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ADVANCES IN WISHART-TYPE MODELLING OF CHANNEL CAPACITY

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Abstract:

- This paper paves the way when the assumption of normality is challenged within the wireless communications systems arena. Innovative results pertaining to the distributions of quadratic forms and their associated eigenvalue density functions for the complex elliptical family are derived, which includes an original Rayleigh-type representation of channels. The presented analytical framework provides computationally convenient forms of these distributions. The results are applied to evaluate an important information-theoretic measure, namely channel capacity. Superior performance in terms of higher capacity of the wireless channel is obtained when considering the underlying complex matrix variate t distribution compared to the usual complex matrix variate normal assumption.

Key-Words:

- *channel capacity; complex matrix variate t; complex Wishart; eigenvalues; quadratic form; Rayleigh-type MIMO channel.*

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1. INTRODUCTION

In wireless communications, systems with multiple-input-multiple-output (MIMO) design have become very popular since they allow higher bit rate and because of their applications in the analysis of signal-to-noise ratio (SNR). In the analysis of channel capacity, the formation of complex channel coefficients play a deterministic role and been taken to be complex matrix variate normal distributed so far, to the best of our knowledge. However, this normality assumption has not been challenged. [17] mentioned that the Rayleigh density function is usually derived based on the assumption that from the central limit theorem for large number of partial waves, the resultant process can be decomposed into two orthogonal zero-mean and equal-standard deviation normal random processes. This is an approximation and the restriction of complex normal is unnecessary — it is not always a large number of interfering signals. Thus a more general assumption than complex matrix variate normal may not be that far from reality (see also [12]). This speculative research challenges this assumption of a channel being fed by normal inputs, and sets the platform for introducing our newly proposed models to the MIMO wireless systems arena, and to provide deeper insight into these systems.

The performance of these MIMO systems relies on the quadratic form of the complex normal channel matrix, with n "inputs" and p "outputs", colloquially referred to as "receivers" and "transmitters" respectively. Thus, the distribution of quadratic forms of the underlying complex normal channel matrix is of particular interest. Distributions of quadratic forms of complex normal matrix variates is a topic that has been studied to a wide extent in literature ([7], [6], [15]). In this paper the distribution of $\boldsymbol{S} = \boldsymbol{X}^H \boldsymbol{A} \boldsymbol{X}$ is of interest[1], where $\boldsymbol{X} \in \mathbb{C}_1^{n\times p}$ is taken to be the complex matrix variate *elliptical* distribution to address the criticism against the questionable use of the normal model ($\boldsymbol{A} \in \mathbb{C}_2^{n\times n}$, where $\mathbb{C}_1^{n\times p}$ denotes the space of $n\times p$ complex matrices, and $\mathbb{C}_2^{p\times p}$ denotes the space of Hermitian positive definite matrices of dimension p). This complex matrix variate elliptical distribution, which contains the well-studied complex matrix variate normal distribution as a special case, is defined next.

The complex matrix variate $\boldsymbol{X} \in \mathbb{C}_1^{n\times p}$, whose distribution is absolutely continuous, has the complex matrix variate elliptical distribution with parameters $\boldsymbol{M} \in \mathbb{C}_1^{n\times p}$, $\boldsymbol{\Phi} \in \mathbb{C}_2^{n\times n}$, $\boldsymbol{\Sigma} \in \mathbb{C}_2^{p\times p}$, denoted by $\boldsymbol{X} \sim \mathcal{C}E_{n\times p}(\boldsymbol{M}, \boldsymbol{\Phi}\otimes\boldsymbol{\Sigma}, g)$, if it has the following density function[2] (see also [10]):

$$h_{\boldsymbol{X}}(\boldsymbol{X}) = \frac{1}{|\boldsymbol{\Sigma}|^n\,|\boldsymbol{\Phi}|^p}\; g\Big[-\operatorname{tr}\Big(\boldsymbol{\Sigma}^{-1}(\boldsymbol{X}-\boldsymbol{M})^H\,\boldsymbol{\Phi}^{-1}(\boldsymbol{X}-\boldsymbol{M})\Big)\Big]. \tag{1.1}$$

In (1.1), $g(\cdot)$ denotes the density generator[3] $g\colon \mathbb{R}^+ \to \mathbb{R}^+$, which should be a function of a quadratic form (see also [6]).

[2] and [6] demonstrates that real elliptical distributions can always be expanded as an integral of a set of normal densities. Similar to [13], we present the following lemma to define the complex matrix variate elliptical distribution as a weighted representation of complex matrix variate normal density functions. This representation can be used to explore the distribution of $\boldsymbol{S}$ when the distribution of $\boldsymbol{X}$ can be that of any member of the complex matrix variate elliptical class.

[1] $\boldsymbol{X}^H$ denotes the conjugate transpose of $\boldsymbol{X}$.
[2] $|\boldsymbol{X}|$ denotes the determinant of matrix $\boldsymbol{X}$.
[3] $\mathbb{R}^+$ denotes the positive real line.

Lemma 1.1. *If* $\boldsymbol{X} \sim \mathcal{C}E_{n\times p}(\boldsymbol{M}, \boldsymbol{\Phi}\otimes\boldsymbol{\Sigma}, g)$ *with density function* $h_{\boldsymbol{X}}(\boldsymbol{X})$*, then there exists a scalar weight function* $\mathcal{W}(\cdot)$ *on* $\mathbb{R}^+$ *such that*

$$h_{\boldsymbol{X}}(\boldsymbol{X}) \;=\; \int_{\mathbb{R}^+} \mathcal{W}(t)\, f_{\mathcal{C}N_{n\times p}(\boldsymbol{M},\boldsymbol{\Phi}\otimes t^{-1}\boldsymbol{\Sigma})}\big(\boldsymbol{X}\,|t\big)\, dt\,,$$

where[4] $f_{\mathcal{C}N_{n\times p}(\boldsymbol{M},\boldsymbol{\Phi}\otimes t^{-1}\boldsymbol{\Sigma})}(\boldsymbol{X}|t) = \frac{1}{\pi^{pn}|\boldsymbol{\Phi}|^p\,|t^{-1}\boldsymbol{\Sigma}|^n}\ \mathrm{etr}\big[-\big(t\,\boldsymbol{\Sigma}^{-1}(\boldsymbol{X}-\boldsymbol{M})^H\,\boldsymbol{\Phi}^{-1}(\boldsymbol{X}-\boldsymbol{M})\big)\big]$ *is the density function of* $\boldsymbol{X}|t \sim \mathcal{C}N_{n\times p}(\boldsymbol{M}, \boldsymbol{\Phi}\otimes t^{-1}\boldsymbol{\Sigma})$*, with*

$$\mathcal{W}(t) \;=\; \pi^{np}\, t^{-np}\, \mathcal{L}^{-1}\Big\{g\Big[-\mathrm{tr}\Big(\boldsymbol{\Sigma}^{-1}(\boldsymbol{X}-\boldsymbol{M})^H\,\boldsymbol{\Phi}^{-1}(\boldsymbol{X}-\boldsymbol{M})\Big)\Big]\Big\}\,,$$

where $\mathcal{L}$ *is the Laplace transform operator.*

Proof: Let $s = \mathrm{tr}\big(\boldsymbol{\Sigma}^{-1}(\boldsymbol{X}-\boldsymbol{M})^H\,\boldsymbol{\Phi}^{-1}(\boldsymbol{X}-\boldsymbol{M})\big)$. Using (1.1) we have

$$\begin{aligned}
h_{\boldsymbol{X}}(\boldsymbol{X}) \;&=\; |\boldsymbol{\Sigma}|^{-n}\,|\boldsymbol{\Phi}|^{-p}\, g[-s] \\
&=\; |\boldsymbol{\Sigma}|^{-n}\,|\boldsymbol{\Phi}|^{-p}\, \mathcal{L}\left[\mathcal{W}(t)\,\pi^{-np}\,t^{np}\right] \\
&=\; |\boldsymbol{\Sigma}|^{-n}\,|\boldsymbol{\Phi}|^{-p} \int_{\mathbb{R}^+} \mathcal{W}(t)\,\pi^{-np}\,t^{np}\,e^{-ts}\,dt \\
&=\; \int_{\mathbb{R}^+} \mathcal{W}(t)\,\pi^{-np}\,\left|t^{-1}\boldsymbol{\Sigma}\right|^{-n}|\boldsymbol{\Phi}|^{-p}\,e^{-ts}\,dt\,,
\end{aligned}$$

from where the result follows. □

Remark 1.1. Under the assumptions of Lemma 1.1, using Fubbini's Theorem, we have

$$1 \;=\; \int_{\mathbb{C}_1^{n\times p}} h_{\boldsymbol{X}}(\boldsymbol{X})\,d\boldsymbol{X} \;=\; \int_{\mathbb{R}^+} \mathcal{W}(t) \left(\int_{\mathbb{C}_1^{n\times p}} f_{\boldsymbol{X}}(\boldsymbol{X})\,d\boldsymbol{X}\right) dt \;=\; \int_{\mathbb{R}^+} \mathcal{W}(t)\,dt\,.$$

Thus for a non-negative weight function $\mathcal{W}(\cdot)$, the function $\mathcal{W}(\cdot)$ is a density function of t. Therefore Lemma 1.1 can only be interpreted as a representation of a scale mixture of complex matrix variate normal distributions. However, $\mathcal{W}(\cdot)$ is not always positive and can be negative on some domains (see [13] for some examples). The only limitation of Lemma 1.1 is that it defines those complex matrix variate elliptical distributions whose inverse Laplace transform exist. There are some mild sufficient conditions that ensure the inverse Laplace transform exists for most of the well-known complex matrix variate elliptical distributions.

In this paper two special cases of the complex matrix variate elliptical model is of interest. Firstly, the complex random matrix $\boldsymbol{X} \in \mathbb{C}_1^{n\times p}$ has the complex matrix variate normal distribution with weight function $\mathcal{W}(\cdot)$ in Lemma 1.1 given by

$$\mathcal{W}(t) \;=\; \delta\,(t-1)\,, \tag{1.2}$$

where $\delta(\cdot)$ is the Dirac delta function (see [2] and [13]).

[4] $e^{\mathrm{tr}(\cdot)} = \mathrm{etr}(\cdot)$ where $\mathrm{tr}(\boldsymbol{X})$ denotes the trace of matrix $\boldsymbol{X}$, and $\boldsymbol{X}^{-1}$ denotes the inverse of matrix $\boldsymbol{X}$.

Secondly, $\boldsymbol{X} \in \mathbb{C}_1^{n\times p}$ has the *complex matrix variate t distribution* with the parameters $\boldsymbol{M} \in \mathbb{C}_1^{n\times p}$, $\boldsymbol{\Phi} \in \mathbb{C}_2^{n\times n}$, $\boldsymbol{\Sigma} \in \mathbb{C}_2^{p\times p}$ and degrees of freedom $\upsilon > 0$, denoted by $\boldsymbol{X} \sim \mathcal{C}t_{n\times p}(\boldsymbol{M}, \boldsymbol{\Phi}\otimes\boldsymbol{\Sigma}, \upsilon)$, with the following density function:

$$f_{\boldsymbol{X}}(\boldsymbol{X}) = \frac{\upsilon^{np}\,\mathcal{C}\Gamma(np+\upsilon)}{\pi^{np}\,\mathcal{C}\Gamma_p(\upsilon)} \left\{1 + \frac{1}{\upsilon}\,\mathrm{tr}\Big(\boldsymbol{\Sigma}^{-1}(\boldsymbol{X}-\boldsymbol{M})^H\,\boldsymbol{\Phi}^{-1}(\boldsymbol{X}-\boldsymbol{M})\Big)\right\}^{-(np+\upsilon)}, \tag{1.3}$$

where the complex multivariate gamma function is given by (see [7])

$$\mathcal{C}\Gamma_p(a) = \pi^{\frac{1}{2}p(p-1)} \prod_{i=1}^{p} \Gamma\big(a-(i-1)\big). \tag{1.4}$$

In this case the weight function $\mathcal{W}(\cdot)$ in Lemma 1.1 is given by

$$\mathcal{W}(t) = \frac{(t\upsilon)^{\upsilon}\, e^{-t\upsilon}}{t\,\Gamma(\upsilon)}, \tag{1.5}$$

where $\Gamma(\cdot)$ denotes the well-known gamma function.

This paper is organized as follows: in Section 2 the distribution of the quadratic form within the complex elliptical class for the nonsingular- and singular case is derived, along with the density functions of the eigenvalues of these quadratic forms. The distribution of the eigenvalues of the quadratic forms are of particular interest in the MIMO environment as it describes the underlying distribution for many of the performance measures for these MIMO systems. In Section 3 this newly developed theory in the complex elliptical class is used to evaluate the capacity of MIMO wireless systems for a specific channel environment; by particularly assuming the complex matrix variate t distribution. Furthermore, a Rayleigh-type distribution stemming from the underlying elliptical assumption, is also defined. Section 4 highlights the advantages of the complex matrix variate t distribution in the MIMO environment and includes some conclusions.

2. DISTRIBUTIONS OF QUADRATIC FORMS FROM THE COMPLEX ELLIPTICAL CLASS

In this section the necessary theoretical development is presented to set the platform for Section 3. The density functions of the nonsingular and singular quadratic forms of complex elliptical random matrices are derived and particular cases of them are of special focus. In addition, the density functions for the joint eigenvalues are also derived; these densities are of particular importance when calculating performance measures of MIMO systems. For the reader's convenience, Remark 2.1 provides background regarding matrix spaces.

Remark 2.1. Matrix spaces: The set of all $n\times p$ $(n\geq p)$ matrices, $\boldsymbol{E}$, with orthonormal columns is called the Stiefel manifold, denoted by $\mathcal{C}V_{p,n}$. Thus $\mathcal{C}V_{p,n} = \big\{\boldsymbol{E}(n\times p)\,;\, \boldsymbol{E}^H\boldsymbol{E} = \boldsymbol{I}_p\big\}$. The volume of this manifold is given by $\mathrm{Vol}\,(\mathcal{C}V_{p,n}) = \int\limits_{\mathcal{C}V_{p,n}} \big(\boldsymbol{E}^H d\boldsymbol{E}\big) = \frac{2^p\,\pi^{np}}{\mathcal{C}\Gamma_p(n)}$. If $n = p$ then a special case of the Stiefel manifold is obtained, the so-called unitary manifold, defined as $\mathcal{C}V_{n,n} = \big\{\boldsymbol{E}(n\times n)\,;\, \boldsymbol{E}^H\boldsymbol{E} = \boldsymbol{I}_n\big\} \equiv U(n)$ where $U(n)$ denotes the group of unitary $n\times n$ matrices. The volume of $U(n)$ is given by $\mathrm{Vol}\big(U(n)\big) = \int\limits_{U(n)} \big(\boldsymbol{E}^H d\boldsymbol{E}\big) = \frac{2^n\,\pi^{n^2}}{\mathcal{C}\Gamma_n(n)}$.

2.1. Nonsingular case

Theorem 2.1. *Suppose that $n \geq p$ and $\boldsymbol{X} \sim \mathcal{C}E_{n\times p}(\boldsymbol{0}, \boldsymbol{\Phi}\otimes\boldsymbol{\Sigma}, g)$, and let $\boldsymbol{\Phi}, \boldsymbol{A} \in \mathbb{C}_2^{n\times n}$ and $\boldsymbol{\Sigma} \in \mathbb{C}_2^{p\times p}$. Then the quadratic form $\boldsymbol{S} = \boldsymbol{X}^H\boldsymbol{A}\boldsymbol{X} \in \mathbb{C}_2^{p\times p}$ has the integral series complex Wishart-type (ISCW) distribution with density function*

$$f_{\boldsymbol{S}}(\boldsymbol{S}) = \frac{|\boldsymbol{S}|^{n-p}\,\mathcal{G}(\boldsymbol{S})}{\mathcal{C}\Gamma_p(n)\,|\boldsymbol{\Phi}\boldsymbol{A}|^p\,|\boldsymbol{\Sigma}|^n}\,, \tag{2.1}$$

where

$$\mathcal{G}(\boldsymbol{S}) = \int_{\mathbb{R}^+} t^{np}\;{}_0\mathcal{C}F_0^{(p)}(\boldsymbol{B}, -t\,\boldsymbol{\Sigma}^{-1}\boldsymbol{S})\,\mathcal{W}(t)\,dt$$

and $\boldsymbol{B} = \boldsymbol{A}^{-\frac{1}{2}}\,\boldsymbol{\Phi}^{-1}\boldsymbol{A}^{-\frac{1}{2}}$. This distribution is denoted as $\boldsymbol{S} \sim \mathrm{ISCW}_p(n, \boldsymbol{\Phi}\otimes\boldsymbol{\Sigma}, \mathcal{G}(\cdot))$, where ${}_0\mathcal{C}F_0^{(p)}(\cdot,\cdot)$ denotes the complex hypergeometric function with two Hermitian matrix arguments (see [7], [9]).

