observations. In biology, they are used to model random polymerizations of macro-molecules, in chemical solvents. In physics, they also describe the evolution of a Markov particle in an medium, with absorbing obstacles related to potential functions. More recently, they have been proved to be useful in the modeling of the biological and human learning process, see the recent article of Körding and Wolpert (2004).

These evolutionary particle algorithms have taken various botanical names in the applied literature, such as the "go with the winner", the multi-splitting or the prune enrichment evolution model in biology, as well as the bootstrap or condensation filter, the sampling-importance-resampling, the spawning filter, and the population Monte-Carlo algorithm in signal processing. For more details on the theoretical and the applied side of this subject we refer the reader to Del Moral and Miclo (2000), and Doucet and De Freitas and Gordon (2001), and references therein.

3.   Large deviations for projective limits

A projective (or inverse) spectrum $(M_U, p_{U,V})_{U \geq V}$ of a directed set $(\mathcal{U}, \leq)$ is a family $\mathcal{M} = (M_U, p_{U,V})_{U \geq V}$ of Hausdorff topological spaces M_U and continuous mappings

$$p_{U,V} : M_U \to M_V, \qquad U \geq V$$

with $p_{U,U} = Id$, and satisfying the compatibility conditions

$$U \geq V \geq W \implies p_{U,W} = p_{U,V} \circ p_{V,W}$$

Let p_U be the canonical projection from $\prod_{U \in \mathcal{U}} M_U$ into M_U. The set

$$\lim_{\mathcal{U}} \mathcal{M} = \{m \in \prod_{U \in \mathcal{U}} M_U \; : \; \forall U \geq V \;\; p_V(m) = p_{U,V}(p_U(m))\}$$

equipped with the product topology, is called the projective (or inverse) limit space of the spectrum. We shall always assume that the sets M_U are equipped with the Borel σ-field $B(M_U)$ and the σ-field $\sigma(\lim_{\mathcal{U}} \mathcal{M})$ on the projective limit space contains all the sets $p_U^{-1}(B(M_U))$.

LEMMA 10.1 *A function I is a good rate function on $\lim_{\mathcal{U}} \mathcal{M}$, if and only if, there exists a sequence of good rate functions I_U on M_U, with $U \in \mathcal{U}$, and such that*

$$I(m) = \sup_{U \in \mathcal{U}} I_U(p_U(m)) \tag{10.6}$$

Proof. Suppose I is a good rate function on $\lim_{\mathcal{U}} \mathcal{M}$, in the sense that I is a lower semi-continuous function with compact level sets $I^{-1}([0, a])$, $a > 0$. By the contraction principle (see for instance Theorem 4.2.1 in Dembo and Zeitouni (1993)), the image set-functions $I_U = I \circ p_U^{-1}$ defined by

$$I_U(A) = \inf \{I(m) \; : \; m \in p_U^{-1}(A)\}$$

are good rate functions on M_U. In addition, by the lower semi-continuity property of I we have

$$I(m) = \sup \{I(m) \; : \; m \in p_U^{-1}(A_U), \;\; A_U \text{ open} \subset M_U, \;\; U \in \mathcal{U}\}$$

from which we prove that (10.6) holds true. Inversely, if I_U is a sequence of good rate function on the sets M_U with $U \in \mathcal{U}$, then the function I defined in (10.6) is a good rate function on I. The lower semi-continuity property comes from the fact that the pointwise supremum of a of lower semi-continuous functions is again lower semi-continuous. To prove that I has compact level sets, we first observe that the compact levels sets $I_U^{-1}([0, a])$ of the functions I_U satisfy the compatibility condition $I_V^{-1}([0, a]) = p_{U,V}(I_U^{-1}([0, a]))$, for all $U \geq V$. Since projective limits are inherited by closed sets, the levels sets $I^{-1}([0, a]) = \lim_{\mathcal{U}} \mathcal{M} \cap \prod_{U \in \mathcal{U}} I_U^{-1}([0, a])$ are the projective limits of compact sets; thus, they are compact by Tychonov's Theorem.   □

Let us quote a min-max type theorem for good rate functions on projective limit spaces.

THEOREM 10.2 *Let I be a good rate function on the projective limit space $\lim_{\mathcal{U}} \mathcal{M}$, and let $I_U = I \circ p_U^{-1}$ be the p_U-image function of I on M_U. For any closed set $F \subset \lim_{\mathcal{U}} \mathcal{M}$, we have*

$$I(F) = \sup_{u \in \mathcal{U}} I_U(\overline{p_U(F)}) \tag{10.7}$$

where $\overline{A}$ stands for the closure of a measurable set A.

Proof.   By (10.6), we first notice that (10.7) can be rewritten as

$$I(F) = \inf_{m \in F} \sup_{U \in \mathcal{U}} I_U(p_U(m)) = \sup_{U \in \mathcal{U}} \inf_{m \in \overline{p_U(F)}} I_U(m) =_{def} \tilde{I}(F)$$

Since we have $I_U(p_U(m)) \geq I_U(\overline{p_U(F)})$, for any $m \in F$, we deduce that $I(F) \geq \tilde{I}(F)$. To prove the reverse inequality, we assume that $\tilde{I}(F) < \infty$; otherwise, the desired bound trivially holds true. In this case, for each $\varepsilon > 0$ the sets

$$p_U^{-1}(\overline{p_U(F)}) \cap I^{-1}([0, \tilde{I}(F) + \varepsilon])$$

are non empty compact sets. The compactness property results from the fact that $p_U^{-1}(\overline{p_U(F)})$ is a closed set into the compact level sets $I^{-1}([0, \tilde{I}(F) + \varepsilon])$. On the other hand, if these sets were empty, we would be able to find some $m \in p_U^{-1}(\overline{p_U(F)})$ such that

$$I(m) \geq I(p_U^{-1}(\overline{p_U(F)})) = I_U(\overline{p_U(F)}) \geq \tilde{I}(F) + \varepsilon = \sup_{V \in \mathcal{U}} I_V(\overline{p_V(F)}) + \varepsilon$$

This clearly yields a contradiction. Finally, we observe that

$$U \geq V \Rightarrow p_U^{-1}(\overline{p_U(F)}) \subset p_V^{-1}(\overline{p_V(F)})$$

This readily yields that, for each $\varepsilon > 0$ we have

$$[\cap_{U \in \mathcal{U}} p_U^{-1}(\overline{p_U(F)})] \cap I^{-1}([0, \tilde{I}(F) + \varepsilon]) \neq \emptyset$$

Since F coincide with the projective limit of the sets $(\overline{p_U(F)})_{U \in \mathcal{U}}$, we have $F = \cap_{U \in \mathcal{U}} p_U^{-1}(\overline{p_U(F)})$. From previous considerations, for any $\varepsilon > 0$, there exists some point $m_\varepsilon \in F$, such that

$$I(F) \leq I(m_\varepsilon) \leq \tilde{I}(F) + \varepsilon$$

We end the proof of the theorem, by letting $\varepsilon \to 0$. $\square$

One easily derived consequence of Lemma 10.1 and Theorem 10.2, is the following corollary.

COROLLARY 10.2 *A sequence of probability measures P^N on $\lim_{\mathcal{U}} \mathcal{M}$ satisfy the large deviations principles with some good rate function I, if and only if, the sequence of all image measures $P^N \circ p_U^{-1}$ satisfy the large deviations principles on M_U, for some good rate functions I_U with $U \in \mathcal{U}$. In addition, the rate functions are given by $I_U = I \circ p_U^{-1}$, and they satisfy (10.6).*

Proof. Assume that Q^N satisfy the large deviations principles on $\lim_{\mathcal{U}} \mathcal{M}$ for some good rate function I. By a traditional contraction argument, the image measures $Q^N \circ p_U^{-1}$ also satisfy the large deviations principles on M_U, with good rate function $I_U = I \circ p_U^{-1}$.

In the reverse situation, suppose that the sequence of measures $Q^N \circ p_U^{-1}$ satisfy the large deviations principles upper bound, with the good rate functions I_U. Since a closed set $F \subset \lim_{\mathcal{U}} \mathcal{M}$ coincides with the projective limit of the sets $(\overline{p_U(F)})_{U \in \mathcal{U}}$, we have $F = \cap_{U \in \mathcal{U}} p_U^{-1}(\overline{p_U(F)})$.

Applying the deviation upper bound for $Q^N \circ p_U^{-1}$, we conclude that

$$\limsup_{N \to \infty} \frac{1}{N} \log Q^N(F) \leq \limsup_{N \to \infty} \frac{1}{N} \log Q^N \circ p_U^{-1}(\overline{p_U(F)})$$
$$\leq -I_U(\overline{p_U(F)})$$

We complete the proof, by taking the infimum over all $U \in \mathcal{U}$, and using (10.7).

Suppose that $Q^N \circ p_U^{-1}$ satisfy the deviation lower bound, with the good rate function I_U. For any open subset $A \subset \lim_{\mathcal{U}} \mathcal{M}$, and $m \in A$, there exists an open set $B_U \in M_U$, for some $U \in \mathcal{U}$, such that

$$m \in p_U^{-1}(B_U) \subset A$$

Applying the deviation lower bound for $Q^N \circ p_U^{-1}$, we find that

$$\liminf_{N \to \infty} \frac{1}{N} \log Q^N(A) \geq \liminf_{N \to \infty} \frac{1}{N} \log Q^N \circ p_U^{-1}(B_U)$$
$$\geq -I_U(B_U) \geq -I_U(m)$$

The end of the proof of the corollary is now clear. $\square$

4. A projective approach to Sanov's Theorem

Let $\mathcal{U}$ be the set of all finite and Borel partitions of E. By $\sigma(U)$, we denote the σ-algebra generated by $U \in \mathcal{U}$. We let H be the relative entropy criteria on $\mathbf{P}(E)$, defined by

$$H(\mu|\nu) =_{def.} \sup_{U \in \mathcal{U}} \mathrm{Ent}_U(\mu|\nu)$$

where for each $U = (U^k)_{1 \leq k \leq d} \in \mathcal{U}$, $\text{Ent}_U(.|.)$ denotes the the U-relative entropy defined (with standard conventions) by the formulae

$$\text{Ent}_U(\mu|\nu) = \sum_{k=1}^{d} \mu(U^k) \, \log\left(\mu(U^k)/\nu(U^k)\right)$$

with the convention $0 \log 0 = 0 = 0 \log(0/0)$. We let $V \leq U$ be the partial order on $\mathcal{U}$ induced by the inclusions relation $\sigma(V) \subset \sigma(U)$ between the corresponding σ-algebras. We slight abuse the notation, and we let $\mathcal{P}(U)$ and $\mathcal{B}_b(U)$ be respectively, the set of probability measures on $(E, \sigma(U))$, and the set of bounded and $\sigma(U)$-measurable functions on E. For each pair of partitions $V \leq U$, we let q_V and $q_{U,V}$ be the canonical projections from $\mathbf{P}(E)$ into $\mathcal{P}(V)$, and from $\mathcal{P}(U)$ into $\mathcal{P}(V)$. Notice that $\text{Ent}_U(.|\nu)$ is finite and continuous on the compact sets $\{\eta \in \mathcal{P}(U) \; : \; \eta \ll q_U(\nu)\}$, and $\text{Ent}_U(\mu|.)$ is continuous for every fixed μ.

LEMMA 10.2 *The projective limit topological space* $\lim_{\mathcal{U}} \mathcal{P}$ *associated to the set* $(\mathcal{P}(U), q_{U,V})_{V \leq U}$ *is compact and homeomorphic to* $\mathbf{P}(E)$. *In addition, for any* $(\mu, \nu) \in (\mathbf{P}(E) \times \mathcal{P}(E))$, *with* $H(\mu|\nu) < \infty$, *we have* $\mu \in \mathcal{P}(E)$ *and*

$$H(\mu|\nu) = \text{Ent}(\mu|\nu) \tag{10.8}$$

Proof. The set $\mathcal{P} = ((\mathcal{P}(U), d_U), q_{U,V})_{U \geq V}$ forms a projective inverse spectrum of $\mathcal{U}$, with compact metric spaces $(\mathcal{P}(U), d_U)$, and connecting maps $q_{U,V}$. The Hausdorff property ensures that $\lim_{\mathcal{U}} \mathcal{P}$ is a closed subset of $\prod_{U \in \mathcal{U}} \mathcal{P}(U)$, which is compact by Tychonov's Theorem. Let

$$h : \lim_{\mathcal{U}} \mathcal{P} \to \mathbf{P}(E)$$

be the mapping which associates to a point $\mu = (\mu^U)_{U \in \mathcal{U}} \in \lim_{\mathcal{U}} \mathcal{P}$ the set function $h(\mu) \in \mathbf{P}(E)$ defined for any $A \in \mathcal{E}$ by $h(\mu)(A) = \mu^U(A)$, where $U \in \mathcal{U}$ is some finite partition of E such that $A \in \sigma(U)$. Then, h is an homeomorphism between the compact spaces $\lim_{\mathcal{U}} \mathcal{P}$ and $\mathbf{P}(E)$. To prove this claim, we first check that h is well defined. This assertion is easily proved by noting that

$$A \in (\sigma(U) \cap \sigma(V)) \implies A \in \sigma(U \vee V)$$

where

$$(U \vee V) = \{A \cap B \; : \; (A, B) \in (U \times V)\}$$

is the smallest partition such that $\sigma(U) \vee \sigma(V) = \sigma(U \vee V)$. By the compatibility conditions in the definition of $\lim_{\mathcal{U}} \mathcal{P}$, we have

$$\mu^{(U \vee V)}(A) = \mu^U(A) = \mu^V(A)$$

To prove that $h(\mu)$ is an additive set function on $\mathcal{E}$, we choose a pair of disjoint Borel sets A, B, and a pair U, V of partitions with $A \in U$, and $B \in V$. Since A and B are disjoint, we have

$$
\begin{aligned}
A &= A \cap (E - B) = A \cap (\cup_{C \in V, C \neq B} C) \\
&= \cup_{C \in V, C \neq B} (A \cap C) \in \sigma(U \vee V)
\end{aligned}
$$

and by symmetry arguments, $B \in \sigma(U \vee V)$. Using the fact that $\mu^{(U \vee V)} \in \mathcal{P}(U \vee V)$, we conclude that

$$
\begin{aligned}
h(\mu)(A \cup B) &= \mu^{(U \vee V)}(A \cup B) = \mu^{(U \vee V)}(A) + \mu^{(U \vee V)}(B) \\
&= h(\mu)(A) + h(\mu)(B)
\end{aligned}
$$

Let us prove that h is an injection. Let $\mu, \nu \in \lim_{\mathcal{U}} \mathcal{P}$ be a pair of points such that $h(\mu) = h(\nu)$. By definition of h, we find that $\mu^U = \nu^U$ for any $U \in \mathcal{U}$, from which we conclude that $\mu = \nu$. On the other hand, for any $\mu \in \mathbf{P}(E)$ we have $(q_U(\mu))_{U \in \mathcal{U}} \in \lim_{\mathcal{U}} \mathcal{P}$, and

$$h((q_U(\mu))_{U \in \mathcal{U}})(A) = q_U(\mu)(A) = \mu \circ e_U^{-1}(A) = \mu(A)$$

for any $A \in \sigma(U)$, for some $U \in \mathcal{U}$. We conclude that h is a bijective map from $\lim_{\mathcal{U}} \mathcal{P}$ into $\mathbf{P}(E)$, and $h^{-1}(\mu) = (q_U(\mu))_{U \in \mathcal{U}}$.

It remains to prove that h and h^{-1} are continuous. To prove this final step, we observe that for any sequence $\mu = (\mu^U)_{U \in \mathcal{U}}$ of points in $\lim_{\mathcal{U}} \mathcal{P}$, and $\mu = (\mu^U)_{U \in \mathcal{U}} \in \lim_{\mathcal{U}} \mathcal{P}$, we have the following series of equivalent assertions

$$
\begin{aligned}
\lim_{n \to \infty} \mu = \mu \text{ in } \lim_{\mathcal{U}} \mathcal{P} &\Leftrightarrow \forall U \in \mathcal{U} \quad \lim_{n \to \infty} \mu^U = \mu^U \text{ (in } \mathcal{P}(U)) \\
&\Leftrightarrow \forall A \in \mathcal{E} \quad \lim_{n \to \infty} h(\mu)(A) = h(\mu)(A)
\end{aligned}
$$

This ends the proof of the first part of the lemma. The proof of the second part can be found in Groeneboom, Oosterhoff and Ruymgaart (1979), and in Pinsker (1964)). ☐

The next technical lemma provides large deviations probabilities for independent and identically distributed sequences, on finite state space models.

LEMMA 10.3 *Let S be a finite state space, and let $Y = (Y^i)_{1 \leq i \leq N}$ be a collection of N independent, and S-valued random variables, identically*

distributed according to a measure $\eta \in \mathcal{P}(S)$. For any $\mu \in m_N(S^N)$, we have

$$(N+1)^{-|S|} \leq \exp\{N\mathrm{Ent}(\mu|\eta)\} \, \mathbb{P}_\eta(m_N(Y) = \mu) \leq 1$$

Proof.   This result is rather well known, see for instance Lemma 2.1.9 p. 15 in Dembo and Zeitouni (1993). Its proof is rather elementary. We notice that for $y \in m_N^{-1}(\mu)$ with $\mu \in m_N(S^N)$, we have

$$\mathbb{P}_\eta(Y = y) = \prod_{u \in S} \eta(u)^{N\mu(u)} = \exp N \sum_{u \in S} \mu(u) \log \eta(u)$$

This yields that

$$\begin{aligned}
\mathbb{P}_\eta(m_N(Y) = \mu) &= \mathbb{P}_\eta(Y \in m_N^{-1}(\mu)) \\
&= |m_N^{-1}(\mu)| \, \exp N \sum_{u \in S} \mu(u) \log \eta(u) \quad (10.9)
\end{aligned}$$

Using the fact that $\mathbb{P}_\mu(m_N(Y) = \mu) \leq 1$, we find that

$$|m_N^{-1}(\mu)| \leq \exp -N \sum_{u \in S} \mu(u) \log \mu(u)$$

from which we conclude that $\mathbb{P}_\eta(m_N(Y) = \mu) \leq \exp\{-N\mathrm{Ent}(\mu|\eta)\}$. Since $n!/p! \geq p^{n-p}$, for any $n, p \geq 0$, one checks that for any $\eta \ll \mu$

$$\frac{\mathbb{P}_\mu(m_N(Y) = \mu)}{\mathbb{P}_\mu(m_N(Y) = \eta)} = [\prod_{u \in S} \frac{(N\eta(u))!}{(N\mu(u))!}] \, \mu(u)^{N(\mu(u)-\eta(u))} \geq 1$$

Recalling that $\mathrm{Ent}(\mu|\eta) \geq 0$, this also yields that

$$\mathbb{P}_\mu(m_N(Y) = \eta) \vee \mathbb{P}_\eta(m_N(Y) = \mu) \leq \mathbb{P}_\mu(m_N(Y) = \mu)$$

This implies that

$$1 = \mathbb{P}_\mu(m_N(Y) \in m_N(S^N)) \leq |m_N(S^N)| \mathbb{P}_\mu(m_N(Y) = \mu)$$

Using the fact that any $m_N(y) \in m_N(S^N)$ can be rewritten as

$$m_N(y) = \frac{1}{N} \sum_{u \in S} |\{i \ : \ y^i = u\}| \, \delta_u$$

we find that $|m_N(S^N)| \leq (N+1)^{|S|}$, from which we conclude that

$$|m_N^{-1}(\mu)| \geq (N+1)^{-|S|} \, \exp -N \sum_{u \in S} \mu(u) \log \mu(u)$$

This, together with (10.9), ends the proof of the lemma.   □

THEOREM 10.3 *Let $(X^i)_{i \geq 1}$ be a sequence of independent, E-valued random variables, identically distributed according to a measure $\eta \in \mathcal{P}(E)$. For any N, we denote by Q^N the law on $\mathcal{P}(E)$ of the N-empirical measures $m_N(X)$. For any $U \in \mathcal{U}$, the sequence of distributions $Q^N \circ q_U^{-1}$ satisfy the large deviations principles on $(\mathcal{P}(U), d_U)$, with the good entropy rate function*

$$I_U = \text{Ent}_U(\,.\,|\eta)$$

Combining Corollary 10.2 with Lemma 10.2, and recalling that the relative entropy is a good rate function for the τ-topology on $\mathcal{P}(E)$ (see for instance Groeneboom, Oosterhoff and Ruymgaart (1979) or p. 240-243 in Dembo and Zeitouni (1993)), we easily obtain the strong version of Sanov's Theorem, which states that Q^N satisfy the large deviations principles on $\mathcal{P}(E)$, equipped with the τ-topology, and with the good entropy rate function $\text{Ent}(\,.\,|\eta)$.

In the reverse angle, by a simple contraction argument, Sanov's Theorem implies Corollary 10.2. To check that $I_U \geq \text{Ent}_U(\nu|\eta)$, we use the fact that for any $\nu \in \mathcal{P}(U)$ we have

$$\text{Ent}(\Omega_\eta(\nu)|\eta) = \text{Ent}_U(\nu|\eta)$$

where Ω_η is the mapping from $\mathcal{P}(U)$ into $q_U^{-1}(\mathcal{P}(U))$, which associate with any $\nu \in \mathcal{P}(U)$, the measure $\Omega_\eta(\nu)$ defined for any $A \in \mathcal{E}$ and $i \leq d$ by

$$\Omega_\eta(\nu)(A \cap U^i) = \begin{cases} \eta(A \cap U^i)\,\nu(U^i)/\eta(U^i) & \text{if } \eta(U^i) > 0 \\ \nu(A \cap U^i) & \text{if } \eta(U^i) = 0 \end{cases} \quad (10.10)$$

Proof of Theorem 10.3

Let $\Lambda_U : \mathcal{B}_b(U) \to \mathbb{R}$ be the logarithmic moment generating function defined for any $f \in \mathcal{B}_b(U)$ by

$$\begin{aligned} \Lambda_U(f) &= \frac{1}{N} \log \int e^{N <f,\mu>} (Q^N \circ q_U^{-1})(d\mu) \\[2mm] &= \frac{1}{N} \log \mathbb{E}_\eta^N(e^{N m_N(X)(f)}) \\[2mm] &= \log \eta(\exp f) = \log q_U(\eta)(\exp f) < \infty \end{aligned}$$

By Cramér's Theorem, the deviation upper bound follows from the fact that $\mathcal{P}(U)$ is compact, and $\text{Ent}_U(\,.\,|\eta)$ is the Fenchel-Legendre transform of the function Λ_U.

To prove the lower bound, we let $A \subset \mathcal{P}(U)$ be a open set such that $\mathrm{Ent}_U(A|\eta)$ is finite (otherwise the proof of the lower bound is trivial). For any $\delta > 0$, there exists a point $\mu \in A$ such that

$$\mathrm{Ent}_U(\mu|\eta) \leq \mathrm{Ent}_U(A|\eta) + \delta \qquad (10.11)$$

Since $\mu \in A$, and A is open in $(\mathcal{P}(U), d_U)$, there exists some $\varepsilon > 0$, such that

$$\mathcal{V}_U(\mu,\varepsilon) = \{\nu \in \mathcal{P}(U) \ : \ d_U(\nu,\mu) < \varepsilon\} \subset A$$

Up to a change of index, we suppose that $\mu(U^d) = \vee_{i=1}^d \mu(U^i)(> 0)$ and we associate with μ, the N-approximating distributions $\mu^N \in \mathcal{P}(U)$ defined by

$$\mu^N(U^i) = \begin{cases} [N\mu(U^i)]/N & \text{if} \ \ 1 \leq i < d \\ 1 - \sum_{i=1}^{d-1}[N\mu(U^i)]/N & \text{if} \ \ i = d \end{cases}$$

By construction, we note that

$$\mu^N \ll \mu \ (\ll q_U(\eta)) \quad \text{and} \quad \mathrm{Ent}_U(\mu^N|\eta) < \infty$$

Since $d_U(\mu^N,\mu) \leq (d-1)/N$, then we have $\mu^N \in \mathcal{V}_U(\mu,\varepsilon)$ for any $N > N_1 = (d-1)/\varepsilon$. On the other hand, we have

$$q_U^{-1}(\{\eta \in \mathcal{P}(U) \ : \ d_U(\eta,\mu^N) = 0\}) \ \subset \ q_U^{-1}(\mathcal{V}_U(\mu,\varepsilon))$$

and by Lemma 10.3, we get

$$\begin{aligned} Q^N(q_U^{-1}(\mathcal{V}_U(\mu,\varepsilon))) \ &\geq \ \mathbb{P}_\eta^N(d_U(m_N(X),\mu^N) = 0) \\ &= \ \frac{N!}{(N\mu^N(U^1))! \dots (N\mu^N(U^d))!} \prod_{i=1}^d \eta(U^i)^{(N\mu^N(U^i))} \\ &\geq \ (N+1)^{-d} \exp\{-N\mathrm{Ent}_U(\mu^N|\eta)\} \end{aligned}$$

The continuity of the entropy function $\mathrm{Ent}_U(.|\eta)$ on the set of measures $\{\mu \in \mathcal{P}(U) \ : \ \mu \ll q_U(\eta)\}$, now implies that for any $N \geq N_2$, and some $N_2 \geq 1$,

$$\mathrm{Ent}_U(\mu^N \mid \eta) \leq \mathrm{Ent}_U(\mu \mid \eta) + \delta$$

We finally conclude that for any $N \geq (N_1 \vee N_2)$

$$\begin{aligned} \frac{1}{N} \log Q^N(q_U^{-1}(A)) \ &\geq \ \frac{1}{N} \log \mathbb{Q}^N(q_U^{-1}(\mathcal{V}_U(\mu,\varepsilon))) \\ &\geq \ -\mathrm{Ent}_U(A|\eta) - d\,\frac{\log(N+1)}{N} - 2\delta \end{aligned}$$

Letting $N \to \infty$, and then $\delta \to 0$, the end of the proof of the lower bound is completed. This ends the proof of Theorem 10.3. $\qquad\qquad \square$

5.   Large deviations for interacting processes

5.1   Some topological preliminaries

We equip the set $\mathcal{U}^n = \prod_{p=0}^{n} \mathcal{U}_p$ with the partial ordering defined by

$$(U_p)_{p \le n} \le (V_p)_{p \le n} \iff (U_p \le V_p, \quad \forall 0 \le p \le n)$$

We associate with each $U^n = (U_p)_{p \le n} \in \mathcal{U}^n$, the Cartesian product $\mathcal{P}^n(U) = \prod_{p=0}^{n} \mathcal{P}(U_p)$. For any $U^n \ge V^n$, we denote respectively by q_{U^n}, and q_{U^n,V^n}, the continuous and canonical projections from $\mathbf{P}^n(E)$, and respectively from $\mathcal{P}^n(U)$, into $\mathcal{P}^n(V)$. From the projective limit Theorem 10.2, it is easily established that the Cartesian product space $\mathbf{P}^n(E)$, equipped with the product τ-topology, is homeomorphic to the projective limit $\lim_{\mathcal{U}^n} \mathcal{P}^n$ of the set

$$\mathcal{P}^n = (\mathcal{P}^n(U), q_{U^n,V^n})_{U^n \ge V^n}.$$

For any $n \ge 0$, we denote by J_n, the function on $\mathbf{P}^n(E) = \prod_{p=0}^{n} \mathbf{P}(E_p)$ defined by

$$J_n((\mu_p)_{0 \le p \le n}) = H(\mu_0|\eta_0) + \sum_{p=1}^{n} H(\mu_p|\Phi_p(\mu_{p-1}))$$

with the convention $\Phi_0(\mu_{-1}) = \eta_0$ for $p = 0$. Observe that J_n is lower semi-continuous, since it can be obtained as the supremum of continuous functions

$J_n((\mu_p)_{0 \le p \le n})$

$= \sup \left\{ \sum_{p=0}^{n} [\mu_p(f_p) - \log \Phi_p(\mu_{p-1})(e^{f_p})] \ (f_p)_{p \le n} \in \cup_{U^n \in \mathcal{U}^n} \mathcal{B}_b^n(U) \right\}$

where $\mathcal{B}_b^n(U) = \prod_{p=0}^{n} \mathcal{B}_b(U_p)$.

On the other hand, by Theorem 10.2, and using a simple induction on the time parameter, we prove that the domain $\{\mu; J_n(\mu) < \infty\}$ of J_n is included in $\mathcal{P}^n(E)$. In addition for any $(\mu_p)_{p \le n} \in \mathcal{P}^n(E)$ we have

$$J_n((\mu_p)_{0 \le p \le n}) = \text{Ent}(\mu_0|\eta_0) + \sum_{p=1}^{n} \text{Ent}(\mu_p|\Phi_p(\mu_{p-1}))$$

This implies that for any τ_1-closed, or τ_1-open subset, A of $\mathbf{P}^n(E)$, we have $J_n(A \cap \mathcal{P}^n(E)) = J_n(A)$.

The above observations, combined with Theorem 10.1, imply that Q_n^N satisfies the large deviations principles on $\mathcal{P}^n(E)$, equipped with the relative τ-topology, with rate function J_n. To prove that J_n is a good rate

function, we use the lower semi-continuity property of J_n on $\mathbf{P}^n(E)$ to check that the level sets $J_n^{-1}([0, a])$, $a > 0$, are τ_1-closed, thus τ_1-compact in the compact set $\mathbf{P}^n(E)$. Since we proved that $J_n^{-1}([0, a]) \subset \mathcal{P}^n(E)$, we conclude that these level sets are also τ-compact subsets of $\mathcal{P}^n(E)$.

It is also convenient to notice that Corollary 10.2, combined with Theorem 10.1, implies that for any $U^n = (U_p)_{p \leq n} \in \mathcal{U}^n$, the image measures $Q_n^N \circ q_{U^n}^{-1}$ satisfy the large deviations principles on $\mathcal{P}^n(U)$, with the good rate function defined for any $\nu = (\nu_p)_{p \leq n} \in \mathcal{P}^n(U)$ by

$$J_n^U(\nu) = J_n(q_{U^n}^{-1}(\nu)) \; (= \inf_{q_{U^n}^{-1}(\nu)} J_n)$$

Furthermore, arguing as in (10.10), we find that

$$J_n^U(\nu) = \sum_{p=0}^{n} \inf_{\mu_{p-1} \in q_{U_{p-1}}^{-1}(\nu_{p-1})} \mathrm{Ent}_{U_p}(\nu_p | \Phi_p(\mu_{p-1}))$$

with the conventions $q_{U_{-1}}^{-1}(\nu_{-1}) = \{\eta_0\}$, and $\Phi_0 = Id$ for $p = 0$.

We end this section with an elementary proof of Corollary 10.1. We first observe that for any flow $\mu = (\mu_p)_{p \leq n} \in \mathcal{P}^n(E)$, we have

$$d_{U_n}(\mu_n, \eta_n) \leq \|\mu_n - \nu_n\|_{tv}$$

Using the triangular inequality, and condition (L), we find that

$$\begin{aligned}
\|\mu_n - \eta_n\|_{tv} &\leq \sum_{p=0}^{n} \|\Phi_{p,n}(\mu_p) - \Phi_{p,n}(\Phi_p(\mu_{p-1}))\|_{tv} \\
&\leq \sum_{p=0}^{n} \beta(\Phi_{p,n}) \|\mu_p - \Phi_p(\mu_{p-1})\|_{tv}
\end{aligned}$$

with the convention $\Phi_0(\mu_{-1}) = \eta_0$ for $p = 0$. This readily yields that

$$d_{U_n}(\mu_n, \eta_n)^2 \leq \beta(\Phi) \sum_{p=0}^{n} \|\mu_p - \Phi_p(\mu_{p-1})\|_{tv}^2 \leq \beta(\Phi) \, J_n(\mu)$$

In the last inequality, we have used the fact that the relative entropy dominates the square of the total variation distance (see for instance Csiszar (1967), Theorem 4.1). From the additive structure of J_n, we conclude that

$$\sup_{p \leq n} d_{U_p}(\mu_p, \eta_p)^2 \leq \beta(\Phi) \, J_n(\mu)$$

The end of the proof of the corollary is now clear.

5.2   Proof of Theorem 10.1

To prepare the proof of the upper bound, we again recall that any closed F of $\mathbf{P}^n(E)$ has the form $F = \cap_{U^n \in \mathcal{U}^n} q_{U^n}^{-1}(F_{U^n})$, where F_{U^n} stands for the τ_1-closure of the set $q_{U^n}(F)$. Since $\mathbf{P}^n(E)$ is compact, the sets $q_{U^n}^{-1}(F_{U^n})$ are compact, and for any $\varepsilon > 0$, one can find a finite and open ε-covering

$$q_{U^n}^{-1}(F_{U^n}) \subset \cup_{i=1}^m \mathcal{V}_n^{U^n}(\mu^i, \varepsilon)$$

with $\mu^i = (\mu_p^i)_{p \leq n} \in F$ and $\mathcal{V}_p^{U^n}(\mu^i, \varepsilon) = (\prod_{0 \leq q \leq p} \mathcal{V}_p^{U^n}(\mu_q^i, \varepsilon))$, for any $p \leq n$. Under our continuity assumptions, we can choose these open neighborhoods such that for any $\eta_p \in \mathcal{V}_p^{U^n}(\mu_p^i, \varepsilon)$.

$$d_{U_p}(\eta_p, \mu_p^i) \vee d_{U_{p+1}}(\Phi_{p+1}(\eta_p), \Phi_{p+1}(\mu_p^i)) \leq \varepsilon$$

In this case, we have for each $(f_p)_{p \leq n} \in \mathcal{B}_b^n(U_n)$

$$\mathbb{P}((\eta_p^N)_{p \leq n} \in \mathcal{V}_n^{U^n}(\mu^i, \varepsilon))$$

$$= \mathbb{E}(e^{N(\eta_n^N - \mu_n^i)(f_n) - N(\eta_n^N - \mu_n^i)(f_n)} \, 1_{\mathcal{V}_{n-1}^{U^n}(\mu^i, \varepsilon)}((\eta_p^N)_{p<n}))$$

$$\leq e^{\varepsilon N \|f_n\|} \, \mathbb{E}(e^{N(\eta_n^N - \mu_n^i)(f_n)} \, 1_{\mathcal{V}_{n-1}^{U^n}(\mu^i, \varepsilon)}((\eta_p^N)_{p<n}))$$

By definition of the particle approximating model, we arrive at

$$\mathbb{P}((\eta_p^N)_{p \leq n} \in \mathcal{V}_n^{U^n}(\mu^i, \varepsilon))$$

$$\leq e^{\varepsilon N \|f_n\|} \, \mathbb{E}(e^{-N(\mu_n^i(f_n) - \log \Phi_n(\eta_{n-1}^N)(e^{f_n}))} \, 1_{\mathcal{V}_{n-1}^{U^n}(\mu^i, \varepsilon)}((\eta_p^N)_{p<n}))$$

$$\leq e^{\varepsilon N c(f_n) - N(\mu_n^i(f_n) - \log \Phi_n(\mu_{n-1}^i)(e^{f_n}))} \, \mathbb{P}((\eta_p^N)_{p<n} \in \mathcal{V}_{n-1}^{U^n}(\mu^i, \varepsilon))$$

for some finite constant $c(f_n) < \infty$, whose values only depend on the supremum norm of f_n. A simple induction now yields that

$$\frac{1}{N} \log \mathbb{P}((\eta_p^N)_{p \leq n} \in \mathcal{V}_n^{U^n}(\mu^i, \varepsilon))$$

$$\leq \varepsilon \sum_{p \leq n} c(f_p) - \sum_{p \leq n}(\mu_p^i(f_p) - \log \Phi_p(\mu_{p-1}^i)(e^{f_p}))$$

from which we conclude that

$$\limsup_{\varepsilon \to 0} \limsup_{N \to \infty} \frac{1}{N} \log \mathbb{P}((\eta_p^N)_{p \leq n} \in \mathcal{V}_n^{U^n}(\mu^i, \varepsilon))$$

$$\leq - \sum_{p \leq n}(\mu_p^i(f_p) - \log \Phi_p(\mu_{p-1}^i)(e^{f_p}))$$

Taking the infimum over all $(f_p)_{p \leq n} \in \mathcal{B}_b^n(U_n)$ in the r.h.s of the above display, we conclude that

$$\limsup_{\varepsilon \to 0} \limsup_{N \to \infty} \tfrac{1}{N} \log \mathbb{P}((\eta_p^N)_{p \leq n} \in \mathcal{V}_n^{U^n}(\mu^i, \varepsilon))$$

$$\leq - \sum_{p \leq n} \mathrm{Ent}_{U_n}(\mu_p^i | \log \Phi_p(\mu_{p-1}^i))$$

$$\leq -J_n^U(q_{U^n}(\mu^i)) \leq -J_n^U(F_{U^n})$$

By the union of events bounds, we find that

$$\limsup_{N \to \infty} \frac{1}{N} \log \mathbb{P}((\eta_p^N)_{p \leq n} \in q_{U^n}^{-1}(F_{U^n})) \leq -J_n^U(F_{U^n})$$

and therefore

$$\limsup_{N \to \infty} \frac{1}{N} \log \mathbb{P}((\eta_p^N)_{p \leq n} \in F) \leq -J_n^U(F_{U^n}) \leq -J_n^U(F_{U^n})$$

We end the proof of the upper bound by taking the infimum over all U^n, and invoking the min-max Theorem 10.2.

Our final objective is to prove that the rate function J_n governs the large deviations principles lower bounds. To this end, we let $A \subset \mathbf{P}^n(E)$ be a τ_1-open set such that $J_n(A) = \inf_A J_n < \infty$ (otherwise the proof of the lower bound is as usually trivial). For any $\delta > 0$, there exists a point $\mu \in A \cap \mathcal{P}^n(E)$, such that

$$J_n(\mu) \leq J_n(A) + \delta \qquad\qquad (10.12)$$

Since $\mu = (\mu_p)_{0 \leq p \leq n} \in A$, we can find a collection of strictly positive numbers $(\varepsilon_p)_{0 \leq p \leq n}$, and a sequence of finite partitions $U_p = (U_p^i)_{1 \leq i \leq d_p}$ of the sets E_p, such that

$$\mathcal{C}_{\varepsilon,n}^U(\mu) = \prod_{0 \leq p \leq n} B_{U_p}(\mu_p, \varepsilon_p) \subset A$$

with the open neighborhood $B_{U_p}(\mu_p, \varepsilon_p)$ of $\mu_p \in \mathbf{P}(E_p)$ given by

$$B_{U_p}(\mu_p, \varepsilon_p) = \{\nu_p \in \mathbf{P}(E_p) \ : \ d_{U_p}(\mu_p, \nu_p) < \varepsilon_p\}$$

Up to a change of index, we suppose that $\mu_n(U_n^d) = \vee_{i=1}^{d_n} \mu_n(U_n^i)(> 0)$, and we associate with $\mu_n \in \mathbf{P}(E_n)$, the N-approximating distributions $\mu_n^N \in \mathcal{P}(U_n)$ defined by

$$\mu_n^N(U_n^i) = \begin{cases} [N\mu_n(U_n^i)]/N & \text{if} \ \ 1 \leq i < d_n \\ 1 - \sum_{i=1}^{d_n-1} [N\mu_n(U_n^i)]/N & \text{if} \ \ i = d_n \end{cases}$$

By construction, we note that

$$\mu_n^N \ll q_{U_n}(\mu_n) \ll q_{U_n}(\Phi_n(\mu_{n-1})) \quad \text{and} \quad \text{Ent}_{U_n}(\mu_n^N | \Phi_n(\mu_{n-1})) < \infty$$

Under our assumptions, we also have for any $\nu_{n-1} \in B_{U_{n-1}}(\mu_{n-1}; \varepsilon_{n-1})$, and $1 \le i \le d_n$,

$$\mu_n^N(U_n^i) > 0 \Longrightarrow \Phi_n(\nu_{n-1})(U_n^i) > 0$$

Since $d_{U_n}(\mu_n, \mu_n^N) \le (d_n - 1)/N$, we find that $\mu_n^N \in B_{U_n}(\mu_n, \varepsilon_n)$ as soon as $N > N_n^1 = (d_n - 1)/\varepsilon_n$, and hence

$$\mathcal{C}_{\varepsilon,n-1}^U((\mu_k)_{k<n}) \times \{\nu_n \in \mathbf{P}(E_n) \; : \; d_{U_n}(\mu_n^N, \nu_n) = 0\} \subset A$$

By definition of the N-particle model, and using Lemma 10.3, it is also clear that

$$\mathbb{P}(d_{U_n}(\mu_n^N, \eta_n^N) = 0 \mid \eta_{n-1}^N)$$

$$= \frac{N!}{(N\mu_n^N(U_n^1))! \dots (N\mu_n^N(U_n^{d_n}))!} \prod_{i=1}^{d_n} \Phi_n(\eta_{n-1}^N)(U_n^i)^{(N\mu_n^N(U_n^i))}$$

$$\ge \exp\left[-N \, \text{Ent}_{U_n}(\mu_n^N \mid \Phi_n(\eta_{n-1}^N)) - d\log(N+1)\right]$$

On the other hand, we have for any $\nu_{n-1} \in B_{U_{n-1}}(\mu_{n-1}, \varepsilon_{n-1}) \cap \mathcal{P}(E_{n-1})$ the inequality

$$\text{Ent}_{U_n}(\mu_n^N \mid \Phi_n(\nu_{n-1}))$$

$$\le \text{Ent}_{U_n}(\mu_n^N \mid \Phi_n(\mu_{n-1})) + \sum_i \sum_{\mu_n^N(U_n^i)>0} \mu_n^N(U_n^i) \log \frac{d\Phi_n(\mu_{n-1})(U_n^i)}{d\Phi_n(\nu_{n-1})(U_n^i)}$$

Under our assumptions, we have

$$\text{Ent}_{U_n}(\mu_n^N \mid \Phi_n(\nu_{n-1}))$$

$$\le \text{Ent}_{U_n}(\mu_n^N \mid \Phi_n(\mu_{n-1})) + \frac{2}{\rho_n \, \lambda_n^\star(U_n)} \; d_{U_n}(\Phi_n(\nu_{n-1}), \Phi_n(\mu_{n-1}))$$

with $\lambda_n^\star(U_n) = \wedge_i \lambda_n(U_n^i) > 0 \lambda_n(U_n^i)$. Since Φ_n represents a τ_1-continuous mapping, for every $\delta > 0$, there exists some τ_1-open neighborhood $\mathcal{O}_\delta(\mu_{n-1}) \subset \mathbf{P}(E_{n-1})$ of μ_{n-1} (which may depend on U_n), such that

$$\mathcal{O}_\delta(\mu_{n-1}) \subset B_{U_{n-1}}(\mu_{n-1}, \varepsilon_{n-1})$$

and on the set of events $\{\eta_{n-1}^N \in \mathcal{O}_\delta(\mu_{n-1})\}$, we have

$$\text{Ent}_{U_n}(\mu_n^N \mid \Phi_n(\eta_{n-1}^N)) \le \text{Ent}_{U_n}(\mu_n^N \mid \Phi_n(\mu_{n-1})) + \delta \; (< \infty)$$

The continuity of the function $\mathrm{Ent}_{U_n}(.\mid \Phi_n(\mu_{n-1}))$, on the set of measures $\{\nu_n \in \mathcal{P}(U_n) : \nu_n \ll q_{U_n}(\Phi_n(\mu_{n-1}))\}$, now implies that

$$
\begin{aligned}
\mathrm{Ent}_{U_n}(\mu_n^N \mid \Phi_n(\mu_{n-1})) &\leq \mathrm{Ent}_{U_n}(\mu_n \mid \Phi_n(\mu_{n-1})) + \delta \\
&\leq H(\mu_n \mid \Phi_n(\mu_{n-1})) + \delta
\end{aligned}
$$

for any $N \geq N_n^2$, and some $N_n^2 \geq 1$. It is now convenient to observe that

$$
\begin{aligned}
Q_n^N(A) &= \mathbb{P}_{\eta_0}^N((\eta_0^N,\ldots,\eta_n^N) \in A) \\
&\geq \mathbb{P}_{\eta_0}^N\big(d_{U_n}(\mu_n^N,\eta_n^N) = 0 , \ \eta_{n-1}^N \in \mathcal{O}_\delta(\mu_{n-1}) \\
&\qquad\qquad \text{and } (\eta_k^N)_{p<n-1} \in \mathcal{C}_{\varepsilon,n-2}^U((\mu_p)_{p\leq n-2})
\end{aligned}
$$

Using a simple calculation, we deduce the following lower bound

$$
Q_n^N(A)
$$

$$
\geq \inf_{\nu\in\mathcal{O}_\delta(\mu_{n-1})} \mathbb{P}\big(d_{U_n}(\mu_n^N,\eta_n^N) = 0 \mid \eta_{n-1}^N = \nu\big) \ Q_{n-1}^N\big(\mathcal{D}_{(\delta,\varepsilon),n-1}(\mu)\big)
$$

with the τ_1-open neighborhood $\mathcal{D}_{(\delta,\varepsilon),n-1}(\mu) \in \mathbf{P}^{n-1}(E)$ of $(\mu_p)_{p\leq n-1}$ defined by

$$
\mathcal{D}_{(\delta,\varepsilon),n-1}(\mu) = \mathcal{C}_{\varepsilon,n-2}^U((\mu_p)_{p\leq n-2}) \times \mathcal{O}_\delta(\mu_{n-1})
$$

From previous estimations, we find that, for any $N \geq N_n^1 \vee N_n^2$

$$
\begin{aligned}
\frac{1}{N}\log Q_n^N(A) &\geq -H(\mu_n\mid\Phi_n(\mu_{n-1})) - \frac{d\log(N+1)}{N} - 2\delta \\
&\quad + \frac{1}{N}\log Q_{n-1}^N\big(\mathcal{D}_{(\delta,\varepsilon),n-1}(\mu)\big) \\
&= -J_n(\mu) - \frac{d\log(N+1)}{N} - 2\delta + J_{n-1}((\mu_p)_{p\leq n}) \\
&\quad + \frac{1}{N}\log Q_{n-1}^N\big(\mathcal{D}_{(\delta,\varepsilon),n-1}(\mu)\big)
\end{aligned}
$$

Furthermore by (10.12), and using our induction hypothesis, we have

$$
\begin{aligned}
\liminf_{N\to\infty} \frac{1}{N}\log Q_n^N(A) &\geq -J_n(A) - 3\delta + [J_{n-1}((\mu)_{p<n}) \\
&\qquad - J_{n-1}(\mathcal{D}_{(\delta,\varepsilon),n-1}(\mu))] \\
&\geq -J_n(A) - 3\delta
\end{aligned}
$$

Letting δ tends to 0, we conclude that J_n governs the lower bounds. $\qquad\square$

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Chapter 11

ASYMPTOTIC DISTRIBUTION OF A SIMPLE LINEAR ESTIMATOR FOR VARMA MODELS IN ECHELON FORM

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Abstract   In this paper, we study the asymptotic distribution of a simple two-stage (Hannan-Rissanen-type) linear estimator for stationary invertible vector autoregressive moving average (VARMA) models in the echelon form representation General conditions for consistency and asymptotic normality are given A consistent estimator of the asymptotic covariance matrix of the estimator is also provided, so that tests and confidence intervals can easily be constructed

1.   Introduction

Multivariate time series analysis is widely based on vector autoregressive models (VAR), especially in econometric studies (see Lütkepohl (1991, 2001) and Hamilton (1994, Chapter 11)). One reason for this popularity is that VAR models are easy to estimate and can account for relatively complex dynamic phenomena. On the other hand, very large numbers of parameters are often required to obtain a good fit, and the class of VAR models is not robust to disaggregation: if a vector process satisfies a VAR scheme, its subvectors (such as individual components) do not follow VAR processes. Instead, the subvectors of VAR processes follow vector autoregressive moving average (VARMA) processes. The latter class, indeed, includes VAR models as a special case, and can reproduce in a parsimonious way a much wider class of autocovariance structures. So they can lead to improvements in estimation and forecast precision. Further, VARMA modelling is theoretically consistent, in the sense that the subvectors of a VARMA model also satisfy VARMA schemes (usually of different order). Similarly, the VARMA

class of models is not affected by temporal aggregation, while a VAR model may cease to be a VAR after it has been aggregated over time (see Lütkepohl (1987)).

VARMA modelling has been proposed a long time ago (see Hillmer and Tiao (1979), Tiao and Box (1981), Lütkepohl (1991), Boudjellaba, Dufour and Roy (1992, 1994), Reinsel (1997)), but has remained little used in practical work. Although the process of building VARMA models is, in principle, similar to the one associated with univariate ARMA modelling, the difficulties involved are compounded by the multivariate nature of the data.

At the specification level, new identification issues (beyond the possible presence of common factors) arise and must be taken into account to ensure that unique parameter values can be associated with a given autocovariance structure (compatible with a VARMA model); see Hannan (1969, 1970, 1976b, 1979), Deistler and Hannan (1981), Hannan and Deistler (1988, Chapter 2), Lütkepohl (1991, Chapter 7) and Reinsel (1997, Chapter 3). An important finding of this work is the importance of the concepts of dynamic dimension and Kronecker indices in the formulation of identifiable VARMA structures. Further, specifying such models involves the selection of several autoregressive and moving average orders: in view of achieving both identifiability and efficiency, it is important that a reasonably parsimonious model be formulated. Several methods for that purpose have been proposed. The main ones include: (1) techniques based on canonical variate analysis (Akaike (1976), Cooper and Wood (1982), Tiao and Tsay (1985, 1989), Tsay (1989a)); (2) methods which specify an echelon form through the estimation of Kronecker indices (Hannan and Kavalieris (1984b), Tsay (1989b), Nsiri and Roy (1992, 1996), Poskitt (1992), Lütkepohl and Poskitt (1996), Bartel and Lütkepohl (1998)); (3) scalar-component models (Tiao and Tsay (1989), Tsay (1991)).

At the estimation level, once an identifiable specification has been formulated, the most widely proposed estimation method is maximum likelihood (ML) derived under the assumption of i.i.d. (independent and identically distributed) Gaussian innovations; see Hillmer and Tiao (1979), Tiao and Box (1981), Shea (1989), Mauricio (2002), and the review of Mélard, Roy and Saïdi (2002). This is mainly due to the presence of a moving average part in the model, which makes the latter fundamentally nonlinear. For example, in the Gaussian case, maximizing the likelihood function of a VARMA(p, q) model is typically a burdensome numerical exercise, as soon as the model includes a moving average part. Even numerical convergence may be problematic. Note also that, in the case of weak white noise innovations, quasi-maximum likelihood

estimates may not be consistent. These problems also show up (at a smaller scale) in the estimation of univariate ARMA models.

From the viewpoint of making VARMA modelling, it appears crucial to have estimation methods that are both quick and simple to implement with standard statistical software, even if this may involve an efficiency cost. Another reason for putting a premium on such estimation methods is that large-sample distributional theory tends to be quite unreliable in high-dimensional dynamic models, so that tests and confidence sets based on asymptotic approximations are also unreliable (for example, the actual size of test procedures may be far larger than their nominal size). This suggests that simulation-based procedures – for example, bootstrap techniques – should be used, but simulation may be impractical if calculation of the estimators involved is difficult or time consuming.

In the case of univariate ARMA models, a relatively simple estimation procedure was originally proposed by Hannan and Rissanen (1982); see also Durbin (1960), Hannan and Kavalieris (1984a), Zhao-Guo (1985), Hannan, Kavalieris and Mackisack (1986), Poskitt (1987), Koreisha and Pukkila (1990a, 1990b, 1995), Pukkila, Koreisha and Kallinen (1990), and Galbraith and Zinde-Walsh (1994, 1997). This approach is based on estimating (by least squares) the innovations of the process through a long autoregression; after that, the lagged innovations are replaced by the corresponding residuals in the ARMA equation, which may then be also estimated by least squares.

Extensions of this method to VARMA models have been studied by Hannan and Kavalieris (1984b, 1986), Hannan and Deistler (1988), Koreisha and Pukkila (1989), Huang and Guo (1990), Poskitt (1992), Poskitt and Lütkepohl (1995), Lütkepohl and Poskitt (1996), Lütkepohl and Claessen (1997), and Flores de Frutos and Serrano (2002). Work on VARMA estimation has focused on preliminary use of such linear estimators for model selection purposes. It is then suggested that other estimation procedures (such as ML) be used. Although consistency is proved, the asymptotic distribution of the basic two-step estimator has not apparently been supplied.

In this paper, we consider the problem of estimating the parameters of stationary VARMA models in echelon form using only linear least squares methods. The echelon form is selected because it tends to deliver relatively parsimonious parameterizations. In particular, we study a simple two-step estimator that can be implemented only through single equation linear regressions and thus is remarkably simple to apply. Such an estimator was previously considered in the above mentioned work on linear VARMA estimation, but its asymptotic distribution has not

apparently been established. Given the Kronecker indices of the VARMA process, we derive the asymptotic distribution of this estimator under standard regularity conditions. In particular, we show that the latter has an asymptotic normal distribution (which entails its consistency), and we provide a simple consistent estimator for its asymptotic covariance matrix, so that asymptotically valid tests and confidence tests can be built for the parameters of the model.

The paper is organized as follows. In Section 2, we formulate the background model, where the echelon form VARMA representation is considered to ensure unique parametrization, and we define the assumptions which will be used in the rest of the paper. The two-step linear estimation procedure studied in the paper is described in Section 3, and we derive its asymptotic distribution in Section 4. We conclude in Section 5. The proofs of the propositions and theorems appear in the Appendix.

2.   Framework

In this section, we describe the theoretical framework and the assumptions we will consider in the sequel. We will first define the standard VARMA representation. As the latter may involve identification problems, we will then define the echelon form on the VARMA model, which ensures uniqueness of model parameters. Finally, we shall formulate the basic regularity assumptions we shall consider.

2.1   Standard form

A k-dimensional regular vector process $\{Y_t : t \in \mathbb{Z}\}$ has a VARMA(p, q) representation if it satisfies an equation of the form.

$$Y_t = \sum_{i=1}^{p} A_i Y_{t-i} + u_t + \sum_{j=1}^{q} B_j u_{t-j} , \qquad (11.1)$$

for all t, where $Y_t = (Y_{1,t}, \ldots, Y_{k,t})'$, p and q are non-negative integers (respectively, the autoregressive and moving average orders), A_i and B_j the $k \times k$ coefficient matrices, and $\{u_t : t \in \mathbb{Z}\}$ is a (second order) white noise $WN(0, \Sigma_u)$, where Σ_u is a $k \times k$ positive definite symmetric matrix. Under the stationary and invertibility conditions the coefficients A_i and B_j satisfy the constraints

$$\det\{A(z)\} \neq 0 \text{ and } \det\{B(z)\} \neq 0 \text{ for all } |z| \leq 1 \qquad (11.2)$$

where z is a complex number, $A(z) = I_k - \sum_{i=1}^{p} A_i z^i$ and $B(z) = I_k + \sum_{j=1}^{q} B_j z^j$. This process has the following autoregressive and moving average representations:

$$Y_t = \sum_{\tau=1}^{\infty} \Pi_\tau Y_{t-\tau} + u_t \,, \tag{11.3}$$

$$Y_t = u_t + \sum_{\tau=1}^{\infty} \Psi_\tau u_{t-\tau} \,, \quad t = 1, \ldots, T \,, \tag{11.4}$$

where

$$\Pi(z) = B(z)^{-1} A(z) = I_k - \sum_{\tau=1}^{\infty} \Pi_\tau z^\tau \,, \tag{11.5}$$

$$\Psi(z) = A(z)^{-1} B(z) = I_k + \sum_{\tau=1}^{\infty} \Psi_\tau z^\tau \,, \tag{11.6}$$

$$\det\{\Pi(z)\} \neq 0 \text{ and } \det\{\Psi(z)\} \neq 0 \,, \text{ for all } |z| \leq 1 \,. \tag{11.7}$$

Note also that we can find real constants $C > 0$ and $\rho \in (0, 1)$ such that

$$\|\Pi_\tau\| \leq C\rho^\tau \text{ and } \|\Psi_\tau\| \leq C\rho^\tau \,, \tag{11.8}$$

hence

$$\sum_{\tau=1}^{\infty} \|\Pi_\tau\| < \infty \,, \quad \sum_{\tau=1}^{\infty} \|\Psi_\tau\| < \infty \,, \tag{11.9}$$

where $\|.\|$ is the Schur norm for a matrix (see Horn and Johnson (1985)), i.e.

$$\|M\|^2 = \operatorname{tr}(M'M) \,. \tag{11.10}$$

2.2 Echelon form

It is well known that the standard VARMA(p, q) representation given by (11.1) is not unique, in the sense that different sets of coefficients A_i and B_j may represent the same autocovariance structure. To ensure a unique parameterization, we shall consider the stationary invertible VARMA(p, q) process in echelon form representation. Such a representation can be defined as follows:

$$\Phi(L) Y_t = \Theta(L) u_t \,, \tag{11.11}$$

$$\Phi(L) = \Phi_0 - \sum_{i=1}^{\bar{p}} \Phi_i L^i \,, \quad \Theta(L) = \Theta_0 + \sum_{j=1}^{\bar{p}} \Theta_j L^j \,, \tag{11.12}$$

where L denotes the lag operator, $\Phi_i = [\phi_{lm\,i}]_{l,m=1,\ldots,k}$ and $\Theta_j = [\theta_{lm,j}]_{l,m=1,\ldots,k}$, $\bar{p} = \max(p, q)$, $\Theta_0 = \Phi_0$, and Φ_0 is a lower-triangular

matrix whose diagonal elements are all equal to one. The VARMA representation (11.11) has an echelon form if $\Phi(L) = [\phi_{lm}(L)]_{l,m=1,\ ,k}$ and $\Theta(L) = [\theta_{lm}(L)]_{l,m=1,\ ,k}$ satisfy the following conditions: given a vector of orders $(p_1,\ ,p_k)$ called the *Kronecker indices*, the operators $\phi_{lm}(L)$ and $\theta_{lm}(L)$ on any given row l of $\Phi(L)$ and $\Theta(L)$ have the same degree p_l $(1 \leq l \leq k)$ and

$$
\begin{aligned}
\phi_{lm}(L) \quad &= 1 - \sum_{i=1}^{p_l} \phi_{ll,i} L^i \qquad \text{if } l = m \,, \\
&= - \sum_{i=p_l-p_{lm}+1}^{p_l} \phi_{lm,i} L^i \quad \text{if } l \neq m \,,
\end{aligned}
\tag{11 13}
$$

$$
\theta_{lm}(L) = \sum_{j=0}^{p_l} \theta_{lm,j} L^j \quad \text{with } \Theta_0 = \Phi_0 \,, \tag{11.14}
$$

for $l, m = 1,\ .\ , k$, where

$$
\begin{aligned}
p_{lm} \quad &= \min(p_l+1, p_m) \quad \text{for } l \geq m \,, \\
&= \min(p_l, p_m) \qquad \text{for } l < m
\end{aligned}
\tag{11.15}
$$

Clearly, $p_{ll} = p_l$ is the order of the polynomial (i e., the number of free coefficients) on the l-th diagonal element of $\Phi(L)$ as well as the order of the polynomials on the corresponding row of $\Theta(L)$, while p_{lm} specifies the number of free coefficients in the operator $\phi_{lm}(L)$ for $l \neq m$ The sum of the Kronecker indices $\sum_{l=1}^{k} p_l$ is called the McMillan degree The P matrix formed by the Kronecker indices associated with the model is $P = [p_{lm}]_{l,m=1,\ ,k}$ This leads to $\sum_{l=1}^{k}\sum_{m=1}^{k} p_{lm}$ autoregressive and $k\sum_{l=1}^{k} p_l$ moving average free coefficients, respectively. Obviously, for the VARMA orders we have $\bar{p} = \max(p_1,\ , p_k)$. Note that this identified parameterization for VARMA(p,q) models ensures the uniqueness of left-coprime operators $\Phi(L)$ and $\Theta(L)$ Although other identifiable parameterizations could be used – such as the final equations form – the echelon form tends to be more parsimonious and can lead to efficiency gains For proofs of the uniqueness of the echelon form and for other identification conditions, the reader should consult to Hannan (1969, 1970, 1976a, 1979), Deistler and Hannan (1981), Hannan and Deistler (1988) and Lütkepohl (1991, Chapter 7).

The stationarity and invertibility conditions for echelon form of (11 11) are the same as usual, namely

$$
\det\{\Phi(z)\} \neq 0 \quad \text{for all } |z| \leq 1 \,, \tag{11 16}
$$

for stationarity, and

$$
\det\{\Theta(z)\} \neq 0 \quad \text{for all } |z| \leq 1 \,, \tag{11 17}
$$

for invertibility, where

$$\Phi(z) = \Phi_0 - \sum_{i=1}^{\bar{p}} \Phi_i z^i, \quad \Theta(z) = \Theta_0 + \sum_{j=1}^{\bar{p}} \Theta_j z^j, \tag{11.18}$$

with $\Pi(z) = \Theta(z)^{-1}\Phi(z)$ and $\Psi(z) = \Phi(z)^{-1}\Theta(z)$ It will be useful to observe that (11 11) can be rewritten in the following form

$$Y_t = (I_k - \Phi_0)V_t + \sum_{i=1}^{\bar{p}} \Phi_i Y_{t-i} + \sum_{j=1}^{\bar{p}} \Theta_j u_{t-j} + u_t, \tag{11 19}$$

where

$$V_t = Y_t - u_t = \Phi_0^{-1}\Big[\sum_{i=1}^{\bar{p}} \Phi_i Y_{t-i} + \sum_{j=1}^{\bar{p}} \Theta_j u_{t-j}\Big]. \tag{11 20}$$

Note that V_t is a function of *lagged* values of Y_t and u_t, so that the error term u_t in (11.19) is uncorrelated with all the other variables on the right-hand side of the equation
    Set

$$X_t = \begin{bmatrix} V_t', Y_{t-1}', & , Y_{t-\bar{p}}', u_{t-1}', & . , u_{t-\bar{p}}' \end{bmatrix}', \tag{11 21}$$
$$D = \begin{bmatrix} I_k - \Phi_0, \Phi_1, & , \Phi_{\bar{p}}, \Theta_1, & , \Theta_{\bar{p}} \end{bmatrix}'. \tag{11.22}$$

The vector X_t has dimension $(kh) \times 1$ where $h = 2\bar{p} + 1$ while D is a $(kh) \times k$ matrix of coefficients In view of (11 20), it is clear the covariance matrix of X_t is singular, so it is crucial that (identifying) restrictions be imposed on model coefficients Under the restrictions of the echelon form (11 12)–(11.15), we can find a unique $(k^2 h) \times \nu$ full rank matrix R such that $\beta = R\eta$, where η is a $\nu \times 1$ vector of free coefficients and $\nu < k^2 h$ Thus Y_t in (11.19) can be expressed as

$$Y_t = D'X_t + u_t = \left(I_k \otimes X_t'\right)R\eta + u_t \tag{11 23}$$

The structure of R is such that

$$\beta = \text{vec}(D) = R\eta, \tag{11 24}$$

$$R = \text{diag}(R_1, \quad . , R_k) = \begin{bmatrix} R_1 & 0 & \cdot\cdot & 0 \\ 0 & R_2 & \cdot & \vdots \\ & & & 0 \\ 0 & 0 & \cdot & R_k \end{bmatrix}, \tag{11 25}$$

where R_i, $i = 1, 2, \ldots, k$, are $(kh) \times \nu_i$ full-rank selection (zero-one) matrices, each one of which selects the non-zero elements of the corresponding equation, and ν_i is the number of freely varying coefficients present in the i-th equation. The structure of R_i is such that $R_i' R_i = I_{\nu_i}$ and $\beta_i = R_i \eta_i$ where β_i and η_i are respectively a $(kh) \times 1$ and $\nu_i \times 1$ vectors so that β_i is the unconstrained parameter vector in the i-th equation of (11.19) – on which zero restrictions are imposed – and η_i is the corresponding vector of free parameters.

$$\beta = \left(\beta_1', \beta_2', \ldots, \beta_k'\right)', \quad \eta = \left(\eta_1', \eta_2', \ldots, \eta_k'\right)'. \tag{11 26}$$

Note also that successful identification entails that

$$\mathrm{rank}\left\{\mathsf{E}\left[R'\left(I_k \otimes X_t\right)\left(I_k \otimes X_t'\right)R\right]\right\} = \mathrm{rank}\left\{R'\left(I_k \otimes \Gamma\right)R\right\} = \nu \tag{11 27}$$

where $\Gamma = \mathsf{E}(X_t X_t')$, or equivalently

$$\mathrm{rank}\left\{\mathsf{E}\left[R_i' X_t X_t' R_i\right]\right\} = \mathrm{rank}\left\{R_i' \Gamma R_i\right\} = \nu_i, \quad i = 1, \ldots, k. \tag{11.28}$$

Setting

$$X(T) = [X_1, \ldots, X_T]', \tag{11.29}$$

$$Y(T) = [Y_1, \ldots, Y_T]' = [y_1(T), \ldots, y_k(T)], \tag{11.30}$$

$$U(T) = [u_1, \ldots, u_T]' = [U_1(T), \ldots, U_k(T)], \tag{11.31}$$

$$y(T) = \mathrm{vec}[Y(T)], \quad u(T) = \mathrm{vec}[U(T)], \tag{11.32}$$

(11 23) can be put in any one of the two following matrix forms:

$$Y(T) = X(T)D + U(T), \tag{11.33}$$

$$y(T) = [I_k \otimes X(T)]R\eta + u(T), \tag{11.34}$$

where $[I_k \otimes X(T)]R$ is a $(kT) \times \nu$ matrix. In the sequel, we shall assume that

$$\mathrm{rank}\left([I_k \otimes X(T)]R\right) = \nu \text{ with probability 1.} \tag{11.35}$$

Under the assumption that the process is a regular process with continuous distribution, it is easy that the latter must hold

To see better how the echelon restrictions should be written, consider the following VARMA$(2, 1)$ model in echelon form:

$$Y_{1,t} = \phi_{11,1} Y_{1,t-1} + \phi_{11,2} Y_{1,t-2} + u_{1,t}, \tag{11.36}$$

$$Y_{2,t} = \phi_{21,0}\left(Y_{1,t} - u_{1,t}\right) + \phi_{21,1} Y_{1,t-1} + \phi_{22,1} Y_{2,t-1} + \theta_{22,1} u_{2,t-1} + u_{2,t}. \tag{11 37}$$

In this case, we have:

$$\Phi(L) = \begin{bmatrix} 1 - \phi_{11,1}L - \phi_{11,2}L^2 & -\phi_{12,2}L^2 \\ -\phi_{21,0} - \phi_{21,1}L & 1 - \phi_{22,1}L \end{bmatrix}, \tag{11.38}$$

$$\Theta(L) = \begin{bmatrix} 1 + \theta_{11,1}L + \theta_{11,2}L^2 & \theta_{12,1}L + \theta_{12,2}L^2 \\ \theta_{21,1}L & 1 + \theta_{22,1}L \end{bmatrix}, \tag{11.39}$$

with $\phi_{12,2} = 0$, $\theta_{11,1} = 0$, $\theta_{11,2} = 0$, $\theta_{12,1} = 0$, $\theta_{12,2} = 0$, $\theta_{21,1} = 0$, so that the Kronecker indices are $p_1 = p_{11} = 2$, $p_2 = p_{22} = 1$, $p_{21} = 2$ and $p_{12} = 1$ Setting $X_t = \left[V_t', Y_{t-1}', Y_{t-2}', u_{t-1}'\right]'$, $V_t = (V_{1,t}, V_{2,t})'$, $V_{1,t} = (Y_{1,t} - u_{1,t})$ and $V_{2,t} = (Y_{2,t} - u_{2,t})$, we can then write·

$$\begin{bmatrix} Y_{1,t} \\ Y_{2,t} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ \phi_{21,0} & 0 \end{bmatrix} \begin{bmatrix} V_{1,t} \\ V_{2,t} \end{bmatrix} + \begin{bmatrix} \phi_{11,1} & 0 \\ \phi_{21,1} & \phi_{22,1} \end{bmatrix} \begin{bmatrix} Y_{1,t-1} \\ Y_{2,t-1} \end{bmatrix}$$
$$+ \begin{bmatrix} \phi_{11,2} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Y_{1,t-2} \\ Y_{2,t-2} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \theta_{22,1} \end{bmatrix} \begin{bmatrix} u_{1,t-1} \\ u_{2,t-1} \end{bmatrix} + \begin{bmatrix} u_{1,t} \\ u_{2,t} \end{bmatrix} \tag{11.40}$$

Here we have·

$$\beta = (0, 0, \phi_{11,1}, 0, \phi_{11,2}, 0, 0, 0, \phi_{21,0}, 0, \phi_{21,1}, \phi_{22,1}, 0, 0, 0, \theta_{22,1})', \tag{11.41}$$

$$\eta = (\phi_{11,1}, \phi_{11,2}, \phi_{21,0}, \phi_{21,1}, \phi_{22,1}, \theta_{22,1})', \tag{11.42}$$

$$[I_k \otimes X_t'] R = \begin{bmatrix} Y_{1,t-1} & Y_{1,t-2} & 0 & 0 & 0 & 0 \\ 0 & 0 & V_{1,t} & Y_{1,t-1} & Y_{2,t-1} & u_{2,t-1} \end{bmatrix}, \tag{11.43}$$

and

$$[I_k \otimes X(T)] R = \begin{bmatrix} Y_{1,0} & Y_{1,-1} & 0 & 0 & 0 & 0 \\ 0 & 0 & V_{1,1} & Y_{1,0} & Y_{2,0} & u_{2,0} \\ Y_{1,1} & Y_{1,0} & 0 & 0 & 0 & 0 \\ 0 & 0 & V_{1,2} & Y_{1,1} & Y_{2,1} & u_{2,1} \\ & & \vdots & & & \\ Y_{1,T-1} & Y_{1,T-2} & 0 & 0 & 0 & 0 \\ 0 & 0 & V_{1,T} & Y_{1,T-1} & Y_{2,T-1} & u_{2,T-1} \end{bmatrix} \tag{11.44}$$

The appropriate matrix R is given by·

$$R' = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{11.45}$$

2.3   Regularity assumptions

In order to establish the asymptotic distribution of the linear estimator defined below, we will need further assumptions on the innovation process and the truncation lag of the first step autoregression We now state the assumptions we shall consider.

ASSUMPTION 11 1 STRONG WHITE NOISE INNOVATIONS. *The vectors* u_t, $t \in \mathbb{Z}$, *are independent and identically distributed (i i d.) with mean zero, covariance matrix* Σ_u *and continuous distribution.*

ASSUMPTION 11 2 UNIFORM BOUNDEDNESS OF FOURTH MOMENTS *There is a finite constant* m_4 *such that, for all* $1 \leq i, j, r, s \leq k$ *and for all* t,

$$\mathsf{E} \left| u_{it} u_{jt} u_{rt} u_{st} \right| \leq m_4 < \infty$$

ASSUMPTION 11 3 AUTOREGRESSIVE TRUNCATION LAG OF ORDER LESS THAN $T^{1/2}$ n_T *is a function of* T *such that*

$$n_T \to \infty \ \text{and} \ n_T^2 / T \to 0 \ as \ T \to \infty \tag{11.46}$$

and, for some $c > 0$ *and* $0 < \bar{\delta} < 1/2$,

$$n_T \geq c T^{\bar{\delta}} \ \text{for} \ T \ \text{sufficiently large.} \tag{11.47}$$

ASSUMPTION 11.4 DECAY RATE OF TRUNCATED AUTOREGRESSIVE COEFFICIENTS. *The coefficients of the autoregressive (11.3) representation*

$$n_T^{1/2} \sum_{\tau = n_T + 1}^{\infty} \| \Pi_\tau \| \to 0 \ as \ T \to \infty. \tag{11.48}$$

Assumption 11.1 means that we have a strong VARMA process, while Assumption 11.2 on moments of order four will ensure the empirical autocovariances of the process have finite variances. Assumption 11.3 implies that n_T goes to infinity at a rate slower than $T^{1/2}$; for example, the assumption is satisfied if $n_T = c T^\delta$ with $0 < \bar{\delta} \leq \delta < 1/2$. Assumption 11.4 characterizes the rate of decay of autoregressive coefficients in relation with n_T.

Although the above assumptions are sufficient to show consistency of the two-stage linear estimator, we will need another assumption to show that the asymptotic distribution is normal with a distribution which is unaffected by the use of estimated innovations.

ASSUMPTION 11.5 AUTOREGRESSIVE TRUNCATION LAG OF ORDER
LESS THAN $T^{1/4}$. n_T *is a function of* T *such that*

$$n_T \to \infty \quad \text{and} \quad n_T^4/T \to 0 \quad \text{as } T \to \infty. \tag{11.49}$$

The latter assumption means that n_T goes to infinity at a rate slower than $T^{1/4}$; for example, it is satisfied if $n_T = cT^\delta$ with $0 < \bar{\delta} \le \delta < 1/4$. It is easy to see that the condition (11.49) entails (11.46). Finally, it is worthwhile to note that (11.48) holds for VARMA processes whenever $n_T = cT^\delta$ with $c > 0$ and $\delta > 0$, i.e.

$$T^\delta \sum_{\tau=n_T+1}^{\infty} \|\Pi_\tau\| \to 0 \text{ as } T \to \infty, \quad \text{for all } \delta > 0. \tag{11.50}$$

This is easy to see from the exponential decay property of VARMA processes (see (11.8)).

3. Two-step linear estimation

In this section, we describe a simple estimation procedure for a VARMA models in echelon form with known order. The Kronecker indices characterizing the echelon form VARMA model are taken as given, and we focus our attention on the estimation of the autoregressive and moving average coefficients.

Let $(Y_{-n_T+1}, \dots, Y_T)$ be a random sample of size $T + n_T$, where n_T goes to infinity as T goes to infinity. We consider first a "long" multivariate linear vector autoregression:

$$Y_t = \sum_{\tau=1}^{n_T} \Pi_\tau Y_{t-\tau} + u_t(n_T), \quad t = 1, \dots, T, \tag{11.51}$$

and the corresponding least squares estimates:

$$\tilde{\Pi}(n_T) = \left[\tilde{\Pi}_1(n_T), \dots, \tilde{\Pi}_{n_T}(n_T)\right]. \tag{11.52}$$

Such an estimation can be performed by running k separate univariate linear regressions (one for each variable in Y_t). Yule-Walker estimates of the corresponding theoretical coefficients Π_τ could also be considered. Then, under model (11.3) and the Assumptions 11.1 to 11.4, it follows from the results of Paparoditis (1996, Theorem 2.1) and Lewis and Reinsel (1985, proof of Theorem 1) that:

$$\|\tilde{\Pi}(n_T) - \Pi(n_T)\| = O_p(n_T^{1/2}/T^{1/2}) \tag{11.53}$$

where

$$\Pi\left(n_T\right) = \left[\Pi_1, \ldots, \Pi_{n_T}\right]. \qquad (11.54)$$

As usual, for any sequence of random variables Z_T and positive numbers r_T, $T = 1, 2, \ldots$, the notation $Z_T = O_p(r_T)$ means that Z_T/r_T is asymptotically bounded in probability (as $T \to \infty$), while $Z_T = o_p(r_T)$ means that Z_T/r_T converges to zero in probability. When Y_t satisfies a VARMA scheme, the Assumptions 11.3 and 11.4 are satisfied by any truncation lag of the form $n_T = cT^\delta$ with $c > 0$ and $0 < \delta < 1/2$. If, furthermore, the Assumptions 11.3 and 11.4 are replaced by stronger ones, namely

$$n_T \to \infty \text{ and } n_T^3/T \to 0 \text{ as } T \to \infty, \qquad (11.55)$$

$$T^{1/2} \sum_{\tau=n_T+1}^{\infty} \|\Pi_\tau\| \to 0 \text{ as } T \to \infty, \qquad (11.56)$$

then asymptotic normality also holds:

$$T^{1/2} l\left(n_T\right)' \left[\tilde\pi\left(n_T\right) - \pi\left(n_T\right)\right] \xrightarrow[T\to\infty]{} \mathrm{N}\left[0, l\left(n_T\right)' Q(n_T) l\left(n_T\right)\right], \quad (11.57)$$

where $l\left(n_T\right)$ is a sequence of $k^2 n_T \times 1$ vectors such that $0 < M_1 \le \|l\left(n_T\right)\| \le M_2 < \infty$ for $n_T = 1, 2, \ldots$, and

$$\tilde\pi\left(n_T\right) - \pi\left(n_T\right) = \mathrm{vec}\left[\tilde\Pi\left(n_T\right) - \Pi\left(n_T\right)\right], \qquad (11.58)$$

$$Q(n_T) = \Gamma(n_T)^{-1} \otimes \Sigma_u, \ \ \Gamma(n_T) = \mathsf{E}[Y_t(n_T)Y_t(n_T)'], \qquad (11.59)$$

$$Y_t(n_T) = \left[Y_{t-1}', Y_{t-2}', \ldots, Y_{t-n_T}'\right]'. \qquad (11.60)$$

Note that a possible choice for the sequence n_T that satisfies both $n_T^3/T \to 0$ and $T^{1/2} \sum_{\tau=n_T+1}^{\infty} \|\Pi_\tau\| \to 0$ is for example $n_T = T^{1/\varepsilon}$ with $\varepsilon > 3$. On the other hand $n_T = \ln(\ln T)$, as suggested by Hannan, and Kavalieris (1984*b*), is not a permissible choice because in general $T^{1/2} \sum_{\tau=n_T+1}^{\infty} \|\Pi_\tau\|$ does not approach zero as $T \to \infty$.

Let

$$\tilde{u}_t(n_T) = Y_t - \sum_{\tau=1}^{n_T} \tilde\Pi_\tau(n_T) Y_{t-\tau} = Y_t - \tilde\Pi\left(n_T\right) Y_t(n_T) \qquad (11.61)$$

be the estimated residuals obtained from the first stage estimation procedure.

$$\tilde\Sigma_u(n_T) = \frac{1}{T} \sum_{t=1}^{T} \tilde{u}_t(n_T)\tilde{u}_t(n_T)' \qquad (11.62)$$

the corresponding estimator of the innovation covariance matrix, and

$$\hat{\Sigma}_T = \frac{1}{T} \sum_{t=1}^{T} u_t u_t' \tag{11.63}$$

the covariance "estimator" based on the true innovations. Then, we have the following equivalences and convergences.

PROPOSITION 11.1   INNOVATION COVARIANCE ESTIMATOR CONSISTENCY. *Let* $\{Y_t : t \in \mathbb{Z}\}$ *be a* k-*dimensional stationary invertible stochastic process with the VARMA echelon representation given by (11.11)–(11.15). Then, under the Assumptions 11.1 to 11.4, we have:*

$$\left\| \frac{1}{T} \sum_{t=1}^{T} u_t [\tilde{u}_t(n_T) - u_t]' \right\| = O_p\left(\frac{n_T}{T}\right), \tag{11.64}$$

$$\frac{1}{T} \sum_{t=1}^{T} \|\tilde{u}_t(n_T) - u_t\|^2 = O_p\left(\frac{n_T^2}{T}\right), \tag{11.65}$$

$$\left\| \frac{1}{T} \sum_{t=1}^{T} [\tilde{u}_t(n_T) - u_t][\tilde{u}_t(n_T) - u_t]' \right\| = O_p\left(\frac{n_T^2}{T}\right), \tag{11.66}$$

$$\|\tilde{\Sigma}_u(n_T) - \hat{\Sigma}_T\| = O_p\left(\frac{n_T^2}{T}\right), \quad \|\tilde{\Sigma}_u(n_T) - \Sigma_u\| = O_p\left(\frac{n_T^2}{T}\right). \tag{11.67}$$

The asymptotic equivalence between $\tilde{u}_t(n_T)$ and u_t stated in the above proposition suggests we may be able to consistently estimate the parameters of the VARMA model in (11.19) after replacing the unobserved lagged innovations $u_{t-1}, \ldots, u_{t-\bar{p}}$ with the corresponding residuals $\tilde{u}_{t-1}(n_T), \ldots, \tilde{u}_{t-\bar{p}}(n_T)$ from the above long autoregression. So, in order to estimate the coefficients Φ_i and Θ_j of the VARMA process, we consider a linear regression of the form

$$Y_t = \sum_{i=1}^{\bar{p}} \Phi_i Y_{t-i} + \sum_{j=1}^{\bar{p}} \Theta_j \tilde{u}_{t-j}(n_T) + e_t(n_T) \tag{11.68}$$

imposing the (exclusion) restrictions associated with the echelon form. Setting

$$\check{V}_t(n_T) = Y_t - \tilde{u}_t(n_T), \tag{11.69}$$

this regression can also be put in a regression form similar to (11.19):

$$Y_t = (I_k - \Phi_0)\,\check{V}_t(n_T) + \sum_{i=1}^{\bar{p}} \Phi_i Y_{t-i} + \sum_{j=1}^{\bar{p}} \Theta_j \tilde{u}_{t-j}(n_T) + e_t(n_T), \tag{11.70}$$

where

$$e_t(n_T) = \tilde{u}_t(n_T) + \sum_{j=0}^{\bar{p}} \Theta_j [u_{t-j} - \tilde{u}_{t-j}(n_T)] . \tag{11.71}$$

Note that (11.70) can be written as

$$Y_t = \left[I_k \otimes \tilde{X}_t(n_T)' \right] R\eta + e_t(n_T), \quad t = 1, \ldots, T , \tag{11.72}$$

where

$$\tilde{X}_t(n_T) = \left[\tilde{V}_t(n_T)', Y_{t-1}', \ldots, Y_{t-p}', \tilde{u}_{t-1}(n_T)', \ldots, \tilde{u}_{t-\bar{p}}(n_T)' \right]' . \tag{11.73}$$

Therefore the second step estimators $\tilde{\eta}$ can be obtained by running least squares on the equations (11.72). Setting

$$\tilde{X}(n_T) = \left[\tilde{X}_1(n_T), \tilde{X}_2(n_T), \ldots, \tilde{X}_T(n_T) \right]' \tag{11.74}$$

we get, after some manipulations,

$$\begin{aligned}
\tilde{\eta} &= \{ R' \left[I_k \otimes \tilde{X}(n_T)' \tilde{X}(n_T) \right] R \}^{-1} R' [I_k \otimes \tilde{X}(n_T)'] y(T) \\
&= (\tilde{\eta}_1', \tilde{\eta}_2', \ldots, \tilde{\eta}_k')'
\end{aligned} \tag{11.75}$$

where

$$\tilde{\eta}_i = [R_i' \tilde{X}(n_T)' \tilde{X}(n_T) R_i]^{-1} R_i' \tilde{X}(n_T)' y_i(T) . \tag{11.76}$$

$\tilde{\eta}$ can be easily obtained by stacking the single equation LS estimators $\tilde{\eta}_i$ which are obtained by regressing y_i on $\tilde{X}(n_T)R_i$.

4.   Asymptotic distribution

We will now study the asymptotic distribution of the linear estimator described in the previous section. For that purpose, we note first that the estimator $\tilde{\eta}$ in (11.75) can be expressed as

$$\tilde{\eta} = \{ R'[I_k \otimes \tilde{\Gamma}(n_T)] \} R \}^{-1} \{ \frac{1}{T} \sum_{t=1}^{T} R'[I_k \otimes \tilde{X}_t(n_T)] Y_t \} \tag{11.77}$$

where

$$\tilde{\Gamma}(n_T) = \frac{1}{T} \sum_{t=1}^{T} \tilde{X}_t(n_T) \tilde{X}_t(n_T)' . \tag{11.78}$$

Let also

$$\tilde{\Upsilon}(n_T) = I_k \otimes \tilde{\Gamma}(n_T), \quad \tilde{Q}(n_T) = [R' \tilde{\Upsilon}(n_T) R]^{-1} , \tag{11.79}$$

$$\tilde{\Omega}(n_T) = \frac{1}{T} \sum_{t=1}^{T} R'[I_k \otimes \tilde{X}_t(n_T)]e_t(n_T) \,. \tag{11.80}$$

It is then easy to see that

$$\tilde{\eta} - \eta = \tilde{Q}(n_T)\tilde{\Omega}(n_T) \tag{11.81}$$

hence

$$\|\tilde{\eta} - \eta\| \leq \|\tilde{Q}(n_T)\|_1 \|\tilde{\Omega}(n_T)\| \leq \|\tilde{Q}(n_T)\| \|\tilde{\Omega}(n_T)\| \tag{11.82}$$

where $\|A\|_1 = \sup\limits_{x \neq 0} \left\{ \frac{\|Ax\|}{\|x\|} \right\}$ stands for the largest eigenvalue of $A'A$ and we used the inequality $\|AB\|^2 \leq \|A\|_1^2 \|B\|^2$ for any two conformable matrices A and B (see Horn, and Johnson (1985), Section 5.6).

Define

$$\Gamma = \mathsf{E}\left(X_t X_t'\right), \quad \Upsilon = I_k \otimes \Gamma, \quad Q = (R'\Upsilon R)^{-1}, \tag{11.83}$$

$$\Gamma_T = \frac{1}{T} \sum_{t=1}^{T} X_t X_t', \quad \Upsilon_T = I_k \otimes \Gamma_T = \frac{1}{T} \sum_{t=1}^{T} I_k \otimes X_t X_t', \tag{11.84}$$

$$Q_T = (R'\Upsilon_T R)^{-1}, \quad \Omega_T = \frac{1}{T} \sum_{t=1}^{T} R'(I_k \otimes X_t)u_t \,. \tag{11.85}$$

Note that $R'\Upsilon R$ is positive definite by the regularity assumption. To study the convergence and distributional properties of $\tilde{\eta} - \eta$, we need first to establish the following proposition.

PROPOSITION 11.2 *Let* $\{Y_t : t \in \mathbb{Z}\}$ *be a k-dimensional stationary invertible stochastic process with the VARMA echelon representation given by (11.11)–(11.15). Then, under the Assumptions 11.1 to 11.4, we have the following equivalences:*

$$\frac{1}{T}\|\tilde{X}(n_T) - X(T)\|^2 = O_p\left(\frac{n_T^2}{T}\right), \tag{11.86}$$

$$\|\tilde{\Gamma}(n_T) - \Gamma_T\| = O_p\left(\frac{n_T}{T^{1/2}}\right), \tag{11.87}$$

$$\|\tilde{\Upsilon}(n_T) - \Upsilon_T\| = O_p\left(\frac{n_T}{T^{1/2}}\right), \tag{11.88}$$

$$\|\tilde{Q}(n_T)^{-1} - Q^{-1}\| = O_p\left(\frac{n_T}{T^{1/2}}\right), \tag{11.89}$$

$$\|\tilde{Q}(n_T) - Q\| = O_p\left(\frac{n_T}{T^{1/2}}\right). \tag{11.90}$$

The latter proposition shows that the matrices $\tilde{\Gamma}(n_T), \tilde{\Upsilon}(n_T), \tilde{Q}(n_T)^{-1}$ and $\tilde{Q}(n_T)$ – based on approximate innovations (estimated from a long autoregression) – are all asymptotically equivalent to the corresponding matrices based on true innovations, according to the rate $n_T/T^{1/2}$. Similarly the norm of the difference between the approximate regressor matrix $\tilde{X}(n_T)$ and $X(T)$ has order $O_p(n_T/T^{1/2})$. This suggests that $\tilde{\eta}$ converges to η, and we give the appropriate rate of convergence in the following theorem.

THEOREM 11.1 CONSISTENCY OF SECOND STEP HR ESTIMATES. *Let* $\{Y_t : t \in \mathbb{Z}\}$ *be a k-dimensional stationary invertible stochastic process with the VARMA echelon representation given by (11.11)–(11.15). Then, under the Assumptions 11.1 to 11.4, we have*

$$\|\Omega_T\| = O_p\left(\frac{1}{T^{1/2}}\right), \quad \|\Omega(n_T) - \Omega_T\| = O_p\left(\frac{n_T^2}{T}\right), \qquad (11.91)$$

$$\|\tilde{\eta} - \eta\| = O_p\left(\frac{1}{T^{1/2}}\right) + O_p\left(\frac{n_T^2}{T}\right). \qquad (11.92)$$

If, furthermore,

$$n_T^4/T \to 0 \ as \ T \to \infty, \qquad (11.93)$$

then

$$\|\tilde{\eta} - \eta\| = O_p\left(\frac{1}{T^{1/2}}\right). \qquad (11.94)$$

The latter theorem shows that $\tilde{\eta}$ is a consistent estimator. If furthermore, $n_T^4/T \to 0$ as $T \to \infty$, then $\tilde{\eta}$ converges at the rate $T^{-1/2}$ which is typically expected to get asymptotic normality. In order to derive an asymptotic distribution for $\tilde{\eta}$, we shall establish that the following random matrices

$$\tilde{S}(n_T) = T^{1/2}\tilde{Q}(n_T)\tilde{\Omega}(n_T), \quad S_T = T^{1/2}Q\Omega_T, \qquad (11.95)$$

are asymptotically equivalent.

PROPOSITION 11.3 ASYMPTOTIC EQUIVALENCE. *Let* $\{Y_t : t \in \mathbb{Z}\}$ *be a k-dimensional stationary invertible stochastic process with the VARMA echelon representation given by (11.11)–(11.15). Then, under the Assumptions 11.1 to 11.4, the following equivalence holds*

$$\|\tilde{S}(n_T) - S_T\| = O_p\left(\frac{n_T^2}{T^{1/2}}\right).$$

Finally, we can give the asymptotic distribution of $\sqrt{T}\,(\tilde{\eta} - \eta)$.