Proof: From Lemma 1.1, $\boldsymbol{X}|t \sim \mathcal{C}N(0, \boldsymbol{\Phi}\otimes t^{-1}\boldsymbol{\Sigma})$. The result follows from Theorem 1 of [15] and integrating with respect to the weight function $\mathcal{W}(t)$. □

Remark 2.2. We know that if $\boldsymbol{X} \sim \mathcal{C}N_{n\times p}(\boldsymbol{0}, \boldsymbol{\Phi}\otimes\boldsymbol{\Sigma})$ then $\boldsymbol{X}^H\boldsymbol{A}\boldsymbol{X}$ has the complex matrix variate quadratic distribution, denoted by $\mathcal{C}Q_{n\times p}(\boldsymbol{A}, \boldsymbol{\Phi}\otimes\boldsymbol{\Sigma})$. Assuming that $\boldsymbol{X} \sim \mathcal{C}E_{n\times p}(\boldsymbol{0}, \boldsymbol{\Phi}\otimes\boldsymbol{\Sigma}, g)$, it then follows from Lemma 1.1 that

$$\boldsymbol{S} = \boldsymbol{X}^H\boldsymbol{A}\boldsymbol{X} \overset{d}{=} \boldsymbol{Z}^H\boldsymbol{A}\boldsymbol{Z}\,, \qquad \text{where} \quad \boldsymbol{Z}|t \sim \mathcal{C}N_{n\times p}\big(\boldsymbol{0}, \boldsymbol{\Phi}\otimes t^{-1}\boldsymbol{\Sigma}\big)\,,$$

with

$$\boldsymbol{Z}^H\boldsymbol{A}\boldsymbol{Z}\,|\,t \;\sim\; \mathcal{C}Q_{n\times p}\big(\boldsymbol{A}, \boldsymbol{\Phi}\otimes t^{-1}\boldsymbol{\Sigma}\big)\,.$$

Therefore

$$f_{\boldsymbol{S}}(\boldsymbol{S}) = \int_{\mathbb{R}^+} \mathcal{W}(t)\, f_{\mathcal{C}Q_{n\times p}(\boldsymbol{A}, \boldsymbol{\Phi}\otimes t^{-1}\boldsymbol{\Sigma})}\big(\boldsymbol{Z}^H\boldsymbol{A}\boldsymbol{Z}\,|\,t\big)\,dt\,.$$

Particular cases of the density function (2.1) will be focussed on, since they form part of the investigation in Section 3.

Remark 2.3. If $\boldsymbol{A} = \boldsymbol{I}_n$ and $\boldsymbol{\Phi} = \boldsymbol{I}_n$ then $\boldsymbol{S} \in \mathbb{C}_2^{p\times p}$ has the complex Wishart-type distribution with the following density function

$$f_{\boldsymbol{S}}(\boldsymbol{S}) = \frac{|\boldsymbol{S}|^{n-p}\,\mathcal{G}(\boldsymbol{S})}{\mathcal{C}\Gamma_p(n)\,|\boldsymbol{\Sigma}|^n}\,, \tag{2.2}$$

where

$$\mathcal{G}(\boldsymbol{S}) = \int_{\mathbb{R}^+} t^{np}\,\operatorname{etr}\big(-t\,\boldsymbol{\Sigma}^{-1}\boldsymbol{S}\big)\,\mathcal{W}(t)\,dt\,.$$

If $\boldsymbol{\Sigma} = \sigma^2\boldsymbol{I}_p$ (thus, uncorrelated with variance σ^2), (2.2) simplifies to

$$f_{\boldsymbol{S}}(\boldsymbol{S}) = \frac{|\boldsymbol{S}|^{n-p}\,\mathcal{G}(\boldsymbol{S})}{\mathcal{C}\Gamma_p(n)\,\sigma^{2np}}\,,$$

where

$$\mathcal{G}(\boldsymbol{S}) = \int_{\mathbb{R}^+} t^{np}\,\operatorname{etr}\big(-t\,\sigma^{-2}\boldsymbol{S}\big)\,\mathcal{W}(t)\,dt\,.$$

Next, an expression for the density function of the joint eigenvalues of $\boldsymbol{S} = \boldsymbol{X}^H \boldsymbol{A} \boldsymbol{X}$ is given, when $\boldsymbol{S} \sim \text{ISCW}_p(n, \boldsymbol{\Phi} \otimes \boldsymbol{\Sigma}, \mathcal{G}(\cdot))$ (see (2.1)).

Theorem 2.2. *Suppose that* $\boldsymbol{S} \sim \text{ISCW}_p(n, \boldsymbol{\Phi} \otimes \boldsymbol{\Sigma}, \mathcal{G}(\cdot))$, *and let* $\lambda_1 > \lambda_2 > \cdots > \lambda_p > 0$ *represent the ordered eigenvalues of* $\boldsymbol{S} \in \mathbb{C}_2^{p \times p}$. *Then the eigenvalues of* $\boldsymbol{S}$, $\boldsymbol{\Lambda} = \text{diag}(\lambda_1, \lambda_2, ..., \lambda_p)$, *has density function*[5]

$$f(\boldsymbol{\Lambda}) = K \int_{\mathbb{R}^+} t^{np} \int_{\boldsymbol{E} \in U(p)} {}_0\mathcal{C}F_0^{(p)}\left(\boldsymbol{B}, -t\boldsymbol{\Sigma}^{-1}\boldsymbol{E}\boldsymbol{\Lambda}\boldsymbol{E}^H\right) d\boldsymbol{E}\mathcal{W}(t)\, dt \tag{2.3}$$

$$= K \int_{\mathbb{R}^+} t^{np} \sum_{k=0}^{\infty} \sum_{\kappa} \frac{\mathcal{C}C_\kappa(\boldsymbol{B})}{k!\, C_\kappa(\boldsymbol{I}_n)} \frac{\mathcal{C}C_\kappa\left(-t\boldsymbol{\Sigma}^{-1}\right) \mathcal{C}C_\kappa(\boldsymbol{\Lambda})}{C_\kappa(\boldsymbol{I}_p)}\, \mathcal{W}(t)\, dt\,, \tag{2.4}$$

where $\boldsymbol{B} = \boldsymbol{A}^{-\frac{1}{2}} \boldsymbol{\Phi}^{-1} \boldsymbol{A}^{-\frac{1}{2}}$ *and* $K = \dfrac{\pi^{p(p-1)} \left(\prod_{i=1}^{p} \lambda_i^{n-p}\right) \left(\prod_{k<l}^{p} (\lambda_k - \lambda_l)^2\right)}{\mathcal{C}\Gamma_p(n)\, \mathcal{C}\Gamma_p(p)\, |\boldsymbol{\Phi}\boldsymbol{A}|^p\, |\boldsymbol{\Sigma}|^n}$.

Proof: Using Eq. 93 of [7] and (2.1), the joint density function of the eigenvalues $\lambda_1 > \lambda_2 > ... > \lambda_p > 0$ of $\boldsymbol{S}$ is given by

$$f(\boldsymbol{\Lambda}) = \frac{\pi^{p(p-1)} \left(\prod_{k<l}^{p} (\lambda_k - \lambda_l)^2\right) |\boldsymbol{\Lambda}|^{n-p}}{\mathcal{C}\Gamma_p(n)\, \mathcal{C}\Gamma_p(p)\, |\boldsymbol{\Phi}\boldsymbol{A}|^p\, |\boldsymbol{\Sigma}|^n} \int_{\boldsymbol{E} \in U(p)} \mathcal{G}(\boldsymbol{E}\boldsymbol{\Lambda}\boldsymbol{E}^H)\, d\boldsymbol{E}\,.$$

By using Definition 2.6 from [3], (2.4) follows directly. □

Particular cases of the density function in (2.3) are focussed on next, since they form part of the investigation in Section 3.

Remark 2.4. If $\boldsymbol{A} = \boldsymbol{I}_n$ and $\boldsymbol{\Phi} = \boldsymbol{I}_n$ then the joint density function of the eigenvalues of the complex Wishart-type distribution, $f(\boldsymbol{\Lambda})$, simplifies to

$$f(\boldsymbol{\Lambda}) = \frac{\pi^{p(p-1)} \left(\prod_{i=1}^{p} \lambda_i^{n-p}\right) \left(\prod_{k<l}^{p} (\lambda_k - \lambda_l)^2\right)}{\mathcal{C}\Gamma_p(n)\, \mathcal{C}\Gamma_p(p)\, |\boldsymbol{\Sigma}|^n} \int_{\mathbb{R}^+} t^{np}\, {}_0\mathcal{C}F_0^{(p)}\left(\boldsymbol{\Lambda}, -t\boldsymbol{\Sigma}^{-1}\right) \mathcal{W}(t)\, dt\,. \tag{2.5}$$

If $\boldsymbol{\Sigma} = \sigma^2 \boldsymbol{I}_p$ (thus, uncorrelated with variance σ^2), (2.5) simplifies to

$$f(\boldsymbol{\Lambda}) = \frac{\pi^{p(p-1)} \left(\prod_{i=1}^{p} \lambda_i^{n-p}\right) \left(\prod_{k<l}^{p} (\lambda_k - \lambda_l)^2\right)}{\mathcal{C}\Gamma_p(n)\, \mathcal{C}\Gamma_p(p)\, \sigma^{2np}} \int_{\mathbb{R}^+} t^{np} \exp\left(-t\, \sigma^{-2} \sum_{i=1}^{p} \lambda_i\right) \mathcal{W}(t)\, dt\,.$$

Remark 2.5. It is known that expressions containing hypergeometric functions of matrix argument and zonal polynomials may be cumbersome to compute, and that software packages have limitations to handle such computations. In this paper only cases with specific interest in MIMO systems will be focussed on. The reader is referred to [1], [5], and [9] for some analytical expressions to compute such hypergeometric functions of matrix arguments.

[5] $\mathcal{C}C_\kappa(\boldsymbol{Z})$ denotes the complex zonal polynomial of $\boldsymbol{Z}$ corresponding to the partition $\kappa = (k_1, ..., k_p)$, $k_1 \geq \cdots \geq k_p \geq 0$, $k_1 + \cdots + k_p = k$ and $\sum_\kappa$ denotes summation over all partitions κ.

The following table gives the density function for the special cases (see (2.2) and (2.5)) for the complex matrix variate normal and complex matrix variate t distribution (see (1.5)) case respectively. The expressions for the complex matrix variate normal case reflects the results of [7].

Table 1: Density functions of certain cases of complex matrix variate elliptical quadratic form.

Distribution of $\boldsymbol{X}$	**Density function**
	$f_{\boldsymbol{S}}(\boldsymbol{S})$ (see (2.2))
Normal	$\left(\mathcal{C}\Gamma_p(n)\,\lvert\boldsymbol{\Sigma}\rvert^n\right)^{-1}\lvert\boldsymbol{S}\rvert^{n-p}\,\mathrm{etr}(-\boldsymbol{\Sigma}^{-1}\boldsymbol{S})$
t	$\left(\Gamma(\upsilon)\,\mathcal{C}\Gamma_p(n)\,\lvert\boldsymbol{\Sigma}\rvert^n\right)^{-1}\upsilon^{\upsilon}\,\lvert\boldsymbol{S}\rvert^{n-p}\,\Gamma(np+\upsilon)\,(\mathrm{tr}\,\boldsymbol{\Sigma}^{-1}\boldsymbol{S}+\upsilon)^{(np+\upsilon)}$
	$f(\boldsymbol{\Lambda})$ (see (2.5))
Normal	$\left(\mathcal{C}\Gamma_p(n)\,\mathcal{C}\Gamma_p(p)\,\lvert\boldsymbol{\Sigma}\rvert^n\right)^{-1}\pi^{p(p-1)}\left(\prod_{i=1}^{p}\lambda_i^{n-p}\right)$ $\times\left(\prod_{k<l}^{p}(\lambda_k-\lambda_l)^2\right)\,{}_0\mathcal{C}F_0^{(p)}(\boldsymbol{\Lambda},-\boldsymbol{\Sigma}^{-1})$
t	$\left(\mathcal{C}\Gamma_p(n)\,\mathcal{C}\Gamma_p(p)\,\lvert\boldsymbol{\Sigma}\rvert^n\,\Gamma(\upsilon)\,\upsilon^{np}\right)^{-1}\pi^{p(p-1)}\left(\prod_{i=1}^{p}\lambda_i^{n-p}\right)$ $\times\left(\prod_{k<l}^{p}(\lambda_k-\lambda_l)^2\right)\sum_{k=0}^{\infty}\sum_{\kappa}\frac{\mathcal{C}C_\kappa(-\boldsymbol{\Sigma}^{-1})\;\mathcal{C}C_\kappa(\boldsymbol{\Lambda})}{\upsilon^k\,k!\,C_\kappa(\boldsymbol{I}_p)}\;\Gamma(np+\upsilon+k)$

2.2. Singular case

In this section the *singular* case of the quadratic form of the complex matrix variate elliptical distribution is also considered, where $0 < n < p$.

Theorem 2.3. *Suppose that $0 < n < p$ and $\boldsymbol{X} \sim \mathcal{C}E_{n\times p}(\boldsymbol{0}, \boldsymbol{\Phi}\otimes\boldsymbol{\Sigma}, g)$, and let $\boldsymbol{\Phi}, \boldsymbol{A} \in \mathbb{C}_2^{n\times n}$ and $\boldsymbol{\Sigma} \in \mathbb{C}_2^{p\times p}$. Let $\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2, ..., \lambda_p)$. Then the quadratic form $\boldsymbol{S} = \boldsymbol{X}^H\boldsymbol{A}\boldsymbol{X} \in \mathbb{C}_2^{p\times p}$ has the integral series complex singular Wishart-type (ISCSW) distribution with density function*

$$f_{\boldsymbol{S}}(\boldsymbol{S}) = \frac{\pi^{n(n-p)}\,\lvert\boldsymbol{\Lambda}\rvert^{n-p}\,\mathcal{G}(\boldsymbol{S})}{\mathcal{C}\Gamma_n(n)\,\lvert\boldsymbol{\Phi}\boldsymbol{A}\rvert^p\,\lvert\boldsymbol{\Sigma}\rvert^n}, \tag{2.6}$$

where

$$\mathcal{G}(\boldsymbol{S}) = \int_{\mathbb{R}^+} t^{np}\,{}_0\mathcal{C}F_0^{(n)}\left(\boldsymbol{B}, -t\,\boldsymbol{\Sigma}^{-1}\boldsymbol{S}\right)\mathcal{W}(t)\,dt$$

and $\boldsymbol{B} = \boldsymbol{A}^{-\frac{1}{2}}\,\boldsymbol{\Phi}^{-1}\boldsymbol{A}^{-\frac{1}{2}}$. This distribution is denoted as $\boldsymbol{S} \sim \mathrm{ISCSW}_n(p, \boldsymbol{\Phi}\otimes\boldsymbol{\Sigma}, \mathcal{G}(\cdot))$.

Proof: See that

$$f(\boldsymbol{X}) = \int_{\mathbb{R}^+} t^{np}\,\lvert\boldsymbol{\Phi}\boldsymbol{A}\rvert^{-p}\,\lvert\boldsymbol{\Sigma}\rvert^{-n}\,\pi^{-np}\,\mathrm{etr}\left(-t\,\boldsymbol{B}\boldsymbol{X}\boldsymbol{\Sigma}^{-1}\boldsymbol{X}^H\right)\mathcal{W}(t)\,dt\,,$$

where $\boldsymbol{X}|t \sim \mathcal{C}N\big(\boldsymbol{0}, \boldsymbol{\Phi} \otimes t^{-1}\boldsymbol{\Sigma}\big)$. Let $\boldsymbol{X}^H\boldsymbol{A}^{\frac{1}{2}} = \boldsymbol{E}_1\boldsymbol{\Upsilon}\boldsymbol{H}$ (where $\boldsymbol{A}^{\frac{1}{2}}\boldsymbol{A}^{\frac{1}{2}} = \boldsymbol{A}$), and note $\boldsymbol{S} = \boldsymbol{X}^H\boldsymbol{A}^{\frac{1}{2}}\boldsymbol{A}^{\frac{1}{2}}\boldsymbol{X} = \boldsymbol{E}_1\boldsymbol{\Upsilon}\boldsymbol{H}\boldsymbol{H}^H\boldsymbol{\Upsilon}\boldsymbol{E}_1^H = \boldsymbol{E}_1\boldsymbol{\Upsilon}^2\boldsymbol{E}_1^H = \boldsymbol{E}_1\boldsymbol{\Lambda}\boldsymbol{E}_1^H$ (where $\boldsymbol{\Upsilon}^2 = \boldsymbol{\Lambda}$). From Remark 2.1 follows:

$$f(\boldsymbol{S}) = \frac{\pi^{-np}\,|\boldsymbol{\Lambda}|^{n-p}}{\mathcal{C}\Gamma_n(n)\,|\boldsymbol{\Phi}\boldsymbol{A}|^p\,|\boldsymbol{\Sigma}|^n} \int_{\mathcal{C}V_{n,n}} \int_{\mathbb{R}^+} t^{np}\,{}_0\mathcal{C}F_0^{(n)}\big(\boldsymbol{B}, -t\boldsymbol{\Sigma}^{-1}\boldsymbol{S}\big)\,\mathcal{W}(t)\,dt\,d\boldsymbol{H}\,,$$

from where the result follows after some simplification. □

Particular cases of the density function (2.6) will be focussed on, since they form part of the investigation in Section 3.