THEOREM 11.2 ASYMPTOTIC DISTRIBUTION OF TWO-STAGE ESTIMA-
TOR. *Let $\{Y_t : t \in \mathbb{Z}\}$ be a k-dimensional stationary invertible stochastic process with the VARMA echelon representation given by (11.11)–(11.15). If the Assumptions 11.1 to 11.5 are satisfied, then the asymptotic distribution of the estimator $\tilde{\eta}$ is the following:*

$$\sqrt{T}\,(\tilde{\eta} - \eta) \xrightarrow[T \to \infty]{} \mathrm{N}(0, \Sigma_\eta)$$

where

$$\Sigma_\eta = Q\Sigma_{Xu}Q', \quad \Sigma_{Xu} = R'\left[\Sigma_u \otimes \Gamma\right]R, \qquad (11.96)$$

$$Q = (R'\Upsilon R)^{-1}, \quad \Upsilon = I_k \otimes \Gamma, \quad \Gamma = \mathsf{E}\left(X_t X_t'\right), \qquad (11.97)$$

$$X_t = \left[V_t', Y_{t-1}', \ldots, Y_{t-\bar{p}}', u_{t-1}', \ldots, u_{t-\bar{p}}'\right]' \ and \ V_t = Y_t - u_t\,.$$

An important consequence of the above theorem is the fact that the asymptotic distribution of $\tilde{\eta}$ is the same as in the case where the innovations $u_{t-1}', \ldots, u_{t-\bar{p}}'$ are known rather than approximated by a long autoregression. Furthermore, the covariance matrix Σ_η can be consistently estimated by

$$\hat{\Sigma}_\eta = \tilde{Q}(n_T)\{R'\left[\tilde{\Sigma}_u(n_T) \otimes \tilde{\Gamma}(n_T)\right]R\}\tilde{Q}(n_T)', \qquad (11.98)$$

where

$$\tilde{Q}(n_T) = [R'\tilde{\Upsilon}(n_T)R]^{-1}, \quad \tilde{\Upsilon}(n_T) = I_k \otimes \tilde{\Gamma}(n_T), \qquad (11.99)$$

$$\tilde{\Gamma}(n_T) = \frac{1}{T}\sum_{t=1}^{T}\tilde{X}_t(n_T)\tilde{X}_t(n_T)'. \qquad (11.100)$$

Standard t and F-type tests may then be performed in the usual way.

5. Conclusion

In this paper, we have provided the asymptotic distribution of a simple two-stage estimator for VARMA models in echelon form. The estimator is consistent when the auxiliary long autoregression used to generate first step estimates of model innovations has an order n_T which increases to infinity at a rate inferior to T^δ with $0 < \delta_0 \leq \delta < 1/2$. Further, it has an asymptotic normal distribution provided n_T increases at a rate inferior to T^δ with $0 < \delta_0 \leq \delta < 1/4$. In the latter case, the asymptotic

distribution is not affected by the fact that estimated lagged residuals are used.

The above results can be exploited in several ways. First, the two-stage estimates and the associated distributional theory can be directly used for inference on the VARMA model. In particular, they can be used for model selection purposes and to simplify the model (e.g., by eliminating insignificant coefficients). Second, two-stage estimates can be exploited to get more efficient estimators, such as ML estimators or estimators that are asymptotically to ML. This can be done, in particular, to achieve efficiency with Gaussian innovations. Note, however, that such gains of efficiency may not obtain if the innovations are not Gaussian. Thirdly, because of its simplicity, the two-stage linear estimator is especially well adapted for being used in the context of simulation-based inference procedures, such as bootstrap tests. Further, the asymptotic distribution provided above can be useful in order to improve the validity of the bootstrap. Several of these issues will be studied in a subsequent paper.

Appendix: Proofs

PROOF OF PROPOSITION 11.1

Let us write·

$$\|\tilde{\Sigma}_u(n_T) - \Sigma_u\| = \|\tilde{\Sigma}_u(n_T) - \hat{\Sigma}_T\| + \|\hat{\Sigma}_T - \Sigma_u\| \tag{A.1}$$

where

$$\hat{\Sigma}_T - \Sigma_u = \frac{1}{T} \sum_{t=1}^{T} [u_t u_t' - \Sigma_u], \tag{A.2}$$

$$\begin{aligned}
\tilde{\Sigma}_u(n_T) - \hat{\Sigma}_T &= \frac{1}{T} \sum_{t=1}^{T} \left\{ \tilde{u}_t(n_T) \tilde{u}_t(n_T)' - u_t u_t' \right\} \\
&= \frac{1}{T} \sum_{t=1}^{T} \left\{ [\tilde{u}_t(n_T) - u_t] \bar{u}_t(n_T)' + u_t [\tilde{u}_t(n_T) - u_t]' \right\} \\
&= \frac{1}{T} \sum_{t=1}^{T} \left\{ [\bar{u}_t(n_T) - u_t] u_t' + u_t [\tilde{u}_t(n_T) - u_t]' + [\tilde{u}_t(n_T) - u_t][\bar{u}_t(n_T) - u_t]' \right\}
\end{aligned}$$

$$\tag{A.3}$$

By the Assumptions 11.1 and 11.2,

$$\hat{\Sigma}_T - \Sigma_u = \frac{1}{T} \sum_{t=1}^{T} [u_t u_t' - \Sigma_u] = O_p\left(\frac{1}{T}\right), \tag{A.4}$$

$$\frac{1}{T} \sum_{t=1}^{T} \|u_t\| = O_p(1), \quad \frac{1}{T} \sum_{t=1}^{T} \|u_t\|^2 = O_p(1). \tag{A.5}$$

Now

$$\tilde{u}_t(n_T) - u_t = [\Pi(n_T) - \tilde{\Pi}(n_T)]Y_t(n_T) + \sum_{\tau=n_I+1}^{\infty} \Pi_\tau Y_{t-\tau}, \tag{A.6}$$

hence

$$\frac{1}{T}\sum_{t=1}^{T}[\tilde{u}_t(n_T) - u_t]u_t^{'} = [\Pi(n_T) - \tilde{\Pi}(n_T)]C_{Yu}(n_T) + S_{Yu}(n_T) \tag{A.7}$$

where $Y_t(n_T) = \left[Y_{t-1}^{'}, \ldots, Y_{t-n_I}^{'}\right]^{'}$, and

$$C_{Yu}(n_T) = \frac{1}{T}\sum_{t=1}^{T}Y_t(n_T)u_t^{'} = [C_{Yu}(1,T)^{'}, \ldots, C_{Yu}(n_T,T)^{'}]^{'}, \tag{A.8}$$

$$C_{Yu}(\tau,T) = \frac{1}{T}\sum_{t=1}^{T}Y_{t-\tau}u_t^{'}, \tag{A.9}$$

$$S_{Yu}(n_T) = \frac{1}{T}\sum_{t=1}^{T}\sum_{\tau=n_T+1}^{\infty}\Pi_\tau Y_{t-\tau}u_t^{'}. \tag{A.10}$$

Using the fact that u_t is independent of $X_t, u_{t-1}, \ldots, u_1$, we see that

$$\mathsf{E}\|C_{Yu}(\tau,T)\|^2 = \mathsf{E}[C_{Yu}(\tau,T)C_{Yu}(\tau,T)^{'}] = \frac{1}{T^2}\sum_{t=1}^{T}\mathsf{E}[\text{tr}(Y_{t-\tau}u_t^{'}u_t Y_{t-\tau}^{'})]$$

$$= \frac{1}{T^2}\sum_{t=1}^{T}\text{tr}[\mathsf{E}(u_t^{'}u_t)\mathsf{E}(Y_{t-\tau}^{'}Y_{t-\tau})] = \frac{1}{T}\text{tr}(\Sigma_u)\text{tr}[\Gamma(0)], \tag{A.11}$$

$$\mathsf{E}[S_{Yu}(n_T)] = 0, \tag{A.12}$$

where $\Gamma(0) = \mathsf{E}(Y_t Y_t^{'})$, hence

$$\mathsf{E}\|C_{Yu}(n_T)\|^2 = \mathsf{E}[C_{Yu}(n_T)^{'}C_{Yu}(n_T)] = \sum_{\tau=1}^{n_T}\mathsf{E}\|C_{Yu}(\tau,T)\|^2$$

$$= \frac{n_T}{T}\text{tr}(\Sigma_u)\text{tr}[\Gamma(0)], \tag{A.13}$$

$$\sum_{\tau=1}^{n_T}\|C_{Yu}(\tau,T)\|^2 = O_p\left(\frac{n_T}{T}\right), \tag{A.14}$$

and

$$\|[\tilde{\Pi}(n_T) - \Pi(n_T)]C_{Yu}(n_T)\| \leq \|\tilde{\Pi}(n_T) - \Pi(n_T)\|\|C_{Yu}(n_T)\| = O_p\left(\frac{n_T}{T}\right). \tag{A.15}$$

Using the stationarity of Y_t and (11.8), we have:

$$\mathsf{E}\left[\|S_{Yu}(n_T)\|\right] \leq \mathsf{E}\left[\frac{1}{T}\sum_{t=1}^{T}\left(\sum_{\tau=n_I+1}^{\infty}\|\Pi_\tau\|\|Y_{t-\tau}\|\|u_t\|\right)\right]$$

$$\leq \left[\mathsf{E}\left(\|Y_t\|^2\right)\right]^{1/2}\left[\mathsf{E}\left(\|u_t\|^2\right)\right]^{1/2}\frac{1}{T}\sum_{t=1}^{T}\sum_{\tau=n_I+1}^{\infty}\|\Pi_\tau\|$$

$$\leq \left[\mathsf{E}\left(\|Y_t\|^2\right)\right]^{1/2}\left[\mathsf{E}\left(\|u_t\|^2\right)\right]^{1/2}\frac{C}{T}\sum_{t=1}^{T}\sum_{\tau=n_I+1}^{\infty}\rho^\tau$$

$$\leq \quad \left[\mathsf{E}\left(\|Y_t\|^2\right)\right]^{1/2}\left[\mathsf{E}\left(\|u_t\|^2\right)\right]^{1/2}\frac{C}{T}\sum_{t=1}^{T}\frac{\rho^{n_T+1}}{1-\rho}$$

$$= \quad \left[\mathsf{E}\left(\|Y_t\|^2\right)\right]^{1/2}\left[\mathsf{E}\left(\|u_t\|^2\right)\right]^{1/2}\left(\frac{C\rho}{1-\rho}\right)\rho^{n_T}$$

$$= \quad O(\rho^{n_T}) \tag{A.16}$$

hence

$$\left\|S_{Yu}(n_T)\right\| = O_p(\rho^{n_T})\,. \tag{A.17}$$

Consequently,

$$\left\|\frac{1}{T}\sum_{t=1}^{T}u_t[\tilde{u}_t(n_T)-u_t]'\right\| = \left\|\frac{1}{T}\sum_{t=1}^{T}[\tilde{u}_t(n_T)-u_t]u_t'\right\|$$

$$\leq \left\|[\tilde{\Pi}(n_T)-\Pi(n_T)]C_{Yu}(n_T)\right\| + \left\|S_{Yu}(n_T)\right\|$$

$$= O_p\left(\frac{n_T}{T}\right)\,, \tag{A.18}$$

and (11.64) is established. Finally,

$$\left\|\frac{1}{T}\sum_{t=1}^{T}[\tilde{u}_t(n_T)-u_t][\tilde{u}_t(n_T)-u_t]'\right\| \leq \frac{1}{T}\sum_{t=1}^{T}\left\|[\tilde{u}_t(n_T)-u_t][\tilde{u}_t(n_T)-u_t]'\right\|$$

$$\leq \frac{1}{T}\sum_{t=1}^{T}\left\|\tilde{u}_t(n_T)-u_t\right\|^2 \tag{A.19}$$

where

$$\frac{1}{T}\sum_{t=1}^{T}\|\tilde{u}_t(n_T)-u_t\|^2 \quad \leq \quad \frac{3}{T}\sum_{t=1}^{T}\left\{\|\tilde{\Pi}(n_T)-\Pi(n_T)\|^2\|Y_t(n_T)\|^2\right.$$

$$+\left.\left(\sum_{\tau=n_T+1}^{\infty}\|\Pi_\tau\|\|Y_{t-\tau}\|\right)^2\right\}$$

$$\leq \quad 3\|\tilde{\Pi}(n_T)-\Pi(n_T)\|^2\frac{1}{T}\sum_{t=1}^{T}\|Y_t(n_T)\|^2$$

$$+\frac{3}{T}\sum_{t=1}^{T}\left(\sum_{\tau=n_T+1}^{\infty}\|\Pi_\tau\|\|Y_{t-\tau}\|\right)^2\,. \tag{A.20}$$

Since

$$\mathsf{E}\left[\frac{1}{T}\sum_{t=1}^{T}\|Y_t(n_T)\|^2\right] = \mathsf{E}\left[\frac{1}{T}\sum_{t=1}^{T}\sum_{\tau=1}^{n_T}\|Y_{t-\tau}\|^2\right] = n_T\mathsf{E}\left(\|Y_t\|^2\right)\,, \tag{A.21}$$

we have

$$\frac{1}{T}\sum_{t=1}^{T}\|Y_t(n_T)\|^2 = O_p(n_T)\,. \tag{A.22}$$

Further,

$$\mathsf{E}\left[\frac{1}{T}\sum_{t=1}^{T}\left(\sum_{\tau=n_T+1}^{\infty}\|\Pi_\tau\|\|Y_{t-\tau}\|\right)\right] \quad = \quad \mathsf{E}\|Y_t\|\frac{1}{T}\sum_{t=1}^{T}\sum_{\tau=n_T+1}^{\infty}\|\Pi_\tau\|$$

$$\leq \quad \mathsf{E}\,\|Y_t\|\,\frac{C}{T}\sum_{t=1}^{T}\frac{\rho^{n_I+1}}{1-\rho} = \left(\frac{C\,\mathsf{E}\,\|Y_t\|\,\rho}{1-\rho}\right)\rho^{n_T}$$

$$= \quad O(\rho^{n_I})\,, \tag{A.23}$$

hence

$$\frac{1}{T}\sum_{t=1}^{T}\left(\sum_{\tau=n_I+1}^{\infty}\|\Pi_\tau\|\,\|Y_{t-\tau}\|\right) \quad = \quad O_p(\rho^{n_I})\,, \tag{A.24}$$

$$\frac{1}{T}\sum_{t=1}^{T}\left(\sum_{\tau=n_T+1}^{\infty}\|\Pi_\tau\|\,\|Y_{t-\tau}\|\right)^2 \quad \leq \quad T\left[\frac{1}{T}\sum_{t=1}^{T}\left(\sum_{\tau=n_I+1}^{\infty}\|\Pi_\tau\|\,\|Y_{t-\tau}\|\right)\right]^2$$

$$= \quad O_p(T\rho^{2n_I}) \tag{A.25}$$

and

$$\frac{1}{T}\sum_{t=1}^{T}\|\tilde{u}_t(n_T)-u_t\|^2 \leq O_p\left(\frac{n_T}{T}\right)O_p(n_T)+O_p(T\rho^{2n_I}) = O_p\left(\frac{n_T^2}{T}\right)\,, \tag{A 26}$$

$$\left\|\frac{1}{T}\sum_{t=1}^{T}[\tilde{u}_t(n_T)-u_t][\tilde{u}_t(n_T)-u_t]'\right\| = O_p\left(\frac{n_T^2}{T}\right) \tag{A 27}$$

We can thus conclude that

$$\|\tilde{\Sigma}_u(n_T)-\hat{\Sigma}_T\| = O_p(\frac{n_T}{T})+O_p\left(\frac{n_T^2}{T}\right) = O_p\left(\frac{n_T^2}{T}\right)\,, \tag{A.28}$$

$$\|\tilde{\Sigma}_u(n_T)-\Sigma_u\| = O_p\left(\frac{n_T^2}{T}\right)\,. \tag{A.29}$$

PROOF OF PROPOSITION 11.2
Using (11 78) and (11 84), we see that

$$\tilde{\Gamma}(n_T)-\Gamma_T = \frac{1}{T}\sum_{t=1}^{T}\left[\tilde{X}_t(n_T)\tilde{X}_t(n_T)'-X_tX_t'\right]$$

$$= \frac{1}{T}\sum_{t=1}^{T}\left\{[\tilde{X}_t(n_T)-X_t]X_t'+X_t[\tilde{X}_t(n_T)-X_t]'\right\}$$

$$+ \frac{1}{T}\sum_{t=1}^{T}\left\{[\tilde{X}_t(n_T)-X_t][\tilde{X}_t(n_T)-X_t]'\right\} \tag{A 30}$$

hence, using the triangular and Cauchy-Schwarz inequalities,

$$\|\tilde{\Gamma}(n_T)-\Gamma_T\| \quad \leq \quad 2\left(\frac{1}{T}\sum_{t=1}^{T}\|X_t\|^2\right)^{1/2}\left(\frac{1}{T}\sum_{t=1}^{T}\|\tilde{X}_t(n_T)-X_t\|^2\right)^{1/2}$$

$$+ \frac{1}{T}\sum_{t=1}^{T}\|\tilde{X}_t(n_T)-X_t\|^2$$

$$= \quad 2\left(\frac{1}{T}\|X(T)\|^2\right)^{1/2}\left(\frac{1}{T}\|\tilde{X}(n_T)-X(T)\|^2\right)^{1/2}$$

$$+ \frac{1}{T} \| \tilde{X}(n_T) - X(T) \|^2 \qquad \text{(A 31)}$$

where

$$\tilde{X}_t(n_T) - X_t = \begin{bmatrix} u_t - \bar{u}_t(n_T) \\ 0 \\ \vdots \\ 0 \\ \tilde{u}_{t-1}(n_T) - u_{t-1} \\ \vdots \\ \tilde{u}_{t-\bar{p}}(n_T) - u_{t-\bar{p}} \end{bmatrix}, \qquad \text{(A 32)}$$

$$
\begin{aligned}
\frac{1}{T} \| \tilde{X}(n_T) - X(T) \|^2 &= \frac{1}{T} \sum_{t=1}^{T} \| \tilde{X}_t(n_T) - X_t \|^2 \\
&= \sum_{j=0}^{p} \Big[\frac{1}{T} \sum_{t=1}^{T} \| \tilde{u}_{t-j}(n_T) - u_{t-j} \|^2 \Big] = O_p \left(\frac{n_T^2}{T} \right) \quad \text{(A 33)}
\end{aligned}
$$

and, by the stationarity assumption,

$$\frac{1}{T} \| X(T) \|^2 = \frac{1}{T} \sum_{t-1}^{T} \| X_t \|^2 = O_p(1) . \qquad \text{(A 34)}$$

It follows from the above orders that

$$\| \tilde{\Gamma}(n_T) - \Gamma_T \| = O_p \left(\frac{n_T}{T^{1/2}} \right) . \qquad \text{(A 35)}$$

Consequently, we have

$$
\begin{aligned}
\| \tilde{\Upsilon}(n_T) - \Upsilon_T \| &= \| I_k \otimes \tilde{\Gamma}(n_T) - I_k \otimes \Gamma_T \| \\
&= \| I_k \otimes (\tilde{\Gamma}(n_T) - \Gamma_T) \| \\
&= k^{1/2} \| \tilde{\Gamma}(n_T) - \Gamma_T \| = O_p \left(\frac{n_T}{T^{1/2}} \right) , \qquad \text{(A.36)}
\end{aligned}
$$

$$
\begin{aligned}
\| \tilde{Q}(n_T)^{-1} - Q_T^{-1} \| &= \| R' \big[\tilde{\Upsilon}(n_T) - \Upsilon_T \big] R \| \\
&\leq \| R \|^2 \| \tilde{\Upsilon}(n_T) - \Upsilon_T \| = O_p \left(\frac{n_T}{T^{1/2}} \right) . \qquad \text{(A 37)}
\end{aligned}
$$

Further, since

$$\| \tilde{Q}(n_T)^{-1} - Q^{-1} \| \leq \| \tilde{Q}(n_T)^{-1} - Q_T^{-1} \| + \| Q_T^{-1} - Q^{-1} \| \qquad \text{(A 38)}$$

and

$$
\begin{aligned}
\| Q_T^{-1} - Q^{-1} \| &= \| R'(\Upsilon_T - \Upsilon) R \| \leq \| R \|^2 \| \Upsilon_T - \Upsilon \| \\
&\leq \| R \|^2 \| I_k \otimes (\Gamma_T - \Gamma) \| = k^{1/2} \| R \|^2 \| \Gamma_T - \Gamma \| \\
&= k^{1/2} \| R \|^2 \left\| \frac{1}{T} \sum_{t=1}^{T} X_t X_t' - \mathsf{E}(X_t X_t') \right\| = O_p \left(\frac{1}{T^{1/2}} \right) , \qquad \text{(A.39)}
\end{aligned}
$$

we have

$$\|\tilde{Q}(n_T)^{-1} - Q^{-1}\| = O_p\left(\frac{n_T}{T^{1/2}}\right) \tag{A 40}$$

Finally, using the triangular inequality, we get

$$\|\tilde{Q}(n_T)\| \leq \|\tilde{Q}(n_T) - Q\| + \|Q\|, \tag{A.41}$$

$$
\begin{aligned}
\|\tilde{Q}(n_T) - Q\| &= \|\tilde{Q}(n_T)[\tilde{Q}(n_T)^{-1} - Q^{-1}]Q\| \\
&\leq \|\tilde{Q}(n_T)\|\|\tilde{Q}(n_T)^{-1} - Q^{-1}\|\|Q\| \\
&\leq \left[\|\tilde{Q}(n_T) - Q\| + \|Q\|\right]\|\tilde{Q}(n_T)^{-1} - Q^{-1}\|\|Q\|, \tag{A 42}
\end{aligned}
$$

hence, for $\|\tilde{Q}(n_T)^{-1} - Q^{-1}\|\|Q\| < 1$ (an event whose probability converges to 1 as $T \to \infty$)

$$\|\tilde{Q}(n_T) - Q\| \leq \frac{\|Q\|^2\|\tilde{Q}(n_T)^{-1} - Q^{-1}\|}{1 - \|\tilde{Q}(n_T)^{-1} - Q^{-1}\|\|Q\|} = O_p\left(\frac{n_T}{T^{1/2}}\right) \tag{A 43}$$

PROOF OF THEOREM 11.1

Recall that $\tilde{\eta} - \eta = \tilde{Q}(n_T)\tilde{\Omega}(n_T)$ Then, we have

$$
\begin{aligned}
\|\tilde{\eta} - \eta\| &\leq \|Q\|_1\|\Omega_T\| + \|\tilde{Q}(n_T) - Q\|_1\|\Omega_T\| + \left\|\tilde{Q}(n_T)\right\|_1\|\tilde{\Omega}(n_T) - \Omega_T\| \\
&\leq \|Q\|\|\Omega_T\| + \|\tilde{Q}(n_T) - Q\|\|\Omega_T\| + \|\tilde{Q}(n_T)\|\|\tilde{\Omega}(n_T) - \Omega_T\|. \tag{A.44}
\end{aligned}
$$

By Proposition 11.2,

$$\|\tilde{Q}(n_T) - Q\| = O_p\left(\frac{n_T}{T^{1/2}}\right), \quad \|\tilde{Q}(n_T)\| = O_p(1) \tag{A 45}$$

Now

$$\Omega_T = \frac{1}{T}\sum_{t=1}^{T} R'\left[I_k \otimes X_t\right]u_t = R'\text{vec}\left[\frac{1}{T}\sum_{t=1}^{T} X_t u_t'\right], \tag{A.46}$$

so that

$$\mathsf{E}\|\Omega_T\|^2 \leq \|R\|^2\,\mathsf{E}\|W_T\|^2 \tag{A.47}$$

where

$$W_T = \frac{1}{T}\sum_{t=1}^{T} X_t u_t'. \tag{A 48}$$

Then, using the fact that u_t is independent of $X_t, u_{t-1}, \ldots, u_1$,

$$
\begin{aligned}
\mathsf{E}\|W_T\|^2 &= \mathsf{E}[\text{tr}(W_T W_T')] \\
&= \frac{1}{T^2}\left\{\sum_{t=1}^{T}\mathsf{E}\left(\text{tr}\left[X_t u_t' u_t X_t'\right]\right) + 2\sum_{t=1}^{T-1}\sum_{l=1}^{T-l}\left\{\mathsf{E}\left(\text{tr}\left[X_t u_t' u_{t+l} X_{t+l}'\right]\right)\right\}\right\} \\
&= \frac{1}{T^2}\left\{\sum_{t=1}^{T}\mathsf{E}\left(\text{tr}\left[u_t' u_t X_t' X_t\right]\right) + 2\sum_{t=1}^{T-1}\sum_{l=1}^{T-l}\left\{\mathsf{E}\left(\text{tr}\left[u_{t+l} X_{t+l}' X_t u_t'\right]\right)\right\}\right\} \\
&= \frac{1}{T^2}\left\{\sum_{t=1}^{T}\text{tr}\left[\mathsf{E}(u_t' u_t)\mathsf{E}(X_t' X_t)\right]\right.
\end{aligned}
$$

$$+2 \sum_{t=1}^{T-1} \sum_{l=1}^{T-l} \left\{ \mathsf{E}\left(\mathfrak{t}_1 \left[\mathsf{E}(u_{t+l}) \mathsf{E}(X'_{l+l} X_t u'_l) \right] \right) \right\}$$

$$= \frac{1}{T^2} \left\{ \sum_{t=1}^{T} \operatorname{tr} \left[\mathsf{E}\left(u_t u'_t \right) \mathsf{E}\left(X'_t X_t \right) \right] \right\} = \frac{1}{T} \operatorname{tr}(\Sigma_u) \mathfrak{t}_1(\Gamma) \qquad (\text{A } 49)$$

hence

$$\|W_T\| = O_p\left(T^{-1/2} \right), \quad \|\Omega_T\| = O_p\left(T^{-1/2} \right). \qquad (\text{A } 50)$$

Now, consider the term $\|\tilde{\Omega}(n_T) - \Omega_T\|$. We have:

$$\tilde{\Omega}(n_T) - \Omega_T = \frac{1}{T} R' \sum_{l=1}^{T} \left\{ \left[I_k \otimes \tilde{X}_t(n_T) \right] e_t(n_T) - \left[I_k \otimes X_t \right] u_t \right\}$$

$$= R' \operatorname{vec}\left[\frac{1}{T} \sum_{t=1}^{T} \left\{ \tilde{X}_t(n_T) e_t(n_T)' - X_t u_t' \right\} \right]$$

$$= R' \operatorname{vec}\left\{ \tilde{\Omega}_1(n_T) + \tilde{\Omega}_2(n_T) \right\} \qquad (\text{A.51})$$

where

$$\tilde{\Omega}_1(n_T) = \frac{1}{T} \sum_{l=1}^{T} X_t \left[e_t(n_T) - u_t \right]', \qquad (\text{A.52})$$

$$\tilde{\Omega}_2(n_T) = \frac{1}{T} \sum_{t=1}^{T} \left[\tilde{X}_t(n_T) - X_t \right] e_t(n_T)', \qquad (\text{A.53})$$

$$e_t(n_T) = \tilde{u}_t(n_T) + \sum_{j=0}^{\bar{p}} \Theta_j \left[u_{t-j} - \tilde{u}_{t-j}(n_T) \right]. \qquad (\text{A.54})$$

We can also write

$$e_t(n_T) - u_t = \sum_{j=0}^{\bar{p}} \bar{\Theta}_j \left[\tilde{u}_{t-j}(n_T) - u_{t-j} \right] \qquad (\text{A.55})$$

where $\bar{\Theta}_0 = I_k - \Theta_0$ and $\bar{\Theta}_j = -\Theta_j$, $j = 1, 2, \ldots, \bar{p}$, and

$$\tilde{u}_t(n_T) - u_t = \left[\Pi(n_T) - \tilde{\Pi}(n_T) \right] Y_t(n_T) + \sum_{\tau = n_T + 1}^{\infty} \Pi_\tau Y_{t-\tau}$$

$$= \sum_{\tau=1}^{n_T} \left[\Pi_\tau - \tilde{\Pi}_\tau(n_T) \right] Y_{t-\tau} + \sum_{\tau = n_T + 1}^{\infty} \Pi_\tau Y_{t-\tau}, \qquad (\text{A } 56)$$

hence

$$\tilde{\Omega}_1(n_T) = \frac{1}{T} \sum_{t=1}^{T} X_t \left[e_l(n_T) - u_t \right]'$$

$$= \sum_{j=0}^{\bar{p}} \left\{ \frac{1}{T} \sum_{t=1}^{T} \left\{ \sum_{\tau=1}^{n_T} X_t Y'_{t-j-\tau} \left[\Pi_\tau - \tilde{\Pi}_\tau(n_T) \right]' \right. \right.$$

$$\left. \left. + \sum_{\tau = n_T + 1}^{\infty} X_t Y'_{t-j-\tau} \Pi'_\tau \right\} \right\} \bar{\Theta}'_j$$

$$
= \sum_{j=0}^{\bar{p}} \left\{ \sum_{\tau=1}^{n_T} \left\{ \frac{1}{T} \sum_{t=1}^{T} X_t Y'_{t-j-\tau} \right\} \left[\Pi_\tau - \tilde{\Pi}_\tau(n_T) \right]' \right.
$$
$$
\left. + \frac{1}{T} \sum_{t=1}^{T} \sum_{\tau=n_T+1}^{\infty} X_t Y'_{t-j-\tau} \Pi'_\tau \right\} \bar{\Theta}'_j
$$
$$
= \tilde{\Omega}_{11}(n_T) + \tilde{\Omega}_{12}(n_T) \tag{A.57}
$$

where

$$
\tilde{\Omega}_{11}(n_T) = \sum_{j=0}^{\bar{p}} \left\{ \sum_{\tau=1}^{n_T} \tilde{\Gamma}_{j+\tau}(n_T) \left[\Pi_\tau - \Pi_\tau(n_T) \right]' \right\} \bar{\Theta}'_j, \tag{A.58}
$$

$$
\tilde{\Gamma}_{j+\tau}(n_T) = \frac{1}{T} \sum_{t=1}^{T} X_t Y'_{t-j-\tau}, \tag{A.59}
$$

$$
\tilde{\Omega}_{12}(n_T) = \sum_{j=0}^{\bar{p}} \left\{ \frac{1}{T} \sum_{t=1}^{T} \sum_{\tau=n_T+1}^{\infty} X_t Y'_{t-j-\tau} \Pi'_\tau \right\} \bar{\Theta}'_j. \tag{A.60}
$$

Now, using the linearity and the VARMA structure of Y_t, it is easy to see that

$$
\mathsf{E} \| \tilde{\Gamma}_{j+\tau}(n_T) \|^2 \leq \frac{1}{T} C_1 \rho_1^{j+\tau} \tag{A.61}
$$

for some constants $C_1 > 0$ and $0 < \rho_1 < 1$, hence

$$
\mathsf{E} \left[\sum_{\tau=1}^{n_T} \| \tilde{\Gamma}_{j+\tau}(n_T) \|^2 \right] \leq \frac{1}{T} C_1 \sum_{\tau=1}^{n_T} \rho_1^{j+\tau} \leq \frac{1}{T} \frac{C_1}{1-\rho_1} = O_p \left(\frac{1}{T} \right). \tag{A.62}
$$

Thus

$$
\| \tilde{\Omega}_{11}(n_T) \| \leq \sum_{j=0}^{p} \left\{ \sum_{\tau=1}^{n_T} \| \tilde{\Gamma}_{j+\tau}(n_T) \| \| \Pi_\tau - \tilde{\Pi}_\tau(n_T) \| \right\} \| \bar{\Theta}_j \|
$$
$$
\leq \sum_{j=0}^{\bar{p}} \left\{ \left[\sum_{\tau=1}^{n_T} \| \tilde{\Gamma}_{j+\tau}(n_T) \|^2 \right]^{1/2} \left[\sum_{\tau=1}^{n_T} \| \Pi_\tau - \tilde{\Pi}_\tau(n_T) \|^2 \right]^{1/2} \right\} \| \bar{\Theta}_j \|
$$
$$
\leq \sum_{j=0}^{\bar{p}} \left\{ \left[\sum_{\tau=1}^{n_T} \| \tilde{\Gamma}_{j+\tau}(n_T) \|^2 \right]^{1/2} \| \tilde{\Pi}(n_T) - \Pi(n_T) \| \right\} \| \bar{\Theta}_j \|
$$
$$
= O_p \left(\frac{n_T^{1/2}}{T} \right), \tag{A.63}
$$

while

$$
\mathsf{E} \| \tilde{\Omega}_{12}(n_T) \| \leq \sum_{j=0}^{\bar{p}} \left\{ \mathsf{E} \left[\frac{1}{T} \sum_{t=1}^{T} \sum_{\tau=n_T+1}^{\infty} \| X_t \| \| Y_{t-j-\tau} \| \| \Pi_\tau \| \right] \right\} \| \bar{\Theta}_j \|
$$
$$
\leq \sum_{j=0}^{\bar{p}} \left\{ \frac{1}{T} \sum_{t=1}^{T} \sum_{\tau=n_T+1}^{\infty} \| \Pi_\tau \| \mathsf{E} \left[\| X_t \| \| Y_{t-j-\tau} \| \right] \right\} \| \bar{\Theta}_j \|
$$
$$
\leq \sum_{j=0}^{\bar{p}} \left\{ \left[\mathsf{E}(\| X_t \|^2) \mathsf{E}(\| Y_t \|^2) \right]^{1/2} \frac{1}{T} \sum_{t=1}^{T} \sum_{\tau=n_T+1}^{\infty} \| \Pi_\tau \| \right\} \| \bar{\Theta}_j \|
$$

$$= O_p(\rho^{n_T}), \tag{A.64}$$

hence $\|\tilde{\Omega}_{12}(n_T)\| = O_p(\rho^{n_T})$ and

$$\|\tilde{\Omega}_1(n_T)\| \leq \|\tilde{\Omega}_{11}(n_T)\| + \|\tilde{\Omega}_{12}(n_T)\| = O_p\left(\frac{n_T^{1/2}}{T}\right). \tag{A.65}$$

Now, using (A.55), $\tilde{\Omega}_2(n_T)$ can be decomposed as :

$$\tilde{\Omega}_2(n_T) = \tilde{\Omega}_{21}(n_T) + \tilde{\Omega}_{22}(n_T) \tag{A.66}$$

where

$$\tilde{\Omega}_{21}(n_T) = \frac{1}{T}\sum_{t=1}^{T}\left[\tilde{X}_t(n_T) - X_t\right]u_t', \tag{A.67}$$

$$\tilde{\Omega}_{22}(n_T) = \sum_{j=0}^{\bar{p}}\left\{\frac{1}{T}\sum_{t=1}^{T}\left[\tilde{X}_t(n_T) - X_t\right]\left[\tilde{u}_{t-j}(n_T) - u_{t-j}\right]'\right\}\bar{\Theta}_j'. \tag{A.68}$$

Now, in view of (A.32), consider the variables:

$$C_i(n_T) = \frac{1}{T}\sum_{t=1}^{T}\left[\tilde{u}_{t-i}(n_T) - u_{t-i}\right]u_t'$$

$$= \sum_{\tau=1}^{n_T}\left[\Pi_\tau - \tilde{\Pi}_\tau(n_T)\right]\left(\frac{1}{T}\sum_{t=1}^{T}Y_{t-i-\tau}u_t'\right) + \frac{1}{T}\sum_{t=1}^{T}\sum_{\tau=n_T+1}^{\infty}\Pi_\tau Y_{t-i-\tau}u_t', \tag{A.69}$$

$$C_{ij}(n_T) = \frac{1}{T}\sum_{t=1}^{T}\left[\tilde{u}_{t-i}(n_T) - u_{t-i}\right]\left[\tilde{u}_{t-j}(n_T) - u_{t-j}\right]', \tag{A.70}$$

for $i = 0, 1, \ldots, \bar{p}$. We have:

$$\mathsf{E}\|\frac{1}{T}\sum_{t=1}^{T}Y_{t-i-\tau}u_t'\|^2 = \frac{1}{T^2}\sum_{t=1}^{T}\mathsf{E}\mathrm{tr}[Y_{t-i-\tau}u_t'u_t Y_{t-i-\tau}']$$

$$= \frac{1}{T^2}\sum_{t=1}^{T}\mathrm{tr}[\mathsf{E}(u_t'u_t)\mathsf{E}(Y_{t-i-\tau}'Y_{t-i-\tau})]$$

$$= \frac{1}{T}\mathrm{tr}(\Sigma_v)\mathrm{tr}[\Gamma(0)] \tag{A.71}$$

where $\Gamma(0) = \mathsf{E}(Y_t Y_t')$. hence

$$\sum_{\tau=1}^{n_T}\mathsf{E}\|\frac{1}{T}\sum_{t=1}^{T}Y_{t-i-\tau}u_t'\|^2 = \frac{n_T}{T}\mathrm{tr}(\Sigma_v)\mathrm{tr}[\Gamma(0)], \tag{A.72}$$

$$\sum_{\tau=1}^{n_T}\|\frac{1}{T}\sum_{t=1}^{T}Y_{t-i-\tau}u_t'\|^2 = O_p\left(\frac{n_T}{T}\right), \tag{A.73}$$

and

$$\|C_i(n_T)\| \leq \sum_{\tau=1}^{n_T}\|\Pi_\tau - \tilde{\Pi}_\tau(n_T)\|\|\frac{1}{T}\sum_{t=1}^{T}Y_{t-i-\tau}u_t'\|$$

$$+\frac{1}{T}\sum_{t=1}^{T}\sum_{\tau=n_I+1}^{\infty}\|\Pi_\tau\|\|Y_{l-i-\tau}\|\|u_t\|$$

$$\leq\quad\Big[\sum_{\tau=1}^{n_I}\|\Pi_\tau-\tilde{\Pi}_\tau(n_T)\|^2\Big]^{1/2}\Big[\sum_{\tau=1}^{n_T}\|\frac{1}{T}\sum_{t=1}^{T}Y_{t-i-\tau}u_t'\|^2\Big]^{1/2}$$

$$+\frac{1}{T}\sum_{t=1}^{T}\sum_{\tau=n_{I'}+1}^{\infty}\|\Pi_\tau\|\|Y_{t-i-\tau}\|\|u_t\|$$

$$=\quad\|\tilde{\Pi}(n_T)-\Pi(n_T)\|\Big[\sum_{\tau=1}^{n_I}\|\frac{1}{T}\sum_{t=1}^{T}Y_{t-i-\tau}u_t'\|^2\Big]^{1/2}$$

$$+\frac{1}{T}\sum_{t=1}^{T}\sum_{\tau=n_I+1}^{\infty}\|\Pi_\tau\|\|Y_{t-i-\tau}\|\|u_t\|$$

$$=\quad O_p\left(\frac{n_T}{T}\right). \tag{A.74}$$

Further,

$$\|C_{ij}(n_T)\|\quad\leq\quad\frac{1}{T}\sum_{t=1}^{T}\|\left[\tilde{u}_{t-i}(n_T)-u_{t-i}\right]\|\|\left[\tilde{u}_{t-j}(n_T)-u_{t-j}\right]'\|$$

$$\leq\quad\Big[\frac{1}{T}\sum_{t=1}^{T}\|\tilde{u}_{t-i}(n_T)-u_{t-i}\|^2\Big]^{1/2}\Big[\frac{1}{T}\sum_{t=1}^{T}\|\tilde{u}_{t-j}(n_T)-u_{t-j}\|^2\Big]^{1/2}$$

$$=\quad O_p\left(\frac{n_T^2}{T}\right). \tag{A.75}$$

Thus

$$\|\tilde{\Omega}_{21}(n_T)\|=O_p(n_T/T),\quad\|\tilde{\Omega}_{22}(n_T)\|=O_p\left(\frac{n_T^2}{T}\right), \tag{A.76}$$

hence

$$\|\tilde{\Omega}_2(n_T)\|\leq\|\tilde{\Omega}_{21}(n_T)\|+\|\tilde{\Omega}_{22}(n_T)\|=O_p\left(\frac{n_T^2}{T}\right), \tag{A.77}$$

$$\|\tilde{\Omega}(n_T)-\Omega_T\|\leq\|R\|\big(\|\tilde{\Omega}_1(n_T)\|+\|\tilde{\Omega}_2(n_T)\|\big)$$

$$=O_p\left(\frac{n_T^{1/2}}{T}\right)+O_p\left(\frac{n_T^2}{T}\right)=O_p\left(\frac{n_T^2}{T}\right). \tag{A.78}$$

Consequently,

$$\|\tilde{\eta}-\eta\|\quad\leq\quad O_p\left(\frac{1}{T^{1/2}}\right)+O_p\left(\frac{n_T}{T}\right)+O_p\left(\frac{n_T^2}{T}\right)$$

$$=\quad O_p\left(\frac{1}{T^{1/2}}\right)+O_p\left(\frac{n_T^2}{T}\right)=o_p(1). \tag{A.79}$$

If furthermore $n_T^4/T\longrightarrow 0$ as $T\to\infty$, the latter reduces to

$$\|\tilde{\eta}-\eta\|=O_p\left(\frac{1}{T^{1/2}}\right). \tag{A.80}$$

$\square$

PROOF OF PROPOSITION 11.3

We have:

$$\|\tilde{S}(n_T) - S_T\| = T^{1/2}\|\tilde{Q}(n_T)\tilde{\Omega}(n_T) - Q\Omega_T\|$$
$$\leq T^{1/2}\|\tilde{Q}(n_T)\|\|\tilde{\Omega}(n_T) - \Omega_T\| + T^{1/2}\|\tilde{Q}(n_T) - Q\|\|\Omega_T\|. \quad (A.81)$$

By Proposition 11.2 and Theorem 11.1, the following orders hold:

$$\|\tilde{Q}(n_T) - Q\| = O_p\left(\frac{n_T}{T^{1/2}}\right), \quad \|\tilde{Q}(n_T)\| = O_p(1), \quad (A.82)$$

$$\|\tilde{\Omega}(n_T) - \Omega_T\| = O_p\left(\frac{n_T^2}{T}\right), \quad \|\Omega_T\| = O_p\left(\frac{1}{T^{1/2}}\right). \quad (A.83)$$

Therefore,

$$\|\tilde{S}(n_T) - S_T\| = O_p\left(\frac{n_T^2}{T^{1/2}}\right). \quad (A.84)$$

$\square$

PROOF OF THEOREM 11.2

By the standard central limit theorem for stationary processes (see Anderson (1971, Section 7.7), Lewis and Reinsel (1985, Section 2)) and under the assumption of independence between u_t and X_t, we have:

$$T^{1/2}\Omega_T = \frac{1}{T^{1/2}}\sum_{t=1}^{T} R'(I_k \otimes X_t)u_t = \frac{1}{T^{1/2}}\sum_{t=1}^{T} R'(u_t \otimes X_t) \xrightarrow[T\to\infty]{} N(0, \Sigma_{Xu}) \quad (A.85)$$

where

$$\Sigma_{Xu} = E\left\{R'(u_t \otimes X_t)(u_t \otimes X_t)'R\right\} = E\left\{R'\left[u_t u_t' \otimes X_t X_t'\right]R\right\}$$
$$= R'\left[E(u_t u_t') \otimes E(X_t X_t')\right]R = R'\left[\Sigma_u \otimes \Gamma\right]R. \quad (A.86)$$

Then

$$S_T = T^{1/2}Q\Omega_T \xrightarrow[T\to\infty]{} N(0, \Sigma_\eta) \quad (A.87)$$

where

$$\Sigma_\eta = Q\Sigma_{Xu}Q'. \quad (A.88)$$

Finally, by Proposition 11.3, we can conclude that

$$\sqrt{T}(\tilde{\eta} - \eta) = \tilde{S}(n_T) \xrightarrow[T\to\infty]{} N(0, \Sigma_\eta). \quad (A.89)$$

$\square$

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Chapter 12

RECENT RESULTS FOR LINEAR TIME SERIES MODELS WITH NON INDEPENDENT INNOVATIONS

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Abstract   In this paper, we provide a review of some recent results for ARMA models with uncorrelated but non independent errors. The standard so-called Box-Jenkins methodology rests on the errors independence. When the errors are suspected to be non independent, which is often the case in real situations, this methodology needs to be adapted. We study in detail the main steps of this methodology in the above-mentioned framework.

1.   Introduction

Among the great diversity of stochastic models for time series, it is customary to make a sharp distinction between linear and non-linear models. It is often argued that linear ARMA models do not allow to deal with data which exhibit nonlinearity features. This is true if, as is usually done, strong assumptions are made on the noise governing the ARMA equation. There are numerous data sets from the fields of biology, economics and finance, which appear to be hardly compatible with these so-called strong ARMA models (see Tong (1990) for examples). When these assumptions are weakened, it can be shown that many non linear processes admit a finite order ARMA representation. A striking feature of the ARMA class is that it is sufficiently flexible and rich enough to accommodate a variety of non-linear models. In fact, these two classes of processes, linear and non-linear, are not incompatible and can even be complementary.

A key question, of course, is how to fit linear ARMA models to data which exhibit non-linear behaviours. The validity of the different steps

of the traditional methodology of Box and Jenkins, identification, estimation and validation, crucially depends on the noise properties. If the noise is not independent, most of the tools (such as parameters confidence intervals, autocorrelation significance limits, portmanteau tests for white noise, and goodness-of-fit statistics) provided by standard softwares relying on the Box-Jenkins methodology can be quite misleading, as will be seen below. The consequences in terms of order selection, model validation, prediction, can be dramatic. It is therefore of great importance to develop tests and methods allowing to work with a broad class of ARMA models.

Section 2 of this paper deals with some preliminary definitions and interpretations. Examples of nonlinear processes admitting a linear representation are given in Section 3. Section 4 describes the asymptotic behaviour of the empirical autocovariances of a large class of stationary processes. We show how these results can be used for identifying the ARMA orders. In Section 5 we consider the estimation of the ARMA coefficients based on a least-squares criterion, with emphasis on the limiting behaviour of the estimators under mild dependence assumptions. In Section 6 we consider goodness-of-fit tests. Section 7 concludes. All proofs are collected in an appendix.

The main goal of this paper is to provide a review of recent results for ARMA models with uncorrelated but non independent errors. This paper also contains new results.

2.   Basic definitions

In this paper, a second-order stationary real process $X = (X_t)_{t\in\mathbb{Z}}$, is said to admit an ARMA(p,q) representation, where p and q are integers, if for some constants $a_1, \ldots, a_p, b_1, \ldots, b_q$,

$$\forall t \in \mathbb{Z}, \quad X_t - \sum_{i=1}^{p} a_i X_{t-i} = \epsilon_t - \sum_{j=1}^{q} b_j \epsilon_{t-j}, \qquad (12.1)$$

where $\epsilon = (\epsilon_t)$ is a white noise, that is, a sequence of centered uncorrelated variables, with common variance σ^2. It is convenient to write (12.1) as $\phi(L)X_t = \psi(L)\epsilon_t$, where L is the lag operator, $\phi(z) = 1 - \sum_{i=1}^{p} a_i z^i$ is the AR polynomial and $\psi(z) = 1 - \sum_{j=1}^{q} b_j z^j$ is the MA polynomial.

Different sub-classes of ARMA models can be distinguished depending on the noise assumptions. If in (12.1), ϵ is a strong white noise, that is a sequence of independent and identically distributed (iid) variables, then it is customary to call X a *strong* ARMA(p,q), and we will do this henceforth. If ϵ is a martingale difference (m.d.), that is a sequence such that $E(\epsilon_t|\epsilon_{t-1}, \epsilon_{t-2}, \ldots) = 0$, then X is called a *semi-strong* ARMA(p,q).

If no additional assumption is made on ϵ, that is if ϵ is only a weak white noise (not necessarily iid, nor a m.d.), X is called a *weak* ARMA(p,q). It is clear from these definitions that the following inclusions hold:

$$\{\text{strong ARMA}\} \subset \{\text{semi-strong ARMA}\} \subset \{\text{weak ARMA}\}.$$

It is often necessary to constrain the roots of the AR and MA polynomials. The following assumption is standard:

$$\phi(z)\psi(z) = 0 \Rightarrow |z| > 1. \tag{12.2}$$

Under (12.2): (i) a solution X_t of (12.1) is obtained as a linear combination of $\epsilon_t, \epsilon_{t-1}, \ldots$ (this solution is called non anticipative or causal), and (ii) ϵ_t can be written as a linear combination of $X_t, X_{t-1}, \ldots$ (equation (12.1) is said to be invertible). Moreover, it can be shown that if X satisfies (12.1) with $\phi(z)\psi(z) = 0 \Rightarrow |z| \neq 1$, then there exist a weak white noise ϵ^*, and some polynomials ϕ^* and ψ^*, with no root inside the unit disk, such that $\phi^*(B)X_t = \psi^*(B)\epsilon_t^*$. Therefore, (12.2) is not restrictive for weak ARMA models whose AR and MA polynomials have no root on the unit circle. The next example shows that this property does not hold for strong ARMA models.

EXAMPLE 12.1 (NON CAUSAL STRONG AR(1)) Let the AR(1) model

$$X_t = aX_{t-1} + \eta_t, \quad \eta_t \text{ iid } (0, \sigma^2)$$

where $|a| > 1$. This equation has a stationary yet anticipative solution, of the form $X_t = -\sum_{i=1}^{\infty} a^{-i}\eta_{t+i}$, from which the autocovariance function of (X_t) is easily obtained as $\gamma_X(h) := \text{Cov}(X_t, X_{t+h}) = \frac{\sigma^2}{a^{|h|}} \frac{1}{a^2-1}$. Now let $\epsilon_t^* = X_t - (1/a)X_{t-1}$. Then $E\epsilon_t^* = 0$, $\text{Var}(\epsilon_t^*) = \sigma^2/a^2$, and it is straightforward to show that (ϵ_t^*) is uncorrelated. Therefore X admits the causal AR(1) representation $X_t = (1/a)X_{t-1} + \epsilon_t^*$. This AR(1) is not strong in general because, for example, it can be seen that $E\epsilon_t^* X_{t-1}^2 = E\eta_t^3/\{a^2(1 + a + a^2)\}$. Thus when $E\eta_t^3 \neq 0$, ϵ^* is not even a m.d.

The different assumptions on the noise have, of course, different consequences in terms of prediction. Assume that (12.2) holds. When the ARMA is semi-strong the optimal predictor is linear: that is, the best predictor of X_t in the mean-square sense is a linear function of its past values, and it can be obtained by inverting the MA polynomial. When the ARMA is weak, the same predictor is optimal among the linear functions of the past, and it is called optimal linear predictor, but not necessarily among all functions of the past.

The generality of the weak ARMA class can be assessed through the so-called Wold decomposition. Wold (1938) has shown that any purely

non deterministic, second-order stationary process admits an infinite MA representation of the form

$$X_t = \epsilon_t + \sum_{i=1}^{\infty} c_i \epsilon_{t-i}, \tag{12.3}$$

where (ϵ_t) is the linear innovation process of X and $\sum_i c_i^2 < \infty$. Defining the MA(q) process $X_t(q) = \epsilon_t + \sum_{i=1}^{q} c_i \epsilon_{t-i}$, it is straightforward that

$$\|X_t(q) - X_t\|_2^2 = E \epsilon_t^2 \sum_{i>q} c_i^2 \to 0, \quad \text{when } q \to \infty.$$

Therefore any purely non deterministic, second-order stationary process is the limit, in the mean-square sense, of weak finite-order ARMA processes.

The principal conclusion of this section is that the linear model (12.3), which consists of the ARMA models and their limits, is very general under the noise uncorrelatedness, but can be restrictive if stronger assumptions are made.

3.   Examples of exact weak ARMA representations

Many nonlinear processes admit ARMA representations. Examples of bilinear processes, Markov switching processes, threshold processes, deterministic processes, processes obtained by temporal aggregation of a strong ARMA, or by linear combination of independent ARMA processes can be found in Francq and Zakoïan (1998a, 2000). In this section, we will show that the powers of a GARCH(1,1) process (ϵ_t) admit an ARMA representation.

Consider the GARCH(1,1) model

$$\begin{cases} \epsilon_t &= \sqrt{h_t}\,\eta_t \\ h_t &= \omega + \alpha \epsilon_{t-1}^2 + \beta \sigma_{t-1}^2 \end{cases} \tag{12.4}$$

where α and β are nonnegative constants, ω is a positive constant, (η_t) is a strong white noise with unit variance. Under the constraint $\alpha + \beta < 1$, there exists a strictly stationary solution (ϵ_t), nonanticipative (i.e. such that ϵ_t is a function of the η_{t-i} with $i \geq 0$), and with a second order moment. This solution is clearly a semi-strong white noise. Since $E(\epsilon_t^2 | \epsilon_{t-1}, \epsilon_{t-2}, \ldots) = h_t$, the innovation process of ϵ_t^2 is defined by $\nu_t = \epsilon_t^2 - h_t$. The second equation in (12.4) can be written as

$$\epsilon_t^2 = \omega + (\alpha + \beta)\epsilon_{t-1}^2 + \nu_t - \beta \nu_{t-1}. \tag{12.5}$$

This equation shows that, provided $E(\epsilon_t^4) < \infty$, the process (ϵ_t^2) admits an ARMA(1,1) representation. This representation is semi-strong because $E(\nu_t | \epsilon_{t-1}, \epsilon_{t-2}, \ldots) = 0$. The next theorem generalizes this well-known result.

THEOREM 12.1 *Suppose that (ϵ_t) is strictly stationary nonanticipative solution of Model (12.4) with $E\epsilon_t^{4m} < \infty$, where m is an integer. Then (ϵ_t^{2m}) admits a weak ARMA(m, m) representation*

REMARK 12.1 A similar theorem was proved in the framework of Markov-switching GARCH(p, q) models by Francq and Zakoïan (2003). This class encompasses the standard GARCH model so the theorem of the present paper can be seen as a corollary of a more general theorem. However, the result was obtained for the general class with a more complex proof requiring vector representations. The proof presented in the appendix gives an alternative (simpler) way to show the existence of the ARMA representations in the GARCH(1,1) case.

REMARK 12.2 As can be seen in the appendix, the ARMA coefficients can be derived from the coefficients of model (12.4) and from moments of η_t.

REMARK 12.3 Contrary to the representation (12.5), the ARMA representations for $m > 1$ are not semi-strong in general. The noises involved in these representations are not m.d.'s. This can be seen from tedious computations involving numerical calculations.

4.   Sample ACVF and related statistics

In time series analysis, the autocovariance function (ACVF) is an important tool because it provides the whole linear structure of the series. More precisely, it is easy to compute the ACVF from the Wold representation of a regular stationary process. Conversely, the knowledge of the ACVF is sufficient to determine the ARMA representation (when existing).

Consider observations $X_1, \ldots, X_n$ of a centered second-order stationary process. The sample ACVF and autocorrelation function (ACF) are defined, respectively, by

$$\hat{\gamma}(h) = \hat{\gamma}(-h) = \frac{1}{n} \sum_{t=1}^{n-h} X_t X_{t+h}, \quad \hat{\rho}(h) = \frac{\hat{\gamma}(h)}{\hat{\gamma}(0)}, \quad 0 \le h < n.$$

We know that for strictly stationary ergodic processes, $\hat{\gamma}(h)$ and $\hat{\rho}(h)$ are strongly consistent estimators of the theoretical autocovariance $\gamma(h)$

and the theoretical autocorrelation $\rho(h)$. For $0 \leq m < n$, let $\hat{\gamma}_{0\,m} := \{\hat{\gamma}(0), \hat{\gamma}(1), \ldots, \hat{\gamma}(m)\}'$ and $\gamma_{0\,m} := \{\gamma(0), \gamma(1), \ldots, \gamma(m)\}'$. Similarly, denote by $\hat{\rho}_{1\,m}$ and $\rho_{1:m}$ the vectors of the first m sample autocorrelations and theoretical autocorrelations.

4.1 Asymptotic behaviour of the sample ACVF

Extending the concept of second-order stationarity, a real-valued process (X_t) is said to be stationary up to the order k if $E|X_t|^k < \infty$ for all t, and $EX_{t_1}X_{t_2}\ldots X_{t_k} = EX_{t_1+h}X_{t_2+h}\ldots X_{t_k+h}$ for all $k \in \{1, 2, \ldots, m\}$ all $h, t_1, \ldots, t_k \in \mathbb{Z}$.

THEOREM 12.2 *If* (X_t) *is centered and stationary up to the order 4, and if*

$$\sum_{\ell=-\infty}^{+\infty} |\sigma_{h,k}(\ell)| < \infty, \quad \text{for all } k, h \in \{0, 1 \ldots, m\}$$

where $\sigma_{h,k}(\ell) = Cov(X_t X_{t+h}, X_{t+\ell}X_{t+\ell+k})$, *then*

$$\lim_{n \to \infty} n\text{Var}\left(\hat{\gamma}_{0\cdot m}\right) = \Sigma_{\hat{\gamma}_{0\,m}}, \quad \text{where } \Sigma_{\hat{\gamma}_{0\,n}} = \left(\sum_{\ell=-\infty}^{+\infty} \sigma_{h,k}(\ell)\right)_{0 \leq h,k \leq m}.$$

REMARK 12.4 We have $\Sigma_{\hat{\gamma}_{0\,m}} = \sum_{\ell=-\infty}^{+\infty} \text{Cov}(\Upsilon_t, \Upsilon_{t+\ell})$ where $\Upsilon_t := X_t(X_t, X_{t+1}, \ldots, X_{t+m})'$. Thus $(2\pi)^{-1}\Sigma_{\hat{\gamma}_{0\,m}}$ can be interpreted as the spectral density of (Υ_t) at the zero frequency.

To show the asymptotic normality of the sample ACV's, additional moment conditions and weak dependence conditions are needed. Denote by $(\alpha_X(k))_{k \in N^*}$ the sequence of strong mixing coefficients of any process $(X_t)_{t \in \mathbb{Z}}$. Romano and Thombs (1996) showed that under the assumption

A1: $\sup_t E|X_t|^{4+2\nu} < \infty$ and $\sum_{k=0}^{\infty}\{\alpha_X(k)\}^{\nu/(2+\nu)} < \infty$

for some $\nu > 0$, $\sqrt{n}\left(\hat{\gamma}_{0\,m} - \gamma_{0:m}\right)$ is asymptotically normal with mean 0 and variance $\Sigma_{\hat{\gamma}_{0\,m}}$. The mixing condition in **A1** is valid for large classes of processes (see Pham (1986), Carrasco and Chen (2002)) for which the (stronger) condition of β-mixing with exponential decay can be shown. If the mixing coefficients tend to zero at an exponential rate, ν can be chosen arbitrarily small. The moment condition is mild since $EX_t^4 < \infty$ is required for the existence of $\Sigma_{\hat{\gamma}_{0\,m}}$. Romano and Thombs (1996) proposed resampling methods to obtain confidence intervals and to perform tests on the ACVF and ACF. Berlinet and Francq (1997, 1999) employed HAC type estimators to estimate $\Sigma_{\hat{\gamma}_{0\,m}}$ (see *e.g.* Andrews (1991) for details about HAC estimators). In view of Remark 12.4, alternative

estimators of $\Sigma_{\hat{\gamma}_0\ m}$ can be obtained by smoothing the periodogram of Υ_t at the zero frequency (see *e.g.* Brockwell and Davis, 1991, Sections 10.4 and 11.7) or by using an AR spectral density estimator (see *e.g.* Brockwell and Davis, 1991, Section 10.6, and Berk, 1974). In this paper we use the AR spectral density estimator, studied in Francq, Roy and Zakoïan (2004), and defined by

$$\hat{\Sigma}_{\hat{\gamma}_0\ m} = \hat{\mathcal{A}}_r(1)^{-1}\hat{\Sigma}_r\hat{\mathcal{A}}_r(1)^{-1}, \tag{12.6}$$

where $\hat{\mathcal{A}}_r(\cdot)$ and $\hat{\Sigma}_r$ denote the fitted AR polynomial and the variance of the residuals in the multivariate regression of Υ_t on $\Upsilon_{t-1},\dots,\Upsilon_{t-r}$, for $t = r+1,\dots,n-m$. The AR polynomial is fitted using the Durbin-Levinson algorithm. The order r is selected minimizing the BIC information criteria.

Using the delta method, it is easy to obtain the asymptotic distribution of differentiable functions of $\hat{\gamma}_{0\ m}$. In particular, we have

$$\sqrt{n}\,(\hat{\rho}_{1:m} - \rho_{1:m}) \Rightarrow \mathcal{N}\left(0, \Sigma_{\hat{\rho}_1\ m}\right), \quad \Sigma_{\hat{\rho}_1\ m} = J_m\Sigma_{\hat{\gamma}_0\ m}J'_m \tag{12.7}$$

and $J_m = \partial\rho_{1:m}/\partial\gamma'_{0:m}$. For strong ARMA processes, Matrix $\Sigma_{\hat{\rho}_1\ m}$ is given by the so-called Bartlett's formula, which involves the theoretical autocorrelation function $\rho(\cdot)$ only. In particular, for an iid sequence, $\hat{\rho}(1),\dots,\hat{\rho}(h)$ are approximately independent and $\mathcal{N}(0, n^{-1})$ distributed, for large n. This can be used to detect whether a given series is an iid sequence or not. For a strong MA(q), $\sqrt{n}\hat{\rho}(h)$ is asymptotically normal with mean 0 and variance $\sum_{k=-q}^{q}\rho^2(k)$, for any $h > q$. Replacing $\rho(k)$ by $\hat{\rho}(k)$, this can be used to select the order of a strong MA.

Unfortunately, in the case of weak MA or ARMA models, $\Sigma_{\hat{\rho}_1\ m}$ is much more complicated, and involves not only $\rho(\cdot)$, but also fourth order cumulants.

4.2 Misuse of the Bartlett formula

The usual text book formula for $\Sigma_{\hat{\rho}_1\ m}$, the above-mentioned Bartlett's formula, is based on strong assumptions (see Mélard and Roy, 1987, Mélard, Paesmans and Roy, 1991, and Roy, 1989). In particular, the Bartlett formula is not valid when the linear innovations are not iid. It can be shown that the value given by the Bartlett formula can deviate markedly from the true value of $\Sigma_{\hat{\rho}_0\ m}$. As can be seen in the following example, this result is essential in the identification stage of the Box-Jenkins methodology.

EXAMPLE 12.2 Figure 12.1 displays the sample ACF of a simulation of length 5000 of the GARCH(1,1) model (12.4) where (η_t) is i.i.d $\mathcal{N}(0,1)$,

$\omega = 1$, $\alpha = 0.3$ and $\beta = 0.55$. The solution of (12.4) is a white noise with fourth-order moments, but the ϵ_t's are not independent (the ϵ_t^2's are correlated). The Bartlett formula applied to a strong white noise gives $\Sigma_{\hat{\rho}_1 \, m} = I_m$. We deduce that, asymptotically, the sample auto-correlations of a strong white noise are between the bounds $\pm 1.96/\sqrt{n}$ with probability 0.95. The usual procedure consists in rejecting the white noise assumption and fitting a more complex ARMA model when numerous sample autocorrelations lie outside the bounds $\pm 1.96/\sqrt{n}$ (or when one sample autocorrelation is quite outside the bounds). This procedure is absolutely valid for testing the independence assumption, but may lead to incorrect conclusions when applied for testing the weak white noise assumption. In the left graph of Figure 12.1, it can be seen that numerous sample autocorrelations lie outside the bounds $\pm 1.96/\sqrt{n}$. The sample autocorrelations at lag 2 and 3 are much less that $-1.96/\sqrt{n}$. This leads us to reject the strong white noise assumption. However, this does not mean that the weak white noise must be rejected, i.e. that some sample autocorrelations are significant. Actually, all the sample autocorrelations are inside the true significance limits (in thick dotted lines). The true 5% significance limits for the sample ACF are of course unknown in practice. In the right graph of Figure 12.1, an estimate (based on the AR spectral density estimator of $\Sigma_{\hat{\rho}_1 \, m}$ described in Section 4.1) of these significance limits is plotted. From the right graph, there is no evidence against the weak white noise assumption (but from the left graph the strong white noise model is rejected). We draw the conclude that, to detect weak ARMA models, it is important to use more robust estimators of $\Sigma_{\hat{\rho}_1 \, m}$ than those given by the Bartlett formula.
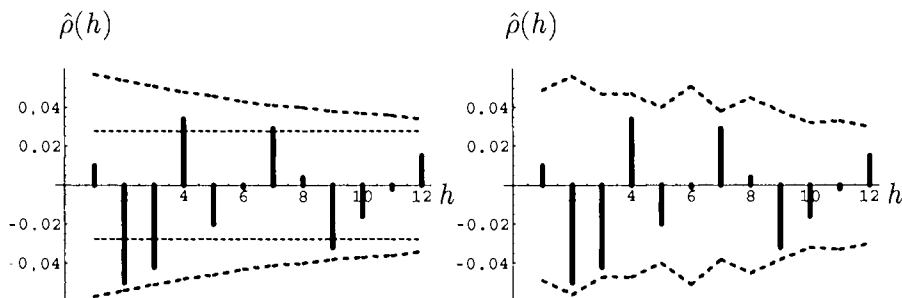
Figure 12.1.   Sample ACF of a simulation of length $n = 5000$ of the weak (semi-strong) white noise (12.4). In the left graph, the horizontal dotted lines $\pm 1.96/\sqrt{n}$ correspond to the asymptotic 5% significance limits for the sample autocorrelations of a strong white noise. The thick dotted lines about zero represent the asymptotic 5% significance limits for the sample autocorrelations of ϵ_t. In the right graph, the thick dotted lines about zero represent an estimate of the 5% significance limits for the sample autocorrelations of ϵ_t.

4.3 Behaviour of the sample partial autocorrelations

The partial autocovariance function (PACF), denoted by $r(\cdot)$, is a very convenient tool to detect $AR(p)$ processes. Since $r(h)$ is a differentiable function of $\rho(1), \rho(2), \ldots, \rho(h)$, the asymptotic behaviour of the sample PACF $\hat{r}(\cdot)$ is given by a formula similar to (12.7).

It is known that, for strong $AR(p)$ processes, $\sqrt{n}\hat{r}(h)$ is asymptotically $\mathcal{N}(0,1)$ distributed, for each $h > p$. This is very convenient to detect the order of strong AR processes. Of course, the limiting distribution is no more $\mathcal{N}(0,1)$ for weak AR models.

The following result shows that a comparison between the sample ACF and sample PACF can be useful to detect a weak white noise.

THEOREM 12.3 *If (X_t) is a stationary weak white noise satisfying* **A1**, *then*

$$\hat{\rho}(h) - \hat{r}(h) = O_p(n^{-1}). \qquad (12.8)$$

REMARK 12.5 This result indicates that, for a weak white noise, the sample ACF and sample PACF should be very close. To our knowledge, however, no formal test based on this principle exists. Theorem 12.3 also entails that, for a weak white noise, the asymptotic distributions of $\sqrt{n}\hat{\rho}_{1:m}$ and $\sqrt{n}\hat{r}_{1:m} := \sqrt{n}\{\hat{r}(1), \ldots, \hat{r}(m)\}$ are the same.

4.4 Portmanteau tests for weak white noise assumption

It is possible to test the assumption $H_0 : \rho(1) = \cdots = \rho(m) = 0$ by a so-called portmanteau test. The initial version of the test is based on the Box and Pierce (1970) statistic $Q_m = n \sum_{h=1}^{m} \hat{\rho}^2(h)$. Under the assumption H'_0 that (X_t) is a strong white noise, we know from the Bartlett formula that the asymptotic distribution of $\sqrt{n}\hat{\rho}_{1:m}$ is $\mathcal{N}(0, I_m)$. Therefore the asymptotic distribution of Q_m is χ^2_m under H'_0. The standard test procedure consists in rejecting the null hypothesis H_0 if $Q_m > \chi^2_m(1-\alpha)$, where $\chi^2_m(1 - \alpha)$ denotes the $(1 - \alpha)$-quantile of a χ^2 distribution with m degrees of freedom. Ljung and Box (1978) argued that, in the case of a Gaussian white noise, the finite sample distribution of the test statistic is more accurately approximated by a χ^2_m when Q_m is replaced by $\tilde{Q}_m = n(n + 2) \sum_{h=1}^{m} \frac{\hat{\rho}^2(h)}{n-h}$. Nowadays, all the time series packages incorporate the Ljung-Box version of the portmanteau test.

It is easy to see that the asymptotic distribution of Q_m (and $\tilde{Q}_m$) can be very different from the χ^2_m when H_0 is satisfied, but H'_0 is not (see Lobato (2001) and Francq, Roy and Zakoïan (2004)). Therefore the standard portmanteau test is rather an independence test than an

uncorrelatedness test. Thus, when the standard portmanteau test leads to the rejection, *i.e.* $Q_m > \chi_m^2(1 - \alpha)$, the practitioner does not know whether (i) H_0 is actually false, or (ii) H_0 is true but H_0' is false. The problem can be solved by using the estimators of $\Sigma_{\hat{\gamma}_{0\ m}}$ mentioned in Section 4.1.

THEOREM 12.4 *Let* (X_t) *be a stationary process and let* $\Upsilon_t := (X_t^2, X_t X_{t+1}, \ldots, X_t X_{t+m})$. *Assume that* $\mathrm{Var}(\Upsilon_t)$ *is non-singular. If* (X_t) *is a weak white noise satisfying* **A1** *and if* $\hat{\Sigma}_{\hat{\rho}_1\ m}$ *is a weakly consistent estimator of* $\Sigma_{\hat{\rho}_1\ m}$, *then the limit law of the statistics*

$$Q_m^\rho = n\hat{\rho}_{1\ m}'\hat{\Sigma}_{\hat{\rho}_1\ m}^{-1}\hat{\rho}_{1\ m} \quad and \quad Q_m^r = n\hat{r}_{1,m}'\hat{\Sigma}_{\hat{\rho}_1\ m}^{-1}\hat{r}_{1\ m} \qquad (12.9)$$

is the χ_m^2 *distribution.*

REMARK 12.6 Replacing Q_m by Q_m^ρ in the standard portmanteau test for strong white noise, we obtain a portmanteau test for weak white noise. Another portmanteau test for weak white noise, based on the sample PACF, is obtained when the statistic Q_m^r is used. Monte Carlo experiments reveal that the portmanteau test based on the sample PACF may be more powerful than that based on the sample ACF. Intuitively, this is the case for alternatives such that the magnitude of the PACF is larger than that of the ACF (in particular, for MA models).

EXAMPLE 12.3 *(Example 12.2 continued)* The sample PACF is displayed in Figure 12.2 It is seen that this PACF is very close to the sample ACF displayed in the right graph of Figure 12.1. This is not surprising in view of Theorem 12.3. The results of the standard portmanteau tests are not presented but lead to reject the strong white noise assumption ($P(\chi_m^2 > Q_m)$ and $P(\chi_m^2 > \tilde{Q}_m)$ are less than 0.001 for $m > 1$). Figure 12.3 shows that the weak white noise assumption is not rejected by the portmanteau tests based on the statistic Q_m^ρ (the portmanteau tests based on the PACF lead to similar results).

4.5   Application to the identification stage

To detect the order of a MA, a common practice is to draw the sample ACF, as in Figure 12.1. If for some not too large integer q_0, almost all the $\hat{\rho}(h)$, $h > q_0$ are inside the bounds $\pm 1.96n^{-1/2}\left\{\sum_{j=-h+1}^{j=h-1}\hat{\rho}^2(j)\right\}^{1/2}$, practitioners consider that a MA(q_0) is a reasonable model. Although meaningful for detecting the order of a strong MA process, this procedure is not valid for identifying weak MA models. Indeed, we have seen that the bounds given by the Bartlett formula are not correct in
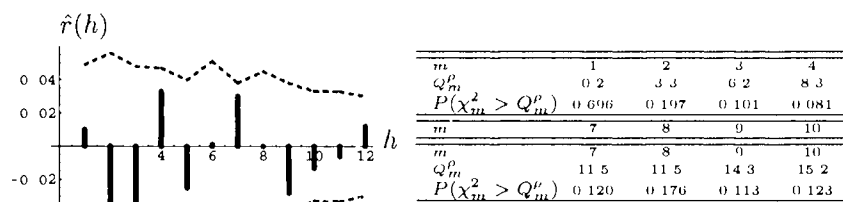
$\hat{r}(h)$

m	1	2	3	4
Q^ρ_m	0 2	3 3	6 2	8 3
$P(\chi^2_m > Q^\rho_m)$	0 696	0 197	0 101	0 081

m	7	8	9	10
m	7	8	9	10
Q^ρ_m	11 5	11 5	14 3	15 2
$P(\chi^2_m > Q^\rho_m)$	0 120	0 176	0 113	0 123

Figure 12.3. Portmanteau tests of the weak white noise assumption (based on (12.9)) for a simulation of length $n = 5000$ of Model (12.4).

Figure 12.2. As for the right graph in Figure 12.1, but for the Sample PACF.

this framework. A procedure which remains valid for weak models, is obtained by replacing $\sum_{j=-h+1}^{j=h-1} \hat{\rho}^2(j)$ by the h-th diagonal term of the matrix $\hat{\Sigma}_{\hat{\rho}1\,m}$ given in (12.7) and (12.6). With this modification, the identification of (weak) MA models can be done in the usual way.

Similarly, the asymptotic distribution of $\hat{r}_{1:m}$, given in Section 4.3 can be used to detect the order of an AR model. For mixed ARMA processes, different statistics have been introduced in the literature (*e.g.* the corner method (Béguin, Gouriéroux and Monfort, 1980), the epsilon algorithm (Berlinet, 1984), Glasbey's generalized autocorrelations (1982)). Initially the methods based on these statistics were developed for strong ARMA models, using the conventional Bartlett formula. Without any modification, their application to weak ARMA models can misguide the analyst and result in an inappropriate model being selected. However, all the above-mentioned statistics are differentiable functions of $\hat{\rho}_{1\,m}$. Thus their asymptotic distributions can be derived from (12.7). Using this correction, these methods remain valid for selecting weak ARMA models.

Other popular approaches for identifying the ARMA orders are founded on information criteria such as AIC and BIC. It was shown in Francq and Zakoïan (1998b) that, asymptotically, the orders are not underestimated when these criteria are applied to weak ARMA models. The consistency of the BIC criterion is an open issue in the weak ARMA framework.

5. Estimation

Following the seminal papers by Mann and Wald (1943) and Walker (1964), numerous works have been devoted to the estimation of ARMA models. Hannan (1973) showed the strong consistency of several estimators, under the ergodicity assumption for the observed process, and the asymptotic normality under the m.d. assumption for the noise.

Dunsmuir and Hannan (1976) and Rissanen and Caines (1979) extended these results to multivariate processes. Tiao and Tsay (1983) considered a nonstationary case with an iid noise. Mikosch et al. (1995) considered ARMA with infinite variance and iid noise. Kokoszka and Taqqu (1996) considered fractional ARIMA with infinite variance and iid noise. Following Dickey and Fuller (1979), the estimation of ARMA models with unit roots have been extensively investigated. All these authors assumed (at least for the asymptotic normality) that the linear innovations constitute a m.d. This assumption is not satisfied for ARMA representations of non linear processes.

We will investigate the asymptotic behaviour of the ordinary least squares (OLS) estimator when the linear innovation process is not a m.d. Alternative estimators, such as those obtained from the generalized method of moments (see Hansen (1982), have been proposed (see Broze, Francq and Zakoïan (2002)). Denote by $\theta_0 = (a_1, \ldots, a_p, b_1, \ldots, b_q)'$ the true value of the unknown parameter.

5.1   Consistency

The assumptions are the following.

A2: X is strictly stationary and ergodic.

A3: The polynomials $\phi(z) = 1 - a_1 z + \ldots - a_p z^p$ and $\psi(z) = 1 - b_1 z + \ldots - b_q z^q$ have all their zeros outside the unit disk and have no zero in common.

A4: $p + q > 0$ and $a_p^2 + b_q^2 \neq 0$ (by convention $a_0 = b_0 = 1$).

A5: $\sigma^2 > 0$.

A6: $\theta_0 \in \Theta^*$ where Θ^* is a compact subspace of the parameter space

$$\Theta \; := \; \big\{ \theta = (\theta_1, \ldots, \theta_{p+q}) \in \mathbb{R}^{p+q} : \; \phi_\theta(z) = 1 - \theta_1 z - \cdots - \theta_p z^p$$
$$\text{and } \psi_\theta(z) = 1 - \theta_{p+1} z - \cdots - \theta_{p+q} z^q$$
$$\text{have all their zeros outside the unit disk} \big\}.$$

Note that **A2** is equivalent to **A2'**: ϵ is strictly stationary and ergodic.
For all $\theta \in \Theta$, let

$$\epsilon_t(\theta) = \psi_\theta^{-1}(B) \phi_\theta(B) X_t = X_t + \sum_{i=1}^{\infty} c_i(\theta) X_{t-i}.$$

Given a realization of length n, $X_1, X_2, \ldots, X_n$, $\epsilon_t(\theta)$ can be approximated, for $0 < t \le n$, by $e_t(\theta)$ defined recursively by

$$e_t(\theta) = X_t - \sum_{i=1}^{p} \theta_i X_{t-i} + \sum_{i=1}^{q} \theta_{p+i} e_{t-i}(\theta) \tag{12.10}$$

where the unknown starting values are set to zero: $e_0(\theta) = e_{-1}(\theta) = \ldots = e_{-q+1}(\theta) = X_0 = X_{-1} = \ldots = X_{-p+1} = 0$. The random variable $\hat{\theta}_n$ is called least squares (LS) estimator if it satisfies, almost surely,

$$Q_n(\hat{\theta}_n) = \min_{\theta \in \Theta^*} Q_n(\theta), \qquad Q_n(\theta) = \frac{1}{n} \sum_{t=1}^{n} e_t^2(\theta). \tag{12.11}$$

Hannan (1973) showed the following result using the spectral analysis. The proof we give in the appendix is quite different.

THEOREM 12.5 *Under Assumptions* **A2-A6**, $\hat{\theta}_n \longrightarrow \theta_0$ *almost surely as $n \to \infty$.*

5.2 Asymptotic normality

The asymptotic normality is established in Francq and Zakoïan (1998a), using the additional assumptions **A1** and

A6 : θ belongs to the interior of Θ^*.

Assumption **A1** can be replaced by

A1' : $E|\epsilon_t|^{4+2\nu} < \infty$ and $\sum_{k=0}^{\infty} [\alpha_\epsilon(k)]^{\frac{\nu}{2+\nu}} < \infty$ for some $\nu > 0$.

Note that Assumptions **A1** and **A1'** are not equivalent.

THEOREM 12.6 *Under Assumption* **A1** *or* **A1'** *and Assumptions* **A2-A6**,

$$\sqrt{n}\left(\hat{\theta}_n - \theta_0\right) \xrightarrow{d} \mathcal{N}(0, J^{-1}IJ^{-1}) \text{ as } n \to \infty, \tag{12.12}$$

where $I = I(\theta_0)$, $J = J(\theta_0)$,

$$I(\theta) = \frac{1}{4} \lim_{n \to \infty} \text{Var}\left\{\sqrt{n}\frac{\partial}{\partial \theta}Q_n(\theta)\right\}, \quad J(\theta) = \frac{1}{2} \lim_{n \to \infty} \frac{\partial^2}{\partial\theta\partial\theta'}Q_n(\theta) \quad a.s.$$

REMARK 12.7 Matrices I and J can be computed explicitly. Indeed, from (12.1) we have

$$-X_{t-i} = \psi(B)\frac{\partial}{\partial\theta_i}\epsilon_t \quad \text{and} \quad 0 = -\epsilon_{t-j} + \psi(B)\frac{\partial}{\partial\theta_{p+j}}\epsilon_t$$

for $i = 1, \ldots, p$ and $j = 1, \ldots, q$. Thus

$$\partial \epsilon_t / \partial \theta = (u_{t-1}, \ldots, u_{t-p}, v_{t-1}, \ldots, v_{t-q})'$$

where

$$u_t = -\phi^{-1}(B)\epsilon_t := -\sum_{i=0}^{\infty} \phi_i^* \epsilon_{t-i} \quad \text{and} \quad v_t = \psi^{-1}(B)\epsilon_t := \sum_{i=0}^{\infty} \psi_i^* \epsilon_{t-i}.$$

Hence

$$
\begin{aligned}
J &= \text{Var}\left(\frac{\partial}{\partial \theta}\epsilon_t\right)_{\theta=\theta_0} = \text{Var}\,(u_{t-1}, \ldots, u_{t-p}, v_{t-1}, \ldots, v_{t-q})' \\
&= \text{Var}\sum_{i=1}^{\infty} \epsilon_{t-i}\lambda_i = \sigma^2 \Lambda_\infty \Lambda_\infty'
\end{aligned}
$$

and

$$
\begin{aligned}
I &= \sum_{h=-\infty}^{+\infty} \text{Cov}\left\{\epsilon_t\frac{\partial}{\partial\theta}\epsilon_t, \epsilon_{t+h}\frac{\partial}{\partial\theta}\epsilon_{t+h}\right\} \\
&= \sum_{i,j=1}^{\infty} \lambda_i \sum_{h=-\infty}^{+\infty} \text{Cov}\,(\epsilon_t\epsilon_{t-i}, \epsilon_{t+h}\epsilon_{t+h-j})\,\lambda_j' = \Lambda_\infty \Sigma_{\hat{\gamma}_\infty} \Lambda_\infty'
\end{aligned}
$$

where, for $m = 1, 2, \ldots, \infty$, the matrix $\Sigma_{\hat{\gamma}_m^\epsilon}$ is the asymptotic variance of $\sqrt{n}\,\{\hat{\gamma}_\epsilon(1), \ldots, \hat{\gamma}_\epsilon(m)\}'$, and

$$
\Lambda_m = (\lambda_1 \ \lambda_2 > \ \cdots \ \lambda_m) =
\begin{pmatrix}
-1 & -\phi_1^* & \cdots & & & & & -\phi_{m-1}^* \\
0 & -1 & & & & & & \vdots \\
\vdots & & & & & & & \\
0 & & & -1 & -\phi_1^* & \cdots & & -\phi_{m-p}^* \\
1 & \psi_1^* & \cdots & & & & & \psi_{m-1}^* \\
0 & 1 & & & & & & \vdots \\
\vdots & & & & & & & \\
0 & & & 1 & \psi_1^* & \cdots & & \psi_{m-q}^*
\end{pmatrix}.
$$

$$(12.13)$$

5.3   Asymptotic accuracy of LSE for weak and strong ARMA

In the strong ARMA case, we have

$$I = \frac{1}{4}\text{Var}\left\{\frac{\partial}{\partial\theta}\epsilon_t^2(\theta_0)\right\} = \text{Var}\left\{\epsilon_t\frac{\partial}{\partial\theta}\epsilon_t(\theta_0)\right\} = \sigma^2 J.$$

The asymptotic covariance matrix of the LSE is then $S = \sigma^2 J^{-1}$. In the weak ARMA case, the true asymptotic variance Σ can be very different from S (see Example 12.4 below). For the statistical inference on the parameter, in particular the Student's t significant test, the standard time series analysis softwares use empirical estimators of S. Under ergodicity and moment assumptions, these estimators converges to S, but, in general, they do not converge to the true asymptotic variance Σ. This can of course be a serious cause of mistake in model selection. Francq and Zakoïan (2000) have proposed an estimator of Σ which is consistent for both weak and strong ARMA cases.

EXAMPLE 12.4 *(Example 12.3 continued)* Consider the AR(1) model $X_t - aX_{t-1} = \epsilon_t$ where ϵ_t is the weak white noise defined by the GARCH(1,1) equation (12.4). The LSE of a is simply $\hat{a} = \sum_{t=2}^{n} X_t X_{t-1} / \sum_{t=2}^{n} X_{t-1}^2$. From Theorem 12.6 we know that $n^{1/2}(\hat{a} - a)$ converges in law to the $\mathcal{N}(0, \Sigma)$ distribution, where Σ depends on a, ω, α and β. It is also well known that, when (ϵ_t) is a strong white noise (*i.e.* when $\alpha = \beta = 0$), $n^{1/2}(\hat{a} - a)$ converges in law to the $\mathcal{N}(0, S)$ distribution, where $S = 1 - a^2$. Figure 12.4 displays the ratio Σ/S for several values of a, α and β. It can be seen that Σ and S can be very different.

$\omega = 1, \alpha = 0.3, \beta = 0.55$ 　　 $a = 0, \omega = 1, \alpha = 0.3$ 　　 $a = 0, \omega = 1, \beta = 0.55$
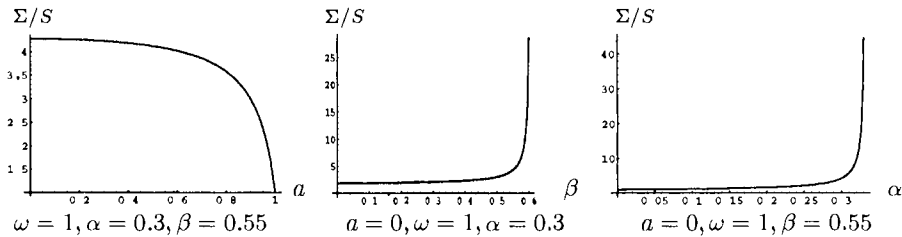
Figure 12.4 Comparison of the true asymptotic covariance Σ and $S = 1 - a^2$ for the LS estimator of a in the model $X_t = aX_{t-1} + \epsilon_t$, where (ϵ_t) follows the GARCH(1,1) equation (12.4)

6. Validation

The goodness of fit of a given ARMA(p, q) model is often judged by studying the residuals $\hat{\epsilon} = (\hat{\epsilon}_t)$. If the model is appropriate, then the residual autocorrelations should not be too large. Box and Pierce (1970) gave the asymptotic distribution of the residual autocorrelations of strong ARMA models. Recently, Francq, Roy and Zakoïan (2004) considered the weak ARMA case. We summarize their results. Let $\hat{\rho}^{\hat{\epsilon}}_{1:m}$ be the vector of the first m residual autocorrelations.

We use the notations of Remark 12.7 and the additional notation

$$\Sigma_{\hat{\gamma}_1^\epsilon \, m \times 1 \, m'} = \lim_{n \to \infty} n \mathrm{Cov}\left[\{\hat{\gamma}_\epsilon(1), \dots, \hat{\gamma}_\epsilon(m)\}', \{\hat{\gamma}_\epsilon(1), \dots, \hat{\gamma}_\epsilon(m')\}'\right].$$

Under the assumptions of Theorem 12.6, it can be shown that $\sqrt{n}\hat{\rho}_{1 \, m}^\epsilon \overset{d}{\rightsquigarrow} \mathcal{N}(0, \Sigma_{\hat{\rho}_{1 \, m}^\epsilon})$, where

$$
\begin{aligned}
\Sigma_{\hat{\rho}_{1 \, m}^\epsilon} &= \sigma^{-4}\Sigma_{\hat{\gamma}_{1 \cdot m}^\epsilon} + \Lambda_m' J^{-1} I J^{-1} \Lambda_m - \sigma^{-2} \Lambda_m' J^{-1} \Lambda_\infty \Sigma_{\hat{\gamma}_1^\epsilon \, \infty \times 1 \, m} \\
&\quad - \sigma^{-2}\Sigma_{\hat{\gamma}_1^\epsilon \, m \times 1 \, \infty} \Lambda_\infty' J^{-1} \Lambda_m.
\end{aligned}
\tag{12.14}
$$

Note that in the strong ARMA case, $\Sigma_{\hat{\gamma}_1^\epsilon \, m} = \sigma^4 I_m$ and

$$\Sigma_{\hat{\rho}_{1 \, m}^\epsilon} = I_m - \Lambda_m'\{\Lambda_\infty \Lambda_\infty'\}^{-1}\Lambda_m \simeq I_m - \Lambda_m'\{\Lambda_m \Lambda_m'\}^{-1}\Lambda_m$$

is close to a projection matrix with $m - (p + q)$ eigenvalues equal to 1, and $(p + q)$ eigenvalues equal to 0, and we retrieve the result given in Box and Pierce (1970). Matrices Λ_m only depend on the ARMA parameters and can be estimated by a plug-in approach. Matrices $\Sigma_{\hat{\gamma}_1^\epsilon \, m}$ can be estimated by the methods described in Section 4.1. This leads to a consistent estimator of $\Sigma_{\hat{\rho}_{1 \, m}^\epsilon}$, which provides estimated significance limits for the sample autocorrelations. This can be used in a graph, similar to that of the right panel of Figure 12.1, to judge whether the selected weak ARMA(p, q) model is adequate or not.