Remark 2.6. If $\boldsymbol{A} = \boldsymbol{I}_n$ and $\boldsymbol{\Phi} = \boldsymbol{I}_n$, then $\boldsymbol{S}$ has the complex singular Wishart-type distribution with the following density function

$$f_{\boldsymbol{S}}(\boldsymbol{S}) = \frac{\pi^{n(n-p)}\,|\boldsymbol{\Lambda}|^{n-p}\,\mathcal{G}(\boldsymbol{S})}{\mathcal{C}\Gamma_n(n)\,|\boldsymbol{\Sigma}|^n}\,, \tag{2.7}$$

where

$$\mathcal{G}(\boldsymbol{S}) = \int_{\mathbb{R}^+} t^{np}\,\operatorname{etr}\big(-t\boldsymbol{\Sigma}^{-1}\boldsymbol{S}\big)\,\mathcal{W}(t)\,dt\,.$$

If $\boldsymbol{\Sigma} = \sigma^2\boldsymbol{I}_p$ (thus, uncorrelated with variance σ^2), (2.7) simplifies to

$$f_{\boldsymbol{S}}(\boldsymbol{S}) = \frac{\pi^{n(n-p)}\,|\boldsymbol{\Lambda}|^{n-p}\,\mathcal{G}(\boldsymbol{S})}{\mathcal{C}\Gamma_n(n)\,\sigma^{2np}}\,,$$

where

$$\mathcal{G}(\boldsymbol{S}) = \int_{\mathbb{R}^+} t^{np}\,\operatorname{etr}\big(-t\sigma^{-2}\boldsymbol{S}\big)\,\mathcal{W}(t)\,dt\,.$$

Next, expressions for the density function of the joint eigenvalues for the singular case are derived.

Theorem 2.4. *Suppose that* $0 < n < p$ *and* $\boldsymbol{S} \sim \mathrm{ISCSW}_n(p, \boldsymbol{\Phi}\otimes\boldsymbol{\Sigma}, \mathcal{G}(\cdot))$ *(see (2.6)), and let* $\lambda_1 > \lambda_2 > \ldots > \lambda_n > 0$ *represent the ordered eigenvalues of* $\boldsymbol{S}$*. Then the joint distribution of the eigenvalues of* $\boldsymbol{S}$*,* $\boldsymbol{\Lambda} = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_p)$*, has density function*

$$\begin{aligned} f(\boldsymbol{\Lambda}) = {} & \frac{\pi^{n(n-1)}\left(\prod_{i=1}^{n}\lambda_i^{p-n}\right)\left(\prod_{k<l}^{n}(\lambda_k-\lambda_l)^2\right)}{\mathcal{C}\Gamma_n(n)\,\mathcal{C}\Gamma_n(p)\,|\boldsymbol{\Phi}\boldsymbol{A}|^p\,|\boldsymbol{\Sigma}|^n} \\ & \times \int_{\mathbb{R}^+} t^{np} \int_{\mathcal{C}V_{p,n}} {}_0\mathcal{C}F_0^{(n)}\big(\boldsymbol{B}, -t\boldsymbol{\Sigma}^{-1}\boldsymbol{E}\boldsymbol{\Lambda}\boldsymbol{E}^H\big)\,(d\boldsymbol{E})\,\mathcal{W}(t)\,dt\,, \end{aligned} \tag{2.8}$$

where $\boldsymbol{B} = \boldsymbol{A}^{-\frac{1}{2}}\,\boldsymbol{\Phi}^{-1}\boldsymbol{A}^{-\frac{1}{2}}$.

Proof: Consider a partial spectral decomposition where $\boldsymbol{S} = \boldsymbol{E}\boldsymbol{\Lambda}\boldsymbol{E}^H$, where $\boldsymbol{E} \in \mathcal{C}V_{p,n}$. The transformation from $\boldsymbol{S}$ to $\boldsymbol{E}, \boldsymbol{\Lambda}$ has volume element

$$(d\boldsymbol{S}) = (2\pi)^{-n}\left|\boldsymbol{\Lambda}^{n-p}\right|^{-2}\prod_{k<l}^{n}(\lambda_k-\lambda_l)^2\,(d\boldsymbol{\Lambda})\,\big(\boldsymbol{E}^H d\boldsymbol{E}\big)\,.$$

Therefore, from (2.6) and Remark 2.1:

$$f(\boldsymbol{\Lambda}) = \frac{\pi^{n(n-p)}}{\mathcal{C}\Gamma_n(n)\,|\boldsymbol{\Phi}\boldsymbol{A}|^p\,|\boldsymbol{\Sigma}|^n}\,(2\pi)^{-n}\left|\boldsymbol{\Lambda}^{n-p}\right|^{-2}|\boldsymbol{\Lambda}|^{n-p}\left(\prod_{k<l}^{n}(\lambda_k-\lambda_l)\right)^2 \times \int_{\mathbb{R}^+} t^{np}\int_{\mathcal{C}V_{p,n}} {}_0\mathcal{C}F_0^{(n)}\left(\boldsymbol{B}, -t\,\boldsymbol{\Sigma}_2^{-1}\boldsymbol{E}\boldsymbol{\Lambda}\boldsymbol{E}^H\right)\left(\boldsymbol{E}^H d\boldsymbol{E}\right)\mathcal{W}(t)\,dt$$

and the result follows. □

Some special cases of the density function in (2.8) are reported next.

Remark 2.7. If $\boldsymbol{A}=\boldsymbol{I}_n$ and $\boldsymbol{\Phi}=\boldsymbol{I}_n$, then the joint density function of the eigenvalues of the complex singular Wishart type distribution, $f(\boldsymbol{\Lambda})$, simplifies to the following density function:

$$f(\boldsymbol{\Lambda}) = \frac{\pi^{n(n-1)}\left(\prod_{i=1}^{n}\lambda_i^{p-n}\right)\left(\prod_{k<l}^{n}(\lambda_k-\lambda_l)^2\right)}{\mathcal{C}\Gamma_n(n)\,\mathcal{C}\Gamma_n(p)\,|\boldsymbol{\Sigma}|^n}\int_{\mathbb{R}^+} t^{np}\,{}_0\mathcal{C}F_0^{(n)}\left(\boldsymbol{\Lambda}, -t\,\boldsymbol{\Sigma}^{-1}\right)\mathcal{W}(t)\,dt. \tag{2.9}$$

If $\boldsymbol{\Sigma}=\sigma^2\boldsymbol{I}_p$ (thus, uncorrelated with variance σ^2), (2.7) simplifies to

$$f(\boldsymbol{\Lambda}) = \frac{\pi^{n(n-1)}\left(\prod_{i=1}^{n}\lambda_i^{p-n}\right)\left(\prod_{k<l}^{n}(\lambda_k-\lambda_l)^2\right)}{\mathcal{C}\Gamma_n(n)\,\mathcal{C}\Gamma_n(p)\,\sigma^{2np}}\int_{\mathbb{R}^+} t^{np}\,\exp\left(-t\,\sigma^{-2}\sum_{i=1}^{n}\lambda_i\right)\mathcal{W}(t)\,dt\,.$$

The following table gives the density function for the special cases (see (2.7) and (2.9)) for weight functions (1.2) and (1.5) respectively.

Table 2: Density functions of certain cases of complex singular matrix variate elliptical quadratic form.

Distribution of $\boldsymbol{X}$	**Density function**
	$f_{\boldsymbol{S}}(\boldsymbol{S})$ (see (2.7))
Normal	$\left(\mathcal{C}\Gamma_n(n)\,|\boldsymbol{\Sigma}|^n\right)^{-1}\pi^{n(n-p)}\,|\boldsymbol{\Lambda}|^{n-p}\,\mathrm{etr}(-\boldsymbol{\Sigma}^{-1}\boldsymbol{S})$
t	$\left(\Gamma(\upsilon)\,\mathcal{C}\Gamma_n(n)\,|\boldsymbol{\Sigma}|^n\right)^{-1}\upsilon^{\upsilon}\,\pi^{n(n-p)}\,|\boldsymbol{\Lambda}|^{n-p}\,\Gamma(np+\upsilon)\,(\mathrm{tr}\,\boldsymbol{\Sigma}^{-1}\boldsymbol{S}+\upsilon)^{-(np+\upsilon)}$
	$f(\boldsymbol{\Lambda})$ (see (2.9))
Normal	$\left(\mathcal{C}\Gamma_n(n)\,\mathcal{C}\Gamma_n(p)\,|\boldsymbol{\Sigma}|^n\right)^{-1}\pi^{n(n-1)}\left(\prod_{i=1}^{n}\lambda_i^{p-n}\right)$ $\times\left(\prod_{k<l}^{n}(\lambda_k-\lambda_l)^2\right)\,{}_0\mathcal{C}F_0^{(n)}(\boldsymbol{\Lambda}, -\boldsymbol{\Sigma}^{-1})$ (see Eq. 25 in [14])
t	$\left(\mathcal{C}\Gamma_n(n)\,\mathcal{C}\Gamma_n(p)\,|\boldsymbol{\Sigma}|^n\,\Gamma(\upsilon)\,\upsilon^{np}\right)^{-1}\pi^{n(n-1)}\left(\prod_{i=1}^{n}\lambda_i^{p-n}\right)$ $\times\left(\prod_{k<l}^{n}(\lambda_k-\lambda_l)^2\right)\sum_{k=0}^{\infty}\sum_{\kappa}\frac{\mathcal{C}C_\kappa\left(-\boldsymbol{\Sigma}^{-1}\right)\mathcal{C}C_\kappa(\boldsymbol{\Lambda})}{\upsilon^k\,k!\,C_\kappa(\boldsymbol{I}_p)}\,\Gamma(np+\upsilon+k)$

3. CHANNEL CAPACITY

Suppose that a communication system is being characterized by the following output relation, as depicted in Figure 1:

$$\boldsymbol{y} = \boldsymbol{H}\boldsymbol{x} + \boldsymbol{v}\,,$$

where $\boldsymbol{y}, \boldsymbol{v} \in \mathbb{C}_1^{n_r \times 1}$, $\boldsymbol{x} \in \mathbb{C}_1^{n_t \times 1}$ and $\boldsymbol{H} \in \mathbb{C}_1^{n_r \times n_t}$. In a correlated Rayleigh channel, the distribution of an $n_r \times n_t$ channel matrix $\boldsymbol{H}$ is usually given by $\boldsymbol{H} \sim \mathcal{C}N_{n_r \times n_t}(\boldsymbol{0}, \boldsymbol{I}_{n_r} \otimes \boldsymbol{\Sigma})$ with $n_r \geq n_t$ (in other words, the channel coefficient from different transmitter antennas to a single receiver antenna is correlated), and note that the off-diagonal elements of $\boldsymbol{\Sigma} \in \mathbb{C}_2^{n_t \times n_t}$ are nonzero for correlated channels. Suppose that the channel matrix $\boldsymbol{H}$ and noise vector $\boldsymbol{v}$ are independently distributed according the complex matrix variate elliptical and complex multivariate normal distributions, respectively, in other words, $\boldsymbol{H} \sim \mathcal{C}E_{n_r \times n_t}(\boldsymbol{0}, \boldsymbol{I}_{n_r} \otimes \boldsymbol{\Sigma}, g)$, and $\boldsymbol{v} \sim \mathcal{C}N_{n_r \times 1}(\boldsymbol{0}, \sigma^2 \boldsymbol{I}_{n_r})$. In this section, the focus is to derive the channel capacity capacity if $\boldsymbol{H} \sim \mathcal{C}t_{n_r \times n_t}(\boldsymbol{0}, \boldsymbol{I}_{n_r} \otimes \boldsymbol{\Sigma}, \upsilon)$, with the weight function (1.5).

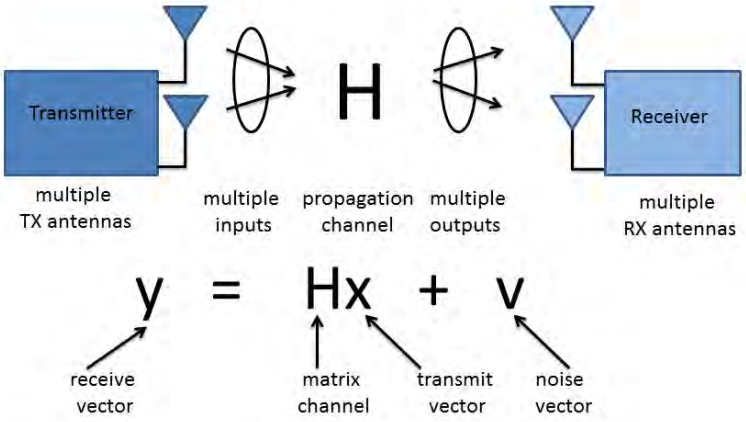

Figure 1: MIMO System.

The input power is distributed equally over all transmitting antennas and is constrained to ρ (the signal to noise ratio) such that (see [15])

$$E(\boldsymbol{x}^H \boldsymbol{x}) \leq \rho\,.$$

For the purpose of this paper we are particularly interested in Rayleigh distributed channels. However, having an underlying complex matrix variate elliptical distribution for $\boldsymbol{H}$ results in having to consider a Rayleigh-*type* channel which is defined next.

Proposition 3.1. *Consider a complex elliptical process, $Z = X + iY$, where X, Y are independent and identically zero-mean elliptical random variates. Let $R = \sqrt{X^2 + Y^2}$ denote an element h_{ij} of $\boldsymbol{H}$. The density function of R emanating from the complex elliptical class is given by*

$$h(r) = \frac{r}{\sigma^2} \int_{\mathbb{R}^+} t \exp\left(-\frac{r^2}{2\,\sigma^2 t^{-1}}\right) \mathcal{W}(t)\, dt\,,$$

where $r > 0$, which is described as a Rayleigh-type density function (see also [11]).

Moreover, if a block-fading model is assumed together with coding over many independent fading intervals, then the ergodic capacity of the random MIMO channel is given by (see [18])

$$\begin{aligned} C &= E_{\boldsymbol{H}}\left(\log\left|\left(\boldsymbol{I}_{n_t}+\frac{\rho}{n_t}\,\boldsymbol{H}^H\boldsymbol{H}\right)\right|\right) \\ &= E_{\boldsymbol{\Lambda}}\left(\log\prod_{k=1}^{n_t}\left(1+\frac{\rho}{n_t}\,\lambda_k\right)\right), \end{aligned} \tag{3.1}$$

where $\lambda_1 > ... > \lambda_{n_t}$ are the eigenvalues of $\boldsymbol{S}$. Hence (3.1) can be evaluated using the joint density functions of the eigenvalues ((2.3) and (2.8) respectively). In the following two sections, the channel capacity is derived for the nonsingular- and singular case, for both correlated- and uncorrelated cases.

3.1. Nonsingular case

In this section the assumption is that the complex channel coefficients are distributed according to the complex matrix variate t distribution. To this end, we first consider the more general complex matrix variate elliptical distribution and subsequently derive the results for the complex matrix variate t distribution. We firstly derive the expressions for the channel capacity of a correlated- and uncorrelated Rayleigh-type $n_r \times 2$ channel environment when the underlying distribution is complex matrix variate elliptical. In particular, a two-input ($n_t = 2$), n_r output communication system is considered and the capacity graphically illustrated.

Theorem 3.1.

1. *For a two-input correlated Rayleigh-type channel* $\boldsymbol{H} \sim \mathcal{C}E_{n_r\times 2}(\boldsymbol{0}, \boldsymbol{I}_{n_r}\otimes\boldsymbol{\Sigma}, g)$, *with* $n_r \geq 2$, *the capacity* C *is given by*

$$\begin{aligned} C = {} & \frac{(a_1a_2)^{n_r}}{\Gamma(n_r)\,\Gamma(n_r-1)\,(a_1-a_2)}\int_0^\infty \log\left(1+\frac{\rho}{2}\,\lambda_1\right) \\ & \times\left\{\lambda_1^{n_r-1}\,\Gamma(n_r-1)\,a_2^{-(n_r-1)}\int_{\mathbb{R}^+} t^{n_r}\exp(-t\,a_1\lambda_1)\,\mathcal{W}(t)\,dt\right. \\ & -\lambda_1^{n_r-1}\,\Gamma(n_r-1)\,a_1^{-(n_r-1)}\int_{\mathbb{R}^+} t^{n_r}\exp(-t\,a_2\lambda_1)\,\mathcal{W}(t)\,dt \\ & -\lambda_1^{n_r-2}\,\Gamma(n_r)\,a_2^{-n_r}\int_{\mathbb{R}^+} t^{n_r-1}\exp(-t\,a_1\lambda_1)\,\mathcal{W}(t)\,dt \\ & \left.+\lambda_1^{n_r-2}\,\Gamma(n_r)\,a_1^{-n_r}\int_{\mathbb{R}^+} t^{n_r-1}\exp(-t\,a_2\lambda_1)\,\mathcal{W}(t)\,dt\right\}\,d\lambda_1\,, \end{aligned} \tag{3.2}$$

where $a_1 > a_2$ *are the ordered eigenvalues of the diagonalized covariance matrix* $\boldsymbol{\Sigma}$.