Other very popular diagnostic checking tools are the portmanteau tests based on the residual autocorrelations. Let $Q_m^{\rho_\epsilon} := n \sum_{i=1}^m \hat{\rho}_\epsilon^2(i)$ be the Box-Pierce portmanteau statistic based on the first m sample autocorrelations. The portmanteau statistic for residuals is not defined as in (12.9), because $\Sigma_{\hat{\rho}_{1 \, m}^\epsilon}$ can be singular. From (12.13), it is easy to see that the statistics $Q_m^{\rho_\epsilon}$ converges in distribution, as $n \to \infty$, to

$$\mathbf{Z}_m(\xi_m) := \sum_{i=1}^m \xi_{i,m} Z_i^2 \tag{12.15}$$

where $\xi_m = (\xi_{1,m}, \dots, \xi_{m,m})'$ is the eigenvalues vector of $\Sigma_{\hat{\rho}_{1 \, m}^\epsilon}$, and $Z_1, \dots, Z_m$ are independent $\mathcal{N}(0, 1)$ variables. The distribution of the quadratic form $\mathbf{Z}_m(\xi_m)$ can be computed using the algorithm by Imhof (1961).

EXAMPLE 12.5 *(Example 12.4 continued)* We simulated a realization of length $n = 5000$ of the AR(1) model $X_t - aX_{t-1} = \epsilon_t$ with $a = 0.5$ and where (ϵ_t) satisfies the GARCH(1,1) equation (12.4). The LS estimate of a is $\hat{a} = 0.483$. Figure 12.5 displays the sample autocorrelations,

$\hat{\rho}_{\hat{\epsilon}}(h)$, $h = 1, \ldots, 12$, of the residuals $\hat{\epsilon}_t = X_t - \hat{a}X_{t-1}$, $t = 2, \ldots, n$. For a strong AR(1) model, we know that $\hat{\rho}_{\hat{\epsilon}}(h)$ should lie between the bounds $\pm 1.96n^{-1/2}\left\{1 - a^{2h-2}(1 - a^2)\right\}$ with probability close to 95%. These 5% significance limits are plotted in thin dotted lines. It can be seen that numerous residual autocorrelations are close or outside the thin dotted lines, which can be considered as an evidence against the strong AR(1) model. This is confirmed by the standard portmanteau tests given in Figure 12.6. For the simulated weak AR(1), the correct 5% significance limits are not the thin dotted lines. Estimates of the true 5% significance limits are plotted in thick dotted lines. Since all the residual autocorrelations are inside these limits, there is no evidence against the weak AR(1) model. This is confirmed by the portmanteau tests (based on the statistic $Q_m^{\rho_{\hat{\epsilon}}}$ and on the limiting distribution (12.15)), presented in Figure 12.7.
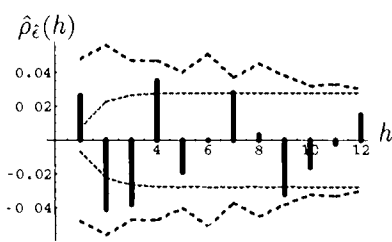
Figure 12.5. Residual ACF of a simulation of the model of Example 12.5

m	1	2	3	12
$P(\chi^2_m > Q_m^{\rho})$	n.d.	0.001	0.000	0.000

Figure 12.6. Portmanteau test for a strong AR(1)

m	1	2	3	12
p-value	0 295	0.187	0.125	0 185

Figure 12.7. Portmanteau test for a weak AR(1)

7.   Conclusion

The principal thrust of this paper is to point out that: (i) the standard Box-Jenkins methodology can lead to erroneous conclusions when the independence assumption on the noise is in failure; (ii) this methodology can be accommodated to handle weak ARMA models. We made a survey of the recent literature on this topic and also presented some complementary new results and illustrations. Of course, many issues remain uncovered, such as efficiency of the inference procedures, testing the different classes of ARMA models, extension to the multivariate framework.

Appendix: Proofs

Proof of Theorem 12.1. Let for $i \geq j \geq 0$,

$$\xi_{i,j} = \binom{i}{j} \omega^{i-j} E(\alpha\eta_t^2 + \beta)^j \frac{\mu_{2i}}{\mu_{2j}} \quad \text{where} \quad \mu_{2i} = E\eta_t^{2i}.$$

We have, for $i = 0, \dots, 2m$

$$E\epsilon_t^{2i} = \mu_{2i} \sum_{j=0}^{i} \binom{i}{j} \omega^{i-j} E(\alpha\eta_{t-1}^2 + \beta)^j E(h_{t-1}^j) = \sum_{j=0}^{i} \xi_{i,j} E(\epsilon_{t-1}^{2j}), \quad \text{(A.1)}$$

using the independence between η_t and h_t. Similarly, for $k > 1$ and $i = 0, \dots, m$

$$E(\epsilon_t^{2i} \epsilon_{t-k}^{2m}) = \sum_{j=0}^{i} \xi_{i,j} E(\epsilon_{t-1}^{2j} \epsilon_{t-k}^{2m}).$$

It follows that for $k > 1$ and $i = 0, \dots, m$

$$\text{Cov}(\epsilon_t^{2i}, \epsilon_{t-k}^{2m}) = \sum_{j=1}^{i} \xi_{i,j} \text{Cov}(\epsilon_{t-1}^{2j}, \epsilon_{t-k}^{2m}). \quad \text{(A.2)}$$

Denoting by L the lag operator and writing, for any bivariate stationary process (X_t, Y_t), $L\text{Cov}(X_t, Y_t) = \text{Cov}(X_{t-1}, Y_t)$, we then have

$$(1 - \xi_{i,i}L)\text{Cov}(\epsilon_t^{2i}, \epsilon_{t-k}^{2m}) = \sum_{j=1}^{i-1} \xi_{i,j}\text{Cov}(\epsilon_{t-1}^{2j}, \epsilon_{t-k}^{2m}), \quad k > 1 \quad \text{(A.3)}$$

Note the right hand side of (A.3) is equal to equal to zero when $i = 1$. Applying to this equality the lag polynomial $1 - \xi_{i-1,i-1}L$ we get

$$(1 - \xi_{i,i}L)(1 - \xi_{i-1,i-1}L)\text{Cov}(\epsilon_t^{2i}, \epsilon_{t-k}^{2m}) = \xi_{i,i-1}(1 - \xi_{i-1,i-1}L)\text{Cov}(\epsilon_{t-1}^{2(i-1)}, \epsilon_{t-k}^{2m})$$
$$+ \sum_{j=1}^{i-2} \xi_{i,j}(1 - \xi_{i-1,i-1}L)\text{Cov}(\epsilon_{t-1}^{2j}, \epsilon_{t-k}^{2m}).$$

Since by stationarity $\text{Cov}(\epsilon_{t-1}^{2(i-1)}, \epsilon_{t-k}^{2m}) = \text{Cov}(\epsilon_t^{2(i-1)}, \epsilon_{t-k+1}^{2m})$, we can use (A.3) to obtain, for $k > 2$,

$$(1 - \xi_{i,i}L)(1 - \xi_{i-1,i-1}L)\text{Cov}(\epsilon_t^{2i}, \epsilon_{t-k}^{2m})$$
$$= \xi_{i,i-1} \sum_{j=1}^{i-2} \xi_{i-1,j}\text{Cov}(\epsilon_{t-2}^{2j}, \epsilon_{t-k}^{2m}) + \sum_{j=1}^{i-2} \xi_{i,j}(1 - \xi_{i-1,i-1}L)\text{Cov}(\epsilon_{t-1}^{2j}, \epsilon_{t-k}^{2m})$$
$$= \sum_{j=1}^{i-2} (\xi_{i,i-1}\xi_{i-1,j} - \xi_{i-1,i-1}\xi_{i,j})\text{Cov}(\epsilon_{t-2}^{2j}, \epsilon_{t-k}^{2m}) + \sum_{j=1}^{i-2} \xi_{i,j}\text{Cov}(\epsilon_{t-1}^{2j}, \epsilon_{t-k}^{2m}).$$

The right hand side of previous equality is zero when $i = 2$. Applying iteratively equation (A.3) we obtain, for $k > i$,

$$\prod_{j=1}^{i} (1 - \xi_{j,j}L)\text{Cov}(\epsilon_t^{2i}, \epsilon_{t-k}^{2m}) = 0.$$

In particular

$$\prod_{j=1}^{m}(1 - \xi_{j,j}L)\mathrm{Cov}(\epsilon_t^{2m}, \epsilon_{t-k}^{2m}) = 0, \qquad k > m. \tag{A.4}$$

In view of the standard result characterizing the existence of an ARMA representation through the autocovariance function (see *e.g.* Brockwell and Davis (1991), Proposition 3.2.1 and Remark p. 90), we conclude that (ϵ_t^{2m}) admits an ARMA(m,m) representation as claimed. $\square$

Derivation of the ARMA(m,m) representation of Theorem 12.1. By (A.4) the AR polynomial of the ARMA representation is $\prod_{j=1}^{m}(1 - \xi_{j,j}L)$. Notice that, by (A.1),

$$(1 - \xi_{i,i})E(\epsilon_t^{2i}) = \sum_{j=0}^{i-1} \xi_{i,j}E(\epsilon_{t-1}^{2j}),$$

which proves that $\xi_{i,i} < 1$ for $i = 1, \dots, m$. The condition $\xi_{i,i} < 1$ can be shown to be necessary and sufficient for the existence of a strictly stationary nonanticipative solution of Model (12 4) with $E\epsilon_t^{2i} < \infty$

The MA part can be derived by computing the first $m + 1$ autocovariances of ϵ_t^{2m} The moments of ϵ_t^2 up to the order $2m$ are obtained recursively from (A.1). Hence the variance of ϵ_t^{2m} Next, the first-order autocovariance can be obtained from

$$E(\epsilon_t^{2i}\epsilon_{t-1}^{2m}) = \sum_{j=0}^{i}\binom{i}{j}\omega^{i-j}E\{(\alpha\eta_{t-1}^2 + \beta)^j\eta_{t-1}^{2m}\}\frac{\mu_{2i}}{\mu_{2(m+j)}}E\epsilon_{t-1}^{2(m+j)},$$

implying, for $i = 1, \dots, m$

$$\mathrm{Cov}(\epsilon_t^{2i}, \epsilon_{t-1}^{2m}) = \sum_{j=1}^{i}\binom{i}{j}\omega^{i-j}\mu_{2i}\left\{ E\{(\alpha\eta_{t-1}^2 + \beta)^j\eta_{t-1}^{2m}\}\frac{1}{\mu_{2(m+j)}}E\epsilon_t^{2(m+j)}\right.$$
$$\left. - E(\alpha\eta_{t-1}^2 + \beta)^j\frac{1}{\mu_{2j}}E\epsilon_t^{2j}E\epsilon_t^{2m}\right\}.$$

The other autocovariances follow from (A 2)

For instance if the ARMA(1,1) representation (12 5) for ϵ_t^2 was not known, it could be obtained as follows. First note that $\xi_{1,1} = \alpha + \beta$, which gives the AR coefficient. To derive the MA coefficient we derive the first-order autocorrelation of ϵ_t^2. From

$$E(\epsilon_t^2) = \frac{\omega}{1 - (\alpha + \beta)}, \quad E(\epsilon_t^4) = \frac{\omega^2\mu_4(1 + \alpha + \beta)}{\{1 - (\alpha + \beta)\}\{1 - (\alpha + \beta)^2 - (\mu_4 - 1)\alpha^2\}},$$

we get

$$\gamma(0) := \mathrm{Var}(\epsilon_t^2) = \frac{\omega^2(\mu_4 - 1)(1 - 2\alpha\beta - \beta^2)}{\{1 - (\alpha + \beta)\}^2\{1 - (\alpha + \beta)^2 - (\mu_4 - 1)\alpha^2\}}$$

$$\gamma(1) := \mathrm{Cov}(\epsilon_t^2, \epsilon_{t-1}^2) = \frac{\omega^2\alpha(\mu_4 - 1)(1 - (\alpha + \beta)\beta)}{\{1 - (\alpha + \beta)\}^2\{1 - (\alpha + \beta)^2 - (\mu_4 - 1)\alpha^2\}}$$

$$\rho(1) := \frac{\gamma(1)}{\gamma(0)} = \frac{\alpha(1 - (\alpha + \beta)\beta)}{1 - 2\alpha\beta - \beta^2}.$$

For an ARMA(1,1) with AR coefficient ϕ and MA coefficient θ, the first-order autocorrelation is

$$\rho(1) = \frac{(\phi - \theta)(1 - \theta\phi)}{1 - 2\theta\phi + \theta^2}.$$

Given that $\phi = \alpha + \beta$ we obtain $\theta = \beta$ or, if $\beta \neq 0$, $\theta = 1/\beta$. Since $0 \leq \beta < 1$, the canonical ARMA representation is therefore given by (12.5) When $\beta = 0$ we obtain an AR(1) model

Proof of Theorem 12.2. For $h \geq 0$, let $\gamma^*(h) = \gamma^*(-h) = \frac{1}{n}\sum_{t=1}^{n} X_t X_{t+h}$. We have

$$n\mathrm{Cov}\{\hat{\gamma}(h), \hat{\gamma}(k)\} - n\mathrm{Cov}\{\gamma^*(h), \gamma^*(k)\} = d_1 + d_2 + d_3,$$

where $d_1 = n\mathrm{Cov}\{\hat{\gamma}(h) - \gamma^*(h), \gamma^*(k)\}$, $d_2 = n\mathrm{Cov}\{\gamma^*(h), \hat{\gamma}(k) - \gamma^*(k)\}$ and $d_3 = n\mathrm{Cov}\{\hat{\gamma}(h) - \gamma^*(h), \hat{\gamma}(k) - \gamma^*(k)\}$ By the fourth-order stationarity,

$$|d_1| = n\left|\mathrm{Cov}\left(\frac{1}{n}\sum_{t=n-h+1}^{n} X_t X_{t+h}, \frac{1}{n}\sum_{s=1}^{n} X_s X_{s+k}\right)\right| \leq \frac{h}{n}\sum_{\ell=-\infty}^{+\infty} |\sigma_{h,k}(\ell)| \to 0.$$

Similarly, it can be shown that d_2 and d_3 tend to zero as $n \to \infty$

This entails that we can replace $\{\hat{\gamma}(h), \hat{\gamma}(k)\}$ by $\{\gamma^*(h), \gamma^*(k)\}$ to show the theorem. By stationarity, we have

$$n\mathrm{Cov}\{\gamma^*(h), \gamma^*(k)\} = \frac{1}{n}\sum_{t,s=1}^{n} \mathrm{Cov}\left(X_t X_{t+h}, X_s X_{s+k}\right)$$

$$= \frac{1}{n}\sum_{\ell=-n+1}^{n-1} (n - |\ell|)\mathrm{Cov}\left(X_1 X_{1+h}, X_{1+\ell} X_{1+\ell+k}\right) \to \sum_{\ell=-\infty}^{+\infty} \sigma_{h,k}(\ell)$$

using the dominated convergence theorem. $\quad\square$

Proof of Theorem 12.3. The result is obvious for $h = 1$. For $h > 1$, we have

$$\hat{r}(h) = \frac{\hat{\rho}(h) - \sum_{i=1}^{h-1} \hat{\rho}(h-i)\hat{a}_{h-1,i}}{1 - \sum_{i=1}^{h-1} \hat{\rho}(i)\hat{a}_{h-1,i}},$$

where $(\hat{a}_{h-1,1}, \ldots, \hat{a}_{h-1,h-1})'$ is the vector of the estimated coefficients in the regression of X_t on $X_{t-1}, \ldots, X_{t-h+1}$, $(t = h, \ldots, n)$. Using the ergodic theorem (stationarity and **A1** imply ergodicity), it can be shown that, $\hat{\rho}(1) \to 0, \ldots, \hat{\rho}(h) \to 0$ and $(\hat{a}_{h-1,1}, \ldots, \hat{a}_{h-1,h-1})' \to 0$ almost surely. From Romano and Thombs (1996), we know that $\sqrt{n}\hat{\rho}(h) = O_p(1)$. Similarly, it can be shown that $\sqrt{n}(\hat{a}_{h-1,1}, \ldots, \hat{a}_{h-1,h-1}) = O_p(1)$ Therefore $\hat{\rho}(k)\hat{a}_{h-1,i} = O_p(n^{-1})$ for $i = 1, \ldots, h-1$ and $k = 1, \ldots, h$. Thus

$$n\{\hat{\rho}(h) - \hat{r}(h)\} = \frac{n\sum_{i=1}^{h-1} \hat{a}_{h-1,i}\{\hat{\rho}(h-i) - \hat{\rho}(i)\hat{\rho}(h)\}}{1 - \sum_{i=1}^{h-1} \hat{\rho}(i)\hat{a}_{h-1,i}} = O_p(1). \quad\square$$

Proof of Theorem 12.4. It can be shown that $\Sigma_{\hat{\rho}_{1:m}}$ is non-singular. So the proof comes from (12.7), Remark 12.5, and a standard result (see e.g Brockwell and Davis, 1991, Problem 6.14). $\quad\square$

Proof of Theorem 12.5. We only give the scheme of the proof A detailed proof is given in an unpublished document (a preliminary version of Francq and Zakoïan,

1998a) which is available on request. It can be shown that the identifiability assumptions, in **A3** − **A6** entail that for all $\theta \in \Theta$ and all $t \in \mathbb{Z}$,

$$\epsilon_t(\theta) = \epsilon_t \ a.s. \quad \Rightarrow \quad \theta = \theta_0. \tag{A.5}$$

It can also be shown that the assumptions on the roots of the AR and MA polynomials, in **A3**, entail that the initial values $e_0(\theta), \ldots, e_{-q+1}(\theta), X_0, \ldots, X_{-p+1}$ are asymptotically negligible. More precisely, we show that

$$\sup_{\theta \in \Theta^*} |c_i(\theta)| = O(\rho^i) \quad \text{for some } \rho \in [0, 1[, \quad \lim_{t \to \infty} \sup_{\theta \in \Theta^*} |\epsilon_t(\theta) - e_t(\theta)| = 0,$$

$$\lim_{n \to \infty} \sup_{\theta \in \Theta^*} |Q_n(\theta) - O_n(\theta)| = 0 \quad \text{where} \quad O_n(\theta) = \frac{1}{n} \sum_{t-1}^{n} \epsilon_t^2(\theta). \tag{A.6}$$

Since $\epsilon_t - \epsilon_t(\theta) = \sum_{i=1}^{\infty} \{c_i(\theta_0) - c_i(\theta)\} X_{t-i}$ belongs to the linear past of X_t, it is uncorrelated with the linear innovation ϵ_t. Hence the limit criterion $Q_\infty(\theta) := E_{\theta_0} \epsilon_t^2(\theta)$ satisfies $Q_\infty(\theta) = E_{\theta_0} \{\epsilon_t(\theta) - \epsilon_t + \epsilon_t\}^2 = E_{\theta_0} \{\epsilon_t(\theta) - \epsilon_t\}^2 + E_{\theta_0} \epsilon_t^2 + 2\mathrm{Cov} \{\epsilon_t(\theta) - \epsilon_t, \epsilon_t\} = E_{\theta_0} \{\epsilon_t(\theta) - \epsilon_t\}^2 + \sigma^2 \geq \sigma^2$, with equality if and only if $\epsilon_t(\theta) = \epsilon_t$ a.s. In view of (A.5), the last equality holds if and only if $\theta = \theta_0$. Thus, we have shown that $Q_\infty(\theta)$ is minimized at θ_0:

$$\sigma^2 = Q_\infty(\theta_0) < Q_\infty(\theta), \quad \forall \theta \neq \theta_0 \tag{A.7}$$

Let $V_m(\theta^*)$ be the sphere with center θ^* and radius $1/m$. It is clear that $S_m(t) = \inf_{\theta \in V_m(\theta^*) \cap \Theta} \epsilon_t^2(\theta)$ is measurable and integrable. The process $\{S_m(t)\}_t$ is stationary and ergodic. The ergodic theorem shows that, almost surely,

$$\inf_{\theta \in V_m(\theta^*) \cap \Theta} O_n(\theta) = \inf_{\theta \in V_n(\theta^*) \cap \Theta} \frac{1}{n} \sum_{t=1}^{n} \epsilon_t^2(\theta) \geq \frac{1}{n} \sum_{t=1}^{n} S_m(t) \to E_{\theta_0} S_m(t),$$

as $n \to \infty$. Since $\epsilon_t^2(\theta)$ is continuous in θ, $S_m(t)$ increases to $\epsilon_t^2(\theta^*)$ as m increases to $+\infty$. By Beppo-Levi's theorem we obtain

$$\lim_{m \to \infty} E_{\theta_0} S_m(t) = E_{\theta_0} \epsilon_t^2(\theta^*) = Q_\infty(\theta^*)$$

From (A.7), we then have

$$\liminf_{m \to \infty} \liminf_{n \to \infty} \inf_{\theta \in V_m(\theta^*)} O_n(\theta) \geq Q_\infty(\theta^*) > \sigma^2 \quad \forall \theta^* \in \Theta, \ \theta^* \neq \theta_0.$$

Thus we have shown that, for all $\theta^* \in \Theta$, $\theta^* \neq \theta_0$, there exists a neighborhood $V(\theta^*)$ of θ^* such that $V(\theta^*) \subset \Theta$ and

$$\liminf_{n \to \infty} \inf_{\theta \in V(\theta^*)} O_n(\theta) > \sigma^2, \quad a.s. \tag{A 8}$$

In view of (A.6), (A 8) and the inequality

$$\inf_{\theta \in \theta^* \in \Theta^*} Q_n(\theta) \geq \inf_{\theta \in \theta \in \Theta^*} O_n(\theta) - \sup_{\theta \in \Theta^*} |O_n(\theta) - Q_n(\theta)|$$

we obtain that, for all $\theta^* \in \Theta^*$, $\theta^* \neq \theta_0$, there exists a neighborhood $V(\theta^*)$ of θ^* such that $V(\theta^*) \subset \Theta$ and

$$\liminf_{n \to \infty} \inf_{\theta \in V(\theta^*)} Q_n(\theta) > \sigma^2, \quad a.s. \tag{A 9}$$

We conclude by a standard compactness argument. Let $V(\theta_0)$ be a neighborhood of θ_0. The compact set Θ^* is covered by $V(\theta_0)$ and the union of the open sets $V(\theta^*)$, $\theta^* \in \Theta^* - V(\theta_0)$, where the $V(\theta^*)$'s satisfy (A.9) Therefore Θ^* is covered by a finite number of these open sets; there exist θ_1, $,\theta_k$ such that $\bigcup_{i=0}^{k} V(\theta_i) \subset \Theta^*$ Inequality (A 9) shows that, almost surely,

$$\inf_{\theta \in \Theta^*} Q_n(\theta) = \min_{i=0,1, \ldots, k} \inf_{\theta \in V(\theta_i) \cap \Theta^*} Q_n(\theta) = \inf_{\theta \in V(\theta_0) \cap \Theta^*} Q_n(\theta),$$

for sufficiently large n Thus, almost surely, $\hat{\theta}_n$ belongs to $V(\theta_0)$ for sufficiently large n Since $V(\theta_0)$ can be chosen arbitrarily small, the proof is complete $\quad\square$

Proof of Theorem 12.6. Under Assumption **A1**, the proof is given in Francq and Zakoïan (1998a) Under Assumption **A1'**, the scheme of the proof is the same It relies on a Taylor expansion of the criterion $Q_n(\theta)$ around θ_0, and on showing that

$$\sqrt{n} \frac{\partial}{\partial \theta} Q_n(\theta_0) \overset{d}{\leadsto} \mathcal{N}(0, 4I) \tag{A 10}$$

To show (A 10), note that $\partial \epsilon_t(\theta_0)/\partial \theta = \sum_{i=1}^{\infty} \epsilon_{t-i} \lambda_i$ for some sequence of vectors (λ_i) (see Remark 12 7 below for an explicit form of these vectors) Thus, we can write

$$n^{1/2} \frac{\partial}{\partial \theta} Q_n(\theta_0) = n^{-1/2} \sum_{t=2}^{n} Y_{t,r} + n^{-1/2} \sum_{t=2}^{n} Z_{t,r} + o_p(1),$$

$$Y_{t,r} = 2\epsilon_t \sum_{i=1}^{r} \lambda_i \epsilon_{t-i}, \quad Z_{t,r} = 2\epsilon_t \sum_{i=r+1}^{\infty} \lambda_i \epsilon_{t-i}$$

Under **A1'**, the process $Y_r = (Y_{t,r})_t$ is strongly mixing, since $\alpha_Y(h) \leq \alpha_\epsilon(h - r - 1)$ From the central limit theorem for mixing processes (see Herrndorf, 1984), we show that $n^{-1/2} \sum_{t=2}^{n} Y_{t,r} \overset{d}{\leadsto} \mathcal{N}(0, 4I_r)$ where $I_r \to I$ as $r \to \infty$ Using the arguments given in Francq and Zakoïan (1998a, Lemma 4), it can be shown that $\lim_{r \to \infty} \sup_n \text{Var} \left\{ n^{-1/2} \sum_{t=2}^{r} Z_{t,r} \right\} = 0$ So the proof comes from a standard result (see e g Billingsley, 1995, Theorem 12 5) $\quad\square$

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Chapter 13

FILTERING OF IMAGES FOR DETECTING MULTIPLE TARGETS TRAJECTORIES

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Abstract   The aim of this paper is to present efficient algorithms for the detection of multiple targets in noisy images. The algorithms are based on the optimal filter of a multidimensional Markov chain signal We also present some simulations, in the case of one, two and three targets, showing the efficiency of the method for detecting the positions of the targets.

1.   Introduction

The problem of detecting targets in a region, using images, is a quite interesting challenge, having a lot of applications. For example, one can try to find a boat lost at sea, or try to track drug smugglers, etc. Unfortunately, images are not crystal clear and can be affected by several parameters, in particular weather conditions.

In what follows, we will assume that the targets move on a lattice, according to a Markov chain. Moreover, the observations are black-and-white noisy images of a finite fixed region. Our setting is different of the setting considered by Ballantyne, Chan and Kouritzin (2001), where they used different kind of noise and a different approach for the motion of targets.

In order to simplify calculations, the following notations will be used.

MODEL FOR TARGETS: Let $(\xi_k)_{k \geq 0}$ be a finite system of m Markovian targets evolving in a countable space $\mathfrak{X}$. The state space is the set of all $\xi \in \{0,1\}^{\mathfrak{X}}$ so that $\sum_{x \in \mathfrak{X}} \xi(x) = m$.

Let $\mathcal{A}$ be the set of all $A \subset \mathfrak{X}$, $|A| = m$. For any $A \in \mathcal{A}$, define

$$F_A(\xi) = \prod_{x \in A} \xi(x),$$

and set $\nu_\xi(A) = E(F_A(\xi_{k+1})|\xi_k = \xi)$. We will use different probabilities laws. Note that, for any $B \in \mathfrak{X}$, $|B| \leq m$,

$$E_P\{F_B(\xi_{k+1})|\xi_k = \xi\} = P(\xi_k(x) = 1, x \in B|\xi_k = \xi) = \sum_{A \in \mathcal{A}, A \supset B} \nu_\xi(A).$$

Further set

$$M(A, B) = E\{F_A(\xi_{k+1})|F_B(\xi_k) = 1\}, \tag{13.1}$$

where $A, B \in \mathcal{A}$. The transition function M is important since it describes exactly the movement of the m targets. We discuss it in Section 3.

MODEL FOR OBSERVATIONS: Observations are denoted by $Y_k \in \{0,1\}^I$, where $I \subset \mathfrak{X}$ is a finite set. Given $\xi_0, \ldots, \xi_k$, we assume the $\{Y_k(x)\}_{x \in I}$ are independent and

$$P(Y_k(x) = 0|\xi_k(x) = 0) = p_0, \tag{13.2}$$
$$P(Y_k(x) = 1|\xi_k(x) = 1) = p_1, \tag{13.3}$$

where $x \in I$ and $0 < p_0, p_1 < 1$.

Two algorithms will be defined to compute the optimal filter according as we know or not the transition function M.

In the next section, we will present a straightforward algorithm when the motion of targets is assumed to be known, i.e. M is known. In Section 3 we will propose an algorithm in the case on an unknown motion. Simulations showing the performance of the algorithms are presented in Section 4 in the case of $m = 1, 2, 3$ targets. Finally, Section 5 contains a discussion of the results and ideas for future work.

2. Optimal filter when the transition mechanism is known

Throughout this section we assume the transition function M to be known. Our aim is to find an easy algorithm to compute

$$P\left(\cap_{x \in B}\{\xi_k(x) = 1\}|\mathcal{Y}_k\right),$$

where $B \in \mathcal{A}$, $|B| \leq m$ and $\mathcal{Y}_k$ is the sigma-algebra generated by observations $Y_1, \ldots, Y_k$. Set $\mathcal{Y}_0 = \{\emptyset, \{0,1\}^I\}$.

The first step is to compute, for any $y \in \{0,1\}^I$, the following conditional probability

$$P(Y_k = y | \xi_k = \xi) = P\left(\cap_{x \in I}\{Y_k(x) = y(x)\} | \xi_k = \xi\right).$$

Using the independence assumption, together with (13.2) and (13.3), one can check that

$$P(Y_k = y | \xi_k = \xi) = \prod_{x \in I} \left\{(1 - p_0)^{1-\xi(x)} p_1^{\xi(x)}\right\}^{y(x)}$$

$$\times \left\{p_0^{1-\xi(x)}(1 - p_1)^{\xi(x)}\right\}^{1-y(x)}$$

$$= p_0^{|I|} \left(\frac{1 - p_0}{p_0}\right)^{<y>} \left(\frac{1 - p_1}{p_0}\right)^{<\xi>}$$

$$\times \left(\frac{p_0 p_1}{(1 - p_0)(1 - p_1)}\right)^{<y\xi>},$$

where $< y > = \sum_{x \in I} y(x)$, $< y\xi > = \sum_{x \in I} y(x)\xi(x)$ and $< \xi > = \sum_{x \in I} \xi(x)$.
We note

$$\Lambda(y, \xi) = p_0^{|I|} \left(\frac{1 - p_0}{p_0}\right)^{<y>} \left(\frac{1 - p_1}{p_0}\right)^{<\xi>} \left(\frac{p_0 p_1}{(1 - p_0)(1 - p_1)}\right)^{<y\xi>}.$$

$$(13.4)$$

Let P be the joint law of the Markovian targets with initial distribution ν, and the observations, and let Q be the joint law of the Markovian targets with initial distribution ν, and independent Bernoulli observations with mean $1/2$.

Further let $\mathcal{G}_k$ be the sigma-algebra generated by $Y_1, \ldots, Y_k, \xi_0, \ldots, \xi_k$. Then one can check that with respect to $\mathcal{G}_k$, P is equivalent to Q and

$$\left.\frac{dP}{dQ}\right|_{\mathcal{G}_k} = \prod_{j=1}^{k} 2^{|I|} \Lambda(Y_j, \xi_j). \tag{13.5}$$

Further define

$$L_k = \prod_{j=1}^{k} \Lambda(Y_j, \xi_j). \tag{13.6}$$

It follows that for any $\mathcal{G}_k$-measurable random variable Z and for any sigma-algebra $\mathcal{F} \subset \mathcal{G}_k$,

$$E_P(Z | \mathcal{F}) = \frac{E_Q(Z L_k | \mathcal{F})}{E_Q(L_k | \mathcal{F})}. \tag{13.7}$$

While this formula is an consequence of the properties of conditional expectations, in the context of filtering, (13.7) is known as the Kallianpur-Striebel formula (see Kallianpur and Striebel (1968)). We note by E_P (resp. E_Q) the expectation under the probability law P (resp. Q) when it is not clear.

The key observation here is to note that expectations relative to Q are much easier to evaluate since the signal and the observations are independent. Moreover all variables $\{Y_i(x)\}_{1 \leq i \leq k, x \in I}$ are independent and identically distributed Bernoulli with mean $1/2$.

For any $A \in \mathcal{A}$, define $q_k(A) = E_Q(F_A(\xi_k)L_k|\mathcal{Y}_k)$. Note that, according to (13.7), we have, for any $B \in \mathfrak{X}$, $|B| \leq m$,

$$
P\left(\cap_{x \in B}\{\xi_k(x) = 1\}|\,\mathcal{Y}_k\right) = \frac{\displaystyle\sum_{A \in \mathcal{A}, A \supset B} q_k(A)}{\displaystyle\sum_{A \in \mathcal{A}} q_k(A)}.
$$

Therefore the conditional law of ξ_k given $\mathcal{Y}_k$ is completely determined by the following set: $\{q_k(A); A \in \mathcal{A}\}$.

Our goal will be attained if one can find a recursive formula for the "unnormalized measure" q_k. To this end, set

$$
D_A(y) = p_0^{|I|}\left(\frac{1-p_0}{p_0}\right)^{<y>}\left(\frac{1-p_1}{p_0}\right)^{|A \cap I|}\left(\frac{p_0 p_1}{(1-p_0)(1-p_1)}\right)^{<y>_{A \cap I}},
$$

where $< y >_{A \cap I} = \displaystyle\sum_{x \in A \cap I} y(x)$.

Using independence and identity (13.4), we have

$$
\begin{aligned}
q_{k+1}(A) &= E_Q\left\{F_A(\xi_{k+1})L_{k+1}|\mathcal{Y}_{k+1}\right\} \\
&= E_Q\left[E_Q\left\{F_A(\xi_{k+1})\Lambda(Y_{k+1}, \xi_{k+1})|Y_{k+1}, \xi_k\right\} L_k|\mathcal{Y}_k\right] \\
&= D_A(Y_{k+1})E_Q\left[E_Q\left\{F_A(\xi_{k+1})|\xi_k\right\} L_k|\mathcal{Y}_k\right] \\
&= D_A(Y_{k+1})E_Q\left[\nu_{\xi_k}(A)L_k|\mathcal{Y}_k\right] \\
&= D_A(Y_{k+1})\sum_{B \in \mathcal{A}} E_Q\left[\nu_{\xi_k}(A)F_B(\xi_k)L_k|\mathcal{Y}_k\right] \\
&= D_A(Y_{k+1})\sum_{B \in \mathcal{A}} M(A, B)E_Q\left[F_B(\xi_k)L_k|\mathcal{Y}_k\right] \\
&= D_A(Y_{k+1})\sum_{B \in \mathcal{A}} M(A, B)q_k(B)
\end{aligned}
$$

Therefore we obtain

$$q_{k+1}(A) = D_A(Y_{k+1}) \sum_{B \in \mathcal{A}} M(A, B) q_k(B), \qquad (13.8)$$

it is called "Zakai" equation.

Note also that for any $B \in \mathfrak{X}$, $|B| \leq m$, one can define $q_k(B)$ by the formula

$$q_k(B) = \sum_{A \in \mathcal{A}, A \supset B} q_k(A).$$

It follows that for any such B

$$q_k(B) = E_Q(F_B(\xi_k) L_k | \mathcal{Y}_k)$$

and

$$E_P \{F_B(\xi_k) | \mathcal{Y}_k\} = P \left(\cap_{x \in B} \{\xi_k(x) = 1\} | \mathcal{Y}_k \right) = \frac{q_k(B)}{\sum_{A \in \mathcal{A}} q_k(A)}.$$

REMARK 13.1 Using the same technique, one can prove that for any $1 \leq k \leq n$,

$$P(Y_k = y | \mathcal{Y}_{k-1}) = \frac{p_k(y)}{\sum_{z \in \{0,1\}^I} p_k(z)}, \qquad (13.9)$$

where

$$p_k(y) = \sum_{A \in \mathcal{A}} \sum_{B \in \mathcal{A}} D_A(y) M(A, B) q_{k-1}(B), \quad 1 \leq k \leq n. \qquad (13.10)$$

Note that, using (13.4) and (13.10) and the definition of $D_A(y)$, one can write

$$\sum_{z \in \{0,1\}^I} p_k(z) = \sum_{z \in \{0,1\}^I} \sum_{A \in \mathcal{A}} \sum_{B \in \mathcal{A}} D_A(z) M(A, B) q_{k-1}(B)$$

$$= \sum_{A \in \mathcal{A}} \sum_{B \in \mathcal{A}} M(A, B) q_{k-1}(B) \sum_{z \in \{0,1\}^I} D_A(z)$$

$$= \sum_{A \in \mathcal{A}} \sum_{B \in \mathcal{A}} M(A, B) q_{k-1}(B).$$

It follows that

$$P(Y_1 = y_1, \ldots, Y_n = y_n) = \prod_{k=1}^{n} P(Y_k = y_k | \mathcal{Y}_{k-1}) \qquad (13.11)$$

can be written in terms of (13.9). This expression can be used to find maximum likelihood estimates of M and p_0, p_1.

In view of applications, one can restrict himself to finite sets $\mathfrak{X}$. However, to be realistic, one should take $\mathfrak{X}$ bigger that I. Think about ships sailing in a certain region, where a satellite take pictures of a subregion. It is quite possible that some ships are outside of satellite reach.

Under this finiteness hypothesis, Zakai equation (13.8) is a finite sum and it can be evaluated (theoretically). Note that by definition, q_0 is determined by the initial law of the targets. Having observed Y_1, one can calculate the measure q_1, and so on. Since the state space is finite, it is recommended to choose the uniform distribution as the initial distribution. In fact, any distribution equivalent to the uniform should also work, because the effect of the initial should vanish after some iterations.

Let us remark that some calculations can be done off-line. The probabilities $M(A, B)$, for $A, B \in \mathfrak{X}$, can be stored as a matrix, prior to starting the observation process. Note also that the computation of q_k is nothing but matrix multiplication.

The location of the m targets after the k-th observation can be estimated by choosing $A \in \mathcal{A}$, $|A| = m$, such that

$$q_k(A) = \max_{B \in \mathcal{A}} q_k(B).$$

3.   Algorithm when the transition mechanism is unknown

Suppose now that we do not know the value of the transition function M defined in (13.1), and we want again to find the position of targets. Throughout the rest of the section, M will be considered as random. In that case, we have to estimate both the positions of targets and the probability law of M.

This case is of course a little more complicated and we need to introduce new notations. For any $A \in \mathcal{A}$ and any $k \geq 0$, define

$$\tilde{r}_k(A) = E(F_A(\xi_k)|\mathcal{Y}_k) = \tilde{\mu}_k(F_A)$$
$$r_{k+1}(A) = E(F_A(\xi_{k+1})|\mathcal{Y}_k) = \mu_{k+1}(F_A)$$
$$\tilde{r}_k^{(M)}(A) = E(F_A(\xi_k)|\mathcal{Y}_k, M) = \tilde{\mu}_k^{(M)}(F_A)$$
$$r_{k+1}^{(M)}(A) = E(F_A(\xi_{k+1})|\mathcal{Y}_k, M) = \mu_{k+1}^{(M)}(F_A),$$

where $\nu(f)$ is a shorthand notation for $\int f(y)\nu(dy)$, for any measure ν. Using the results of Section 2, the following identities hold true:

$$\tilde{r}_k^{(M)}(A) = \frac{q_k(A)}{\displaystyle\sum_{B \in \mathcal{A}} q_k(B)},$$

and

$$\tilde{r}_{k+1}^{(M)}(A) = \frac{1}{C_{k+1}^{(M)}} D_A(Y_{k+1}) \sum_{B \in \mathcal{A}} M(A, B) \tilde{r}_k^{(M)}(B), \quad k \geq 0, \quad (13.12)$$

where

$$C_{k+1}^{(M)} = \sum_{A, B \in \mathcal{A}} D_A(Y_{k+1}) M(A, B) \tilde{r}_k^{(M)}(B).$$

Note also that for any $k \geq 1$,

$$r_{k+1}^{(M)}(A) = \sum_{B \in \mathcal{A}} M(A, B) \tilde{r}_k^{(M)}(B). \quad (13.13)$$

Now, our aim is to find a recursive algorithm to compute $\tilde{r}_k(A)$, for any $A \in \mathcal{A}$.

Using the projection property of conditional expectations, we get

$$\begin{aligned}
\tilde{r}_{k+1}(A) &= E(E(F_A(\xi_{k+1})|\mathcal{Y}_{k+1}, M)|\mathcal{Y}_{k+1}) \\
&= E\left(\tilde{r}_{k+1}^{(M)}(A)|\mathcal{Y}_{k+1}\right) \\
&= \tilde{\eta}_{k+1}\left(\tilde{r}_{k+1}^{()}(A)\right) \\
&= \int \tilde{r}_{k+1}^{(M)}(A) \tilde{\eta}_{k+1}(dM),
\end{aligned}$$

where $\tilde{\eta}_{k+1}$ refers to the probability law of M, given $\mathcal{Y}_{k+1}$.

We have now to find how to compute expectations with respect to the measure $\tilde{\eta}_{k+1}$. This is done using a useful result due to Del Moral and Miclo (2002). See Del Moral (2002) for a general statement of the result.

LEMMA 13.1 (DEL MORAL-MICLO) *For any bounded measurable function ϕ of M, we have*

$$\tilde{\eta}_k(\phi) = \frac{E\left(\phi(M) \prod_{i=1}^{k} \mu_i^{(M)}(\Lambda(Y_i, \cdot)) \,\middle|\, \mathcal{Y}_k\right)}{E\left(\prod_{i=1}^{k} \mu_i^{(M)}(\Lambda(Y_i, \cdot)) \,\middle|\, \mathcal{Y}_k\right)}.$$

Proof. For sake of completeness, we give a proof in our setting. First, for a given M, $(\xi_k)_{k \geq 0}$ is a Markov chain. So $(M, \xi_k)_{k \geq 0}$ is also a Markov

chain. Using Kallianpur-Stridel formula, one can check that for any bounded measurable function ψ of (M, ξ_k),

$$E_P(\psi(M, \xi_k)|\mathcal{Y}_k) = \frac{E_Q(\psi(M, \xi_k)L_k|\mathcal{Y}_k)}{E_Q(L_k|\mathcal{Y}_k)},$$

where L_k is defined by (13.6).

Applying the formula to $\psi(M, \xi_k) = \phi(M)$, one obtains

$$E_P(\phi(M)|\mathcal{Y}_k) = \frac{E_Q(\phi(M)L_k|\mathcal{Y}_k)}{E_Q(L_k|\mathcal{Y}_k)}$$

$$= \frac{E_Q(\phi(M)E_Q(L_k|\mathcal{Y}_k, M)|\mathcal{Y}_k)}{E_Q(E_Q(L_k|\mathcal{Y}_k, M)|\mathcal{Y}_k)}.$$

It is easy to check that

$$E_Q(L_k|\mathcal{Y}_k, M) = \mu_k^{(M)}(\Lambda(Y_k, \cdot))E_Q(L_{k-1}|\mathcal{Y}_{k-1}, M),$$

so that, using induction, one gets

$$E_Q(L_k|\mathcal{Y}_k, M) = \prod_{i=1}^{k-1} \mu_i^{(M)}(\Lambda(Y_i, \cdot)),$$

yielding the result. $\square$

By Lemma 13.1, we have

$$\tilde{\eta}_{k+1}(\phi) = \frac{\tilde{\eta}_k\left(\phi\mu_{k+1}^{()}(\Lambda(Y_{k+1}, \cdot))\right)}{\tilde{\eta}_k\left(\mu_{k+1}^{()}(\Lambda(Y_{k+1}, \cdot))\right)}.$$

From the definition of $\tilde{r}_k^{(M)}$, one gets, using equality (13.13),

$$\mu_{k+1}^{(M)}(\Lambda(Y_{k+1}, \cdot)) = \sum_{A \in \mathcal{A}} D_A(Y_{k+1})r_{k+1}^{(M)}(A)$$

$$= \sum_{A, B \in \mathcal{A}} D_A(Y_{k+1})M(A, B)\tilde{r}_k^{(M)}(B)$$

$$= C_{k+1}^{(M)}.$$

Next, (13.12) yields

$$\tilde{r}_{k+1}(A) = \int \frac{1}{C_{k+1}^{(M)}} D_A(Y_{k+1}) \sum_{B \in \mathcal{A}} M(A, B)\tilde{r}_k^{(M)}(B) \, \tilde{\eta}_{k+1}(dM)$$

$$= \frac{\int D_A(Y_{k+1}) \sum_{B \in \mathcal{A}} M(A, B)\tilde{r}_k^{(M)}(B) \; \tilde{\eta}_k(dM)}{\int C_{k+1}^{(M)} \; \tilde{\eta}_k(dM)}. \tag{13.14}$$

Note that $\int C_{k+1}^{(M)} \; \tilde{\eta}_k(dM)$ is just a normalizing term.

REMARK 13.2 Applying equality (13.14), when the measure $\tilde{\eta}_k$ is the Dirac measure at M_0, we obtain the same formula as the one described in Section 2.

We are now in a position to describe the new algorithm.

3.1   Algorithm

Initialization: As in the first algorithm, $\tilde{r}_o$ and $\tilde{\eta}_0$ are determined by the initial law of the targets.