2. *For a two-input uncorrelated Rayleigh-type channel* $\boldsymbol{H} \sim \mathcal{C}E_{n_r\times 2}(\boldsymbol{0}, \boldsymbol{I}_{n_r} \otimes \sigma^2 \boldsymbol{I}_2, g)$, *with* $n_r \geq 2$, *the capacity* C *is given by*

$$
\begin{aligned}
C \;=\; & \int_0^\infty \log\Big(1+\frac{\rho}{2}\,\lambda_1\Big) \Bigg\{ \int_{\mathbb{R}^+} \frac{\lambda_1^{n_r}\, t^{n_r+1}\, \exp\big(-t\,\sigma^{-2}\lambda_1\big)\, \mathcal{W}(t)}{2\,\Gamma(n_r)\,\sigma^2}\, dt \\
& - \int_{\mathbb{R}^+} \frac{\lambda_1^{n_r-1}\, t^{n_r}\, \exp\big(-t\,\sigma^{-2}\lambda_1\big)\, \mathcal{W}(t)}{\Gamma(n_r-1)}\, dt \\
& + \int_{\mathbb{R}^+} \frac{\lambda_1^{n_r-2}\, t^{n_r-1}\, \Gamma(n_r+1)\, \exp\big(-t\,\sigma^{-2}\lambda_1\big)\, \mathcal{W}(t)}{2\,\Gamma(n_r-1)\,\sigma^{-2}}\, dt \Bigg\}\, d\lambda_1 \,.
\end{aligned} \tag{3.3}
$$

Proof: **1**. The unordered density function of (2.5) is obtained by dividing by $p! = n_t! = 2!$:

$$
f(\lambda_1,\lambda_2) \;=\; \frac{(\lambda_1\lambda_2)^{n_r-2}\,(\lambda_1-\lambda_2)\,(a_1a_2)^{n_r}}{2!\,\Gamma(n_r)\,\Gamma(n_r-1)\,(a_2-a_1)} \int_{\mathbb{R}^+} t^{2n_r-1}\,\big|\exp(-t\,a_i\,\lambda_j)\big|\,\mathcal{W}(t)\,dt\,,
$$

since from (1.4) we have $\mathcal{C}\Gamma_2(2) = \pi\,\Gamma(2)\,\Gamma(1)$, $\mathcal{C}\Gamma_2(n_r) = \pi\,\Gamma(n_r)\,\Gamma(n_r-1)$, and using an expression for the complex hypergeometric function by [8]. Then

$$
\begin{aligned}
\big|\exp(-t\,a_i\,\lambda_j)\big| \;&=\; \begin{vmatrix} \exp(-t\,a_1\lambda_1) & \exp(-t\,a_1\lambda_2) \\ \exp(-t\,a_2\lambda_1) & \exp(-t\,a_2\lambda_2) \end{vmatrix} \\
&=\; \exp\big(-t(a_1\lambda_1+a_2\lambda_2)\big) - \exp\big(-t(a_1\lambda_2+a_2\lambda_1)\big)\,.
\end{aligned}
$$

From (3.1) the capacity for a correlated Rayleigh-type fading model of dimension $n_r\times 2$ under the complex matrix variate elliptical distribution is given by

$$
\begin{aligned}
C \;&=\; 2\int_0^\infty \log\Big(1+\frac{\rho}{2}\,\lambda_1\Big) \int_0^\infty f(\lambda_1,\lambda_2)\,d\lambda_2\,d\lambda_1 \\
&=\; K\int_0^\infty \log\Big(1+\frac{\rho}{2}\,\lambda_1\Big) \int_0^\infty \big(\lambda_1^{n_r-1}\lambda_2^{n_r-2} - \lambda_1^{n_r-2}\lambda_2^{n_r-1}\big) \\
&\quad \times \int_{\mathbb{R}^+} t^{2n_r-1}\Big(\exp\big(-t\,(a_1\lambda_1+a_2\lambda_2)\big) - \exp\big(-t\,(a_1\lambda_2+a_2\lambda_1)\big)\Big)\,\mathcal{W}(t)\,dt\,d\lambda_2\,d\lambda_1 \\
&=\; K\int_0^\infty \log\Big(1+\frac{\rho}{2}\,\lambda_1\Big) \int_{\mathbb{R}^+} t^{2n_r-1} \int_0^\infty \big(\lambda_1^{n_r-1}\lambda_2^{n_r-2} - \lambda_1^{n_r-2}\lambda_2^{n_r-1}\big) \\
&\quad \times \Big(\exp\big(-t\,(a_1\lambda_1+a_2\lambda_2)\big) - \exp\big(-t\,(a_1\lambda_2+a_2\lambda_1)\big)\Big)\,d\lambda_2\,\mathcal{W}(t)\,dt\,d\lambda_1\,,
\end{aligned}
$$

where $K = \frac{(a_1a_2)^{n_r}}{\Gamma(n_r)\,\Gamma(n_r-1)\,(a_2-a_1)}$. The latter integral equals

$$
\begin{aligned}
&\lambda_1^{n_r-1}\exp(-ta_1\lambda_1)\,\Gamma(n_r-1)\,(ta_2)^{-(n_r-1)} - \lambda_1^{n_r-1}\exp(-ta_2\lambda_1)\,\Gamma(n_r-1)\,(ta_1)^{-(n_r-1)} \;- \\
&\qquad - \lambda_1^{n_r-2}\exp(-ta_1\lambda_1)\,\Gamma(n_r)\,(ta_2)^{-n_r} + \lambda_1^{n_r-2}\exp(-ta_2\lambda_1)\,\Gamma(n_r)\,(ta_1)^{-n_r}
\end{aligned}
$$

by using Eq. 3.381.4 from [4]. Result (3.2) follows.

2. The proof follows similarly where $\boldsymbol{\Sigma} = \sigma^2\boldsymbol{I}_2$. □

A particular focus is that of an underlying complex matrix variate t distribution, therefore the weight function (1.5) is substituted into (3.2) and (3.3) to obtain the corresponding capacity.

Corollary 3.1.

1. *For a two-input correlated Rayleigh-type channel,* $\boldsymbol{H} \sim \mathcal{C}t_{n_r\times 2}(\boldsymbol{0}, \boldsymbol{I}_{n_r}\otimes\boldsymbol{\Sigma}, \upsilon)$*, with* $n_r \geq 2$*, the capacity is given by*

$$
\begin{aligned}
C \;=\; & \frac{a_1^{n_r} a_2\, \upsilon^{\upsilon}\, \Gamma(n_r+\upsilon)}{(a_1-a_2)\,\Gamma(\upsilon)\,\Gamma(n_r)} \int_0^{\infty} \log\Big[1+\frac{\rho}{2}\,\lambda_1\Big]\, \lambda_1^{n_r-1}(a_1\lambda_1+\upsilon)^{-(n_r+\upsilon)}\, d\lambda_1 \\
& - \frac{a_1\, a_2^{n_r}\, \upsilon^{\upsilon}\, \Gamma(n_r+\upsilon)}{(a_1-a_2)\,\Gamma(\upsilon)\,\Gamma(n_r)} \int_0^{\infty} \log\Big[1+\frac{\rho}{2}\,\lambda_1\Big]\, \lambda_1^{n_r-1}(a_2\lambda_1+\upsilon)^{-(n_r+\upsilon)}\, d\lambda_1 \\
& - \frac{a_1^{n_r}\, \upsilon^{\upsilon}\, \Gamma(n_r+\upsilon-1)}{(a_1-a_2)\,\Gamma(\upsilon)\,\Gamma(n_r-1)} \int_0^{\infty} \log\Big[1+\frac{\rho}{2}\,\lambda_1\Big]\, \lambda_1^{n_r-2}(a_1\lambda_1+\upsilon)^{-(n_r+\upsilon-1)}\, d\lambda_1 \\
& + \frac{a_2^{n_r}\, \upsilon^{\upsilon}\, \Gamma(n_r+\upsilon-1)}{(a_1-a_2)\,\Gamma(\upsilon)\,\Gamma(n_r-1)} \int_0^{\infty} \log\Big[1+\frac{\rho}{2}\,\lambda_1\Big]\, \lambda_1^{n_r-2}(a_2\lambda_1+\upsilon)^{-(n_r+\upsilon-1)}\, d\lambda_1 .
\end{aligned}
\tag{3.4}
$$

2. *For a two-input uncorrelated Rayleigh-type channel,* $\boldsymbol{H} \sim \mathcal{C}t_{n_r\times 2}(\boldsymbol{0}, \boldsymbol{I}_{n_r}\otimes\sigma^2\boldsymbol{I}_2, \upsilon)$*, with* $n_r \geq 2$*, the capacity* C *is given by*

$$
\begin{aligned}
C \;=\; & \frac{\upsilon^{\upsilon}\, \Gamma(n_r+\upsilon+1)}{\sigma^2\,\Gamma(\upsilon)\,\Gamma(n_r)} \int_0^{\infty} \log\Big[1+\frac{\rho}{2}\,\lambda_1\Big]\, \lambda_1^{n_r}\Big(\frac{\lambda_1}{\sigma^2}+\upsilon\Big)^{-(n_r+\upsilon+1)} d\lambda_1 \\
& - \frac{2\,\upsilon^{\upsilon}\, \Gamma(n_r+\upsilon)}{\Gamma(\upsilon)\,\Gamma(n_r-1)} \int_0^{\infty} \log\Big[1+\frac{\rho}{2}\,\lambda_1\Big]\, \lambda_1^{n_r-1}\Big(\frac{\lambda_1}{\sigma^2}+\upsilon\Big)^{-(n_r+\upsilon)} d\lambda_1 \\
& + \frac{\upsilon^{\upsilon}\, \Gamma(n_r+\upsilon-1)\,\Gamma(n_r+1)}{\sigma^{-2}\,\Gamma(\upsilon)\,\Gamma(n_r-1)} \int_0^{\infty} \log\Big[1+\frac{\rho}{2}\,\lambda_1\Big]\, \lambda_1^{n_r-2}\Big(\frac{\lambda_1}{\sigma^2}+\upsilon\Big)^{-(n_r+\upsilon-1)} d\lambda_1 .
\end{aligned}
$$

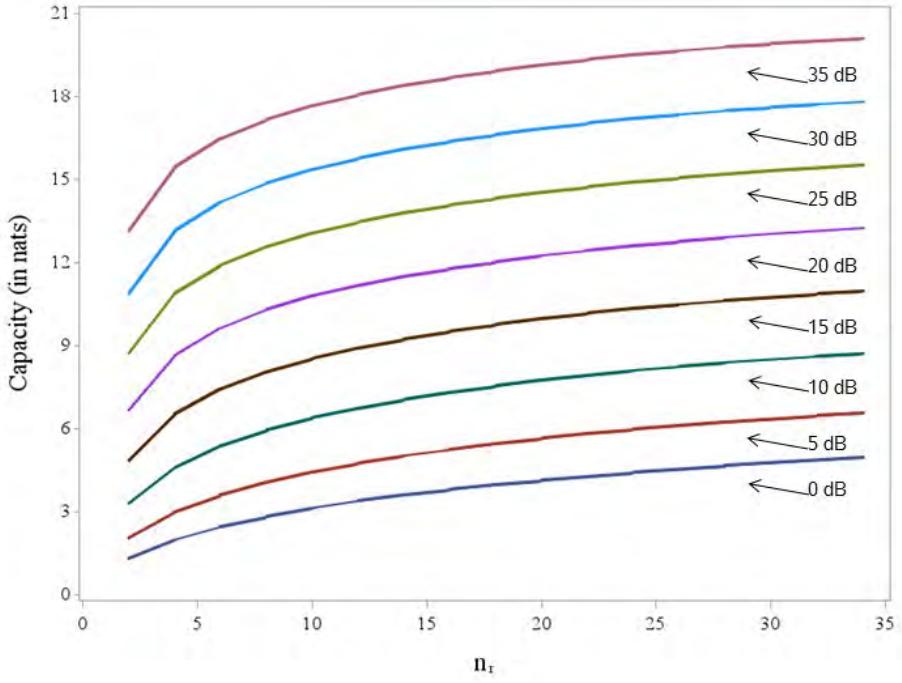

Figure 2: (3.4) against n_r for different values of ρ.

Figure 2 shows the calculated channel capacity (3.4) versus n_r for different values of ρ, assuming a correlation of 0.9, $\sigma^2 = 1$, and $\upsilon = 10$.

Figure 3 shows the calculated channel capacity (3.5) versus n_r for different values of ρ, assuming a correlation of 0, $\sigma^2 = 1$, and $\upsilon = 10$.

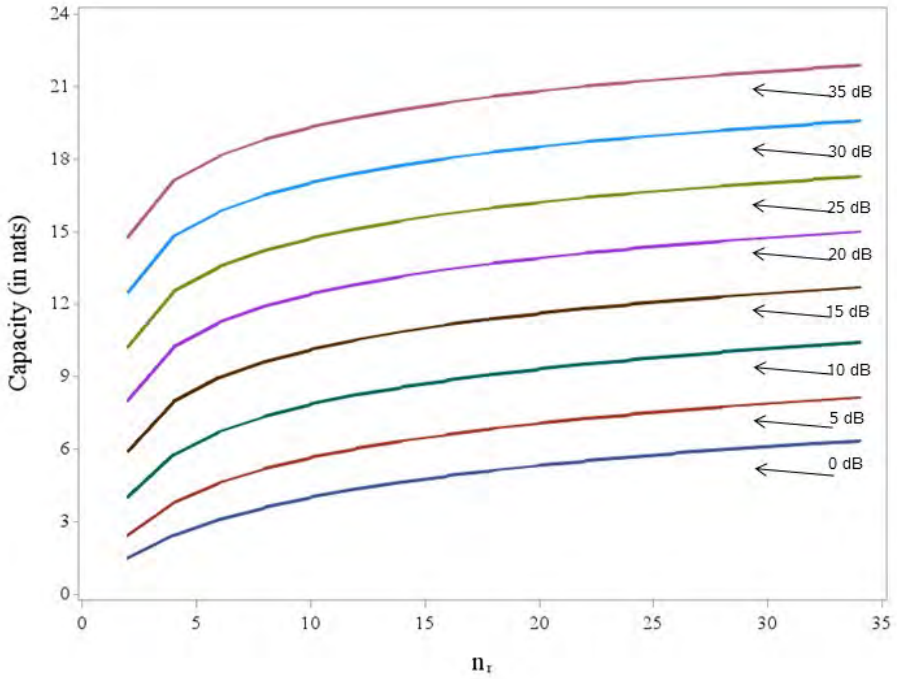

Figure 3: (3.5) against n_r for different values of ρ.

Table 3 shows the capacity in nats[6] for this $n_r \times 2$ correlated Rayleigh-type fading channel matrix (as illustrated in Figure 2). Table 4 shows the capacity in nats for this $n_r \times 2$ uncorrelated Rayleigh-type fading channel matrix (as illustrated in Figure 3). Each column represents different levels of SNR, in decibels (dB). Observe how the capacity is increasing in both Tables 3 and 4 with regards to increasing SNR, as well as increasing number of receivers n_r.

Table 3: Capacity (3.4) in nats for a $n_r \times 2$ system for different values of ρ and $\upsilon = 10$.

n_r	0 dB	5 dB	10 dB	15 dB	20 dB	25 dB	30 dB	35 dB
2	1.2916	2.0609	3.3057	4.8558	6.6852	8.7821	10.9059	13.1656
4	1.9816	2.9984	4.5956	6.5129	8.6450	10.8836	13.1643	15.4598
6	2.4582	3.6126	5.3811	7.4294	9.6327	11.9010	14.1924	16.4914
8	2.8266	4.0737	5.9455	8.0592	10.2922	12.5715	14.8665	17.1666
10	3.1289	4.4445	6.3856	8.5381	10.7872	13.0721	15.368	17.6696
12	3.3862	4.7550	6.7460	8.9240	11.1831	13.4713	15.7691	18.0700
14	3.6105	5.0222	7.0506	9.2467	11.5125	13.8028	16.1012	18.4021
16	3.8095	5.2564	7.3141	9.5234	11.7939	14.0856	16.3842	18.6850
18	3.9882	5.4646	7.5456	9.7650	12.0988	14.3313	16.6298	18.9303
20	4.1502	5.6515	7.7414	9.9786	12.2547	14.5476	16.8458	19.1458

[6] In (3.4) if $\log_e$ is used then the measurement unit for capacity is termed "nats".

Furthermore, note how the capacity for the uncorrelated case (Table 4) is higher for all corresponding entries than that of the correlated case (Table 3). The same is observed for other arbitrarily chosen υ.

Table 4: Capacity (3.5) in nats for a $n_r \times 2$ system for different values of ρ and $\upsilon = 10$.

n_r	0 dB	5 dB	10 dB	15 dB	20 dB	25 dB	30 dB	35 dB
2	1.4843	2.4498	4.0298	5.9281	8.0291	10.2403	12.5045	14.7941
4	2.4402	3.7860	5.7830	7.9676	10.2292	12.5184	14.8167	17.1179
6	3.1083	4.6148	6.7334	8.9714	11.2528	13.5486	15.8490	18.1509
8	3.6156	5.2064	7.3788	9.6373	11.9256	14.2237	16.5284	18.8269
10	4.0228	5.6647	7.8668	10.1360	12.4279	14.7270	17.0285	19.3307
12	4.3622	6.0382	8.2591	10.5948	12.8287	15.1285	17.4302	19.7325
14	4.6583	6.3532	8.5869	10.8670	13.1623	15.4625	17.7643	20.0668
16	4.9069	6.6253	8.8684	11.1516	13.4479	14.7484	18.0503	20.3525
18	5.1324	6.8648	9.1149	11.4004	13.6974	15.9981	18.3000	20.6022
20	5.3350	7.0785	9.3342	11.6214	13.9189	16.2197	18.5215	20.8237

3.2. Singular case

For the *singular* case, the correlated- and uncorrelated Rayleigh-type $2 \times n_t$ channel matrix is considered, and its corresponding capacity derived.

Theorem 3.2.

1. *For a two-input correlated Rayleigh-type channel,* $\boldsymbol{H} \sim \mathcal{C}E_{2\times n_t}(\boldsymbol{0}, \boldsymbol{I}_2 \otimes \boldsymbol{\Sigma}, g)$*, with* $n_t \geq 2$*, the capacity* C *is given by*

$$
\begin{aligned}
C \;=\; & K \int_0^{\infty}\!\!\int_0^{\lambda_1} \left\{ \log\left(1 + \frac{\rho}{n_t}\,\lambda_1\right) + \log\left(1 + \frac{\rho}{n_t}\,\lambda_2\right) \right\} (\lambda_1\lambda_2)^{n_t-2}\,(\lambda_1 - \lambda_2) \\
& \times \int_{\mathbb{R}^+} t^{n_t+1} \det\big(\exp(-t a_i \lambda_j)\big)\, \mathcal{W}(t)\, dt\, d\lambda_2\, d\lambda_1\,,
\end{aligned} \tag{3.5}
$$

where $K = \dfrac{\prod_{i=1}^{n_t} a_i^2}{2\,\Gamma(n_t)\,\Gamma(n_t-1)\prod_{k<l}^{n_t}(a_l - a_k)}$*, and* $a_1 > a_2 > \ldots > a_{n_t} > 0$ *are the eigenvalues of* $\boldsymbol{\Sigma}^{-1}$.

2. *For a two-input uncorrelated Rayleigh-type channel,* $\boldsymbol{H} \sim \mathcal{C}E_{2\times n_t}(\boldsymbol{0}, \boldsymbol{I}_2 \otimes \sigma^2 \boldsymbol{I}_{n_t}, g)$*, with* $n_t \geq 2$*, the capacity* C *is given by*

$$
\begin{aligned}
C \;=\; & \frac{1}{\sigma^{2n_t+2}\,\Gamma(n_t)} \int_0^{\infty} \log\left[1 + \frac{\rho}{n_t}\,\lambda_1\right] \lambda_1^{n_t} \int_{\mathbb{R}^+} t^{n_t+1} \exp\big(-t\,\sigma^{-2}\lambda_1\big)\, \mathcal{W}(t)\, dt\, d\lambda_1 \\
& - \frac{2}{\sigma^{2n_t}\,\Gamma(n_t-1)} \int_0^{\infty} \log\left[1 + \frac{\rho}{n_t}\,\lambda_1\right] \lambda_1^{n_t-1} \int_{\mathbb{R}^+} t^{n_t} \exp\big(-t\,\sigma^{-2}\lambda_1\big)\, \mathcal{W}(t)\, dt\, d\lambda_1 \\
& + \frac{\Gamma(n_t+1)}{\sigma^{2n_t-2}\,\Gamma(n_t)\,\Gamma(n_t-1)} \int_0^{\infty} \log\left[1 + \frac{\rho}{n_t}\,\lambda_1\right] \lambda_1^{n_t-2} \int_{\mathbb{R}^+} t^{n_t-1} \exp\big(-t\,\sigma^{-2}\lambda_1\big)\, \mathcal{W}(t)\, dt\, d\lambda_1\,.
\end{aligned} \tag{3.6}
$$

Proof: 1. The unordered density function of (2.9) is obtained by dividing by $n! = n_r! = 2!$:

$$f(\lambda_1,\lambda_2) = \frac{\pi^{2(2-1)}\left(\prod_{i=1}^{2}\lambda_i^{n_t-2}\right)\left(\prod_{k<l}^{2}(\lambda_k-\lambda_l)^2\right)}{2\,\mathcal{C}\Gamma_2(2)\,\mathcal{C}\Gamma_2(n_t)\,|\boldsymbol{\Sigma}|^2}\int_{\mathbb{R}^+} t^{2n_t}\,{}_0\mathcal{C}F_0^{(2)}\left(\boldsymbol{\Lambda},-t\,\boldsymbol{\Sigma}^{-1}\right)\mathcal{W}(t)\,dt\,.$$

In the same way as Theorem 3.1, integrating with respect to λ_2 and calculating the expectation of (3.1) leads to the final result.

2. The proof follows similarly where $\boldsymbol{\Sigma} = \sigma^2\boldsymbol{I}_2$. □

Corollary 3.2.

1. *For a two-input correlated Rayleigh-type channel,* $\boldsymbol{H} \sim \mathcal{C}t_{2\times n_t}(\boldsymbol{0}, \boldsymbol{I}_2\otimes\boldsymbol{\Sigma}, \nu)$, *with* $n_t \geq 2$, *the capacity* C *is given by*

$$\begin{aligned} C &= K\,\frac{\upsilon^\upsilon}{\Gamma(\upsilon)}\int_0^\infty\int_0^{\lambda_1}\left\{\log\left(1+\frac{\rho}{n_t}\lambda_1\right)+\log\left(1+\frac{\rho}{n_t}\lambda_1\right)\right\}(\lambda_1\lambda_2)^{n_t-2}(\lambda_1-\lambda_2) \\ &\quad\times\int_{\mathbb{R}^+} t^{n_t+\upsilon}e^{-t\upsilon}\det\left(\exp(-t\,a_i\,\lambda_j)\right)dt\,d\lambda_2\,d\lambda_1\,, \end{aligned} \tag{3.7}$$

where $K = \dfrac{\prod_{i=1}^{n_t} a_i^2}{2\,\Gamma(n_t)\,\Gamma(n_t-1)\prod_{k<l}^{n_t}(a_l-a_k)}$, *and* $a_1 > a_2 > \ldots > a_{n_t} > 0$ *are the eigenvalues of* $\boldsymbol{\Sigma}^{-1}$.

2. *For a two-input uncorrelated Rayleigh-type channel,* $\boldsymbol{H} \sim \mathcal{C}t_{2\times n_t}(\boldsymbol{0}, \boldsymbol{I}_2\otimes\sigma^2\boldsymbol{I}_{n_t}, \upsilon)$, *with* $n_t \geq 2$, *the capacity* C *is given by*

$$\begin{aligned} C &= \frac{\upsilon^\upsilon\,\Gamma(n_t+\upsilon+1)}{\sigma^{2n_t+2}\,\Gamma(\upsilon)\,\Gamma(n_t)}\int_0^\infty\log\left[1+\frac{\rho}{n_t}\lambda_1\right]\lambda_1^{n_t}\left(\frac{\lambda_1}{\sigma^2}+\upsilon\right)^{-(n_t+\upsilon+1)}d\lambda_1 \\ &\quad-\frac{2\,\upsilon^\upsilon\,\Gamma(n_t+\upsilon)}{\sigma^{2n_t}\,\Gamma(\upsilon)\,\Gamma(n_t-1)}\int_0^\infty\log\left[1+\frac{\rho}{n_t}\lambda_1\right]\lambda_1^{n_t-1}\left(\frac{\lambda_1}{\sigma^2}+\upsilon\right)^{-(n_t+\upsilon)}d\lambda_1 \\ &\quad+\frac{\upsilon^\upsilon\,\Gamma(n_t+\upsilon-1)\,\Gamma(n_t+1)}{\sigma^{2n_t-2}\,\Gamma(\upsilon)\,\Gamma(n_t)\,\Gamma(n_t-1)}\int_0^\infty\log\left[1+\frac{\rho}{n_t}\lambda_1\right]\lambda_1^{n_t-2}\left(\frac{\lambda_1}{\sigma^2}+\upsilon\right)^{-(n_t+\upsilon-1)}d\lambda_1\,. \end{aligned} \tag{3.8}$$

Figure 4 shows the calculated channel capacity (3.7) (correlation 0.9) and (3.8) (no correlation) versus SNR (ρ) for $n_t = 4$ and $\upsilon = 10$. Figure 5 illustrates the higher capacity for the underlying complex matrix variate t distribution versus the complex matrix variate normal distribution for the correlated nonsingular case.

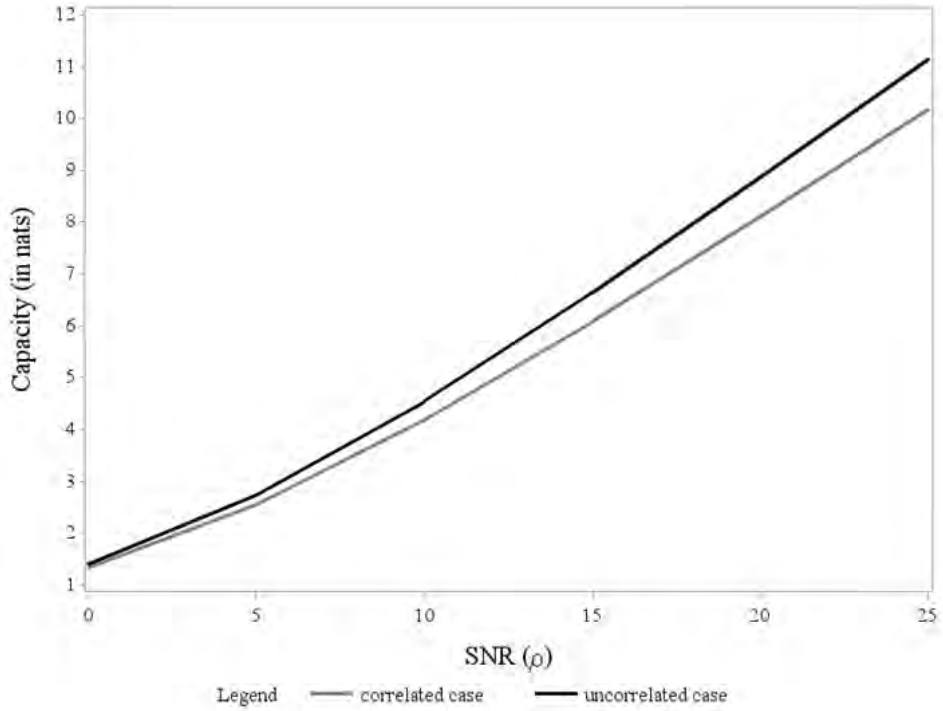

Figure 4: (3.7) and (3.8) against ρ, for $n_t = 4$.

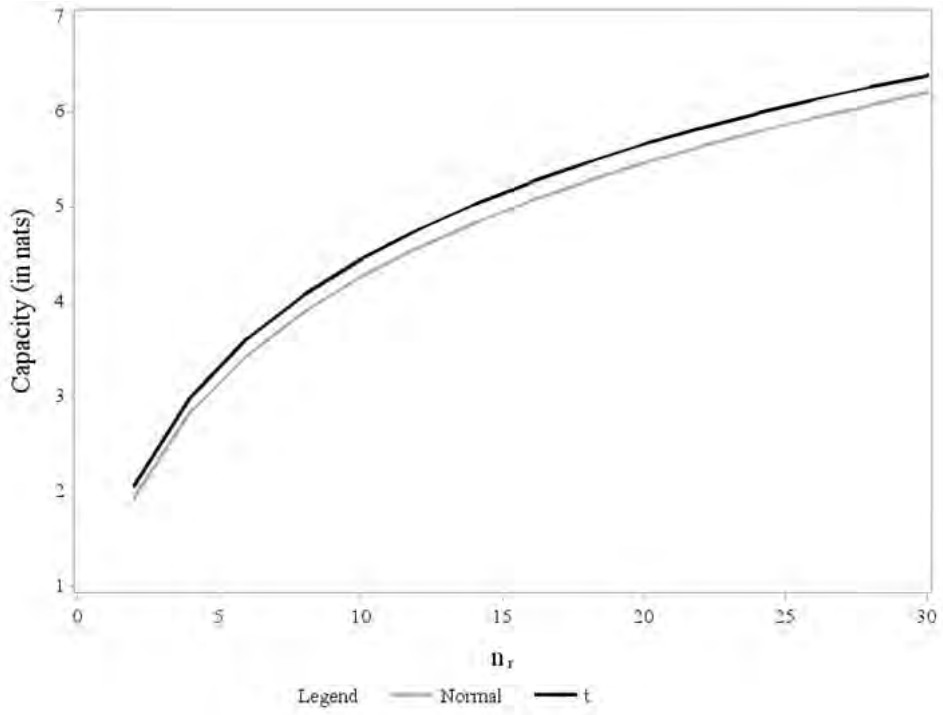

Figure 5: (3.4) and Eq. (29) from [16] against n_r, for $\rho, \upsilon = 10$.

4. CONCLUDING REMARKS

In this paper the distribution of the quadratic form and its associated joint eigenvalues with an underlying complex matrix variate elliptical model was derived. The proposed methodology is based on an integral representation that provides the researcher with expressions for allowing other underlying models than that of the normal, providing new insightful research possibilities. Some special cases were highlighted with the well-known Wishart distribution as a special case when the complex matrix variate normal distribution is under consideration. Another special case is that of no correlation; this case is of specific interest in the performance measure of channel capacity in the MIMO environment.

In particular the complex matrix variate t distribution was applied and the literature is enriched with its representation. The channel capacity within the MIMO environment is investigated for correlated and uncorrelated scenarios in the nonsingular and singular cases. It is observed that

(**1**) Correlation between transmitters/receivers degrade system capacity; and

(**2**) The capacity of the system is higher in the case of underlying complex matrix variate complex t distribution than that compared to an underlying complex matrix variate normal distribution.

When no correlation exists between receivers, the well-known central limit theorem can be assumed which results in $\boldsymbol{H} \sim \mathcal{C}N_{n_r \times n_t}(\mathbf{0}, \boldsymbol{I}_{n_r} \otimes \boldsymbol{\Sigma})$. However, this paper provides new possibilities in the wireless communications systems environment with the elliptical platform. In particular, the complex matrix variate t distribution is considered (as the t is a familiar candidate when placed alongside the normal). These numerical examples (see Figure 5) of the channel capacity show that the derived expressions under the complex matrix variate t distribution provide significant insights on the behaviour of performance measures when the assumption of the complex matrix variate normal distribution is challenged.

If the receivers and transmitters are correlated simultaneously, i.e. $\boldsymbol{H} \sim \mathcal{C}N_{n_r \times n_t}(\mathbf{0}, \boldsymbol{\Phi}_{n_r} \otimes \boldsymbol{\Sigma}_{n_t})$, then the well-known central limit theorem does not apply. In that case the complex matrix variate elliptical distribution may provide greater flexibility in this regard. Although the results in this paper are presented for the $\boldsymbol{I}_{n_r} \otimes \boldsymbol{\Sigma}$ and related cases, in the case of $\boldsymbol{\Phi}_{n_r} \otimes \boldsymbol{\Sigma}_{n_t}$ the covariance structure can be adapted to $\boldsymbol{I}_{n_r} \otimes \boldsymbol{\Sigma}$ via a transformation.

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PARAMETRIC ELLIPTICAL REGRESSION QUANTILES

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Abstract:

- The article extends linear and nonlinear quantile regression to the case of vector responses by generalizing multivariate elliptical quantiles to a regression context. In particular, it introduces parametric elliptical quantile regression in a general nonlinear multivariate heteroscedastic framework and discusses, investigates, and illustrates the new method in some detail, including basic properties, various parametrizations, possible heteroscedastic patterns, related computational issues, model validation, and a real biometric data example. The method seems suitable for multi-response regression models with symmetric errors, especially if the dimension of responses is less than ten and if the right parametrization of the model follows from the context.

Key-Words:

- *multiple-output regression; quantile regression; nonlinear regression; elliptical quantile.*

AMS Subject Classification:

- 62H12, 62J02, 62G05, 62G15, 62G35.

1. INTRODUCTION

Quantiles fully describe univariate probability distributions and may be very useful for statistical inference. Scalar random variables and their quantiles can often be expected to depend on some influential factors whose precise impact can be analyzed in the quantile regression framework, introduced in [23] and surveyed in [22]. Under weak moment assumptions, it models the entire conditional distribution of interest and not only its mean as the least squares approach. Therefore, it can reliably reveal even subtle changes in the conditional distribution that usually remain hidden in a conventional statistical analysis despite their possibly very important consequences. In fact, it is the tails of such conditional distributions that often contain much useful information and are thus very interesting for researchers in various fields such as finance and insurance, meteorology and climatology, labor and public economics, reliability and quality management, developmental studies, and medicine.

The everyday reality is usually intrinsically multivariate, and its successful analysis thus asks for multivariate quantiles. Unfortunately, they cannot be defined in a universally acceptable way because there exists no canonical way of ordering multivariate points and because all the attractive properties of univariate quantiles cannot be met simultaneously in a single multivariate quantile concept. Consequently, there already exist dozens of different multivariate quantile proposals that are usually based on data depth or spatial ranks, norm minimization or M-estimation, inversion of mappings, gradients, or generalized quantile processes; see, e.g., [33] for an overview.

Despite the abundance of the literature on multivariate quantiles (also called location quantiles), their regression generalizations are still scarce; see [18]. They may be either parametric (when the overall regression dependence is supposed to have a particular functional form), or nonparametric (when the overall dependence pattern is unknown). In the latter case, it is often possible to assume that the regression dependence is locally polynomial, which opens the door to the spline or locally polynomial (or, kernel) approach. Therefore, it makes perfect sense to call multivariate regression quantiles after the way they were obtained as parametric, nonparametric, or locally polynomial, for example. On the one hand, the parametric regression approach requires relatively strong assumptions regarding the particular form of regression dependence, on the other hand, it allows for general designs and implies standard consistency rates of related estimators (unlike its nonparametric competitors).