Recursion: For any $k \geq 0$, given $\tilde{r}_k$, $\tilde{r}_k^{(\;)}$, and $\tilde{\eta}_k$, compute $\tilde{r}_{k+1}^{(M)}$, using (13.12), $\tilde{r}_{k+1}$, using (13.14). Then, for any bounded measurable ϕ of M,

$$\tilde{\eta}_{k+1}(\phi) = \frac{\int \phi(M) \sum_{A, B \in \mathcal{A}} D_A(Y_{k+1}) M(A, B)\tilde{r}_k^{(M)}(A) \; \tilde{\eta}_k(dM)}{\int \sum_{A, B \in \mathcal{A}} D_A(Y_{k+1}) M(A, B)\tilde{r}_k^{(M)}(A) \; \tilde{\eta}_k(dM)}.$$

As in the first algorithm, we can locate the m targets at the k-th iteration by choosing $A \in \mathcal{A}$ such that

$$\tilde{r}_k(A) = \max_{B \in \mathcal{A}} \tilde{r}_k(B).$$

4.   Simulations

Animations representing the results of the simulations described below can be obtained at the web site
http://www.ceremade.dauphine.fr/~gentil/ensimulations.html
Calculations were done using C++ and MATLAB.

4.1   Simulation results when M is known

When M is known, one can use the algorithm described in Section 2. For the estimation of the positions of the targets, we chose the sets $A \in \mathcal{A}$

maximizing $q_k(A) = \max\limits_{B \in \mathcal{A}} q_k(B)$. Note that several sets can satisfy this property, due to the lack of precision, especially in the first iterations.

In order to simplify calculations, we assumed that $\mathcal{X} = I$. The Markovian targets are non-intersecting nearest neighbors random walks moving up (resp. down, right and left), with probability α_1 (respectively α_2, α_3 and $\alpha_4 = 1 - \alpha_1 - \alpha_2 - \alpha_3$). The initial distribution q_0 was chosen to be the uniform law on all possible configurations.

For memory and computing time reasons, we restricted the simulations to the cases of one, two and three targets, and images of size 200×200 in the case of one target, size 60×60 for two targets, and size 20×20 for three targets.

In order to estimate the efficiency of our algorithm, we computed the mean error over several time intervals. We found out that the positions predictions were quite good after 10 to 30 steps. We also took into account various values of parameters p_0 and p_1. The error made at each iteration was calculated in the following way: in case of just one estimate A, we calculated the L^1-distance between the targets and the estimate; in case of several estimates, the largest L^1-distance was kept. The first iteration is never considered. The results are reported in Tables 13.1, 13.2 and 13.3.

Table 13.1   Mean error for one target in images of size 200×200.

t	$[2, 100]$	$[10, 100]$	$[30, 100]$
$p_0 = p_1 = 0.9$	8.7	4.1	1.2
$p_0 = p_1 = 0.95$	4.3	0.3	0.3

Table 13.2   Mean error for two targets in images of size 60×60

t	$[2, 100]$	$[10, 100]$	$[30, 100]$
$p_0 = p_1 = 0.9$	6.5	1.7	1.8
$p_0 = p_1 = 0.95$	3.1	1.1	1.2

Note that in each case, the algorithm presents really satisfying results. From the 10-th, or 30-th iteration (depending on the choice of parameters p_0 and p_1), the distance between the estimation and the targets is about one or two pixels. This is due to the fact that the algorithm provides an exact solution to the resolution of the optimal filter. The estimation is of course better in the case of one target.

Table 13 3 Mean error for three targets in images of size 20×20

t	$[2, 100]$	$[10, 100]$	$[30, 100]$
$p_0 = p_1 = 0.9$	4 0	3 1	2 6
$p_0 = p_1 = 0.95$	3 5	2.5	2.0

REMARK 13.3 A natural question to ask is how to track more than two targets for large images? One solution is to use one dimensional optimal filters to try to approximate the optimal filter for several targets. This can be done in the following way. We use the optimal filter for one target. Then we assume that the first target is on the first estimation and we use again the optimal algorithm to find another target, and so on. Tables 13.4, 13.5 and 13.6 below represent the results obtained by simulations.

Table 13.4. Mean error for two targets with the approximation of the algorithm and in images of size 60×60.

t	$[2, 100]$	$[10, 100]$	$[30, 100]$
$p_0 = p_1 = 0\,9$	7.9	3.9	4.4
$p_0 = p_1 = 0.95$	4.1	0.9	0 6

Table 13 5. Mean error for two targets with the approximation of the algorithm in images of size 200×200.

t	$[2, 100]$	$[10, 100]$	$[30, 100]$
$p_0 = p_1 = 0.9$	47	42	45.3
$p_0 = p_1 = 0.95$	5.7	0.5	0.6
$p_0 = p_1 = 0.99$	20.1	17.3	19.0

These results are quite interesting. For two targets and images of size 60×60, the mean errors are almost the same as the one obtained in Table 13.2. However, as can be seen in Tables 13.5 and 13.6, the stability of the approximation of the optimal filter is not as good. Remark that for three targets, when $p_0 = p_1 = 0.99$, the approximation is quite satisfactory.

Table 13 6.   Mean error for three targets with the approximation of the algorithm in images of size 200×200.

t	[2, 100]	[10, 100]	[30, 100]
$p_0 = p_1 = 0.9$	40 7	35.6	31
$p_0 = p_1 = 0.95$	45.9	45.3	44.1
$p_0 = p_1 = 0.99$	15.1	14.1	14.7

4.2   Simulation results when M is unknown

We now present simulations using the algorithm developed in Section 3. For sake of simplicity, we chose to simulate only one target in images of size 200×200.

As in the previous subsection, we use the uniform law on all pixels. The measure $\tilde{\eta}_0$ is a discrete measure with N Dirac measures defined as

$$\tilde{\eta}_0(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = \sum_{i=0}^{N} \frac{1}{N+1} \delta_{(\frac{i}{2N}, \frac{i}{2N}, \frac{1}{2} - \frac{i}{2N}, \frac{1}{2} - \frac{i}{2N})}(\alpha_1, \alpha_2, \alpha_3, \alpha_4).$$

$$(13.15)$$

This is not the best choice for $\tilde{\eta}_0$ but it is very simple for computations and the results obtained are quite interesting. Of course, in simulations, the motion of the target is random and is not in the support of $\tilde{\eta}_0$ defined by (13.15).

For the simulations, we used several values for N and (p_0, p_1). The results are reported in the Table 13.7.

Table 13.7   Mean error for one target in images of size 200×200 for random M.

$p_0 = p_1 = 0.9$	[2, 100]	[10, 100]	[30, 100]
$N = 2$	36	27	20
$N = 10$	21	10.5	0.9
$N = 100$	20	8	0.8
$p_0 = p_1 = 0\ 95$	[2, 100]	[10, 100]	[30, 100]
$N = 2$	6.5	1.4	0.5
$N = 10$	7.1	0 1	0 1
$N = 100$	7.1	0.1	0.1

From these results, one can see that when the measure is initialized by a discrete measure with $N = 10$ or 100, the approximations look

like simulations when we know the transition function M of the targets. When $N = 2$, the measure $\tilde{\eta}_0$ is too bad to estimate the target.

REMARK 13.4 In view of applications, one can either consider that the parameters p_0 and p_1 have been estimated or one can use the maximum likelihood method, (e.g. using (13.11)) to estimate them from the observation of images.

5. Conclusion

We can conclude that the optimal filter is quite easy to implement whether the transition function M of the targets is known or unknown. Simulations results reported in the previous section showed quite convincing arguments in favor of the proposed approach.

On the negative side, the optimal filter method need a lot of memory to compute predictions for 3 targets or 2 targets in large images.

A good solution could be to use an hybrid method combining the optimal filter for one or two targets and "Interacting Particle methods". See e.g. Del Moral and Miclo (2000) for an interesting review of the subject. With this hybrid method used in Section 3, we could compute also the optimal filter to find the positions and the number of targets. This is still work in progress.

Finally, one could replace the hypothesis of conditional independence of the observations by introducing Gibbs measure noise (see Rémillard and Beaudoin 1999 for other applications of Gibbs noise). The only difference would be in the definition of the L_k's.

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Chapter 14

OPTIMAL DETECTION OF PERIODICITIES IN VECTOR AUTOREGRESSIVE MODELS

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Abstract   Locally asymptotically optimal tests for testing stationary against periodic AR(p) dependence have been constructed by Bentarzi and Hallin (1996) in the univariate setting. These tests are generalized here to the multivariate context. A local asymptotic normality property is derived for m-variate d-periodic VAR(p) models in the vicinity of the stationary ones. The central sequence and the locally optimal tests are expressed in terms of a generalized concept of residual cross-covariance matrices

1.   Introduction

Periodic models, where the parameters vary periodically with time, are an attractive alternative to the traditional seasonal ones. In the simple autoregressive case, an m-dimensional periodic autoregressive model of order p and period d (in short, a PVAR(p) model) is a stochastic difference equation of the form

$$\mathbf{X}_t - \sum_{i=1}^{p} \boldsymbol{\Theta}_i(s)\, \mathbf{X}_{t-i} = \boldsymbol{\varepsilon}_t, \quad s = t - d\lceil t/d \rceil, \quad t \in \mathbb{Z}, \qquad (14.1)$$

where $\lceil t/d \rceil$ denotes the largest integer strictly less than t/d, and $\{\boldsymbol{\varepsilon}_t; t \in \mathbb{Z}\}$ is m-variate independent white noise with zero mean and covariance matrix $\boldsymbol{\Sigma}$. The period d is supposed to be the smallest integer such that a periodic representation of $\mathbf{X}_t$ of the form (14.1) is possible; s can be interpreted as the "season", and $t^* := \lceil t/d \rceil + 1$ as the "year".

Such models have been studied by many authors, mainly in the univariate context: Gladyshev (1961) has defined a lumped VAR representation of (14.1); Anderson and Vecchia (1993) have treated the

estimation problem; the asymptotic behaviour of time- and frequency-domain estimators has been studied by Hurd and Gerr (1991), Leskow (1994), and Cambanis et al. (1994). Locally asymptotically optimal tests for stationary autoregressive dependence against periodic autoregression for the univariate case are derived by Bentarzi and Hallin (1996). Other contributions include Pagano (1978), Anděl (1989), Birchenhall et al. (1989), Osborn (1988), Osborn and Smith (1989), Franses (1994), Franses and Paap (1994), Vecchia and Ballerini (1991), Lund and Basawa (2000), Basawa and Lund (2001), Ghysels and Osborn (2001), etc.: see Franses (1996) for a comprehensive review.

Depending on the period d, a periodic model may involve quite a number of parameters. Therefore, before starting with the problem of order identification and estimation of (14.1), one first should make sure that such a model indeed is necessary. On the other hand, in case periodicities are present in the data, this fact should not be missed. The unpleasant effects of overlooking the periodic features and using standard time series analysis with periodically correlated data have been stressed by Osborn (1991), Tiao and Grupe (1980), Tiao and Guttman (1980), and Novales and Flores de Fruto (1997), among others.

Attention so far has been concentrated on the univariate version of model (14.1); the only exceptions, to the best of our knowledge, are Chapter 12 in Lütkepohl (1991), and Franses (1997) with a study of cointegration problems in periodic multivariate time series. Our objective in this paper is to consider the multivariate generalization of model (14.1), and to construct a locally asymptotically optimal test for the hypothesis that an m-variate process is a classical, stationary $VAR(p)$ process against the alternative of a $PVAR(p)$ process with given period d. This test is a generalization of the univariate test proposed by Bentarzi and Hallin (1996), and does not require Gaussian innovations.

The paper is organized as follows. Section 2 describes the model and gives the main technical assumptions. In Section 3, we establish the local asymptotic normality (LAN) of $PVAR(p)$ models in the vicinity of $VAR(p)$ ones. The asymptotic behavior of central sequences is studied in Section 4. The central sequence in the LAN property is expressed in terms of residual cross-covariance matrices, for which a local asymptotic linearity result is proved in Section 5. The optimal tests are derived in Section 6.

Note that likelihoods could be written from the stacked VAR representation of $PVAR(p)$ models proposed by Gladyshev (1961) (see also Tiao and Grupe 1980). In principle, the LAN property of Section 3 then could be deduced from Garel and Hallin (1995)'s general results. However, these VAR representations involve a much larger number of

parameters than the original PVAR(p) model—along with a series of constraints that compensate for this number but make the likelihood-based approach rather tedious. This stacked VAR representation therefore is not considered here.

2. The problem

2.1 Notation and main assumptions

We are interested in testing a null hypothesis of stationary VAR(p) dependence, with unspecified coefficients and unspecified innovation density, against alternatives of PVAR(p) dependence with given period d, characterized by a model of the form (14.1), where $s = 1, \ldots, d$ denotes the *season* and $\boldsymbol{\Theta}_i(s)$ is the matrix of autoregressive coefficients for season s and lag i. The process $\{\boldsymbol{\varepsilon}_t \,;\, t \in \mathbb{Z}\}$ is assumed to be m-variate independent white noise, with density f such that $\int \mathbf{x} f(\mathbf{x}) d\mathbf{x} = \mathbf{0}$ and positive definite covariance matrix $\boldsymbol{\Sigma} := \int \mathbf{x}\mathbf{x}' f(\mathbf{x}) d\mathbf{x}$, with diagonal elements $\Sigma_{ii} := \sigma_i^2$.

Under the null hypothesis of non-periodic dependence, $\boldsymbol{\Theta}_i(s) = \boldsymbol{\Theta}_i$ for all s, so that (14.1) takes the form of a traditional VAR(p) model

$$\mathbf{X}_t - \sum_{i=1}^{p} \boldsymbol{\Theta}_i \mathbf{X}_{t-i} = \boldsymbol{\varepsilon}_t, \quad t \in \mathbb{Z}. \tag{14.2}$$

Letting

$$\begin{aligned}
\boldsymbol{\Theta} \; &:= \; \left([\text{vec}\,\boldsymbol{\Theta}_1]', \ldots, [\text{vec}\,\boldsymbol{\Theta}_p]', \ldots, [\text{vec}\,\boldsymbol{\Theta}_1]', \ldots, [\text{vec}\,\boldsymbol{\Theta}_p]'\right)' \tag{14.3} \\
&= \; \mathbf{1} \otimes \left([\text{vec}\,\boldsymbol{\Theta}_1]', \ldots, [\text{vec}\,\boldsymbol{\Theta}_p]'\right)' \in \mathbb{R}^{dpm^2},
\end{aligned}$$

where $\mathbf{1} := (1, \ldots, 1)' \in \mathbb{R}^d$, denote by $\mathcal{H}_f^{(n)}(\boldsymbol{\Theta})$ the null hypothesis under which an observed series $\mathbf{X}^{(n)} = (\mathbf{X}_1^{(n)}, \ldots, \mathbf{X}_n^{(n)})$ is a finite realization of length n of a solution of (14.2). Whenever f, or both f and $\boldsymbol{\Theta}$ remain unspecified (except for the assumptions listed below), we use the notation $\mathcal{H}^{(n)}(\boldsymbol{\Theta})$ and $\mathcal{H}^{(n)}$, respectively.

In order to obtain locally asymptotically optimal tests for $\mathcal{H}_f^{(n)}(\boldsymbol{\Theta})$, we consider *local* sequences of alternatives, denoted as $\mathcal{H}_f^{(n)}(\boldsymbol{\Theta}^{(n)})$. These alternatives are characterized by sequences of ($m \times m$) matrices

$$\begin{aligned}
\boldsymbol{\Theta}^{(n)} \; := \; &\Big([\text{vec}\,\boldsymbol{\Theta}_1^{(n)}(1)]', \ldots, [\text{vec}\,\boldsymbol{\Theta}_p^{(n)}(1)]', \ldots \\
&\ldots, [\text{vec}\,\boldsymbol{\Theta}_1^{(n)}(d)]', \ldots, [\text{vec}\,\boldsymbol{\Theta}_p^{(n)}(d)]'\Big)'
\end{aligned}$$

of the form $\boldsymbol{\Theta}^{(n)} := \boldsymbol{\Theta} + n^{-\frac{1}{2}}\,\mathbf{K}\boldsymbol{\tau}^{(n)}$, where

$$\boldsymbol{\tau}^{(n)} = ([\text{vec}\,\boldsymbol{\alpha}_1^{(n)}]',\ldots,[\text{vec}\,\boldsymbol{\alpha}_p^{(n)}]',[\text{vec}\,\boldsymbol{\beta}_1^{(n)}(1)]',\ldots,[\text{vec}\,\boldsymbol{\beta}_p^{(n)}(d-1)]')' \tag{14.4}$$

denotes a bounded sequence of dpm^2-dimensional vectors, and

$$\mathbf{K} := \begin{bmatrix} 1 & & & \\ 1 & & \mathbf{I}_{(d-1)\times(d-1)} & \\ \vdots & & & \\ 1 & -1 & \cdots & -1 \end{bmatrix} \otimes \mathbf{I}_{(pm^2\times pm^2)}. \tag{14.5}$$

The p matrices $\boldsymbol{\alpha}_i^{(n)}$, $i = 1,\ldots,p$, can be interpreted as non-seasonal perturbations of the corresponding autoregressive matrices $\boldsymbol{\Theta}_i$, the collection

$$(\boldsymbol{\beta}_i^{(n)}(1),\ldots,\boldsymbol{\beta}_i^{(n)}(d-1),\boldsymbol{\beta}_i^{(n)}(d) := -\sum_{s=1}^{d-1}\boldsymbol{\beta}_i^{(n)}(s))$$

as a periodical perturbation of the same $\boldsymbol{\Theta}_i$'s. Note that these perturbations are such that $\sum_{s=1}^d \boldsymbol{\beta}_i^{(n)}(s) = \mathbf{0}$, $i = 1,\ldots,p$, which allows for identifiable perturbations

$$\boldsymbol{\alpha}^{(n)} := \left([\text{vec}\,\boldsymbol{\alpha}_1^{(n)}]',\ldots,[\text{vec}\,\boldsymbol{\alpha}_p^{(n)}]'\right)'$$

and, writing $\boldsymbol{\beta}^{(n)}(s)$ for $\left(\text{vec}\,\boldsymbol{\beta}_1^{(n)}(s),\ldots,\text{vec}\,\boldsymbol{\beta}_p^{(n)}(s)\right)$, identifiable perturbations

$$\boldsymbol{\beta}^{(n)} := \left(\boldsymbol{\beta}^{(n)\prime}(1),\ldots,\boldsymbol{\beta}^{(n)\prime}(d-1)\right)'.$$

With this notation, $\boldsymbol{\Theta}_i^{(n)}$ has (j,k) entry

$$\boldsymbol{\Theta}_{i;j,k}^{(n)}(s) = \boldsymbol{\Theta}_{i;j,k} + n^{-\frac{1}{2}}\left(\boldsymbol{\alpha}_{i;j,k}^{(n)} + \boldsymbol{\beta}_{i;j,k}^{(n)}(s)\right) \quad j,k = 1,\ldots,m$$

for $i = 1,\ldots,p$ and $s = 1,\ldots,d$. Finally, putting $\mathbf{D}_i^{(n)}(s) := \boldsymbol{\alpha}_i^{(n)} + \boldsymbol{\beta}_i^{(n)}(s)$, let

$$\boldsymbol{\tau}_*^{(n)}(s) := \left([\text{vec}\,\mathbf{D}_1^{(n)}(s)]',\ldots,[\text{vec}\,\mathbf{D}_p^{(n)}(s)]'\right)'$$

and

$$\boldsymbol{\tau}_*^{(n)} := \left(\boldsymbol{\tau}_*^{(n)\prime}(1),\ldots,\boldsymbol{\tau}_*^{(n)\prime}(d)\right)' = \mathbf{K}\boldsymbol{\tau}^{(n)}. \tag{14.6}$$

Note that, for all $\mathbf{v} \in \mathbb{R}^{pm^2}$,

$$[\mathbf{K}'(\mathbf{1} \otimes \mathbf{v})]_i = 0, \quad i = pm^2 + 1,\ldots,dpm^2, \tag{14.7}$$

where $\mathbf{1} := (1,\ldots,1)' \in \mathbb{R}^d$.

2.2   Main assumptions

The LAN property we are establishing in Section 3 requires some technical assumptions.

(A.1) Letting $\boldsymbol{\Theta}(z) := \mathbf{I} - \sum_{i=1}^{p} \boldsymbol{\Theta}_i z^i$, the parameter $\boldsymbol{\Theta}$ is such that $|\boldsymbol{\Theta}_p \neq 0|$, and the roots of the determinantal equation $|\boldsymbol{\Theta}(z)| = 0$, $z \in \mathbb{C}$ all lie outside the unit disk, i.e., the VAR(p) model (14.2) is *causal*.

(A.2) The innovations density f satisfies the following regularity assumptions.

    (i) There exists a square integrable random vector $\mathbf{D}f^{\frac{1}{2}}$ such that for all $\mathbf{0} \neq \mathbf{b} \to \mathbf{0}$,

$$\left(\mathbf{b}'\mathbf{b}\right)^{-1} \int \left[f^{1/2}(\mathbf{x} + \mathbf{b}) - f^{1/2}(\mathbf{x}) - \mathbf{b}'(\mathbf{D}f^{\frac{1}{2}}(\mathbf{x})) \right]^2 d\mu \to \mathbf{0} \, ,$$

    i.e., $f^{\frac{1}{2}}$ is mean square differentiable, with mean square gradient $\mathbf{D}f^{\frac{1}{2}}$.

    (ii) Letting $\boldsymbol{\varphi}(\mathbf{x}) := (\varphi_1(\mathbf{x}), \dots, \varphi_m(\mathbf{x}))' := -2\, \mathbf{D}f^{\frac{1}{2}}(\mathbf{x})/f^{\frac{1}{2}}(\mathbf{x})$, the *information matrix* $\boldsymbol{\mathcal{I}}(f) := \int \boldsymbol{\varphi}(\mathbf{x})\boldsymbol{\varphi}'(\mathbf{x})\, f(\mathbf{x})\, d\mu$ is finite and positive definite.

(A.3) The score function $\boldsymbol{\varphi}$ is piecewise Lipschitz, i.e., there exists a finite, measurable partition of $\mathbb{R}^m$ into J non overlapping subsets I_j, $j = 1, \dots, J$ such that $\|\boldsymbol{\varphi}(\mathbf{x}) - \boldsymbol{\varphi}(\mathbf{y})\| \leq C_f \|\mathbf{x} - \mathbf{y}\|$ for all $\mathbf{x}, \mathbf{y}$ in I_j, $j = 1, \dots, J$.

3.   Local asymptotic normality

3.1   Periodic f-cross-covariance matrices

Assume, for simplicity, that n is a multiple $n = d \times r$ of the period, and let $t^* = \lceil t/d \rceil$, hence $t = dt^* + s$, $s = 1, \dots, d$. Provided that they are $O_p(1)$, it can be assumed, without loss of generality, that the starting values $(\mathbf{X}_0^{(n)}, \mathbf{X}_{-1}^{(n)}, \dots, \mathbf{X}_{1-p}^{(n)})$ are all equal to zero (see, e.g., Hallin and Werker 1998).

Let

$$\mathbf{Z}_t^{(n)}(\boldsymbol{\Theta}^{(n)}) = \mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta}^{(n)}) := \mathbf{X}_{dt^*+s}^{(n)} - \sum_{i=1}^{p} \boldsymbol{\Theta}_i^{(n)}(s)\mathbf{X}_{dt^*+s-i}^{(n)}$$

denote the residuals associated with the periodic model (14.1) with parameter values $\boldsymbol{\Theta}^{(n)}$: under $\mathcal{H}^{(n)}(\boldsymbol{\Theta})$, $\mathbf{Z}_t^{(n)}(\boldsymbol{\Theta})$ coincides with $\boldsymbol{\varepsilon}_t$. The

logarithm of the likelihood ratio for $\mathcal{H}_f^{(n)}(\boldsymbol{\Theta})$ against $\mathcal{H}_f^{(n)}(\boldsymbol{\Theta}^{(n)})$ then takes the form (the $o_p(1)$ term corresponds to the influence as $n \to \infty$ of the starting values)

$$
\Lambda_f^{(n)}(\boldsymbol{\Theta} \; + \; n^{-\frac{1}{2}}\mathbf{K}\,\boldsymbol{\tau}^{(n)}/\boldsymbol{\Theta})
$$

$$
= \sum_{s=1}^{d}\sum_{t^*=0}^{r-1} \log\left(f(\mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta}^{(n)}))/f(\mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta}))\right) + o_p(1).
$$

A basic statistical tool in the Gaussian analysis of univariate time series is the observed (residual) autocovariance function. In a non-Gaussian periodic context, the following natural generalization of this classical concept enters naturally the picture. Define the *periodic residual f-cross-covariance matrix of lag k, $k = 1, \ldots, n-1$ as*

$$
\boldsymbol{\Gamma}_{s,k,f}^{(n)} := (r - \lceil\frac{k-s+1}{d}\rceil)^{-1} \sum_{t^*=\lceil\frac{k-s+1}{d}\rceil}^{r-1} \boldsymbol{\varphi}_f(\mathbf{Z}_{dt^*+s}^{(n)})\mathbf{Z}_{dt^*+s-k}^{(n)\prime}, \quad (14.8)
$$

$s = 1, \ldots, d$. Note that, under Gaussian density f, $\boldsymbol{\varphi}_f = \boldsymbol{\varphi}_G$ takes the form $\boldsymbol{\varphi}_G(\mathbf{Z}_{dt^*+s}^{(n)}) = \mathbf{Z}_{dt^*+s}^{(n)}$, so that Gaussian periodic residual cross-covariance matrices take the form

$$
\boldsymbol{\Gamma}_{s,k,G}^{(n)} = (r - \lceil\frac{k-s+1}{d}\rceil)^{-1} \sum_{t^*=\lceil\frac{k-s+1}{d}\rceil}^{r-1} \mathbf{Z}_{dt^*+s}^{(n)}\mathbf{Z}_{dt^*+s-k}^{(n)\prime}.
$$

3.2   LAN property

In order to state the LAN result below, let us introduce some further notation. Define

$$
\mu_{dt^*+s}^{(n)} := \frac{f^{\frac{1}{2}}\left(\mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta} + n^{-1/2}\mathbf{K}\,\boldsymbol{\tau}^{(n)})\right)}{f^{\frac{1}{2}}\left(\mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta})\right)} - 1
$$

and

$$
\xi_{dt^*+s}^{(n)} := \frac{1}{2}n^{-1/2}\left(\sum_{i=1}^{p}(\boldsymbol{\alpha}_i^{(n)} + \boldsymbol{\beta}_i^{(n)}(s))\mathbf{X}_{dt^*+s-i}^{(n)}\right)' \boldsymbol{\varphi}_f(\mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta})).
$$

Also, put $\boldsymbol{\phi}_f^{(n)} := \left(\boldsymbol{\phi}_f^{(n)\prime}(1), \ldots, \boldsymbol{\phi}_f^{(n)\prime}(d) \right)'$, with (writing $\mathbf{I}_{(m \times m)}$ for the $(m \times m)$ unit matrix)

$$
\boldsymbol{\phi}_f^{(n)}(s) := d^{-1/2} \begin{bmatrix} \displaystyle\sum_{k=1}^{n-1} (\mathbf{H}_{k-1} \otimes \mathbf{I}_{(m \times m)}) \, (r - \lceil \frac{k-s+1}{d} \rceil)^{1/2} \operatorname{vec} \boldsymbol{\Gamma}_{s,k,f}^{(n)} \\ \vdots \\ \displaystyle\sum_{k=p}^{n-1} (\mathbf{H}_{k-p} \otimes \mathbf{I}_{(m \times m)}) \, (r - \lceil \frac{k-s+1}{d} \rceil)^{1/2} \operatorname{vec} \boldsymbol{\Gamma}_{s,k,f}^{(n)} \end{bmatrix}.
$$

$$
\tag{14.9}
$$

Finally, denote by $\boldsymbol{\Gamma}(\boldsymbol{\Theta})$ the $(mp \times mp)$-dimensional covariance matrix, under parameter value $\boldsymbol{\Theta}$, of $(\mathbf{X}_1^{(n)\prime}, \ldots, \mathbf{X}_p^{(n)\prime})'$:

$$
(\boldsymbol{\Gamma}(\boldsymbol{\Theta}))_{ij} = \sum_{l=\max(i,j)}^{\infty} \mathbf{H}_{l-i}(\boldsymbol{\Theta}) \, \boldsymbol{\Sigma} \, \mathbf{H}_{l-j}'(\boldsymbol{\Theta}) \quad i,j = 1, \ldots, p. \tag{14.10}
$$

The matrices $\mathbf{H}_l = \mathbf{H}_l(\boldsymbol{\Theta})$, $l \in \mathbb{Z}$ here are the Green's matrices associated with the difference operator $\boldsymbol{\Theta}(L) = \mathbf{I} - \sum_{i=1}^{p} \boldsymbol{\Theta}_i L^i$, where L stands for the lag operator; these Green's matrices are characterized by $(\boldsymbol{\Theta}(L))^{-1} := \sum_{l=0}^{\infty} \mathbf{H}_l L^l$.

Our LAN result is expressed under two equivalent but distinct forms. In the second form, the central sequence is measurable with respect to the periodic residual covariance matrices (14.8).

PROPOSITION 14.1 *Assume that (A.1) and (A.2) hold. Under $\mathcal{H}_f^{(n)}(\boldsymbol{\Theta})$, as $n \to \infty$, we have*

(i) *(LAN 1)*

$$
\Lambda(\boldsymbol{\Theta}^{(n)} / \boldsymbol{\Theta}) = 2 \sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \xi_{s,t^*}^{(n)}(\boldsymbol{\Theta}) \tag{14.11}
$$

$$
- \frac{1}{2d} \boldsymbol{\tau}^{(n)\prime} \mathbf{K}' \left[\mathbf{I}_{(d \times d)} \otimes \{ \boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}(f) \} \right] \mathbf{K} \boldsymbol{\tau}^{(n)} + o_p(1)
$$

and

$$
\frac{\Lambda(\boldsymbol{\Theta}^{(n)} / \boldsymbol{\Theta}) + \frac{1}{2} \boldsymbol{\tau}^{(n)\prime} \boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta}) \boldsymbol{\tau}^{(n)}}{[\boldsymbol{\tau}^{(n)\prime} \boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta}) \boldsymbol{\tau}^{(n)}]^{1/2}} \xrightarrow{\mathcal{L}} \mathcal{N}(0, 1),
$$

with

$$\boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta}) := d^{-1}\mathbf{K}' \begin{bmatrix} \boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \boldsymbol{\mathcal{I}}(f) & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \boldsymbol{\mathcal{I}}(f) \end{bmatrix} \mathbf{K}.$$

$$(14.12)$$

(ii) *(LAN 2)*

$$\Lambda(\boldsymbol{\Theta}^{(n)}/\boldsymbol{\Theta}) = \boldsymbol{\tau}^{(n)\prime}\boldsymbol{\Delta}_f^{(n)}(\boldsymbol{\Theta}) - \frac{1}{2}\boldsymbol{\tau}^{(n)\prime}\boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta})\,\boldsymbol{\tau}^{(n)} + o_p(1)\,, \quad (14.13)$$

with the central sequence

$$\boldsymbol{\Delta}_f^{(n)}(\boldsymbol{\Theta}) := \mathbf{K}'\boldsymbol{\phi}_f^{(n)} =$$

$$\begin{pmatrix} d^{-\frac{1}{2}}\displaystyle\sum_{s=1}^{d}\sum_{k=1}^{n-1}(\mathbf{H}_{k-1}\otimes\mathbf{I})\,(r - \lceil\frac{k-s+1}{d}\rceil)^{1/2}\,\mathrm{vec}(\boldsymbol{\Gamma}_{s,k,f}^{(n)}) \\[2mm] \vdots \\[2mm] d^{-\frac{1}{2}}\displaystyle\sum_{s=1}^{d}\sum_{k=p}^{n-1}(\mathbf{H}_{k-p}\otimes\mathbf{I})\,(r - \lceil\frac{k-s+1}{d}\rceil)^{1/2}\,\mathrm{vec}(\boldsymbol{\Gamma}_{s,k,f}^{(n)}) \\[2mm] d^{-\frac{1}{2}}\displaystyle\sum_{k=1}^{n-1}(\mathbf{H}_{k-1}\otimes\mathbf{I})\left\{(r - \lceil\frac{k-1+1}{d}\rceil)^{1/2}\,\mathrm{vec}\,(\boldsymbol{\Gamma}_{1,k,f}^{(n)})\right. \\[2mm] \left. -(r - \lceil\frac{k-d+1}{d}\rceil)^{1/2}\,\mathrm{vec}(\boldsymbol{\Gamma}_{d,k,f}^{(n)})\right\} \\[2mm] \vdots \\[2mm] d^{-\frac{1}{2}}\displaystyle\sum_{k=p}^{n-1}(\mathbf{H}_{k-p}\otimes\mathbf{I})\left\{(r - \lceil\frac{k-1+1}{d}\rceil)^{1/2}\,\mathrm{vec}\,(\boldsymbol{\Gamma}_{1,k,f}^{(n)})\right. \\[2mm] \left. -(r - \lceil\frac{k-d+1}{d}\rceil)^{1/2}\,\mathrm{vec}(\boldsymbol{\Gamma}_{d,k,f}^{(n)})\right\} \\[2mm] \vdots \\[2mm] d^{-\frac{1}{2}}\displaystyle\sum_{k=1}^{n-1}(\mathbf{H}_{k-1}\otimes\mathbf{I})\left\{(r - \lceil\frac{k-(d-1)+1}{d}\rceil)^{1/2}\,\mathrm{vec}\,(\boldsymbol{\Gamma}_{d-1,k,f}^{(n)})\right. \\[2mm] \left. -(r - \lceil\frac{k-d+1}{d}\rceil)^{1/2}\,\mathrm{vec}(\boldsymbol{\Gamma}_{d,k,f}^{(n)})\right\} \\[2mm] \vdots \\[2mm] d^{-\frac{1}{2}}\displaystyle\sum_{k=p}^{n-1}(\mathbf{H}_{k-p}\otimes\mathbf{I})\left\{(r - \lceil\frac{k-(d-1)+1}{d}\rceil)^{1/2}\,\mathrm{vec}\,(\boldsymbol{\Gamma}_{d-1,k,f}^{(n)})\right. \\[2mm] \left. -(r - \lceil\frac{k-d+1}{d}\rceil)^{1/2}\,\mathrm{vec}\,(\boldsymbol{\Gamma}_{d,k,f}^{(n)})\right\} \end{pmatrix} ;$$

moreover, $\boldsymbol{\Delta}_f^{(n)}(\boldsymbol{\Theta})$ is asymptotically normal, with mean $\mathbf{0}$ and the covariance matrix $\boldsymbol{\Gamma}_f^\Delta(\boldsymbol{\Theta})$ defined in (14.12).

Proof. We start with establishing (LAN 1) which, via Swensen (1985)'s Lemma 1, follows if the following six conditions are satisfied:

(1) $\displaystyle \lim_{r \to \infty} \mathrm{E}\left(\sum_{s=1}^{d} \sum_{t^*=0}^{r-1} [\mu_{dt^*+s}^{(n)} - \xi_{dt^*+s}^{(n)}]^2 \right) = 0,$

(2) $\displaystyle \sup_r \mathrm{E}\left(\sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \xi_{dt^*+s}^{(n)2} \right) < \infty,$

(3) $\displaystyle \max_s \max_{t^*} \left| \xi_{dt^*+s}^{(n)} \right| = o_p(1),$

(4) $\displaystyle \sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \xi_{dt^*+s}^{(n)2} = \boldsymbol{\tau}^{(n)\prime} \boldsymbol{\Gamma}_f^\Delta(\boldsymbol{\Theta}) \boldsymbol{\tau}^{(n)} + o_p(1),$

(5) $\displaystyle \sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \mathrm{E}\left(\xi_{dt^*+s}^{(n)2} I(|\xi_{dt^*+s}^{(n)}| > \frac{1}{2}) \,|\, \mathcal{F}_{dt^*+s-1}^{(n)} \right) = o_p(1),$

(6) $\displaystyle \mathrm{E}\left(\xi_{dt^*+s}^{(n)} \,|\, \mathcal{F}_{dt^*+s-1}^{(n)} \right) = o_p(1).$

Condition (1). Let $\displaystyle \lambda_{dt^*+s}^{(n)} = n^{-1/2} \sum_{i=1}^{p} (\boldsymbol{\alpha}_i^{(n)} + \boldsymbol{\beta}_i^{(n)}(s)) \mathbf{X}_{dt^*+s-i}^{(n)}.$ Under $\mathcal{H}_f^{(n)}(\boldsymbol{\Theta})$,

$$\mathrm{E}\left[\sum_{s=1}^{d} \sum_{t^*=0}^{r-1} (\mu_{dt^*+s}^{(n)} - \xi_{dt^*+s}^{(n)})^2 \right]$$

$$= \sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \mathrm{E}\left\{ I\left[\left\| \lambda_{dt^*+s}^{(n)} \right\|^2 \le C \right] \left[\mu_{dt^*+s}^{(n)} - \xi_{dt^*+s}^{(n)} \right]^2 \right\}$$

$$+ \sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \mathrm{E}\left\{ I\left[\left\| \lambda_{dt^*+s}^{(n)} \right\|^2 > C \right] \left[\mu_{dt^*+s}^{(n)} - \xi_{dt^*+s}^{(n)} \right]^2 \right\}$$

$$=: a_1 + a_2, \text{ say.}$$

Now,

$$a_1 = \sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \mathrm{E}\left\{ I\left[\left\| \lambda_{dt^*+s}^{(n)} \right\|^2 \le C \right] \right.$$

$$\times \mathrm{E}\left\{[\mu_{dt^*+s}^{(n)} - \xi_{dt^*+s}^{(n)}]^2 \mid \mathbf{Z}_{dt^*+s-1}\mathbf{Z}_{dt^*+s-2},\cdots\right\}\right\}$$

$$= \sum_{s=1}^{d}\sum_{t^*=0}^{r-1}\mathrm{E}\left\{I\left[\left\|\boldsymbol{\lambda}_{dt^*+s}^{(n)}\right\|^2 \leq C\right]\right.$$

$$\times \int\left[\frac{f^{1/2}(\mathbf{Z} - \boldsymbol{\lambda}_{dt^*+s}^{(n)}) - f^{1/2}(\mathbf{Z})}{f^{1/2}(\mathbf{Z})} - \frac{1}{2}(\boldsymbol{\lambda}_{dt^*+s}^{(n)})\varphi(\mathbf{Z})\right]^2 f(\mathbf{Z})d\mathbf{Z}\right\}$$

$$\leq \sum_{s=1}^{d}\sum_{t^*=0}^{r-1}\mathrm{E}\left[\left\|\mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta}^{(n)}) - \mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta})\right\|^2\right]C^{(n)}(C)$$

for all $C > 0$. From Garel and Hallin (1995)'s Lemma 2.2 (ii), $C^{(n)}(C)$ converges to zero as $n \to \infty$, for any fixed C. Thus, it is sufficient to note that

$$\sum_{s=1}^{d}\sum_{t^*=0}^{r-1}\mathrm{E}\left[\left\|\mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta}^{(n)}) - \mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta})\right\|^2\right]$$

$$= \sum_{s=1}^{d}\sum_{t^*=0}^{r-1}\mathrm{E}\left[\left\|n^{-1/2}\sum_{i=1}^{p}(\boldsymbol{\alpha}_i + \boldsymbol{\beta}_i(s))\mathbf{X}_{dt^*+s}^{(n)}\right\|\right]^2$$

is bounded as $n \to \infty$, since the process $\mathbf{X}_{dt^*+s}^{(n)}$ is second-order stationary. Hence, $a_1 \to 0$.

Turning to a_2, Garel and Hallin (1995)'s Lemma 2.1 (i) entails

$$a_2 = \sum_{s=1}^{d}\sum_{t^*=0}^{r-1}\mathrm{E}\left\{I[\|\boldsymbol{\lambda}_{dt^*+s}^{(n)}\|^2 > C]\right.$$

$$\times \int[f^{1/2}(\mathbf{Z} - \boldsymbol{\lambda}_{dt^*+s}^{(n)}) - f^{1/2}(\mathbf{Z}) - (\boldsymbol{\lambda}_{dt^*+s}^{(n)})'\mathbf{D}f^{1/2}(\mathbf{Z})]^2 f(\mathbf{Z})d\mathbf{Z}\right\}$$

$$\leq \sum_{s=1}^{d}\sum_{t^*=0}^{r-1}\mathrm{E}\left\{I[\|\boldsymbol{\lambda}_{dt^*+s}^{(n)}\|^2 > C](\boldsymbol{\lambda}_{dt^*+s}^{(n)})'\boldsymbol{\mathcal{I}}(f)(\boldsymbol{\lambda}_{dt^*+s}^{(n)})\right\}.$$

Since $\displaystyle\sum_{s=1}^{d}\sum_{t^*=0}^{r-1}\mathrm{E}\left[\|\mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta}^{(n)}) - \mathbf{Z}_{dt^*+s}^{(n)}(\boldsymbol{\Theta})\|^2\right]$ is bounded as $n \to \infty$, it follows that, for sufficiently large C, a_2 can be made arbitrary small. Condition (1) follows.

Condition (2). It is sufficient to show that $\mathrm{E} \sum\limits_{s=1}^{d} \sum\limits_{t^*=0}^{r-1} (\xi_{s,t^*}^{(n)})^2 < \infty$ for fixed s. Since

$$
\begin{aligned}
\mathrm{E} \sum_{t^*=0}^{r-1} (\xi_{s,t^*}^{(n)})^2 &= \frac{1}{4n} (\lambda_{dt^*+s}^{(n)})' \varphi(\mathbf{Z}) \varphi'(\mathbf{Z}) \lambda_{dt^*+s}^{(n)} \\
&= \frac{1}{4n} \mathrm{tr} \left\{ \mathcal{I}(f) \mathrm{E} [\lambda_{dt^*+s}^{(n)} \lambda_{dt^*+s}^{(n)'}] \right\},
\end{aligned}
$$

where $\mathrm{E} [\lambda_{dt^*+s}^{(n)} \lambda_{dt^*+s}^{(n)'}]$ is bounded, the result follows.

Condition (3). It is sufficient to show that $\max\limits_{t^*} |\xi_{s,t^*}^{(n)}|$ is $o_p(1)$ for all $s = 1, \ldots, d$. For any $\delta > 0$, any $k = 1, \ldots, m$, we have

$$
\mathrm{P} \left(n^{-1/2} \max_{t^*} \left| \sum_{i=1}^{p} \{(\alpha_i + \beta_i(s)) \mathbf{X}_{s,t^*}^{(n)}\}_k \varphi_k(\mathbf{Z}) \right| > \delta \right)
$$

$$
= \mathrm{P} \left\{ n^{-1} \sum_{t^*} (\lambda_{dt^*+s})_k^2 \varphi_k^2(\mathbf{Z}) . I \left[n^{-1/2} |(\lambda_{dt^*+s})_k \varphi_k(\mathbf{Z})| > \delta \right] \delta^2 \right\}
$$

$$
\leq n^{-1} \delta^{-2} \sum_{t^*=0}^{r-1} \mathrm{E} \left\{ (\lambda_{dt^*+s})_k^2 \varphi_k^2(\mathbf{Z}) I \left[n^{-1/2} |(\lambda_{dt^*+s})_k \varphi_k(\mathbf{Z})| > \delta \right] > \delta^2 \right\}.
$$

The result then follows from the fact that λ_{dt^*+s} is stationary and the uniform integrability of $(\lambda_{dt^*+s})_k^2 \varphi_k^2(\mathbf{Z})$.