Most of the existing definitions of multivariate regression quantiles follow a directional strategy. They first define directional regression quantiles as simple objects (typically points or hyperplanes) and then use the directional objects for all directions to construct the resulting multivariate regression quantile (contour or region). The promising parametric proposals presented in [15, 16] and [29] are quite representative of this category and lead to the same multivariate regression quantile regions. Therefore, they will be considered as an established parametric golden standard and used as a benchmark hereinafter. They define a polyhedral multivariate regression quantile as the intersection of all directional regression quantile halfspaces of the same quantile level. They are implementable by means of [30, 31] and [2, 3], and applied, e.g., in [34] and [35]. The other proposals with directional flavor include [8], [25], [6], [9], [37], [26], [14], [7] and [4].

The alternative approach is not directional but direct (or, global) because it defines multivariate regression quantiles and related contours and regions directly, i.e., without any

auxiliary directional construction. Apart from the very recent (but not affine equivariant) proposal of [5] inspired by [10], this category mainly includes various regression extensions of the two proposals of multivariate quantiles with elliptical shapes (or, elliptical quantiles) that were presented in [20] and [21]. The former proposal was motivated by linear quantile regression, included even a heuristic definition of locally constant elliptical quantiles, and employed only convex optimization that turned out very useful for its analysis. Unfortunately, it could not be extended within its convex optimization setting to include robust or flexible parametric regression quantiles, which is why the latter generalized multivariate elliptical quantile concept was proposed as a remedy in [21]. It could not rely on convex optimization any more, but, on the other hand, it was very general and even covered the former approach as a special case, after a suitable reparametrization.

Now the parametric regression extension of the generalized multivariate elliptical quantiles of [21] is discussed, investigated, and illustrated here in a very general nonlinear heteroscedastic framework. An important particular case with unique features has been briefly introduced in [17] together with its examination by means of convex analysis. It is nicely complemented with the general theory derived in this article.

It should also be mentioned for the sake of completeness, that the generalized parametric elliptical regression quantiles considered here bear some similarity to multivariate regression S-estimators and their modifications (see, e.g., [1], [36], and [32]) that are not used for defining multivariate regression quantiles but also result from some location-scale or regression-scale models where the determinant of the shape-defining matrix plays a crucial role.

As the parametric elliptical regression quantiles also roughly order the regression space, they remotely resemble the depth-like notions for regression observations (see, e.g., [15], [29], [34], and [14]).

In [21], the generalized multivariate elliptical quantiles have been shown useful for symmetric distributions and highly competitive with the benchmark introduced above for elliptical distributions. Their parametric regression extensions appear to preserve most of their properties, but they should also be used only if their conditionally elliptical shape is acceptable and, ideally, if the conditional distribution is at least centrally symmetric, which is fortunately the case of all widely used error distributions. Then they are roughly on par with the benchmark in terms of natural nestedness, equivariance properties, and the ability to change with the quantile level and to capture the symmetry or ellipticity of the underlying conditional distribution.

However, the generalized parametric elliptical regression quantiles then also excel in other important aspects. Indeed, unlike the benchmark,

(**1**) they can easily incorporate homoscedasticity and many other types of a priori information regarding their conditional scales, shapes, and centers,

(**2**) their quantile levels can correspond directly to their probability content,

(**3**) they can be parametrized flexibly and very naturally by means of their conditional centers, shape matrices, and inflation (scaling) factors (whose estimates seem very useful for goodness-of-fit tests or for statistical inference regarding conditional location, dispersion, symmetry, or ellipticity),

(**4**) they can be quite robust to outliers,

(**5**) they can work well even in complicated cases involving nonlinear trend or heteroscedasticity, and

(**6**) their computation can be feasible even in the sample cases involving moderate dimensions and large data sets.

In fact, their development seems motivated by the lack of a multivariate regression quantile concept with such a combination of favorable properties. Of course, some of them hold only under certain assumptions on the joint distribution of responses and regressors and on the parametrization of the model. Nevertheless, (1), (3), and (6) are totally out of reach of any directional multivariate quantile regression method.

Most of the following text only clarifies and demonstrates the vaguely stated properties of the generalized elliptical regression quantiles (and the conditions of their validity). As they generally do not result from convex optimization, their computation in the sample case may be quite complicated and their uniqueness may not be guaranteed. Nevertheless, they must be unique in certain special cases including those of [17], and such a possible ambiguity is common to many popular robust or nonlinear estimators. It might even be viewed as a positive feature in some cases involving multimodal conditional distributions that may arise easily in the context of mixtures; see, e.g., [12]. Until the uniqueness issues are satisfactorily resolved, it is nevertheless recommended to use the generalized parametric elliptical regression quantiles cautiously, to experiment with various initial values for their computation in the sample case, and to prefer linearity in their parametrization whenever possible.

Although the generalized parametric elliptical regression quantiles presented here are still somewhat rigid due to the ellipticity woven into their definition, they are definitely worthy of wide attention and careful investigation because there is apparently no other multivariate quantile regression methodology enabling joint parametric nonlinear modeling of both trend and heteroscedasticity without any specific distributional assumptions. It seems that the parametric elliptical quantile regression presented here has great potential and that it could be used with benefits for vector responses in the same fields as the univariate quantile regression or wherever else the whole conditional response distributions or their tails or covariance structures are of interest. That is to say that (various) multivariate regression quantiles have already proved very useful in several instances, e.g., in investigating the dependence

(**1**) of a few kinds of expenditures on the total income [5],

(**2**) of both systolic and diastolic blood pressures on age [6] or on age and BMI [9],

(**3**) of sales growth and sales profitability on the creativity test score in evaluating the performance of salespersons [6],

(**4**) of weight and height on age [37, 26],

(**5**) of a few product characteristics on the time of production to take the tool wear into consideration in the definition of a precision index [35],

(**6**) of length/height or weight and head circumference on age [27],

(**7**) of female thigh and calf maximum girths on age, height, weight or BMI [15, 14],

(**8**) of male life expectancy and death rate on the GNP per capita [29], or

(**9**) of a few financial time series [11, 4].

Some of the cited articles describe the application and its benefits in detail and should be consulted in case of any remaining doubts.

This article further proceeds as follows. Section 2 presents necessary notation and introduces the definition of generalized elliptical regression quantiles, Section 3 studies their basic properties in the population case, Section 4 discusses their parametrization, Section 5 uses them to classify multivariate heteroscedasticity, Section 6 deals with their computation in the sample case, Section 7 proposes some tools for their validation, Section 8 illustrates them with a few carefully designed demo examples, Section 9 applies them to a referential biometric dataset, and concluding Section 10 comments on the previous results and achievements. Applied statisticians reading the article for the first time may skip the text after Definition 2.1 and go directly to Section 4 or 8.

2. DEFINITIONS AND NOTATION

Consider a general regression setup where an m-variate stochastic vector of responses $\boldsymbol{Y} = \big(Y^{(1)}, ..., Y^{(m)}\big)' \in \mathbb{R}^m$ is to be explained with the aid of the corresponding p-variate regressor $\boldsymbol{Z} \in \mathbb{R}^p$, and $(\boldsymbol{Y}', \boldsymbol{Z}')'$ has an absolutely continuous distribution with a density differentiable almost everywhere.

Recall that the standard location and regression quantiles of [23] can be defined for any $\tau \in (0,1)$ by means of the non-negative convex real-valued check function $\rho_\tau(t) = t\big(\tau - \mathrm{I}(t<0)\big) = \max\big\{(\tau-1)t, \tau t\big\}$ with a unique minimum. This function was also used in [20, 21] for defining two types of location elliptical quantiles. Here the second proposal is extended to a general parametric regression setup.

The next definition is rather complicated because it deals with the whole class of parametric elliptical regression quantiles indexed by quantile levels (τ) and certain monotone functions (g), and because the natural parameters characterizing the shape of possible elliptical regression quantile contours ($\varepsilon_{g,\tau}$) themselves depend on a common parameter vector (θ). Only its optimal value (θ_τ) resulting from a minimization problem is used in the definition.

Definition 2.1. For any $\tau \in (0,1)$ and any function g specified below, the parametric elliptical regression τ-g-quantile (contour) $\varepsilon_{g,\tau}(\boldsymbol{Y}, \boldsymbol{Z})$ and the corresponding lower and upper parametric τ-g-quantile regression regions $\mathcal{E}^-_{g,\tau}(\boldsymbol{Y}, \boldsymbol{Z})$ and $\mathcal{E}^+_{g,\tau}(\boldsymbol{Y}, \boldsymbol{Z})$ can be defined by means of the shape (matrix), trend (vector), and scale (scalar) quantile parameters $\mathbb{A}_\tau(\boldsymbol{\theta}, \boldsymbol{z}) \in \mathbb{R}^{m\times m}$, $\boldsymbol{s}_\tau(\boldsymbol{\theta}, \boldsymbol{z}) \in \mathbb{R}^m$, and $c_\tau(\boldsymbol{\theta}, \boldsymbol{z}) \in \mathbb{R}$ depending on $\boldsymbol{z} \in \mathbb{R}^p$ as well as on a common parameter vector $\boldsymbol{\theta} = (\theta_1, ..., \theta_q)' \in \mathbb{R}^q$:

$$\begin{aligned}
\varepsilon_{g,\tau}(\boldsymbol{Y}, \boldsymbol{Z}) &= \Big\{(\boldsymbol{y}, \boldsymbol{z}) \in \mathbb{R}^{m+p} \colon\ h_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{y}, \boldsymbol{z}) = 0\Big\}, \\
\mathcal{E}^-_{g,\tau}(\boldsymbol{Y}, \boldsymbol{Z}) &= \Big\{(\boldsymbol{y}, \boldsymbol{z}) \in \mathbb{R}^{m+p} \colon\ h_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{y}, \boldsymbol{z}) < 0\Big\}, \\
\mathcal{E}^+_{g,\tau}(\boldsymbol{Y}, \boldsymbol{Z}) &= \Big\{(\boldsymbol{y}, \boldsymbol{z}) \in \mathbb{R}^{m+p} \colon\ h_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{y}, \boldsymbol{z}) \geq 0\Big\},
\end{aligned}$$

where

$$h_\tau(\boldsymbol{\theta}, \boldsymbol{y}, \boldsymbol{z}) = g\Big(\big(\boldsymbol{y} - \boldsymbol{s}_\tau(\boldsymbol{\theta}, \boldsymbol{z})\big)' \mathbb{A}_\tau(\boldsymbol{\theta}, \boldsymbol{z}) \big(\boldsymbol{y} - \boldsymbol{s}_\tau(\boldsymbol{\theta}, \boldsymbol{z})\big)\Big) - c_\tau(\boldsymbol{\theta}, \boldsymbol{z}),$$

$g(t)\colon [0,\infty) \mapsto [0,\infty)$ is a suitable strictly increasing smooth function such that $g(0) = 0$, and $\boldsymbol{\theta}_\tau$ minimizes the objective function

$$\text{(OF)} \qquad \Psi_\tau(\boldsymbol{\theta}) = \mathrm{E}\,\rho_\tau\big(h_\tau(\boldsymbol{\theta}, \boldsymbol{Y}, \boldsymbol{Z})\big)$$

over the whole parametric space $\Theta_\tau \subset \mathbb{R}^q$, $\overline{\Theta}_\tau = \overline{\Theta_\tau^\circ}$, subject to a regularity constraint on $\mathbb{A}_\tau$ ensuring that $\mathbb{A}_\tau(\boldsymbol{\theta}, \boldsymbol{z}) \in \mathbb{R}^{m\times m}$ is always symmetric positive definite (its choice is discussed below). The definition also tacitly assumes that the expectation in (OF) is finite and that its partial derivatives with respect to $\boldsymbol{\theta}$ are exchangeable with the expectation sign.

The sets $\varepsilon_{g,\tau}(\boldsymbol{Y}, \boldsymbol{Z}) \cap \{(\boldsymbol{y}, \boldsymbol{z}) \in \mathbb{R}^{m+p} \colon \boldsymbol{z} = \boldsymbol{z}_0\}$, defined for any fixed $\boldsymbol{z}_0 \in \mathbb{R}^p$, will be conveniently called elliptical τ-g-quantile $\boldsymbol{z}_0$-cuts.

As far as the terminology is concerned, all the quantile-related adjectives, prefixes, indices, and arguments may be omitted on condition that they are either clear from the context or irrelevant to the statement being made.

Note that all the regression τ-g-quantile $\boldsymbol{z}_0$-cuts are ellipsoids and that their definition resembles that of multivariate elliptical quantiles of [21] if $\mathbb{A}_\tau$, $\boldsymbol{s}_\tau$, and c_τ are independent of $\boldsymbol{z}$ and the regularity constraint is of the form $\det \mathbb{A}_\tau(\boldsymbol{\theta}, \boldsymbol{z}) = 1$. This constraint seems optimal for achieving the best possible equivariance properties of the resulting elliptical regression τ-quantile entities and also from the statistical point of view, see [28], which is why it is exclusively considered here. This does not necessarily imply complete uselessness of all the other possible regularizations based on the eigenvalues of either $\mathbb{A}_\tau$ itself or of its product with a positive regressor-dependent scale factor; see [20] for some alternatives.

The definition of multivariate elliptical regression τ-g-quantiles is obviously very general. First of all, it allows for very general trend and heteroscedastic patterns with possible nonlinearity in unknown parameters and with arbitrary τ-dependence of g, q, Θ_τ, and the specifications for $\mathbb{A}_\tau$, $\boldsymbol{s}_\tau$, and c_τ. It also permits quite general interdependencies between $\mathbb{A}_\tau$, $\boldsymbol{s}_\tau$, and c_τ thanks to their common dependence on the same parametric vector. Nevertheless, it is recommended that practitioners invoke simplicity and linearity whenever possible and reduce the use of interdependencies to the absolute minimum.

Of course, if there is any information regarding $\boldsymbol{\theta}_\tau$ available in advance, then it can be used advantageously in the optimization of (OF). This might also give rise to some multipliers that could be useful for statistical inference like $\boldsymbol{\theta}_\tau$, $\Psi_\tau(\boldsymbol{\theta}_\tau)$, $\mathbb{A}_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$, $\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$, and $c_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$, possibly considered as functions of τ and g. That is to say that the choice of g matters in general and may have a huge impact on required moment assumptions as well as on the robustness and rigidity of the resulting elliptical regression quantile contours. In fact, the parametrization of quantile characteristics $\mathbb{A}_\tau$, $\boldsymbol{s}_\tau$, and c_τ is so important that it is repeatedly discussed throughout the next sections.

Unfortunately, the parametric elliptical regression τ-quantiles are not uniquely defined in the instances when $\Psi_\tau(\boldsymbol{\theta})$ attains multiple global minima, which is typical of all nonlinear regression estimators; see [21] for a slightly more detailed discussion of that in the generic multivariate case.

If the lack of robustness is not an issue, then $g_I(t) = t$ seems the best choice because it can often be reasonably expected to minimize the number of local minima of (OF) as well as the overall computational burden. This choice also produces the very special uniquely defined elliptical regression quantiles described and illustrated in [17]. If robustness is of high priority, then one should choose either $g(t) = t^\alpha$ for $\alpha < 1$ to preserve affine equivariance or perhaps g equal to a simple, bounded, and easy to compute function behaving like the identity function close to zero. However, if $\alpha < 0.5$ or g is bounded, then the objective function (OF) may

easily become misbehaving. This is why such choices cannot be recommended before such behavior and its consequences are fully clarified.

Obviously, the elliptical regression quantiles handle response outliers better than the design ones, because their robustness to design outliers may remain in question even for a bounded g due to the possible negative impact of $c_\tau(\boldsymbol{\theta}, \boldsymbol{z})$. This defect is unpleasant although $c_\tau(\boldsymbol{\theta}, \boldsymbol{z})$ unbounded in $\boldsymbol{z}$ need not always spoil the robustness too much and although it can be bounded easily by means of a suitable parametrization; see Figure 3 for a result of such an attempt.

The definition of the parametric elliptical regression quantiles is so general that one can hardly say anything special about them without further assumptions. The next section attempts to point out some of their favorable properties without sacrificing too much generality. The following terminology then comes in handy.

Definition 2.2. The parametrization of the elliptical regression τ-g-quantiles is called:

- **separable** if $\boldsymbol{\theta} = (\boldsymbol{\theta}_{\boldsymbol{s}}', \boldsymbol{\theta}_{\mathbb{A}}', \boldsymbol{\theta}_c')'$ and $\boldsymbol{s}_\tau(\boldsymbol{\theta})$, $\mathbb{A}_\tau(\boldsymbol{\theta})$, and $c_\tau(\boldsymbol{\theta})$ really depend solely on $\boldsymbol{\theta}_{\boldsymbol{s}}$, $\boldsymbol{\theta}_{\mathbb{A}}$, and $\boldsymbol{\theta}_c$, respectively;
- **reducible** in $\boldsymbol{s}_\tau$ if $\boldsymbol{s}_\tau(\boldsymbol{\theta}, \boldsymbol{z}) = \boldsymbol{s}_\tau^0 + \boldsymbol{s}_\tau^1(\boldsymbol{\theta}, \boldsymbol{z})$ where $\boldsymbol{s}_\tau^1$ is some function, and $\boldsymbol{s}_\tau^0$ is an m-dimensional subvector of $\boldsymbol{\theta}$ in which $\mathbb{A}_\tau(\boldsymbol{\theta})$, $c_\tau(\boldsymbol{\theta})$, and $\boldsymbol{s}_\tau^1(\boldsymbol{\theta})$ are constant;
- **reducible** in c_τ if $c_\tau(\boldsymbol{\theta}, \boldsymbol{z}) = c_\tau^0 + c_\tau^1(\boldsymbol{\theta}, \boldsymbol{z})$ where c_τ^1 is some function, and c_τ^0 is a scalar subvector of $\boldsymbol{\theta}$ in which $\boldsymbol{s}_\tau(\boldsymbol{\theta})$, $\mathbb{A}_\tau(\boldsymbol{\theta})$, and $c_\tau^1(\boldsymbol{\theta})$ are constant;
- **admissible** if there exists $\boldsymbol{\theta}_\tau^0 \in \Theta_\tau$ such that

$$\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau^0, \boldsymbol{z}) = \boldsymbol{s}_\tau^0(\boldsymbol{z}), \ \mathbb{A}_\tau(\boldsymbol{\theta}_\tau^0, \boldsymbol{z}) = \mathbb{A}_\tau^0(\boldsymbol{z}), \text{ and } c_\tau(\boldsymbol{\theta}_\tau^0, \boldsymbol{z}) = c_\tau^0(\boldsymbol{z})$$

  for almost all $\boldsymbol{z}$ where $\boldsymbol{s}_\tau^0(\boldsymbol{z})$, $\mathbb{A}_\tau^0(\boldsymbol{z})$, and $c_\tau^0(\boldsymbol{z})$ describe a multivariate elliptical τ-g-quantile of the conditional distribution of $\boldsymbol{Y}$ given $\boldsymbol{Z} = \boldsymbol{z}$, as defined in [21]. It means that $\boldsymbol{s}_\tau^0(\boldsymbol{z})$, $\mathbb{A}_\tau^0(\boldsymbol{z})$, and $c_\tau^0(\boldsymbol{z})$ jointly minimize the expectation (with respect to the conditional distribution)

$$\mathrm{E}_{\boldsymbol{Y}|\boldsymbol{Z}=\boldsymbol{z}}\, \rho_\tau\Big(g\big((\boldsymbol{Y}-\boldsymbol{s})'\mathbb{A}(\boldsymbol{Y}-\boldsymbol{s})\big) - c\Big)$$

  subject to the constraints that $\mathbb{A}$ is positive semidefinite and $\det(\mathbb{A}) = 1$.

The parametrization is therefore admissible if there exists $\boldsymbol{\theta}_\tau^0 \in \Theta_\tau$ such that the $\boldsymbol{z}$-cuts of the corresponding elliptical regression τ-g-quantile are equal to multivariate τ-g-quantiles of the conditional distributions of $\boldsymbol{Y}$ given $\boldsymbol{Z} = \boldsymbol{z}$ for almost all $\boldsymbol{z}$.

Example 2.1. Consider $\tau \in (0, 1)$ and $(\boldsymbol{Y}', \boldsymbol{Z}')'$ with a multivariate normal distribution or with a multivariate elliptical distribution having all required moments finite. Then any separable parametrization of elliptical regression τ-g-quantiles such that

1. $\mathbb{A}_\tau(\boldsymbol{\theta}, \boldsymbol{z})$, $\boldsymbol{\theta} \in \Theta_\tau$, does not depend on $\boldsymbol{z}$ and may become any positive definite matrix with unit determinant,
2. $\boldsymbol{s}_\tau(\boldsymbol{\theta}, \boldsymbol{z})$, $\boldsymbol{\theta} \in \Theta_\tau$, includes any affine function of $\boldsymbol{z}$, and
3. $c_\tau(\boldsymbol{\theta})$, $\boldsymbol{\theta} \in \Theta_\tau$, does not depend on $\boldsymbol{z}$ and may attain any positive value,

is admissible for any permitted g if it leads to the uniquely defined elliptical regression τ-g-quantile; see [13] and Theorem 3.5 below.

3. BASIC PROPERTIES

The justification for elliptical regression quantiles is based on their good properties in the special location case, resulting from the necessary gradient conditions of [21]. The conditions play such a prominent role that they deserve to be paraphrased below using current terminology:

Theorem 3.1. *Consider the special location case (without regressors) when* $(\boldsymbol{Y}', \boldsymbol{Z}') = \boldsymbol{Y}'$ *and the parameters* $\boldsymbol{s}_\tau$, $\mathbb{A}_\tau$, *and* c_τ *are constant. Then the elliptical* τ*-g-quantiles must satisfy the necessary conditions (1) to (4) of [21] that translate to*

$$1 = \det(\mathbb{A}_\tau)\,, \tag{3.1}$$

$$0 = P\big((\boldsymbol{Y}', \boldsymbol{Z}')' \in \mathcal{E}^-_{g,\tau}\big) - \tau\,, \tag{3.2}$$

$$\boldsymbol{0} = \frac{1}{1-\tau}\,\mathrm{E}\Big[\gamma\,\boldsymbol{R}_\tau\,\mathrm{I}_{[(\boldsymbol{Y}',\boldsymbol{Z}')'\in\mathcal{E}^+_{g,\tau}]}\Big] - \frac{1}{\tau}\,\mathrm{E}\Big[\gamma\,\boldsymbol{R}_\tau\,\mathrm{I}_{[(\boldsymbol{Y}',\boldsymbol{Z}')'\in\mathcal{E}^-_{g,\tau}]}\Big]\,, \tag{3.3}$$

and

$$L_\tau \frac{\det(\mathbb{A}_\tau)}{\tau(1-\tau)}\,\mathbb{A}_\tau^{-1} = \frac{1}{1-\tau}\,\mathrm{E}\Big[\gamma\,\boldsymbol{R}_\tau\boldsymbol{R}_\tau'\,\mathrm{I}_{[(\boldsymbol{Y}',\boldsymbol{Z}')'\in\mathcal{E}^+_{g,\tau}]}\Big] - \frac{1}{\tau}\,\mathrm{E}\Big[\gamma\,\boldsymbol{R}_\tau\boldsymbol{R}_\tau'\,\mathrm{I}_{[(\boldsymbol{Y}',\boldsymbol{Z}')'\in\mathcal{E}^-_{g,\tau}]}\Big]\,, \tag{3.4}$$

where $\mathbb{A}_\tau$ *is assumed symmetric positive semidefinite,* L_τ *is the Lagrange multiplier corresponding to the constraint* $-\det(\mathbb{A}_\tau) + 1 = 0$, $\boldsymbol{R}_\tau = \boldsymbol{Y} - \boldsymbol{s}_\tau$, $\dot g(t) := \partial g(t)/\partial t$, *and* $\gamma = \dot g(\boldsymbol{R}_\tau'\mathbb{A}_\tau\boldsymbol{R}_\tau)$.

The probability interpretation of the location elliptical quantiles then results from (3.2). If $g = g_I$, then $\gamma = 1$ and the conditions simplify considerably and become easy to interpret; see [21] for further details.

In the general regression context considered here, $\boldsymbol{s}_\tau$, $\mathbb{A}_\tau$, and c_τ may depend on $\boldsymbol{z}$ and on the common underlying parameter $\boldsymbol{\theta}$. Consequently, one should derive (OF) as a compound function and the derivatives of $\boldsymbol{s}_\tau$, $\mathbb{A}_\tau$, and c_τ with respect to $\boldsymbol{\theta}$ should also enter the scene.

If the properties of elliptical regression quantiles should naturally generalize those of the location ones, then only separable parametrizations reducible both in c_τ and $\boldsymbol{s}_\tau$ should be considered.

The next theorem summarizes some obvious special cases.

Theorem 3.2. *If the parametrization of the elliptical regression* τ*-quantiles*

- *is reducible in* c_τ, *then (3.2) holds;*
- *is reducible in* $\boldsymbol{s}_\tau$ *with* $\boldsymbol{z}$*-independent* $\mathbb{A}_\tau$, *then (3.3) holds;*
- *is separable and* $c_\tau = \boldsymbol{\theta}_L'\boldsymbol{z} + c_\tau^I(\boldsymbol{\theta}_c, \boldsymbol{z})$ *where* $\boldsymbol{\theta}_L$ *is a subvector of* $\boldsymbol{\theta}_c$ *in which* c_τ^I *is constant, then*

$$\boldsymbol{0} = \frac{1}{1-\tau}\,\mathrm{E}\Big[\boldsymbol{Z}\,\mathrm{I}_{[(\boldsymbol{Y}',\boldsymbol{Z}')'\in\mathcal{E}^+_{g,\tau}]}\Big] - \frac{1}{\tau}\,\mathrm{E}\Big[\boldsymbol{Z}\,\mathrm{I}_{[(\boldsymbol{Y}',\boldsymbol{Z}')'\in\mathcal{E}^-_{g,\tau}]}\Big]\,.$$

Assume that all the three conditions are satisfied. Then the population parametric elliptical regression quantiles have a clear probability interpretation, $\mathcal{E}^{-}_{g,\tau}$ is nonempty for $\tau > 0$, and the centers of probability mass of $\mathcal{E}^{-}_{g,\tau}(\boldsymbol{Y}, \boldsymbol{Z})$ and $\mathcal{E}^{+}_{g,\tau}(\boldsymbol{Y}, \boldsymbol{Z})$ have the same $\boldsymbol{z}$-coordinates. The second claim then meaningfully links the probability mass centers of scaled residuals $\gamma(\boldsymbol{Y} - \boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{Z}))$ corresponding to the regression observations in $\mathcal{E}^{-}_{g,\tau}(\boldsymbol{Y}, \boldsymbol{Z})$ and $\mathcal{E}^{+}_{g,\tau}(\boldsymbol{Y}, \boldsymbol{Z})$.

Every reasonable multivariate quantile regression concept should also exhibit good equivariance properties. The parametric elliptical quantile regression need not be an exception in this regard. What really matters is how $\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau)$, $\mathbb{A}_\tau(\boldsymbol{\theta}_\tau)$, and $c_\tau(\boldsymbol{\theta}_\tau)$ change with the transformations of $\boldsymbol{Y}$, and this follows directly from the location case of [21].

Definition 3.1. The parametrization of elliptical regression τ-g-quantiles is called affine equivariant if $g(t) = t^r$ for some $r > 0$ and if, for any $\boldsymbol{a} \in \mathbb{R}^m$, any regular $m \times m$ matrix $\mathbb{B}$ (with determinant d), and any $\boldsymbol{\theta} \in \Theta_\tau$, there exists $\boldsymbol{\theta}_{\mathbb{B},\boldsymbol{a},d} \in \Theta_\tau$ such that

$$\mathbb{A}_\tau(\boldsymbol{\theta}_{\mathbb{B},\boldsymbol{a},d}, \boldsymbol{z}) = d^2\big(\mathbb{B}^{-1}\big)'\mathbb{A}_\tau(\boldsymbol{\theta}, \boldsymbol{z})\,\mathbb{B}^{-1}\,, \tag{3.5}$$

$$\boldsymbol{s}_\tau(\boldsymbol{\theta}_{\mathbb{B},\boldsymbol{a},d}, \boldsymbol{z}) = \boldsymbol{a} + \mathbb{B}\,\boldsymbol{s}_\tau(\boldsymbol{\theta}, \boldsymbol{z})\,, \tag{3.6}$$

and

$$c_\tau(\boldsymbol{\theta}_{\mathbb{B},\boldsymbol{a},d}, \boldsymbol{z}) = g\Big(d^2\, g^{-1}\big(c_\tau(\boldsymbol{\theta}, \boldsymbol{z})\big)\Big) \tag{3.7}$$

for all $\boldsymbol{z}$. If (3.5), (3.6) and (3.7) hold for $d = 1$, then the parametrization is called shift and rotation equivariant, even if g is not a polynomial.

Theorem 3.3. *If the parametrization of elliptical regression τ-quantiles is affine equivariant, then the resulting elliptical regression τ-quantiles are affine equivariant. If it is shift and rotation equivariant, then the resulting elliptical regression τ-quantiles are shift and rotation equivariant.*

Proof: If $\boldsymbol{\theta} \in \Theta_\tau$ minimizes (OF) for random vector $(\boldsymbol{Y}', \boldsymbol{Z}')' \in \mathbb{R}^{m+p}$, then corresponding $\boldsymbol{\theta}_{\mathbb{B},\boldsymbol{a},d} \in \Theta_\tau$ from the above definition of the equivariant parametrization obviously minimizes (OF) for random vector $\big((\boldsymbol{a} + \mathbb{B}\boldsymbol{Y})', \boldsymbol{Z}'\big)' \in \mathbb{R}^{m+p}$ for any $\boldsymbol{a} \in \mathbb{R}^m$ and any regular $m \times m$ matrix $\mathbb{B}$ with determinant d. □

In other words, if the elliptical regression τ-quantile of $(\boldsymbol{Y}', \boldsymbol{Z}')'$ is parametrized with $\mathbb{A}_\tau$, $\boldsymbol{s}_\tau$, and c_τ by means of an affine equivariant parametrization, then the elliptical regression τ-quantile of $\big((\boldsymbol{a} + \mathbb{B}\boldsymbol{Y})', \boldsymbol{Z}'\big)'$ can be parametrized with $d^2\big(\mathbb{B}^{-1}\big)'\mathbb{A}_\tau\mathbb{B}^{-1}$, $\boldsymbol{a} + \mathbb{B}\boldsymbol{s}_\tau$, and $g\big(d^2 g^{-1}\big(c_\tau(\boldsymbol{\theta}, \boldsymbol{z})\big)\big)$.

The graph of $\Psi_\tau(\boldsymbol{\theta})$ crucially influences the process of optimization. The following consequences of convex calculus might serve as a guidance for choosing g and minimizing the troubles with the optimization of $\Psi_\tau(\boldsymbol{\theta})$.

Theorem 3.4. *Assume a separable parametrization of the elliptical regression τ-g-quantiles with $\boldsymbol{\theta} = (\boldsymbol{\theta}'_{\boldsymbol{s}}, \boldsymbol{\theta}'_{\mathbb{A}}, \boldsymbol{\theta}'_c)'$.*

- *If $g = g_I$, then Ψ_τ is convex in $\mathbb{A}_\tau$.*
- *If c_τ is linear in $\boldsymbol{\theta}_c$, then $\Psi_\tau(\boldsymbol{\theta})$ is convex in $\boldsymbol{\theta}_c$.*

In fact, $g = g_I$ may easily lead to uniquely defined parametric elliptical regression quantiles; see [17].

Generally speaking, the good properties of multivariate elliptical quantiles extend to the elliptical regression quantiles with admissible and affine equivariant parametrizations.

Theorem 3.5. *Let $\tau \in (0,1)$ and $f(\boldsymbol{y},\boldsymbol{z}) = f_1(\boldsymbol{y}|\boldsymbol{z})\, f_2(\boldsymbol{z})$ be the density of $(\boldsymbol{Y}', \boldsymbol{Z}')' \in \mathbb{R}^{m+p}$ where $f_2(\boldsymbol{z})$ is the marginal density of $\boldsymbol{Z}$ and $f_1(\boldsymbol{y}|\boldsymbol{z})$ is the regularized version of the density of the conditional distribution of $\boldsymbol{Y}$ given $\boldsymbol{Z} = \boldsymbol{z}$ that is assumed to exist.*

If the parametrization $\mathbb{A}_\tau(\boldsymbol{\theta},\boldsymbol{z})$, $\boldsymbol{s}_\tau(\boldsymbol{\theta},\boldsymbol{z})$, and $c_\tau(\boldsymbol{\theta},\boldsymbol{z})$ of the elliptical regression τ-quantile is admissible, then there exists $\boldsymbol{\theta}_\tau \in \Theta_\tau$ minimizing (OF). If for any orthonormal matrix $\mathbb{O}$ there exists $\widetilde{\boldsymbol{\theta}}_\tau(\mathbb{O}) \in \Theta_\tau$ such that $\mathbb{A}_\tau(\widetilde{\boldsymbol{\theta}}_\tau(\mathbb{O}),\boldsymbol{z}) = \mathbb{O}'\mathbb{A}_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z})\,\mathbb{O}$, $c_\tau(\widetilde{\boldsymbol{\theta}}_\tau(\mathbb{O}),\boldsymbol{z}) = c_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z})$, and $\boldsymbol{s}_\tau(\widetilde{\boldsymbol{\theta}}_\tau(\mathbb{O}),\boldsymbol{z}) = \boldsymbol{\mu}(\boldsymbol{z}) + \mathbb{O}'\big(\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z}) - \boldsymbol{\mu}(\boldsymbol{z})\big)$ for the particular $\boldsymbol{\mu}$ appearing below, and

- [**1**] *if $f_1(\boldsymbol{y}|\boldsymbol{z}) = f_1\big(\boldsymbol{\mu}(\boldsymbol{z}) + \mathbb{O}(\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{z}))\,|\,\boldsymbol{z}\big)$ for some function $\boldsymbol{\mu} = (\mu_1,...,\mu_m)'$ and for an orthonormal matrix $\mathbb{O} = \mathbb{O}^{-1'}$, then there exists an elliptical regression τ-quantile parametrized with $\mathbb{A}_\tau(\widetilde{\boldsymbol{\theta}}_\tau(\mathbb{O}),\boldsymbol{z})$, $\boldsymbol{s}_\tau(\widetilde{\boldsymbol{\theta}}_\tau(\mathbb{O}),\boldsymbol{z})$, and $c_\tau(\widetilde{\boldsymbol{\theta}}_\tau(\mathbb{O}),\boldsymbol{z})$.*