Condition (4). Recall that

$$
\sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \xi_{dt^*+s}^{(n)2} = \frac{1}{4} \sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \lambda_{dt^*+s}^{(n)'} \varphi_f(\mathbf{Z}_{dt^*+s}^{(n)}) \varphi_f'(\mathbf{Z}_{dt^*+s}^{(n)}) \lambda_{dt^*+s}^{(n)},
$$

with $\mathbf{D}_i^{(n)}(s) := \alpha_i^{(n)} + \beta_i^{(n)}(s)$. Hence,

$$
\begin{aligned}
\sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \xi_{dt^*+s}^{(n)2} &= \frac{1}{4d} \sum_{s=1}^{d} \frac{1}{r} \sum_{t^*=0}^{r-1} \left(\varphi_f'(\mathbf{Z}_{dt^*+s}^{(n)}) \sum_{i=1}^{p} \mathbf{D}_i^{(n)}(s) \mathbf{X}_{dt^*+s-i}^{(n)} \right)^2 \\
&= \frac{1}{4d} \sum_{s=1}^{d} \mathrm{E} \left(\varphi_f'(\mathbf{Z}_{d1+s}^{(n)}) \sum_{i=1}^{p} \mathbf{D}_i^{(n)}(s) \mathbf{X}_{d1+s-i}^{(n)} \right)^2 + o_p(1) \\
&= \frac{1}{4d} \sum_{s=1}^{d} \sum_{i=1}^{p} \sum_{j=1}^{p} \mathrm{tr} \left\{ \mathcal{I}(f) \mathbf{D}_j^{(n)}(s) \mathrm{E} (\mathbf{X}_{d1+s-j}^{(n)} \mathbf{X}_{d1+s-i}^{(n)'}) \right. \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad \left. \times \mathbf{D}_i^{(n)'}(s) \right\} + o_p(1).
\end{aligned}
$$

Since $\mathrm{tr}(\mathbf{ABC}) = \mathrm{tr}(\mathbf{CAB})$ and $\mathbf{X}_t^{(n)} = \sum_{k=0}^{t-1}\mathbf{H}_k\mathbf{Z}_{t-k}^{(n)}$, this last quantity is equivalent to

$$\frac{1}{4d}\sum_{s=1}^{d}\sum_{i=1}^{p}\sum_{k=\max(i,j)}^{\infty}\mathrm{tr}\left\{\mathbf{D}_i^{(n)\prime}(s)\boldsymbol{\mathcal{I}}(f)\mathbf{D}_i^{(n)}(s)\mathbf{H}_{k-j}\boldsymbol{\Sigma}\mathbf{H}_{k-i}'\right\} + o_p(1).$$

By relation (3.1), and using the fact that $\mathrm{tr}(\mathbf{AB}) = \mathrm{vec}(\mathbf{A}')'\mathrm{vec}(\mathbf{B})$ and $\mathrm{vec}(\mathbf{ABC}) = (\mathbf{C}' \otimes \mathbf{A})(\mathrm{vec}(\mathbf{B}))$, the latter expression yields

$$\frac{1}{4d}\sum_{s=1}^{d}\sum_{i=1}^{p}\sum_{j=1}^{p}\sum_{k=\max(i,j)}^{\infty}[\mathrm{vec}\,\mathbf{D}_j^{(n)}(s)]'\left(\{\mathbf{H}_{k-i}\boldsymbol{\Sigma}\mathbf{H}_{k-j}'\} \otimes \boldsymbol{\mathcal{I}}(f)\right)$$
$$\times[\mathrm{vec}\,\mathbf{D}_i^{(n)}(s)] + o_p(1)$$
$$= \frac{1}{4d}\sum_{s=1}^{d}\left([\mathrm{vec}\mathbf{D}_1^{(n)}(s)]',\ldots,[\mathrm{vec}\mathbf{D}_p^{(n)}(s)]'\right)$$
$$\times (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \boldsymbol{\mathcal{I}}(f))\left([\mathrm{vec}\mathbf{D}_1^{(n)}(s)]',\ldots,[\mathrm{vec}\mathbf{D}_p^{(n)}(s)]'\right)' + o_p(1).$$

In view of (14.6), we then have

$$\sum_{s=1}^{d}\sum_{t^*=0}^{m-1}\xi_{dt^*+s}^{(n)2} = \frac{1}{4d}\sum_{s=1}^{d}\boldsymbol{\tau}_*^{(n)\prime}(s)\,(\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \boldsymbol{\mathcal{I}}(f))\,\boldsymbol{\tau}_*^{(n)}(s) + o_p(1)$$
$$= \frac{1}{4d}\boldsymbol{\tau}^{(n)\prime}\mathbf{K}'\left[\mathbf{I}_{d\times d} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \boldsymbol{\mathcal{I}}(f))\right]\mathbf{K}\,\boldsymbol{\tau}^{(n)} + o_p(1).$$

Condition (5). This condition is an immediate consequence of the mean square differentiability of $f^{1/2}$.

Condition (6). From the definition of $\xi_{s,t^*}^{(n)}$, and since $\mathrm{E}\,(\boldsymbol{\varphi}(\mathbf{Z})) = 0$,

$$\frac{1}{2}\mathrm{E}\,\left(\boldsymbol{\lambda}_{dt^*+s}'\boldsymbol{\varphi}(\mathbf{Z})\,|\,\mathcal{F}_{dt^*+s-1}\right) = \frac{1}{2}\boldsymbol{\lambda}_{dt^*+s}'\mathrm{E}\,(\boldsymbol{\varphi}(\mathbf{Z})) = 0.$$

Turning to (LAN 2), it is sufficient to show that the quadratic approximation (14.11) can be rewritten as (14.13). Since $\mathbf{X}_t^{(n)} = \sum_{k=0}^{t-1}\mathbf{H}_k\mathbf{Z}_{t-k}^{(n)}$, it follows that $2\sum_{s=1}^{d}\sum_{t^*=0}^{r-1}\xi_{s,t^*}^{(n)}(\boldsymbol{\Theta})$ is equivalent to

$$n^{-1/2} \sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \sum_{i=1}^{p} \sum_{k=0}^{dt^*+s-i-1} \left(\mathbf{D}_i^{(n)}(s) \mathbf{H}_k \mathbf{Z}_{dt^*+s-i-k}^{(n)} \right)' \boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{(n)}) + o_p(1)$$

$$= n^{-1/2} \sum_{s=1}^{d} \sum_{i=1}^{p} \sum_{k=i}^{d(r-1)+s-1} \sum_{t^*=\lceil \frac{k-s+1}{d} \rceil}^{r-1} \left(\mathbf{D}_i^{(n)}(s) \mathbf{H}_{k-i} \mathbf{Z}_{dt^*+s-i-k}^{(n)} \right)'$$
$$\boldsymbol{\varphi}(\mathbf{Z}_{t^*+s}^{(n)}) + o_p(1)$$

$$= n^{-1/2} \sum_{s=1}^{d} \sum_{i=1}^{p} \sum_{k=i}^{d(r-1)+s-1}$$
$$\mathrm{tr} \left\{ \sum_{t^*=\lceil \frac{k-s+1}{d} \rceil}^{r-1} \boldsymbol{\varphi}(\mathbf{Z}_{t^*+s}^{(n)}) \mathbf{Z}_{dt^*s-i-k}^{(n)\prime} \mathbf{H}_{k-i}' \mathbf{D}_i^{(n)\prime}(s) \right\} + o_p(1).$$

Since $\mathrm{tr}\,(\mathbf{AB}) = \mathrm{vec}(\mathbf{A}')'\mathrm{vec}(\mathbf{B})$ and $\mathrm{vec}(\mathbf{AB}) = (\mathbf{B}' \otimes \mathbf{I})\,\mathrm{vec}(\mathbf{A})$, we obtain

$$2 \sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \xi_{s,t^*}^{(n)}(\boldsymbol{\Theta}) = d^{-1/2} \sum_{s=1}^{d} \sum_{i=1}^{p} \sum_{k=i}^{d(r-1)+s-1} \left(\mathrm{vec}\,\mathbf{D}_i^{(n)}(s) \right)'$$
$$\times \mathrm{vec} \left((r - \lceil \frac{k-s+1}{d} \rceil)^{1/2} \boldsymbol{\Gamma}_{s,k,f}^{(n)} \mathbf{H}_{k-i}' \right)$$

$$= d^{-1/2} \sum_{s=1}^{d} \left([\mathrm{vec}\mathbf{D}_1^{(n)}(s)]', \ldots, [\mathrm{vec}\mathbf{D}_p^{(n)}(s)]' \right)$$
$$\times \begin{bmatrix} \sum_{k=1}^{n-1} \left(\mathbf{H}_{k-1} \otimes \mathbf{I}_{(m\times m)} \right) \\ \times (r - \lceil \frac{k-s+1}{d} \rceil)^{1/2} \mathrm{vec}\,\boldsymbol{\Gamma}_{s,k,f}^{(n)} \\ \vdots \\ \sum_{k=p}^{n-1} \left(\mathbf{H}_{k-p} \otimes \mathbf{I}_{(m\times m)} \right) \\ \times (r - \lceil \frac{k-s+1}{d} \rceil)^{1/2} \mathrm{vec}\,\boldsymbol{\Gamma}_{s,k,f}^{(n)} \end{bmatrix} + o_p(1).$$

It follows that $2 \sum_{s=1}^{d} \sum_{t^*=0}^{r-1} \xi_{s,t^*}^{(n)}(\boldsymbol{\Theta}) = \sum_{s=1}^{d} \boldsymbol{\tau}_*^{(n)\prime}(s) \boldsymbol{\phi}_f^{(n)}(s) + o_p(1)$. Finally, one can easily check that $\boldsymbol{\Delta}_f^{(n)}(\boldsymbol{\Theta}) = \mathbf{K}' \boldsymbol{\phi}_f^{(n)}$. In view of (14.6), we have

$$2\sum_{s=1}^{d}\sum_{t^*=0}^{r-1}\xi_{s,t^*}^{(n)}(\mathbf{\Theta}) = \tau^{(n)\prime}\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta}) + o_p(1).$$ The asymptotic normality of $\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta})$ follows. $\square$

4.   Local asymptotic behavior of $\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta})$ under $\mathcal{H}_g^{(n)}(\mathbf{\Theta})$ and $\mathcal{H}_g^{(n)}(\mathbf{\Theta}^{(n)})$

The result given hereafter in Proposition 14.2 will be essential in evaluating the local power of the tests based on $\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta})$. For each couple of densities (f,g), let

$$\mathcal{I}_g^{(f)} := \mathrm{E}\,[\varphi_f(\mathbf{Z}_{dt^*+s}^{(n)})\,\varphi_f'(\mathbf{Z}_{dt^*+s}^{(n)})], \quad \mathcal{I}_g^{(f,g)} := \mathrm{E}\,[\varphi_f(\mathbf{Z}_{dt^*+s}^{(n)})\,\varphi_g'(\mathbf{Z}_{dt^*+s}^{(n)})],$$

and

$$\mathcal{I}(g) := \mathrm{E}\,[\varphi_g(\mathbf{Z}_{dt^*+s}^{(n)})\,\varphi_g'(\mathbf{Z}_{dt^*+s}^{(n)})]$$

(all expectations are taken under $\mathcal{H}_g^{(n)}(\mathbf{\Theta})$). Denote by $\mathcal{G}_f$ the class of densities g under which these integrals converge (for fixed f satisfying (A2)):

$$\mathcal{G}_f := \left\{ g \text{ satisfying (A.2)} \middle| \mathcal{I}_g^{(f)} < \infty \right\} \qquad (14.14)$$

(clearly, if f satisfies (A.2) and $g \in \mathcal{G}_f$, then $\mathcal{I}_g^{(f,g)}$ also is finite).

PROPOSITION 14.2 *Let f satisfy (A.2) and $g \in \mathcal{G}_f$ Then,*

(i) $\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta}) \xrightarrow{\mathcal{L}} \mathcal{N}\left(\mathbf{0}, \Gamma_f^{\Delta}(\mathbf{\Theta})\mathbf{K}^{-1}\left[\mathbf{I}_{(dpmn\times dpmn)} \otimes \{(\mathcal{I}(f))^{-1}\mathcal{I}_g^{(f)}\}\right]\mathbf{K}\right),$
and

(ii) $\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta}) - \boldsymbol{\mu}_{f,g}^{(n)}$
$$\xrightarrow{\mathcal{L}} \mathcal{N}\left(\mathbf{0}, \Gamma_f^{\Delta}(\mathbf{\Theta})\mathbf{K}^{-1}\left[\mathbf{I}_{(dpmn\times dpmn)} \otimes \{(\mathcal{I}(f))^{-1}\mathcal{I}_g^{(f)}\}\right]\mathbf{K}\right),$$

under $\mathcal{H}_g^{(n)}(\mathbf{\Theta})$, *as* $n \to \infty$, *with*

$$\boldsymbol{\mu}_{f,g}^{(n)} := \Gamma_f^{\Delta}(\mathbf{\Theta})\mathbf{K}^{-1}\left[\mathbf{I}_{(dpm\times dpm)} \otimes \{(\mathcal{I}(f))^{-1}\mathcal{I}_g^{(f,g)}\}\right]\mathbf{K}\,\tau^{(n)}.$$

Proof. To prove part (i) of the proposition, we use the Cramér-Wold device in order to obtain the joint asymptotic distribution of $\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta})$ and $\Lambda_g^{(n)}(\mathbf{\Theta}^{(n)})$ under $\mathcal{H}_g^{(n)}(\mathbf{\Theta})$; (ii) then follows from applying Le Cam's Third Lemma.

Consider the arbitrary linear combination $c^{(n)} := \alpha\,\Lambda_g^{(n)} + \boldsymbol{\beta}'\mathbf{\Delta}_f^{(n)}$. Note that $c^{(n)}$, under $\mathcal{H}_g^{(n)}(\mathbf{\Theta})$ as well as under contiguous alternatives, is

equal to $\alpha \tau^{(n)\prime} \Delta_g^{(n)} + \beta' \Delta_f^{(n)} - \frac{1}{2}\alpha v_g^2 + o_p(1)$, where $v_g^2 := \tau^{(n)\prime} \Gamma_g^{\Delta}(\Theta)\tau^{(n)}$.
It follows from the definitions of $\Delta_f^{(n)}$ in (3.2) that

$$
\begin{aligned}
c^{(n)} &= \alpha \tau^{(n)\prime} \mathbf{K}' \phi_g^{(n)}(\Theta) + \beta' \mathbf{K}' \phi_f^{(n)}(\Theta) - \frac{1}{2}\alpha v_g^2 + o_p(1) \\
&= \mathbf{A}^{(n)\prime} \phi_g^{(n)}(\Theta) + \mathbf{B}'\phi_f^{(n)}(\Theta) - \frac{1}{2}\alpha v_g^2 + o_p(1) ,
\end{aligned}
$$

where $\mathbf{A}^{(n)} = (\mathbf{A}_1^{(n)\prime}, \dots, \mathbf{A}_d^{(n)\prime})' = \alpha\mathbf{K}\tau^{(n)}$, and $\mathbf{B} = (\mathbf{B}_1'., \dots, \mathbf{B}_d')' = \mathbf{K}\beta$. The functions $\phi_g^{(n)}$ and $\phi_f^{(n)}$ are given in (14.9); expectations are taken under $\mathcal{H}_g^{(n)}(\Theta)$ and $\mathcal{H}_f^{(n)}(\Theta)$, respectively. Therefore, according to Garel and Hallin's (1995) Lemma 4.12, $\mathbf{A}_s^{(n)\prime}\phi_g^{(n)}(s) + \mathbf{B}_s'\phi_f^{(n)}(s)$ is asymptotically normal, with mean μ and variance V. Since

$$
\mathrm{E}(\mathrm{vec}\,\Gamma_{s,i,g}^{(n)}) = \mathrm{E}(\mathrm{vec}\,\Gamma_{s,i,f}^{(n)}) = \mathbf{0}
$$

for all s and $i \neq 0$, it follows that $\mu = 0$.

Next consider the variance

$$
\begin{aligned}
\mathrm{Var}(c^{(n)}) = \sum_{s=1}^{d}\sum_{s'=1}^{d} \mathrm{E}\Big\{ & \mathbf{A}_s^{(n)\prime}\phi_g^{(n)}(s)\phi_g^{(n)}(s')\mathbf{A}_{s'}^{(n)} + \mathbf{B}_s'\,\phi_f^{(n)}(s)\phi_f^{(n)}(s')\mathbf{B}_{s'} \\
& + \mathbf{A}_{s.}^{(n)\prime}\phi_g^{(n)}(s)\phi_f^{(n)}(s')\mathbf{B}_{s'} + \mathbf{B}_s'\,\phi_f^{(n)}(s)\phi_g^{(n)}(s')\mathbf{A}_{s'}^{(n)}\Big\}
\end{aligned}
$$

It is easy to show that, for $s \neq s'$,

$$
\begin{aligned}
\mathrm{E}(\phi_g^{(n)}(s)\phi_g^{(n)}(s')) &= \mathrm{E}(\phi_g^{(n)}(s)\phi_f^{(n)}(s')) = \mathrm{E}(\phi_f^{(n)}(s)\phi_g^{(n)}(s')) \\
&= \mathrm{E}(\phi_f^{(n)}(s)\phi_f^{(n)}(s')) = \mathbf{0}.
\end{aligned}
$$

Hence,

$$
\begin{aligned}
\mathrm{Var}(c^{(n)}) = \sum_{s=1}^{d} \mathrm{E}\Big\{ & \mathbf{A}_{s.}^{(n)\prime}\phi_g^{(n)}(s)\phi_g^{(n)\prime}(s)\mathbf{A}_s^{(n)} + \mathbf{B}_s'\,\phi_f^{(n)}(s)\phi_f^{(n)\prime}(s)\mathbf{B}_s. \\
& + \mathbf{A}_{s.}^{(n)\prime}\phi_g^{(n)}(s)\phi_f^{(n)\prime}(s)\mathbf{B}_s' + \mathbf{B}_s'\,\phi_f^{(n)}(s)\phi_g^{(n)\prime}(s)\mathbf{A}_s^{(n)}\Big\} .
\end{aligned}
$$

From Lemma 4.12 in Garel and Hallin (1995), for fixed s, we have that

$$
\left\{ \left(r - \left\lceil\frac{1-s+1}{d}\right\rceil\right)^{1/2} \mathrm{vec}(\Gamma_{s,1,g}^{(n)}), \dots, \left(r - \left\lceil\frac{l-s+1}{d}\right\rceil\right)^{1/2} \mathrm{vec}(\Gamma_{s,l,g}^{(n)}) \right\}
$$

is asymptotically multinormal under $\mathcal{H}_g^{(n)}(\boldsymbol{\Theta})$, with mean $\mathbf{0}$ and covariance matrix

$$
\begin{pmatrix}
\boldsymbol{\Sigma} \otimes \mathcal{I}(g) & & \mathbf{0} \\
& \ddots & \\
\mathbf{0} & & \boldsymbol{\Sigma} \otimes \mathcal{I}(g)
\end{pmatrix}.
$$

Putting $\mathbf{V}_1 := \mathrm{E}\left[\boldsymbol{\phi}_g^{(n)}(s)\boldsymbol{\phi}_g^{(n)\prime}(s)\right]$, we have

$$
\mathbf{V}_1(i, i') = d^{-1} \sum_{j=\max(i,i')}^{\infty} \left(\mathbf{H}_{j-i} \otimes \mathbf{I}_{(m \times m)}\right)\left(\boldsymbol{\Sigma} \otimes \mathcal{I}(g)\right)\left(\mathbf{H}_{j-i'} \otimes \mathbf{I}_{(m \times m)}\right)',
$$

$i, i' = 1, \ldots, n-1$. Using twice the identity $(\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}) = \mathbf{AC} \otimes \mathbf{BD}$, by (14.10), we obtain

$$
\mathbf{V}_1(i, i') = d^{-1}(\boldsymbol{\Gamma}(\boldsymbol{\Theta}))_{i,i'} \otimes \mathcal{I}(g)
$$

and $\mathbf{V}_1 = d^{-1}\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}(g)$. Now,

$$
\mathrm{Var}(c^{(n)}) = \sum_{s=1}^{d}\{\mathbf{A}_s^{(n)\prime}\mathbf{V}_1\mathbf{A}_s^{(n)} + \mathbf{B}_s'\,\mathbf{V}_2\mathbf{B}_s + \mathbf{A}_s^{(n)\prime}\mathbf{V}_{12}\mathbf{B}_s' + \mathbf{B}_s'\,\mathbf{V}_{21}\mathbf{A}_s^{(n)}\}
$$

where, analogously to $\mathbf{V}_1$, we define $\mathbf{V}_2 := d^{-1}\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}_g^{(f)}$ and $\mathbf{V}_{12} = \mathbf{V}_{21}' := d^{-1}\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}_g^{(f,g)}$. Consequently,

$$
\begin{aligned}
\mathrm{Var}(c^{(n)}) \;=\; & \mathbf{A}^{(n)\prime}d^{-1}\left[\mathbf{I}_{(d \times d)} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}(g))\right]\mathbf{A}^{(n)} \\
& +\mathbf{B}'d^{-1}\left[\mathbf{I}_{(d \times d)} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}_g^{f})\right]\mathbf{B} \\
& +\mathbf{A}^{(n)\prime}d^{-1}\left[\mathbf{I}_{(d \times d)} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}_g^{(f,g)})\right]\mathbf{B} \\
& +\mathbf{B}'d^{-1}\left[\mathbf{I}_{(d \times d)} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}_g^{(f,g)})\right]\mathbf{A}^{(n)}.
\end{aligned}
$$

Finally, $c^{(n)}$ is asymptotically multinormal, with mean zero and asymptotic covariance matrix

$$
\begin{aligned}
& \alpha^2\boldsymbol{\tau}^{(n)\prime}d^{-1}\mathbf{K}'\left[\mathbf{I}_{(d \times d)} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}(g))\right]\mathbf{K}\,\boldsymbol{\tau}^{(n)} \\
& +\boldsymbol{\beta}'d^{-1}\mathbf{K}'\left[\mathbf{I}_{(d \times d)} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}_g^{(f,g)})\right]\mathbf{K}\,\boldsymbol{\beta} \\
& +\alpha\,\boldsymbol{\tau}^{(n)\prime}d^{-1}\mathbf{K}'\left[\mathbf{I}_{(d \times d)} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}_g^{(f,g)})\right]\mathbf{K}\,\boldsymbol{\beta} \\
& +\alpha\,\boldsymbol{\beta}'d^{-1}\mathbf{K}'\left[\mathbf{I}_{(d \times d)} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \mathcal{I}_g^{(f,g)})\right]\mathbf{K}\,\boldsymbol{\tau}^{(n)}.
\end{aligned}
$$

Since $(\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}) = (\mathbf{AC}) \otimes (\mathbf{BD})$, by (14.12), we obtain

$$d^{-1}\mathbf{K}' \left[\mathbf{I}_{(d \times d)} \otimes (\mathbf{\Gamma}(\mathbf{\Theta}) \otimes \mathcal{I}_g^{(f,g)}) \right] \mathbf{K}$$
$$= \mathbf{\Gamma}_f^{\Delta}(\mathbf{\Theta}) \, \mathbf{K}^{-1} \left[\mathbf{I}_{(dpm \times dpm)} \otimes \{ (\mathcal{I}(f))^{-1} \mathcal{I}_g^{(f,g)} \} \right] \mathbf{K}.$$

Now, $c^{(n)}$ can be written as $(\boldsymbol{\beta}' \; \alpha) \begin{pmatrix} \mathbf{\Delta}_f^{(n)} \\ \Lambda_g^{(n)} \end{pmatrix}$. Hence, under $\mathcal{H}_g^{(n)}(\mathbf{\Theta})$,

$$\left(\mathbf{\Delta}_f^{(n)}, \Lambda_g^{(n)} \right)' \overset{\mathcal{L}}{\longrightarrow} \mathcal{N} \left((0, -\frac{1}{2} v_g^2)', \mathbf{\Gamma}^{\Delta, \Lambda} \right),$$

where

$$\mathbf{\Gamma}^{\Delta, \Lambda} := \begin{pmatrix} \mathbf{\Gamma}_{I,I}^{\Delta, \Lambda} & \mathbf{\Gamma}_{I,II}^{\Delta, \Lambda} \\ \mathbf{\Gamma}_{II,I}^{\Delta, \Lambda} & \mathbf{\Gamma}_{II,II}^{\Delta, \Lambda} \end{pmatrix}$$

with

$$\mathbf{\Gamma}_{I,I}^{\Delta, \Lambda} := \mathbf{\Gamma}_f^{\Delta}(\mathbf{\Theta}) \mathbf{K}^{-1} \left[\mathbf{I}_{dpm} \otimes \{ (\mathcal{I}(f))^{-1} \mathcal{I}_g^{(f,g)} \} \right] \mathbf{K},$$

$$\mathbf{\Gamma}_{I,II}^{\Delta, \Lambda} = \left(\mathbf{\Gamma}_{I,II}^{\Delta, \Lambda} \right)' := \mathbf{\Gamma}_f^{\Delta}(\mathbf{\Theta}) \mathbf{K}^{-1} \left[\mathbf{I}_{dpm} \otimes \{ (\mathcal{I}(f))^{-1} \mathcal{I}_g^{(f,g)} \} \right] \mathbf{K} \boldsymbol{\tau}^{(n)},$$

and $\mathbf{\Gamma}_{II,II}^{\Delta, \Lambda} := v_g^2$. Part (ii) of the proposition then readily follows from Le Cam's Third Lemma. □

5. Local asymptotic linearity

Asymptotic linearity allows for controlling the effects of substituting estimated residuals for the exact ones in the central sequence $\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta})$ under innovation density g.

PROPOSITION 14.3 *Let f satisfy* (A.2) *and* (A.3), *and let $g \in \mathcal{G}_f$. Then, for all sequences $\boldsymbol{\tau}^{(n)}$ such that $\sup_n \boldsymbol{\tau}^{(n)\prime} \boldsymbol{\tau}^{(n)} < \infty$ as $n \to \infty$,*

$$\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta}^{(n)}) - \mathbf{\Delta}_f^{(n)}(\mathbf{\Theta})$$
$$+ \mathbf{\Gamma}_f^{\Delta}(\mathbf{\Theta}) \mathbf{K}^{-1} \left[\mathbf{I}_{(dpm \times dpm)} \otimes \{ (\mathcal{I}(f))^{-1} \mathcal{I}_g^{(f,g)} \} \right] \mathbf{K} \boldsymbol{\tau}^{(n)} = o_p(1),$$

under $\mathcal{H}_g^{(n)}(\mathbf{\Theta})$ as well as under $\mathcal{H}_g^{(n)}(\mathbf{\Theta}^{(n)})$.

The proof of Proposition 14.3 relies on the following lemma.

LEMMA 14.1 *Under the assumptions of Proposition 14.3,*

$$\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta}^{(n)}) - \left(\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta}) - \mathrm{E}_{\mathbf{\Theta}^{(n)}} \left[\mathbf{\Delta}_f^{(n)}(\mathbf{\Theta}) \right] \right) = o_p(1) \quad \text{as } n \to \infty \quad (14.15)$$

under $\mathcal{H}_g^{(n)}(\boldsymbol{\Theta})$ as well as under $\mathcal{H}_g^{(n)}(\boldsymbol{\Theta}^{(n)})$.

Proof. Since central sequences are linear combinations of residual f-cross-covariance matrices, it is sufficient to show that (writing $\mathrm{E}_{\boldsymbol{\Theta}^{(n)}}[\ldots]$ for expectations under $\mathcal{H}_g^{(n)}(\boldsymbol{\Theta}^{(n)})$)

$$n^{1/2}\left(\mathrm{vec}\,\boldsymbol{\Gamma}_{s,k,f}^{(n)}(\boldsymbol{\Theta}^{(n)}) - \mathrm{vec}\,\boldsymbol{\Gamma}_{s,k,f}^{(n)}(\boldsymbol{\Theta})\right) + \mathrm{E}_{\boldsymbol{\Theta}^{(n)}}\left(\mathrm{vec}\,\boldsymbol{\Gamma}_{s,k,f}^{(n)}(\boldsymbol{\Theta})\right) = o_p(1) \tag{14.16}$$

under $\mathcal{H}_g^{(n)}(\boldsymbol{\Theta}^{(n)})$, for $s = 1,\ldots,d$ and $k = 1,\ldots,n-1$.

Write $\mathbf{Z}_t^0$ for $\mathbf{Z}_t^{(n)}(\boldsymbol{\Theta})$ and $\mathbf{Z}_t^{(n)}$ for $\mathbf{Z}_t^{(n)}(\boldsymbol{\Theta}^{(n)})$. Since $\mathbf{Z}_t^{(n)}$ under $\mathcal{H}_g^{(n)}(\boldsymbol{\Theta}^{(n)})$ coincides with $\boldsymbol{\varepsilon}_t$, it is independent from $\mathbf{Z}_{t-k}^{(n)}$ and $\mathbf{Z}_{t-k}^0$ for all $k > 0$, and $\mathrm{E}_{\boldsymbol{\Theta}^{(n)}}\left[\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{(n)})\mathbf{Z}_{dt^*+s-k}^{0\prime}\right] = \mathbf{0}$. Therefore, the left-hand side of (14.16) decomposes into $\mathbf{T}_1^{(n)} + \mathbf{T}_2^{(n)} - \mathrm{E}_{\boldsymbol{\Theta}^{(n)}}\left(\mathbf{T}_2^{(n)}\right)$, where

$$\mathbf{T}_1^{(n)} := r^{-1/2} \sum_{t^* = \lceil \frac{k-s+1}{d}\rceil}^{r-1} \mathrm{vec}\left(\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{(n)})\left[\mathbf{Z}_{dt^*+s-k}^{(n)} - \mathbf{Z}_{dt^*+s-k}^0\right]'\right)$$

and

$$\mathbf{T}_2^{(n)} := r^{-1/2} \sum_{t^* = \lceil \frac{k-s+1}{d}\rceil}^{r-1} \mathrm{vec}\left(\left[\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{(n)}) - \boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^0)\right]\mathbf{Z}_{dt^*+s-k}^{0\prime}\right).$$

Note that $\mathrm{E}_{\boldsymbol{\Theta}^{(n)}}\left[\mathbf{T}_1^{(n)}\right] = \mathbf{0}$. In order to show that $\mathbf{T}_1^{(n)} = o_p(1)$, it is thus sufficient to show that $\mathrm{Var}_{\boldsymbol{\Theta}^{(n)}}\left(\mathbf{T}_1^{(n)}\right) = \mathrm{E}_{\boldsymbol{\Theta}^{(n)}}\left[\mathbf{T}_1^{(n)}\mathbf{T}_1^{(n)\prime}\right]$ tends to zero. Using the fact that $\mathrm{vec}[\mathbf{AB}']\mathrm{vec}[\mathbf{AB}']' = [\mathbf{BB}'] \otimes [\mathbf{AA}']$, we obtain

$$\mathrm{E}_{\boldsymbol{\Theta}^{(n)}}(\mathbf{T}_1^{(n)}\,\mathbf{T}_1^{(n)\prime}) = \frac{r - \lceil \frac{k-s+1}{d}\rceil}{r}$$

$$\times \mathrm{E}_{\boldsymbol{\Theta}^{(n)}}\left[\left(\mathbf{Z}_{dt^*+s-k}^{(n)} - \mathbf{Z}_{dt^*+s-k}^0\right)\left(\mathbf{Z}_{dt^*+s-k}^{(n)} - \mathbf{Z}_{dt^*+s-k}^0\right)'\right] \otimes \mathcal{I}_g^{(f)}.$$

Now,

$$\begin{aligned}
\mathbf{Z}_{dt^*+s}^{(n)} &= \mathbf{X}_{dt^*+s} - \sum_{i=1}^p \boldsymbol{\Theta}_i^{(n)}(s)\mathbf{X}_{dt^*+s-i} \\
&= \mathbf{Z}_{dt^*+s}^0 - n^{-1/2}\sum_{i=1}^p (\boldsymbol{\alpha}_i^{(n)} + \boldsymbol{\beta}_i^{(n)}(s))\mathbf{X}_{dt^*+s-i},
\end{aligned}$$

so that

$$
\mathrm{E}_{\boldsymbol{\Theta}^{(n)}}\left[\left(\mathbf{Z}_{dt^*+s-k}^{(n)}-\mathbf{Z}_{dt^*+s-k}^{0}\right)\left(\mathbf{Z}_{dt^*+s-k}^{(n)}-\mathbf{Z}_{dt^*+s-k}^{0}\right)'\right] \tag{14.17}
$$
$$
= n^{-1}\mathrm{Var}_{\boldsymbol{\Theta}^{(n)}}\left(\sum_{i=1}^{p}(\boldsymbol{\alpha}_i^{(n)}+\boldsymbol{\beta}_i^{(n)}(s))\mathbf{X}_{dt^*+s-i}\right).
$$

The second-order moments (under $\boldsymbol{\Theta}^{(n)}$) of $\{\mathbf{X}_{dt^*+s}\}$ are continuous functions of $\boldsymbol{\Theta}^{(n)}$ converging, as $n \to \infty$, to their values under $\boldsymbol{\Theta}$, and the $\boldsymbol{\alpha}_i$'s and $\boldsymbol{\beta}_i$'s, are uniformly bounded; therefore, the right-hand side of (14.17) tends to zero, as was to be proved.

Turning to $\mathbf{T}_2^{(n)}$, we have

$$
\mathrm{Var}_{\boldsymbol{\Theta}^{(n)}}(\mathbf{T}_2^{(n)}) = \frac{r-\lceil\frac{k-s+1}{d}\rceil}{r}\,\mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(0)
$$
$$
+2\sum_{i=1}^{r-\lceil\frac{k-s+1}{d}\rceil-1}\frac{r-\lceil\frac{k-s+1}{d}\rceil-i}{r}\,\mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(i),
$$

where

$$
\mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(i) \;:=\; \mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}\left(\mathrm{vec}\left[\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{(n)})-\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{0})\right]\mathbf{Z}_{dt^*+s-k}^{0\prime},\right.
$$
$$
\left.\mathrm{vec}\left[\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s-i}^{(n)})-\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s-i}^{0})\right]\mathbf{Z}_{dt^*+s-k-i}^{0\prime}\right).
$$

Now,

$$
\mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(0) = \frac{r-\lceil\frac{k-s+1}{d}\rceil}{r}\mathrm{E}_{\boldsymbol{\Theta}^{(n)}}\left\{\left(\mathbf{Z}_{dt^*+s-k}^{0}\mathbf{Z}_{dt^*+s-k}^{0\prime}\right)\right.
$$
$$
\left.\otimes\left(\left[\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{(n)})-\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{0})\right]\left[\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{(n)})-\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{0})\right]'\right)\right\}.
$$

Using the Lipschitz condition, we obtain that

$$
\mathrm{E}_{\boldsymbol{\Theta}^{(n)}}\left(\left\|\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{(n)})-\boldsymbol{\varphi}(\mathbf{Z}_{dt^*+s}^{0})\right\|^2\right) \le C_f^2\mathrm{E}_{\boldsymbol{\Theta}^{(n)}}\left(\left\|\mathbf{Z}_{dt^*+s}^{(n)}-\mathbf{Z}_{dt^*+s}^{0}\right\|^2\right),
$$
$$
\tag{14.18}
$$

where C_f is the Lipschitz constant in Assumption (A3). The same argument used in proving that $\lim_{n\to\infty}\mathrm{Var}_{\boldsymbol{\Theta}^{(n)}}(\mathbf{T}_1^{(n)}) = 0$ also implies that $\lim_{n\to\infty}\mathrm{E}_{\boldsymbol{\Theta}^{(n)}}\left(\left\|\mathbf{Z}_{dt^*+s}^{(n)}-\mathbf{Z}_{dt^*+s}^{0}\right\|^2\right) = 0$, hence, via a Cauchy-Schwarz argument, that $\lim_{n\to\infty}\mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(0) = \mathbf{0}$.

As for $\mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(i)$, the univariate Lemmas 5.2 and 5.3 of Hallin and Puri (1994) extend to this multivariate context. Under $\mathcal{H}_g^{(n)}(\boldsymbol{\Theta}^{(n)})$,

$\{\mathbf{Z}^0_{dt^*+s} - \mathrm{E}\,\mathbf{Z}^0_{dt^*+s}\}$ is a causal, stationary, invertible ARMA(1,1) process with uniformly (in n) bounded variance. It follows that, under $\mathcal{H}^{(n)}_g(\boldsymbol{\Theta}^{(n)})$, the joint process $\{\mathbf{Z}^0_{dt^*+s}, \mathbf{Z}^{(n)}_{dt^*+s} = \boldsymbol{\varepsilon}_{dt^*+s}\}$ is absolutely regular with the same mixing rates $a_i^{(n)}$ as $\{\mathbf{Z}^0_{dt^*+s}\}$. Yoshihara (1976)'s Lemma 1 then entails that, for any $k, \ell \in \{1, \ldots, m\}$,

$$\left| \left(\mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(i) \right)_{k\ell} \right| \le 4 \max_{k,\ell} \left| \left(\mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(0) \right)_{k\ell} \right| (a_i^{(n)})^{1/2},$$

so that

$$\left| \sum_{i=1}^{r-\lceil \frac{k-s+1}{d} \rceil - 1} \frac{r - \lceil \frac{k-s+1}{d} \rceil - i}{r} \left(\mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(i) \right)_{k\ell} \right|$$

$$\le \sum_{i=1}^{\infty} \left| \left(\mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(i) \right)_{k\ell} \right| \le 4 \left| \left(\mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(0) \right)_{k\ell} \right| \sum_{i=1}^{\infty} (a_i^{(n)})^{1/2}.$$

This and $\lim_{n \to \infty} \mathrm{Cov}_{\boldsymbol{\Theta}^{(n)}}(0) = \mathbf{0}$ implies that $\lim_{n \to \infty} \mathrm{Var}_{\boldsymbol{\Theta}^{(n)}}(\mathbf{T}_2^{(n)}) = \mathbf{0}$, hence that $\mathbf{T}_2^{(n)} - \mathrm{E}_{\boldsymbol{\Theta}^{(n)}}(\mathbf{T}_2^{(n)}) = o_p(1)$, which completes the proof of the lemma.   □

Proof of Proposition 14.3. Letting

$$\boldsymbol{\mu}^{(n)}_{f,g} := \boldsymbol{\Gamma}^{\Delta}_f(\boldsymbol{\Theta}) \mathbf{K}^{-1} \left[\mathbf{I}_{(dpm \times dpm)} \otimes \{ (\mathcal{I}(f))^{-1} \mathcal{I}_g^{(f,g)} \} \right] \mathbf{K} \boldsymbol{\tau}^{(n)},$$

we have, from Lemma 14.1,

$$\boldsymbol{\Delta}^{(n)}_f(\boldsymbol{\Theta}^{(n)}) = \boldsymbol{\Delta}^{(n)}_f(\boldsymbol{\Theta}) - \boldsymbol{\mu}^{(n)}_{f,g} + \left(\boldsymbol{\mu}^{(n)}_{f,g} - \mathrm{E}_{\boldsymbol{\Theta}^{(n)}} \left[\boldsymbol{\Delta}^{(n)}_f(\boldsymbol{\Theta}) \right] \right) + o_p(1)$$

under $\mathcal{H}^{(n)}_g(\boldsymbol{\Theta}^{(n)})$ (hence also under $\mathcal{H}^{(n)}_g(\boldsymbol{\Theta})$). Proposition 14.2 implies that, under $\mathcal{H}^{(n)}_g(\boldsymbol{\Theta}^{(n)})$, $\boldsymbol{\Delta}^{(n)}_f(\boldsymbol{\Theta}^{(n)})$ and $\boldsymbol{\Delta}^{(n)}_f(\boldsymbol{\Theta}) - \boldsymbol{\mu}^{(n)}_{f,g}$ both are asymptotically normal, with mean zero and covariance matrix $\mathbf{V}$, say. The centerings $\boldsymbol{\mu}^{(n)}_{f,g}$ and $\mathrm{E}_{\boldsymbol{\Theta}^{(n)}} \left[\boldsymbol{\Delta}^{(n)}_f(\boldsymbol{\Theta}) \right]$ thus both ensure the asymptotic normality of $\boldsymbol{\Delta}^{(n)}_f(\boldsymbol{\Theta})$ under $\mathcal{H}^{(n)}_g(\boldsymbol{\Theta}^{(n)})$. Hence,

$$\left(\boldsymbol{\mu}^{(n)}_{f,g} - \mathrm{E}_{\boldsymbol{\Theta}^{(n)}} \left[\boldsymbol{\Delta}^{(n)}_f(\boldsymbol{\Theta}) \right] \right) = o(1).$$

The proposition thus follows from (14.15).   □

6. Locally asymptotically most stringent tests

Under LAN, the Le Cam theory allows for constructing locally asymptotically optimal tests for linear restrictions on the parameter $\boldsymbol{\Theta}$. Local asymptotic normality here means local asymptotic *stringency*, under some given innovation density f. The asymptotic linearity property derived in Section 5 under a wide class $\mathcal{G}_f$ of innovation densities, allows for extending the validity of those tests to null hypotheses under which g remains unspecified (within the class $\mathcal{G}_f$ of densities under which asymptotic normality holds), although optimality is achieved at f only (unless estimated scores are considered).

More specifically, denoting by $\mathbf{Q}$ a $(dpm^2 \times \kappa)$ real matrix of full rank pm^2, write $\mathcal{M}(\mathbf{Q})$ for the intersection between the κ-dimensional linear subspace of $\mathbb{R}^{dpm^2}$ spanned by the columns of $\mathbf{Q}$ and the set of all $\boldsymbol{\Theta}$'s such that the corresponding VAR(p) model is a stationary one. The (sequences of) linear null hypotheses and alternatives we are considering are of the form

$$\mathcal{H}^{(n)} := \bigcup_{g \in \mathcal{G}_f} \mathcal{H}_{g;\mathbf{Q}}^{(n)} := \bigcup_{g \in \mathcal{G}_f} \bigcup_{\boldsymbol{\Theta} \in \mathcal{M}(\mathbf{KQ})} \mathcal{H}_g^{(n)}(\boldsymbol{\Theta}) \qquad (14.19)$$

and

$$\mathcal{K}^{(n)} := \bigcup_{g \in \mathcal{G}_f} \bigcup_{\boldsymbol{\Theta} \notin \mathcal{M}(\mathbf{KQ})} \mathcal{H}_g^{(n)}(\boldsymbol{\Theta}) \qquad (14.20)$$

respectively, but optimality will be achieved, asymptotically, at local alternatives of the form

$$\mathcal{K}_f^{(n)} := \bigcup_{\boldsymbol{\Theta} \in \mathcal{M}(\mathbf{KQ})} \bigcup_{\boldsymbol{\tau}^{(n)} \notin \mathcal{M}(\mathbf{Q})} \mathcal{H}_f^{(n)}(\boldsymbol{\Theta} + n^{-1/2}\mathbf{K}\boldsymbol{\tau}^{(n)}) \qquad (14.21)$$

(see (14.4) and (14.14) for the notation), where f is some fixed density.

In the particular problem of testing stationary VAR(p) dependence against periodic PVAR(p) alternatives, the matrix $\mathbf{Q}$ takes the very simple form $\mathbf{Q} = \begin{pmatrix} \mathbf{I} \\ \mathbf{0} \end{pmatrix}$, where $\mathbf{I}$ is the pm^2-dimensional unit matrix (i.e., $\kappa = pm^2$). A locally asymptotically most stringent test for $\mathcal{H}_f^{(n)}(\boldsymbol{\Theta})$ against $\bigcup_{\boldsymbol{\tau}^{(n)} \notin \mathcal{M}(\mathbf{Q})} \mathcal{H}_f^{(n)}(\boldsymbol{\Theta} + n^{-1/2}\mathbf{K}\boldsymbol{\tau}^{(n)})$ (for fixed $\boldsymbol{\Theta}$ and f) is obtained by substituting the central sequence $\boldsymbol{\Delta}_f^{(n)}(\boldsymbol{\Theta})$ into the (exactly) most stringent test for $\boldsymbol{\tau} = \mathbf{0}$ against $\boldsymbol{\tau} \notin \mathcal{M}(\mathbf{Q})$ in the Gaussian shift experiment

$$\mathcal{E}_{f,\boldsymbol{\Theta}} := \left\{ \mathcal{N}\left(\boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta})\boldsymbol{\tau}, \boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta})\right) \Big| \boldsymbol{\tau} \in \mathbb{R}^{dmp^2} \right\}$$

(let $\boldsymbol{\Delta}$ denote the observation from that experiment). This test consists in rejecting the null hypothesis $(\boldsymbol{\tau} = \mathbf{0})$ whenever the quadratic form

$$Q_f(\boldsymbol{\Delta}) := \boldsymbol{\Delta}' \left(\boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta}) \right)^{-1/2} \tag{14.22}$$
$$\times \left[\mathbf{I} - \left(\boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta}) \right)^{1/2} \mathbf{Q} \left(\mathbf{Q}' \left(\boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta}) \right) \mathbf{Q} \right)^{-1} \mathbf{Q}' \left(\boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta}) \right)^{1/2} \right]$$
$$\times \left(\boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta}) \right)^{-1/2} \boldsymbol{\Delta}$$

exceeds the $(1 - \alpha)$ quantile $\chi^2_{dpm^2 - \kappa, 1 - \alpha}$ of a chi-square variable with $(dpm^2 - \kappa)$ degrees of freedom (see, e.g., Le Cam (1986), Chapter 10).

Partitioning $\boldsymbol{\Delta}$ and $\boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta})$ into

$$\boldsymbol{\Delta} := \begin{pmatrix} \boldsymbol{\Delta}_I \\ \boldsymbol{\Delta}_{II} \end{pmatrix} \quad \text{and} \quad \boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta}) := \begin{pmatrix} \boldsymbol{\Gamma}_{f;I}^{\Delta} & \boldsymbol{\Gamma}_{f;I,II}^{\Delta} \\ \boldsymbol{\Gamma}_{f,I,II}^{\Delta} & \boldsymbol{\Gamma}_{f;II}^{\Delta} \end{pmatrix},$$

respectively, where $\boldsymbol{\Delta}_I$ is a (pm^2)-vector, and $\boldsymbol{\Gamma}_{f;I}^{\Delta}$ a $(pm^2) \times (pm^2)$-matrix, the test statistic (14.22), in the particular case under study, due to the fact that $\boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta})$ has the block diagonal form

$$\boldsymbol{\Gamma}_f^{\Delta}(\boldsymbol{\Theta}) = d^{-1} \begin{pmatrix} d & 0 & 0 & \dots & 0 \\ 0 & 2 & 1 & \dots & 1 \\ 0 & 1 & & \ddots & \vdots \\ \vdots & \vdots & \ddots & & 1 \\ 0 & 1 & \dots & 1 & 2 \end{pmatrix} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \boldsymbol{\mathcal{I}}(f))$$

$$= \begin{pmatrix} \boldsymbol{\Gamma}_{f;I}^{\Delta}(\boldsymbol{\Theta}) & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Gamma}_{f;II}^{\Delta}(\boldsymbol{\Theta}) \end{pmatrix},$$

simplifies into $Q_f(\boldsymbol{\Delta}) = \boldsymbol{\Delta}'_{II} \left(\boldsymbol{\Gamma}_{f,II}^{\Delta} \right)^{-1} \boldsymbol{\Delta}_{II}$, with critical $(1 - \alpha)$ value $\chi^2_{(d-1)pm^2; 1 - \alpha}$. A locally asymptotically most stringent test for $\mathcal{H}_f^{(n)}(\boldsymbol{\Theta})$ thus can be based on

$$Q_f(\boldsymbol{\Delta}_f^{(n)}(\boldsymbol{\Theta})) = \boldsymbol{\Delta}_{f;II}^{(n)}(\boldsymbol{\Theta})' \left(\boldsymbol{\Gamma}_{f;II}^{\Delta} \right)^{-1} \boldsymbol{\Delta}_{f,II}. \tag{14.23}$$

The problem with (14.23) is that the test statistic $Q_f(\boldsymbol{\Delta}_f^{(n)}(\boldsymbol{\Theta}))$ still depends on $\boldsymbol{\Theta}$, and that its asymptotic chi square null distribution only holds under density f. In order to palliate this, unknown quantities are to be replaced with adequate estimators. Assume that

(A4) A sequence of estimators $\widehat{\boldsymbol{\Theta}}^{(n)}$ exists, such that

(i) $\widehat{\Theta}^{(n)}$ under any $\mathcal{H}_g^{(n)}(\Theta)$ a.s. takes values in $\mathcal{M}(\mathbf{KQ})$, that is, $\widehat{\Theta}^{(n)}$ is a vector of the form $\mathbf{1} \otimes ([\mathrm{vec}\widehat{\Theta}_1^{(n)}]', \ldots, [\mathrm{vec}\widehat{\Theta}_p^{(n)}]')'$;

(ii) $n^{1/2}\left(\widehat{\Theta}^{(n)} - \Theta\right)$ is $O_p(1)$ under $\bigcup_{\Theta \in \mathcal{M}(\mathbf{KQ})} \mathcal{H}_g^{(n)}(\Theta)$

(iii) $\widehat{\Theta}^{(n)}$ is *locally asymptotically discrete*; that is, the number of possible values of $\widehat{\Theta}^{(n)}$ in balls of the form ($\| . \|$ stands for the Euclidean norm) $\left\{\mathbf{t} \in \mathbb{R}^{dpm^2} : n^{1/2}\|\mathbf{K}^{-1}(\mathbf{t} - \Theta)\| \le b\right\}$ remains bounded, as $n \to \infty$, for any Θ and $b > 0$.

Similarly, denote by $\widehat{\mathbf{\Gamma}}_{f,II}^{\Delta}(\Theta)$ the matrix obtained from $\mathbf{\Gamma}_{f;II}^{\Delta}(\Theta)$ by replacing $\mathcal{I}(f)$ with its empirical counterpart

$$\mathcal{I}^{(n)}(f) := n^{-1}\sum_{t=1}^{n}\varphi_f(\mathbf{Z}_t(\Theta))\varphi_f(\mathbf{Z}_t(\Theta))'.$$

The test we are proposing consists in rejecting the null hypothesis $\mathcal{H}^{(n)}$ of stationary VAR(p) dependence with unspecified innovation density g whenever the quadratic form

$$Q_f^{(n)} := \mathbf{\Delta}_{f,II}^{(n)'}(\widehat{\Theta}^{(n)})\left(\widehat{\mathbf{\Gamma}}_{f;II}^{\Delta}(\widehat{\Theta}^{(n)})\right)^{-1}\mathbf{\Delta}_{f,II}^{(n)}(\widehat{\Theta}^{(n)}) \tag{14.24}$$

exceeds the critical value $\chi^2_{(d-1)pm^2;1-\alpha}$. The properties of this test are summarized in the following proposition.

PROPOSITION 14.4 *Let f satisfy (A.2)-(A.3), and denote by $\widehat{\Theta}^{(n)}$ an estimator of Θ satisfying (A.4). Then, (see (14.19) and (14.21) for the definitions of $\mathcal{H}^{(n)}$ and $\mathcal{K}_f^{(n)}$, respectively)*

(i) *the test statistic (14.24) is asymptotically central chi-square with $(d-1)pm^2$ degrees of freedom under $\mathcal{H}^{(n)}$, and noncentral chi-square, still with $(d-1)pm^2$ degrees of freedom, but noncentrality parameter*

$$\delta := \beta'\mathbf{K}^{-1}\left[\mathbf{I}_{(dpm \times dpm)} \otimes \{(\mathcal{I}(f))^{-1}\mathcal{I}_g^{(f,g)}\}\right]'\mathbf{K}\mathbf{\Gamma}_{f;II}^{\Delta}(\Theta)\mathbf{K}^{-1}$$
$$\times \left[\mathbf{I}_{(dpm \times dpm)} \otimes \{(\mathcal{I}(f))^{-1}\mathcal{I}_g^{(f,g)}\}\right]\mathbf{K}\beta$$

under $\mathcal{H}_g^{(n)}(\Theta^{(n)})$ $g \in \mathcal{G}_f$, reducing to $\delta = \beta'\mathbf{\Gamma}_{f,II}^{\Delta}(\Theta)\beta$ under $g = f$;

(ii) accordingly, the test described in (14.24) has asymptotic level α under $\mathcal{H}^{(n)}$, and local asymptotic power $1 - F^{\chi}_{(d-1)pm^2}(\chi^2_{(d-1)pm^2;1-\alpha}; \delta)$ against $\mathcal{H}^{(n)}_g(\boldsymbol{\Theta}^{(n)})$, $g \in \mathcal{G}_f$ and $\boldsymbol{\Theta}^{(n)} = \boldsymbol{\Theta} + n^{-1/2}\mathbf{K}(\mathbf{0}, \boldsymbol{\beta}')'$, where $F^{\chi}_{(d-1)pm^2}(.\,; \delta)$ stands for the noncentral chi-square distribution function with $(d-1)pm^2$ degrees of freedom and noncentrality parameter δ;

(iii) is locally asymptotically most stringent against $\mathcal{K}^{(n)}_f$ within the class of tests having asymptotic level α under $\mathcal{H}^{(n)}$.

Proof. The convergence, under $\bigcup_{g \in \mathcal{G}_f} \mathcal{H}^{(n)}_g(\boldsymbol{\Theta})$, of $\boldsymbol{\mathcal{I}}^{(n)}(f)$ to $\boldsymbol{\mathcal{I}}(f)$ implies that

$$\left[\left(\widehat{\boldsymbol{\Gamma}}^{\Delta}_{f,II}(\boldsymbol{\Theta}) \right)^{-1/2} - \left(\boldsymbol{\Gamma}^{\Delta}_{f;II}(\boldsymbol{\Theta}) \right)^{-1/2} \right] \boldsymbol{\Delta}^{(n)}_{f;II}(\boldsymbol{\Theta}) = o_p(1).$$

Similarly, due to the continuity of $\boldsymbol{\Theta} \mapsto \boldsymbol{\Gamma}^{\Delta}_{f;II}(\boldsymbol{\Theta})$,

$$\left[\left(\boldsymbol{\Gamma}^{\Delta}_{f;II}(\widehat{\boldsymbol{\Theta}}^{(n)}) \right)^{-1/2} - \left(\boldsymbol{\Gamma}^{\Delta}_{f,II}(\boldsymbol{\Theta}) \right)^{-1/2} \right] \boldsymbol{\Delta}^{(n)}_{f;II}(\boldsymbol{\Theta}) = o_p(1).$$

Consequently,

$$Q^{(n)}_f = Q_f(\boldsymbol{\Delta}^{(n)}_f(\boldsymbol{\Theta})) + \left\| \left(\boldsymbol{\Gamma}^{\Delta}_{f,II}(\boldsymbol{\Theta}) \right)^{-1/2} \left(\boldsymbol{\Delta}^{(n)}_{f,II}(\widehat{\boldsymbol{\Theta}}^{(n)}) - \boldsymbol{\Delta}^{(n)}_f(\boldsymbol{\Theta}) \right) \right\|^2 + o_p(1).$$

Part (i) of Assumption (A.4), the asymptotic linearity property of $\boldsymbol{\Delta}^{(n)}_f(\widehat{\boldsymbol{\Theta}}^{(n)})$ (Proposition 14.3), and Lemma 4.4 of Kreiss (1987) (the latter allowing, under (A.4), for substituting the random perturbation $n^{1/2}(\widehat{\boldsymbol{\Theta}}^{(n)} - \boldsymbol{\Theta})$ for the deterministic one $\mathbf{K}\boldsymbol{\tau}$) imply that

$$\boldsymbol{\Delta}^{(n)}_f(\widehat{\boldsymbol{\Theta}}^{(n)}) - \boldsymbol{\Delta}^{(n)}_f(\boldsymbol{\Theta})$$
$$= n^{1/2}d^{-1}\mathbf{K}' \left[\mathbf{I}_{(d \times d)} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \boldsymbol{\mathcal{I}}^{(f,g)}_g) \right] \left(\widehat{\boldsymbol{\Theta}}^{(n)} - \boldsymbol{\Theta} \right) + o_p(1)$$
$$= n^{1/2}d^{-1}\mathbf{K}' \left[\mathbf{I}_{(d \times d)} \otimes (\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \boldsymbol{\mathcal{I}}^{(f,g)}_g) \right]$$
$$\quad \times \left[\mathbf{1} \otimes \left((\mathrm{vec}\,\widehat{\boldsymbol{\Theta}}^{(n)}_1)' - (\mathrm{vec}\,\boldsymbol{\Theta}_1)', \dots, (\mathrm{vec}\,\widehat{\boldsymbol{\Theta}}^{(n)}_p)' - (\mathrm{vec}\,\boldsymbol{\Theta}_p)' \right)' \right] + o_p(1)$$
$$= n^{1/2}d^{-1}\mathbf{K}' \left[\mathbf{1} \otimes \left\{ \left(\boldsymbol{\Gamma}(\boldsymbol{\Theta}) \otimes \boldsymbol{\mathcal{I}}^{(f,g)}_g \right) \begin{pmatrix} \mathrm{vec}\widehat{\boldsymbol{\Theta}}^{(n)}_1 - \mathrm{vec}\boldsymbol{\Theta}_1 \\ \vdots \\ \mathrm{vec}\widehat{\boldsymbol{\Theta}}^{(n)}_p - \mathrm{vec}\boldsymbol{\Theta}_p \end{pmatrix} \right\} \right] + o_p(1).$$

In view of (14.7), $[\mathbf{K}'\{1 \otimes \mathbf{v}\}]_i = 0$, $i = pm^2 + 1, \dots, dpm^2$, for all $\mathbf{v} \in \mathbb{R}^{pm^2}$. Hence,

$$Q_f^{(n)} - Q_f(\boldsymbol{\Delta}_f^{(n)}(\boldsymbol{\Theta})) = o_p(1) \quad \text{as } n \to \infty \text{ under } \mathcal{H}^{(n)}.$$

This implies that $Q_f^{(n)}$ inherits, under the null $\mathcal{H}^{(n)}$ and under local alternatives, all the asymptotic distributional properties of $Q_f(\boldsymbol{\Delta}_f^{(n)}(\boldsymbol{\Theta}))$; parts (i) and (ii) of the proposition follow. It also implies that $Q_f^{(n)}$ inherits, under the local alternatives in $\mathcal{K}_f^{(n)}$, all the optimality features (stringency) of $Q_f(\boldsymbol{\Delta}_f^{(n)}(\boldsymbol{\Theta}))$; part (iii) of the proposition follows. $\square$

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Chapter 15

THE WILCOXON SIGNED-RANK TEST FOR CLUSTER CORRELATED DATA

Denis Larocque

Abstract   In this paper, we adapt the Wilcoxon signed-rank test to the case of cluster correlated data. A simple modification of the estimator of the asymptotic variance is sufficient to obtain a valid asymptotic procedure. However, the resulting test is no longer distribution-free. We derive the asymptotic null distribution of the statistic. A simulation study is performed in order to investigate the finite sample performance of the test. The results show that the performance of the test is very good for all designs and distributions considered when compared to competitors based on signs and on the overall average. In fact, the test is as powerful as the one based on the overall average for normal data as soon as intra-cluster correlation is present. An example of application with a real data set is also given.

1.   Introduction and motivating example

A lot of research about models involving correlated observations has been done in the last twenty years. The ever growing computing power and the development of efficient algorithms now make possible the computations required for models with complicated correlation structures. Cluster correlated data appear often in practice. This type of correlation may arise for example with family data where members of the same family may form a cluster. Goldstein (1995) gives numerous examples where this structure appears naturally and Aerts et al. (2002) provides an overview of existing methods for continuous and discrete outcomes. Typically, it is assumed that observations from a given cluster are possibly correlated while observations from different clusters are independent.

The following motivating example involving real data will be treated in the last section of the paper. These data come from the ongoing "Québec longitudinal study on child and adolescent development" by

the Research Unit on Children's Psycho-Social Maladjustment. For this study, a sample of children attending kindergarten in public schools in 1986-1987 in the province of Québec in Canada was selected and is followed since then. More details about the data are given in Pagani et al. (1997) and Zoccolillo, Tremblay and Vitaro (1996).

For our example, three scales constructed using questionnaires that were sent to the children's teachers at the start of the study in 1986 and one year later when the children were in grade one will be used: a disruptive behavior scale, an anxiety scale and a prosocial behavior scale. For illustration, our goal will be to see if the transition from kindergarten to grade one has an effect on those variables. We will limit this analysis to children that attended the same school for both grades. Data are available for 2837 children coming from 336 different schools. Moreover, between 1 and 78 children were in each school, the average number being 8.44 children per school. In addition to demographics considerations, the fact that the scales were constructed using a questionnaire completed by the teachers themselves makes it reasonable to allow the possibility that measures from children from a given school are correlated, that is, it is reasonable to consider each school as a cluster. For a given scale, define X_{ij} to be the difference between the grade one and kindergarten scores for the jth children in the ith school. One possible model for those differences is

$$X_{ij} = \mu + a_i + \epsilon_{ij}, \quad i = 1, \ldots, n \quad ; \quad j = 1, \ldots, m_i, \qquad (15.1)$$

where n is the number of schools (clusters), $m_1, \ldots, m_n$ are the number of children in each schools (cluster sizes), μ is a fixed location parameter, the a_i's are independently and identically (iid) distributed random school effects and the ϵ_{ij}'s are iid (and independent of the a_i's) individual (at the children level) error terms. If we assume that the a_i's and the ϵ_{ij}'s are normally distributed, this model is simply the usual one-way random effect model. This is an example of a pretest posttest (before-after) design with cluster correlated data.

In this paper we are interested in testing the hypothesis that the location parameter μ is 0. In the example above, this amounts to testing if there is a difference between the kindergarten and grade one scores. We will come back to this example in Section 4.

The multivariate version of this problem is considered in Larocque (2003) where an affine-invariant multivariate sign test is proposed. In a related problem, Rosner and Grove (1999) proposed a modification of the Mann-Whitney rank test for the two-sample problem with clustered data.

In this paper, we propose a simple modification of the Wilcoxon signed-rank test to handle the case of clustered data. The test statistic and some of its properties are described in Section 2. The results of a simulation study are reported in Section 3. In Section 4, we come back to the motivating example and give some concluding remarks. All the proofs are sketched in the Appendix.

2. Test statistic and properties

To begin, consider the usual one-sample location problem. That is, suppose that we have n independent observations $X_1, \ldots, X_n$ from a symmetric distribution around μ and that we wish to test

$$H_0 : \mu = 0 \quad \text{and} \quad H_1 : \mu \neq 0. \tag{15.2}$$

The Wilcoxon signed-rank test is based on the statistic

$$WSR = \sum_{i=1}^{n} s(X_i) R_i^+ \tag{15.3}$$

where s is the sign function defined by $s(u) = 1$, 0 or -1 as u is greater, equal or less than 0 and where R_i^+ is the rank of $|X_i|$ among $|X_1|, \ldots, |X_n|$. If we assume that the distribution of the observations is continuous, so there are no tied values and no observation equal to 0, then $E(WSR) = 0$ and $\text{Var}(WSR) = n(n+1)(2n+1)/6$ under H_0. The variance of WSR does not depend on the underlying distribution and even more, the statistic WSR is distribution-free. This allows the possibility to compute exact p-values for any sample size. For larger sample sizes, p-values can be computed by using the fact that $WSR/(\text{Var}(WSR))^{1/2}$ converges to the standard normal distribution under H_0.

Now, consider the case of clustered data. Consider a sample of observations arising from n clusters of respective size $m_1, \ldots, m_n$. Suppose that the observations from the same cluster are not necessarily independent while observations from different clusters are independent. More precisely, assume the following model

$$X_{ij} = \mu + \epsilon_{ij}, \quad i = 1, \ldots, n \quad ; \quad j = 1, \ldots, m_i, \tag{15.4}$$

where μ is a fixed location parameter and where ϵ_{ij} and ϵ_{kl} are independent if $i \neq k$ and possibly dependent if $i = k$. That is, the observations are possibly correlated within clusters. Furthermore, assume that $(\epsilon_{ip(1)}, \ldots, \epsilon_{ip(j)})$ and $(\epsilon_{kq(1)}, \ldots, \epsilon_{kq(j)})$ are identically distributed for any $i, k = 1, \ldots, n$ and $j \leq \min(m_i, m_k)$ where $(p(1), \ldots, p(j))$ and $(q(1), \ldots, q(j))$ are sets of j indices chosen in $\{1, \ldots, m_i\}$ and $\{1, \ldots, m_k\}$

respectively. Finally, assume that the distribution of ϵ_{ij} is symmetric around 0. Under these assumptions, we wish to confront the hypotheses (15.2). Define $N = m_1 + \ldots + m_n$ to be the total number of observations. Note that the one-way random effect model (15.1) is a special case of (15.4).

Larocque (2003) considered the multivariate version of this model and proposed an affine-invariant multivariate sign statistic to test the location vector. For univariate data, his test statistic is equivalent to

$$S_N = \sqrt{N} \frac{\bar{S}}{\hat{\sigma}_S} \qquad (15.5)$$

where

$$\bar{S} = \frac{1}{N} \sum_{i=1}^{n} \sum_{j=1}^{m_i} s(X_{ij})$$

is the average of the signs of all observations and where

$$\hat{\sigma}_S^2 = \frac{1}{N} \sum_{i=1}^{n} \left(\sum_{j=1}^{m_i} s(X_{ij}) \right)^2.$$

As showed in Larocque (2003), the quantity $\hat{\sigma}_S^2$ is a consistent estimator of the asymptotic variance of $\sqrt{N}\bar{S}$ under H_0 for the cluster correlated data model. Unlike the ordinary sign statistic in the case of independent observations, this statistic is not distribution-free under H_0 because of the clustered structure. However, its asymptotic distribution (as the number of clusters goes to infinity) is given in Larocque (2003). Specifically, under H_0, suppose that $(\sum_{i=1}^{n} m_i^2)/(\sum_{i=1}^{n} m_i)$ converges to a finite number, then S_N converges to the standard normal distribution as $n \to \infty$. Consequently, in the case of the sign test, it is sufficient to incorporate a consistent estimator of the correct asymptotic variance in order to adapt it to the cluster correlation structure. The same is true for the Wilcoxon signed-rank test.

Define

$$\bar{W} = \frac{1}{N} \sum_{i=1}^{n} \sum_{j=1}^{m_i} s(X_{ij}) \left(\frac{R_{ij}^+}{N+1} \right)$$

where R_{ij}^+ is the rank of $|X_{ij}|$ among $|X_{11}|, |X_{12}|, \ldots, |X_{1m_1}|, \ldots, |X_{n1}|, |X_{n2}|, \ldots, |X_{nm_n}|$. The statistic $\bar{W}$ is just the Wilcoxon signed-rank statistic computed with all the observations. The asymptotic null variance of $\bar{W}$ will be estimated by

$$\hat{\sigma}_W^2 = \frac{1}{N} \sum_{i=1}^{n} \left(\sum_{j=1}^{m_i} s(X_{ij}) \left(\frac{R_{ij}^+}{N+1} \right) \right)^2. \tag{15.6}$$

The proposed Wilcoxon signed-rank statistic for cluster correlated data is then defined as

$$W_N = \sqrt{N} \frac{\bar{W}}{\hat{\sigma}_W}.$$

The statistic W_N is not distribution-free under H_0. However, a test can be based on its asymptotic null distribution as the number of clusters goes to infinity. The proof of the next result is given in the Appendix.

THEOREM 15.1 *Assume that the structure of the observations is given by (15.4) and that their joint distribution is continuous. Further, suppose that $(\sum_{i=1}^{n} m_i^2)/(\sum_{i=1}^{n} m_i)$ converges to a finite number when $n \to \infty$. Then, under H_0,*

$$W_N \xrightarrow{D} N(0,1)$$

as $n \to \infty$.

3. Simulation study

In this section, the performance of six tests are compared. The first three are valid for cluster correlated data. They are the test W_N proposed in this paper, the sign test of Larocque (2003) based on (15.5) and a test based on the overall average which is obtained by replacing the signs $s(X_{ij})$ by the observations themselves, X_{ij}, in (15.5). Namely, this test is based on

$$M_N = \sqrt{N} \frac{\bar{M}}{\hat{\sigma}_M}$$

where

$$\bar{M} = \frac{1}{N} \sum_{i=1}^{n} \sum_{j=1}^{m_i} X_{ij}$$

is the overall average of all observations and where

$$\hat{\sigma}_M^2 = \frac{1}{N} \sum_{i=1}^{n} \left(\sum_{j=1}^{m_i} X_{ij} \right)^2.$$

The other three tests are the usual version of the first three for independent and identically distributed data (no cluster correlation). Namely, they are the Wilcoxon signed-rank test given in (15.3), the sign test and the t-test. Even thought those tests are not valid for clustered data,

they are included in the simulation in order to see how they compare
to their cluster correlated data versions when there is no intra-cluster
correlation. The critical point from the asymptotic $N(0, 1)$ distribution
is used to perform all tests except for the t-test where the critical point
from the F distribution is used.

Three designs are used:

- *Design 1:* 15 clusters of 2 observations for a total of 30 observations.

- *Design 2:* 5 clusters of 2 observations, 5 clusters of 5 observations
  and 5 clusters of 8 observations for a total of 75 observations and
  15 clusters.

- *Design 3:* 3 clusters of 2 observations, 3 clusters of 5 observations,
  3 clusters of 8 observations, 3 clusters of 11 observations and 3
  clusters of 14 observations for a total of 120 observations and 15
  clusters.

The data are generated through the one-way random effect model
(15.1). Six choices of distributions are used. The first two produces iid
observations and the last four produces data with intra-cluster correlation.

- *normal:* The ϵ_{ij}'s are iid $N(0, 1)$ and the a_i's are not used.

- *t_3:* The ϵ_{ij}'s are iid from the t_3 (Student with 3 df) distribution
  and the a_i's are not used.

- *normal-normal:* The ϵ_{ij}'s are iid $N(0, 1)$ and the a_i's are also iid
  $N(0, 1)$.

- *normal-t_3:* The ϵ_{ij}'s are iid from the t_3 distribution and the a_i's
  are iid $N(0, 1)$.

- *t_3-normal:* The ϵ_{ij}'s are iid $N(0, 1)$ and the a_i's are iid from the
  t_3 distribution.

- *t_3-t_3:* The ϵ_{ij}'s are iid from the t_3 distribution and the a_i's are also
  iid from the t_3 distribution.

This produces 18 combinations, 3 designs × 6 choices of distributions.
All tests were performed at the 5% level. The alternatives are constructed by shifting the generated errors by a constant c. Four values
of c are considered for each of the 18 combinations, namely, $c = 0$ (the
null hypothesis) and three different positive values of c each producing
a different alternative. The number of replications is 10000.

The results are reported in Tables 15.1 to 15.4. Table 15.1 gives the observed probability of rejecting H_0 for the 6 tests when there is no cluster correlation, that is when, $a_i=0$ for all i. We thus have independent and identically distributed observations in that case. Table 15.2 to

Table 15 1 Observed probability of rejecting H_0 when there is no intra-cluster correlation.

Design	Distribution	Value of c	Test statistics					
			t-test	sign test	WSR	M_N	S_N	W_N
1	$N(0,1)$	0	0 055	0 042	0 047	0.044	0.041	0.044
		0 24	0 262	0 160	0.234	<u>0 213</u>	0.151	<u>0.212</u>
		0.40	0.585	0.376	0.542	<u>0 508</u>	0 352	<u>0 499</u>
		0.57	0.871	0.654	0.833	<u>0.820</u>	0.615	0.799
1	t_3	0	0 054	0.047	0 053	0 039	0.044	0.047
		0.28	0 196	0.183	0.218	0 153	0 172	<u>0 198</u>
		0.50	0.457	0 465	0.540	0.386	0.431	<u>0 496</u>
		0.74	0.730	0 777	0.838	0.666	0.740	<u>0 801</u>
2	$N(0,1)$	0	0.051	0.062	0.048	0 041	0.045	0 042
		0.15	0.254	0.208	0.235	<u>0 199</u>	0 146	<u>0 194</u>
		0 27	0 648	0.500	0.618	<u>0 541</u>	0 385	<u>0.531</u>
		0 37	0.892	0.749	0.869	<u>0 812</u>	0.631	0.800
2	t_3	0	0.051	0.065	0.050	0.043	0.047	0.047
		0.18	0.174	0.239	0 225	0.135	0.174	<u>0 186</u>
		0.33	0.447	0 587	0.601	0.362	0.460	<u>0.512</u>
		0.47	0 718	0.855	0.879	0.612	0.743	<u>0 800</u>
3	$N(0,1)$	0	0.054	0.061	0 051	0.046	0.049	0.046
		0.12	0.267	0.197	0.252	<u>0.207</u>	0.148	<u>0.201</u>
		0.21	0.621	0.459	0.600	<u>0.517</u>	0.365	0.503
		0.30	0.903	0.747	0.946	<u>0 818</u>	0.628	0 803
3	t_3	0	0.048	0.056	0.05	0.040	0.044	0.043
		0.15	0.179	0.242	0.254	0.140	0 178	<u>0.203</u>
		0.28	0.428	0.562	0.604	0.342	0.450	<u>0 502</u>
		0.38	0.718	0.864	0.898	0.617	0.765	<u>0.827</u>

Note For each alternative, the test (among M_N, S_N and W_N) with the highest power and any other that is not significantly different (at the 5% level) from the one with the highest power are underlined.

15.4 give the same probability when cluster correlation is present but, in order to facilitate the comparisons, only for the 3 tests that are suited to this situation. The 3 other tests (t-test, sign test and Wilcoxon signed-rank) can not maintain their prescribed level in that case. Indeed, the observed levels for these tests vary between 0.075 and 0.144 for Design 1, between 0.238 and 0.382 for Design 2 and between 0.306 and 0.505 for Design 3. Also, for each given alternative, the test (among M_N, S_N and

W_N only) with the highest power and any other that is not significantly different (at the 5% level) from the one with the highest power are underlined. Before going into details, Table 15.5 gives a global measure of performance. It simply reports the number of times that each test is the one with the highest power or is not significantly different from the one with the highest power for all the alternatives considered. We see that the test W_N is the best one for 14 out of the 18 alternatives considered when there is no intra-cluster correlation. Furthermore, it is the best one for 33 out of the 36 alternatives considered when intra-cluster correlation is present. Overall, the test W_N is the best one for 47 out of the 54 alternatives. We see that the test M_N is the second best overall followed closely by the test S_N. It is interesting to note that the test S_N is the best one more often than M_N when intra-cluster correlation is present, but it is never the best one when there is no intra-cluster correlation.

Table 15.2. Observed probability of rejecting H_0 for design 1 when intra-cluster correlation is present.

Design	Distribution	Value of c	Test statistics M_N	S_N	W_N
1	normal-normal	0	0.047	0.043	0.048
		0.40	<u>0.210</u>	0.158	<u>0.210</u>
		0.60	<u>0.512</u>	0.400	<u>0.513</u>
		1.00	<u>0.827</u>	0.686	<u>0.825</u>
1	normal-t_3	0	0.045	0.043	0.051
		0.45	0.184	0.168	<u>0.209</u>
		0.79	0.466	0.422	<u>0.518</u>
		1.12	0.751	0.709	<u>0.812</u>
1	t_3-normal	0	0.038	0.041	0.045
		0.48	0.183	0.166	<u>0.201</u>
		0.85	0.467	0.435	<u>0.511</u>
		1.25	0.753	0.734	<u>0.803</u>
1	t_3-t_3	0	0.042	0.044	0.050
		0.52	0.163	0.168	<u>0.192</u>
		0.92	0.421	0.429	<u>0.490</u>
		1.39	0.726	0.752	<u>0.804</u>

Note: For each alternative, the test with the highest power and any other that is not significantly different (at the 5% level) from the one with the highest power are underlined.

Table 15 3. Observed probability of rejecting H_0 for design 2 when intra-cluster correlation is present.

Design	Distribution	Value of c	M_N	S_N	W_N
		0	0.042	0.046	0.045
2	normal-normal	0.38	0.191	0.177	0.195
		0.68	0.497	0.455	0.502
		0.98	0.810	0.758	0.812
		0	0.044	0.048	0.047
2	normal-t_3	0.40	0.167	0.175	0.184
		0.71	0.440	0.454	0.494
		1.04	0.762	0.764	0.811
		0	0.037	0.048	0.046
2	t_3-normal	0.50	0.196	0.217	0.221
		0.86	0.464	0.505	0.512
		1 28	0 750	0 797	0 793
		0	0 033	0 045	0 042
2	t_3-t_3	0 52	0 177	0.212	0 211
		0 90	0 444	0 505	0 508
		1 40	0 764	0 826	0 814

Note For each alternative, the test with the highest power and any other that is not significantly different (at the 5% level) from the one with the highest power are underlined

Let's have a more detailed look at the results starting with Table 15.1. If we compare each tests M_N, S_N and W_N with their natural counterparts for iid observations, that is, if we compare M_N to the t-test, S_N to the sign test and W_N to the WSR test, we see that their power are always a little lower. Fortunately, the difference is usually not that important. Consequently, if there is a possibility that the observations are cluster-correlated, then, since the t-test, the sign test and the WSR test are not suited for that situation, it is safer to use a test (like S_N or M_N and W_N) that can deal with the correlation because the loss of power will not be that great even if there is no intra-cluster correlation. From now on, we will limit our comparison to the three tests S_N or M_N and W_N. We see that the M_N and W_N tests are the most powerful and are almost equivalent for normally distributed data. For data form the t_3 distribution, the test W_N is the better one, followed by the test S_N.

From Table 15 2, we have that the test W_N is the better one everywhere except for the normal-normal distribution where it is tied with the test M_N. From Table 15.3 and 15.4, we see that the M_N and W_N tests are the most powerful and are almost equivalent for the normal-normal

Table 15 4   Observed probability of rejecting H_0 for design 3 when intra-cluster correlation is present

Design	Distribution	Value of c	Test statistics M_N	S_N	W_N
3	normal-normal	0	0 039	0 047	0.042
		0 39	<u>0 206</u>	0 199	<u>0 211</u>
		0 68	<u>0 523</u>	0 493	<u>0 527</u>
		0 98	<u>0 825</u>	0 787	<u>0 829</u>
3	normal-t_3	0	0.041	0.045	0 045
		0 40	0 186	<u>0 200</u>	<u>0 204</u>
		0 69	0 465	0 480	<u>0 501</u>
		1 03	0 802	0 811	<u>0 837</u>
3	t_3-normal	0	0 036	0 047	0 043
		0.49	0.178	<u>0 209</u>	<u>0 208</u>
		0 88	0 472	<u>0 519</u>	<u>0 520</u>
		1 29	0 737	<u>0 796</u>	0 781
3	t_3-t_3	0	0 035	0 046	0 045
		0 48	0 163	<u>0 199</u>	<u>0 195</u>
		0 88	0 448	<u>0.512</u>	<u>0 505</u>
		1 40	0 779	<u>0 839</u>	0 827

Note. For each alternative, the test with the highest power and any other that is not significantly different (at the 5% level) from the one with the highest power are underlined

Table 15 5.   Number of times that each test is either the one with the highest power (among M_N, S_N and W_N) or is not significantly different (at the 5% level) from the one with the highest power for all alternatives considered

	M_N	S_N	W_N
No intra-cluster correlation (18 alternatives)	9	0	14
With intra-cluster correlation (36 alternatives)	9	14	33
Total (54 alternatives)	18	14	47

distribution. The S_N and W_N tests are the better ones for the t_3-normal and t_3-t_3 distributions. Finally, the test W_N is the better one, except for the first shift alternative where it is tied with the test S_N, for the normal-t_3 distribution.

From these results we see that the test W_N offers a very good performance across all the cases considered. In particular, it is as good as the test based on the overall average for normal data when intra-cluster correlation is present.

Table 15 6   Analysis results for the example

	Disruptive behavior	Prosocial behavior	Anxiety	Anxiety altered
t-test	-0 110 (.912)	-3.20 (.0014)	6.70 ($<$.0001)	3.05 (0023)
M_N test	-0.07 (.941)	-1.70 (.090)	4.11 ($<$.0001)	1 69 (.091)
S_N test	-0.06 (.950)	-1.57 (.117)	3.74 (.0002)	3 74 (0002)
W_N test	-0.07 (.941)	-1 66 (098)	3 94 ($<$.0001)	3.41 (0006)
Maximum likelihood analysis				
$\hat{\mu}$	0.037	-0.302	0 379	0.190
SE of $\hat{\mu}$	0 126	0 178	0.073	0.099
Wald test	0.30 (766)	-1 70 (.090)	5.20 ($<$ 0001)	1 92 (.055)
MLE of intra-class correlation	0 107	0 186	0 123	0 227

Note· numbers between parentheses are p-values of associated tests

4.   Example and concluding remarks

We start this section by going back to the motivating example presented in the Introduction. The analysis that was performed in Larocque (2003) (see Table 5 of that article) is reproduced here by adding the test W_N. More precisely, the M_N, S_N and W_N tests and a maximum likelihood analysis (using PROC MIXED in SAS) were applied to each variables (scales) separately. Moreover, in order to investigate what happens when we ignore the clustering effect (treating the 2837 observations as if they were iid), ordinary t-tests were also performed on each variable. The results are presented in Table 15.6.

To be precise, the observed values of the test statistics that are reported in Larocque (2003) are the square of M_N and S_N as defined in the present article. In Table 15.6, the values reported are the ones of M_N, S_N and W_N as defined in this article. The p-values reported are the same however. The five tests agree for the disruptive and anxiety scales: a significant difference is found for anxiety but none is found for disruptive behavior. For the prosocial scale, the t-test rejects the null hypothesis while the four other tests (that are suited for clustered data) do not reject. It is well known, and it was also observed in the simulation study, that a test that neglects to take into account a positive intra-class correlation can be highly liberal. Consequently, we can easily argue that the four other tests give a more accurate picture and that the t-test detects something that is probably not there.

The last column of Table 15.6 is an illustration of the vulnerability of the MLE and average-based tests in the presence of extreme observa-

tions. The range of possible values for the difference between grade one and kindergarten anxiety is $[-10, 10]$. The first 60 negative observations in the data set were changed to -10. They were already strictly negative and we only modified them to -10 which is the smallest value possible for that variable. We thus changed only $60/2837=2.1\%$ of the points. We see that, obviously as no signs have changed, the test S_N is unaffected by this modification. Moreover, the p-value of the test W_N increases a little bit but remains highly significant. However, the M_N and MLE tests are affected a lot more. In fact, they are not significant anymore at the 5% level. We note that in this example, the t-test remains significant but it is pointless because we know that we can not trust it for this kind of data.

In conclusion, we considered the one-sample location problem with cluster correlated data. We showed how to adapt the Wilcoxon signed-rank test to that situation by using a valid estimator of the asymptotic null variance. A simulation study was performed to investigate the merits of the proposed test. The findings indicate that the test is a good procedure in all scenarios considered. It is even as powerful as a test based on the overall average for normally distributed data when intra-cluster correlation is present.

Appendix: Proof of Theorem 15.1

Let F^+ be the cumulative distribution function of $|X_{11}|$. To simplify the notation, define $s_{ij} = S(X_{ij})$ and $F_{ij}^+ = F^+(|X_{ij}|)$ $\forall i, j$. Let

$$\bar{W}^* = \frac{1}{N} \sum_{i=1}^{n} \sum_{j=1}^{m_i} s(X_{ij}) F_{ij}^+$$

The proof goes as follow: first we show that $\bar{W}$ and $\bar{W}^*$ are asymptotically equivalent under H_0 and then we show the asymptotic normality of $\bar{W}^*$.

LEMMA A.1 *Assume that the structure of the observations is given by (15.4) and that their joint distribution is continuous. Further, suppose that $(\sum_{i=1}^{n} m_i^2)/(\sum_{i=1}^{n} m_i)$ converges to a finite number when $n \to \infty$. Then, under H_0,*
a) $\sqrt{N}|\bar{W} - \bar{W}^*| \xrightarrow{P} 0$ *as* $n \to \infty$
b) $E(\sqrt{N}\bar{W}^*) = 0$ *and* $\mathrm{Var}(\sqrt{N}\bar{W}^*) = \frac{1}{3} + \frac{c}{N} \sum_{i=1}^{n} m_i(m_i - 1)$ *where*
$c = E(s_{11} s_{12} F_{11}^+ F_{12}^+)$.

Proof. Note first that the condition, $(\sum_{i=1}^{n} m_i^2)/(\sum_{i=1}^{n} m_i)$ converges to a finite number when $n \to \infty$, implies that

$$\frac{1}{N} \sum_{i=1}^{n} m_i(m_i - 1) = \frac{\sum_{i=1}^{n} m_i^2}{\sum_{i=1}^{n} m_i} - 1$$

converges to a finite number when $n \to \infty$, that

$$\frac{\max_i m_i(m_i - 1)}{N} \leq \frac{1}{N} \sum_{i=1}^{n} m_i(m_i - 1)$$

is bounded away from ∞ when $n \to \infty$ and that

$$\frac{\max_i m_i}{N}$$

converges to 0 when $n \to \infty$.

a) Let

$$\bar{W}^{**} = \frac{1}{N} \sum_{i=1}^{n} \sum_{j=1}^{m_i} s(X_{ij}) \left(\frac{R_{ij}^{+*}}{N+1} \right)$$

where R_{ij}^{+*} is the rank of $|X_{ij}|$ among all observations except those from cluster i, that is,

$$R_{ij}^{+*} = \sum_{\substack{k=1 \\ k \neq i}}^{n} \sum_{l=1}^{m_k} \phi(|X_{ij}| > |X_{kl}|)$$

where ϕ is the indicator function Clearly,

$$\left| \sqrt{N} \bar{W} - \sqrt{N} \bar{W}^{**} \right| \leq \frac{1}{\sqrt{N}} \frac{\sum_{i=1}^{n} m_i^2}{N+1}$$

converges to 0 when $n \to \infty$. Thus, $\bar{W}$ and $\bar{W}^{**}$ are asymptotically equivalent and, consequently, part a) will be established if we show that $E(\sqrt{N} \bar{W}^{**} - \sqrt{N} \bar{W}^*)^2 \to 0$ as $n \to \infty$. We have

$$E(\sqrt{N} \bar{W}^{**} - \sqrt{N} \bar{W}^*)^2$$
$$= \frac{1}{N} \sum_{i=1}^{n} \sum_{j=1}^{m_i} \sum_{k=1}^{n} \sum_{l=1}^{m_k} E \left[s_{ij} s_{kl} \left(\frac{R_{ij}^{+*}}{N+1} - F_{ij}^+ \right) \left(\frac{R_{kl}^{+*}}{N+1} - F_{kl}^+ \right) \right] \quad \text{(A.1)}$$

When $i \neq k$. the expectation on the right hand side of the equation above equals 0. When $i = k$ and $j \neq l$, the same expectation equals

$$\frac{E[s_{ij} s_{il} F_{ij}^+ F_{il}^+]}{(N+1)^2} \left(\frac{(N - m_i)^2}{(N+1)^2} - 2 \frac{(N - m_i)}{N+1} + 1 \right) = h(i),$$

say. Moreover, the total contribution of those terms ($i = k$ and $j \neq l$) is

$$\frac{1}{N} \sum_{i=1}^{n} h(i) m_i (m_i - 1) \to 0 \quad \text{as} \quad n \to \infty.$$

When $i = k$ and $j = l$, we have

$$E \left(F_{ij}^+ - \frac{R_{ij}^{+*}}{N+1} \right)^2 = E(F_{ij}^{+2}) + \frac{1}{(N+1)^2} E(R_{ij}^{+*2}) - \frac{2}{N+1} E(F_{ij}^+ R_{ij}^+)$$

$$= \frac{1}{3} + \frac{1}{(N+1)^2} \frac{1}{3} \sum_{\substack{k=1 \\ k \neq i}}^{n} \sum_{\substack{r=1 \\ r \neq k, i}}^{n} m_k m_r + \frac{1}{(N+1)^2} \frac{1}{2} (N - m_i) +$$

$$\frac{1}{(N+1)^2} O(1) \sum_{\substack{k=1 \\ k \neq i}}^{n} m_k (m_k - 1) - \frac{2}{N+1} \frac{1}{3} (N - m_i)$$

where $O(1)$ is a positive function bounded by 1 independently of i and j. Clearly, $max_{i,j}$ of the third and fourth term on the right side of the last equation converges

to 0, and $max_{i,j}$ of the sum of the first, second and fifth term converges to 0 as $n \to \infty$. Putting all this together, we have that (A 1) converges to 0 as $n \to \infty$ and this concludes the proof of Lemma A 1 a).

b) The symmetry of the distribution implies that s_{ij} and $|X_{ij}|$ are independent. This entails that $E(\sqrt{N}\bar{W}^*) = 0$ since $E(s_{ij}) = 0$. For the variance, a straightforward calculation shows that

$$
\begin{aligned}
\mathrm{Var}(\sqrt{N}\bar{W}^*) &= \frac{1}{N}\sum_{i=1}^{n} E\left(\sum_{j=1}^{m_i} s_{ij}F_{ij}^{+}\right) \\
&= \frac{1}{N}\sum_{i=1}^{n}\left(\sum_{j=1}^{m_i} E(F_{ij}^{+2}) + \sum_{j=1}^{m_i}\sum_{\substack{k-1 \\ k \neq j}}^{m_i} E(s_{ij}s_{ik}F_{ij}^{+}F_{ik}^{+})\right) \\
&= \frac{1}{3} + \frac{c}{N}\sum_{i=1}^{n} m_i(m_i - 1)
\end{aligned}
$$

We can now conclude the proof of Theorem A.1. The Central Limit Theorem for independent but not identically distributed random variables entails that $\sqrt{N}\bar{W}^*$ converges to the $N(0, \sigma_W^2)$ distribution where $\sigma_W^2 = \frac{1}{3} + c\lim_{n \to \infty}\frac{1}{N}\sum_{i=1}^{n} m_i(m_i - 1)$. From Lemma A 1 a), this is also true for $\sqrt{N}\bar{W}$. The only thing remaining to show is that the estimator of the asymptotic variance defined by (15.6) is consistent, that is $E(\hat{\sigma}_W^2) \to \sigma_W^2$ under H_0. This can be easily done by using the same type of argument as above, that is, by using the approximation of $\hat{\sigma}_W^2$ defined by replacing $R_{ij}^{+}/(N + 1)$ by F_{ij}^{+}. This concludes the proof of Theorem 15.1. $\qquad \square$

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