If the elliptical regression τ-quantile is moreover uniquely defined, then

- [**2**] *if $\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z}) = (s_1,...,s_m)(\boldsymbol{z})'$, $\mathbb{A}_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z}) = (a_{ij}(\boldsymbol{z}))_{i,j=1}^m$, and $f_1(\boldsymbol{y}|\boldsymbol{z}) = f_1\big(\boldsymbol{\mu}(\boldsymbol{z}) + \mathbb{J}(\boldsymbol{y} - \boldsymbol{\mu}(\boldsymbol{z}))\,|\,\boldsymbol{z}\big)$ for all $\boldsymbol{z}$ and a sign-change matrix $\mathbb{J} = \mathbb{J}' = \mathbb{J}^{-1} = \mathrm{diag}(j_1,...,j_m)$ with diagonal elements ± 1, then $s_i(\boldsymbol{z}) = \mu_i(\boldsymbol{z})$ whenever $j_i = -1$, $i \in \{1,...,m\}$, and $a_{ij}(\boldsymbol{z}) = 0$ whenever $j_i j_j = -1$, $i,j \in \{1,...,m\}$;*
- [**3**] *if all the conditional distributions of $\boldsymbol{Y}$ given $\boldsymbol{Z} = \boldsymbol{z}$ are centrally symmetric around their center of symmetry $\boldsymbol{\mu}(\boldsymbol{z})$, then $\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z}) = \boldsymbol{\mu}(\boldsymbol{z})$;*
- [**4**] *if all the conditional distributions of $\boldsymbol{Y}$ given $\boldsymbol{Z} = \boldsymbol{z}$ centered with $\boldsymbol{\mu}(\boldsymbol{z})$ are symmetric around a common hyperplane H, then $\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z}) - \boldsymbol{\mu}(\boldsymbol{z})$ lies on H;*
- [**5**] *if all the conditional distributions of $\boldsymbol{Y}$ given $\boldsymbol{Z} = \boldsymbol{z}$ centered with $\boldsymbol{\mu}(\boldsymbol{z})$ are symmetric along a common axis o, then $\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z}) - \boldsymbol{\mu}(\boldsymbol{z})$ lies on that axis.*

Proof: As for [1], the assumed admissible parametrization guarantees that there exists $\boldsymbol{\theta}_\tau \in \Theta_\tau$ such that $\mathbb{A}_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z})$, $\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z})$, and $c_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z})$ minimize $\Phi_\tau^{\boldsymbol{z}}(\mathbb{A},\boldsymbol{s},c) := \mathrm{E}_{\boldsymbol{Y}|\boldsymbol{Z}=\boldsymbol{z}}\,\rho_\tau\big(g\big((\boldsymbol{Y}-\boldsymbol{s})'\,\mathbb{A}(\boldsymbol{Y}-\boldsymbol{s})\big) - c\big)$ for almost all $\boldsymbol{z}$. Therefore, they minimize (OF) as well. The assumption on the conditional density further implies $\Phi_\tau^{\boldsymbol{z}}(\mathbb{A}_\tau,\boldsymbol{s}_\tau,c_\tau) = \Phi_\tau^{\boldsymbol{z}}\big(\mathbb{O}'\mathbb{A}_\tau\mathbb{O}, \boldsymbol{\mu}(\boldsymbol{z}) + \mathbb{O}'(\boldsymbol{s}_\tau - \boldsymbol{\mu}(\boldsymbol{z})), c_\tau\big)$, and thus $\mathbb{O}'\mathbb{A}_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z})\,\mathbb{O}$, $\boldsymbol{\mu}(\boldsymbol{z}) + \mathbb{O}'\big(\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z}) - \boldsymbol{\mu}(\boldsymbol{z})\big)$ and $c_\tau(\boldsymbol{\theta}_\tau,\boldsymbol{z})$ also minimize not only the same conditional expectation for almost all $\boldsymbol{z}$, but also (OF) as well, and, therefore, they also describe an elliptical regression τ-quantile thanks to the assumed existence of $\widetilde{\boldsymbol{\theta}}_\tau(\mathbb{O})$.

As for [2], it follows directly from [1] because matrix $\mathbb{J}$ is orthonormal. Only the two elliptical regression τ-quantiles from [1] must now coincide due to the uniqueness assumption. This fact implies $s_i(\boldsymbol{z}) = \mu_i(\boldsymbol{z})$ whenever $j_i = -1$, and $a_{ij}(\boldsymbol{z}) = 0$ whenever $j_i j_j = -1$, $i,j \in \{1,...,m\}$. Furthermore, [2] implies [3] for $\mathbb{J} = -\mathbb{I}$. The rest ([4] and [5]) analogously results from [1] and [2] for certain orthonormal matrices. □

Note 3.1. In [1], [2], and [3], it would be enough to assume the existence of $\widetilde{\boldsymbol{\theta}}_\tau(\mathbb{O}) \in \Theta_\tau$ only for the particular orthonormal matrices $\mathbb{O}$ considered there. In fact, the statements [2] to [5] could be proved directly by generalizing the location case with similar behavior regarding symmetry, only with the requirement of an admissible parametrization and without any need of $\widetilde{\boldsymbol{\theta}}_\tau(\mathbb{O})$ for some orthonormal matrices $\mathbb{O}$.

Note 3.2. The somewhat analogous Theorem 1 of [21] and its proof unfortunately contain a couple of misprints and one error. First, any occurrence of $\mathbb{O}\boldsymbol{s}_\tau$ should be replaced with $\mathbb{O}'\boldsymbol{s}_\tau$ there. Second, the proof should apply (2) to (6), not (2)–(6). And most importantly, the natural behavior of generalized elliptical quantiles under affine transformations of the response vector, postulated by Theorem 1 (1), is there falsely interpreted as full affine equivariance for any function g, which invalidates the proofs of further statements (3), (4), (5), and (10). While the generalized elliptical quantiles are always shift and rotation equivariant, they are certain to be fully affine equivariant only for $g(t) = t^\alpha$, $\alpha > 0$. Consequently, the statements (3), (4), (5), and (10) there hold only for such functions g or for spherical distributions. The claims (6)–(9) there really require only rotation and shift equivariance and, therefore, remain valid for any function g as they stand.

The uniqueness assumption used in Theorem 3.5 is not as severe as it might seem at first sight. That is to say that what really matters is only the uniqueness of $\mathbb{A}_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$, $\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$ and $\boldsymbol{c}_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$ in the population case.

Any admissible parametrization by definition guarantees the existence of such $\boldsymbol{\theta}_0 \in \Theta_\tau$ that (for almost all $\boldsymbol{z}$) minimizes the (non-negative finite) conditional expectation of $\rho_\tau(h_\tau(\boldsymbol{\theta}, \boldsymbol{Y}, \boldsymbol{Z}))$ (with respect to the conditional distribution of $\boldsymbol{Y}$ given $\boldsymbol{Z} = \boldsymbol{z}$). This implies that the same $\boldsymbol{\theta}_0$ also minimizes its unconditional (finite) expectation (OF). Therefore, the parameter vector $\boldsymbol{\theta}_0 \in \Theta_\tau$ also defines an elliptical regression τ-quantile that is uniquely defined if all the purely multivariate elliptical τ-quantiles of $\mathcal{L}(\boldsymbol{Y} \,|\, \boldsymbol{Z} = \boldsymbol{z})$ are uniquely defined. The uniqueness of multivariate elliptical τ-quantiles has been studied in [20, 21] and established for $g(t) = t$ under very mild conditions. Consequently, the aforementioned considerations extend the uniqueness result even to elliptical regression quantiles with $g(t) = t$ and admissible parametrizations. This is why $g(t) = t$ is generally preferred to other possibilities for the time being.

Unfortunately, ill-specified models for elliptical regression quantiles generally need not lead to a unique solution even for $g(t) = t$. This is typical of all nonlinear regression methods. Nevertheless, there exist certain natural parametrizations with $g(t) = t$ that lead to unique elliptical regression quantiles even if the model is misspecified; see [17].

4. THE ART OF PARAMETRIZATION

The parametrization of $\boldsymbol{s}_\tau$ follows directly from available preconceptions regarding the multivariate trend, and that of c_τ also often results from the context quite easily. One choice can be nevertheless much better than its formal equivalents from the computational point of view; see Section 6.

On the contrary, it need not be that clear how to parametrize $\mathbb{A}_\tau$ to keep it positive definite with unit determinant so that one could avoid all the restrictions and constrained optimization. In the case of bivariate responses with $m = 2$, there are several possibilities at hand, e.g.

$$\mathbb{A}_\tau(\boldsymbol{\theta}, \boldsymbol{z}) = \begin{pmatrix} a_{11}^2 & a_{12} \\ a_{12} & (1 + a_{12}^2)/a_{11}^2 \end{pmatrix}, \tag{4.1}$$

$$\mathbb{A}_\tau(\boldsymbol{\theta}, \boldsymbol{z}) = \begin{pmatrix} c_1 & c_2 \\ 0 & \frac{1}{c_1} \end{pmatrix}' \begin{pmatrix} c_1 & c_2 \\ 0 & \frac{1}{c_1} \end{pmatrix} = \begin{pmatrix} c_1^2 & c_1 c_2 \\ c_1 c_2 & c_2^2 + \frac{1}{c_1^2} \end{pmatrix}, \tag{4.2}$$

or

$$\mathbb{A}_\tau(\boldsymbol{\theta}, \boldsymbol{z}) = \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{pmatrix}' \begin{pmatrix} d^2 & 0 \\ 0 & \frac{1}{d^2} \end{pmatrix} \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{pmatrix}, \tag{4.3}$$

where the obvious dependence of a_{11}, a_{12}, c_1, c_2, α, and d^2 on τ, $\boldsymbol{\theta}$, and $\boldsymbol{z}$ is not emphasized for the sake of brevity. Of course, one could also consider $\exp(a_{11})$ and $\exp(d)$ instead of a_{11}^2 and d^2, not to mention other alternatives in the same spirit.

Clearly, (4.1) is the most straightforward possibility but it can hardly be generalized beyond dimension $m = 2$ or $m = 3$. On the other hand, (4.2) follows from the Choleski decomposition advocated in [21] and it can be easily adjusted to any dimension of the responses. The third example (4.3) results from the spectral decomposition and it also can be extended to general multivariate response settings, though in a rather complicated way.

The optimal choice of parametrization for $\mathbb{A}_\tau$ crucially depends on the type of expected heteroscedasticity. The spectral decomposition in (4.3) appears very appealing due to its easy and natural interpretation. Unfortunately, such a parametrization of a positive definite matrix is not unique without further assumptions regarding the angles and/or the diagonal elements of the sandwiched matrix. Sometimes one can give up the uniqueness, find a solution, and then transform it to a canonical form without any harm. One could also use the well-worn tricks how to enforce one parameter higher than the other or in a certain range. The choices may depend on the expected model, which shifts the modeling from a boring routine to sophisticated art.

In the cases of homoscedasticity and multiplicative heteroscedasticity described below and corresponding to constant $\mathbb{A}_\tau$, one can simply avoid all such problems by using the parametrization based on the Choleski decomposition, which is generally recommended in such situations.

5. CLASSIFICATION OF HETEROSCEDASTICITY

Assume that a correctly specified elliptical quantile regression model for bivariate responses leads to a unique solution $\mathbb{A}_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$, $\boldsymbol{s}_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$, and $c_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$, with $\mathbb{A}_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$ parametrized by means of $\alpha_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$ and $d_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$ as in (4.3). Then it makes sense to speak of τ-level homoscedasticity when $\alpha_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$, $c_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$, and $d_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$ are all independent of $\boldsymbol{z}$. Furthermore, it is possible to distinguish three canonical τ-level heteroscedastic patterns corresponding to the cases when only one of the characteristics $\alpha_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$, $c_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$, and $d_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$ depends on $\boldsymbol{z}$:

(**1**) rotational heteroscedasticity (if only $\alpha_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$ is $\boldsymbol{z}$-dependent),

(**2**) multiplicative (or scale) heteroscedasticity (if only $c_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$ is $\boldsymbol{z}$-dependent), and

(**3**) proportional heteroscedasticity (if only $d_\tau(\boldsymbol{\theta}_\tau, \boldsymbol{z})$ is $\boldsymbol{z}$-dependent).

Any type of bivariate heteroscedasticity can then be decomposed into the three canonical forms. See Figure 1 for an illustration of this classification.

If these heteroscedastic patterns are observed for all $\tau \in (0, 1)$, then one can speak of τ-independent heteroscedastic patterns. If they are observed only locally in τ or $\boldsymbol{z}$, then one can speak of local heteroscedastic patterns. This terminology can be adopted even informally when the true underlying model is unknown but its heteroscedastic profile slightly resembles that of elliptical quantile regression.

The situation becomes more complicated in case of multivariate responses, but even then the classification can still be used for any couple of their coordinates and the terms like overall rotational/proportional/multiplicative heteroscedasticity still make perfect sense.

Although the multiplicative heteroscedasticity seems by far the most common, the others are not necessarily extinct but maybe only hidden because the ways available for their detection and modeling are rather limited and unpopular, at least for the time being. For example, the rotational heteroscedasticity may be dormant in the data observed by the satellites orbiting the Earth. And it is demonstrated below in Section 9 that it might be present even in biometric data.

6. COMPUTATION

The sample elliptical regression τ-g-quantiles can be obtained directly from the definition if the expectation in (OF) is taken with respect to the discrete empirical probability distribution. Consider n responses $\boldsymbol{Y}_i$'s accompanied with corresponding regressor vectors $\boldsymbol{Z}_i$'s, $i = 1, ..., n$, from the population distribution assumed above. Even if all the constraints on $\mathbb{A}_\tau$ are removed in the way described in Section 4, then it still remains to solve the unconstrained optimization problem

$$\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \rho_\tau\big(h_\tau(\boldsymbol{\theta}, \boldsymbol{Y}_i, \boldsymbol{Z}_i)\big)$$

for appropriate h_τ where the objective function is generally neither smooth nor convex. Of course, it could be done with a suitable general solver for non-convex optimization. Fortunately, this problem can also be viewed as a nonlinear quantile regression task with zero responses and regressors $(\boldsymbol{Y}_i', \boldsymbol{Z}_i')'$, $i = 1, ..., n$, that has already been studied successfully, see [22], and can be solved for differentiable h_τ with the special algorithm developed in [24] whose MATLAB implementation in IPQR.M, available at http://sites.stat.psu.edu/~dhunter/code/qrmatlab, had been tuned up and used for the computation of all the sample parametric elliptical regression g-quantiles presented in the next sections. In other words, the parametric elliptical regression quantiles can be computed like their location predecessors of [21].

Unfortunately, the algorithm of [24] must be initialized with a preliminary estimate of $\boldsymbol{\theta}_\tau$.

This is a stage when any available information about the estimated vector parameter can be employed advantageously. Of course, one should experiment with several wise choices of initial parameters and then choose the solution according to the final parameter estimators and corresponding values of the minimized objective function. If some not-so-complicated regression models were considered, then one might also fit each response component by means of single-response quantile regression and use the resulting parameter estimates to initialize the algorithm. A few multivariate quantile cuts obtained from other multi-response quantile regression method(s) could also be mined for some information leading to the initial parameter estimates.

The parametrization of the problem also matters as one can lead to the successful end much more quickly and easily than another. From this point of view, it is strongly recommended to avoid nonlinearities whenever possible. If the Jacobian derived from h_τ is singular from the very beginning or becomes singular or close to singular during the computation, then insuperable numerical problems can be expected, which also speaks for using well-thought-out parametrizations and parameter initializations. For example, such a situation may happen for $d^2 = 1$ if the parametrization (4.3) is used for $\mathbb{A}_\tau$.

The computational side of many nonlinear regression methods is not ideal and the parametric elliptical quantile regression is no exception in this regard. But one can hardly hope for anything else if the model is genuinely nonlinear and non-convex in its parameters.

7. MODEL VALIDATION

This section suggests a few heuristic ways how to validate the resulting elliptical quantile regression models before the topic is treated elsewhere in full detail and exactness. The first two are commonly used in the ordinary least squares regression.

Suppose that n regression observations $(\boldsymbol{Y}_i', \boldsymbol{Z}_i')'$, $i = 1, ..., n$, were fitted with a generalized parametric elliptical (τ-g-)quantile regression model leading to unique quantile parameter estimates $\mathbb{A}(\widehat{\boldsymbol{\theta}}, \boldsymbol{z})$, $\boldsymbol{s}(\widehat{\boldsymbol{\theta}}, \boldsymbol{z})$, $c(\widehat{\boldsymbol{\theta}}, \boldsymbol{z})$, and to homogenized (pseudo)residuals $r_i(\widehat{\boldsymbol{\theta}}) := h(\widehat{\boldsymbol{\theta}}, \boldsymbol{Y}_i, \boldsymbol{Z}_i)$, $i = 1, ..., n$; see Definition 2.1 for the origin of h.

One can then use the cross-validation approach to look for outliers or influential observations. In other words, the impact of some observation(s) can be evaluated by means of the differences $\widehat{\boldsymbol{\theta}} - \widehat{\boldsymbol{\theta}}_-$, $\Psi(\widehat{\boldsymbol{\theta}}) - \Psi(\widehat{\boldsymbol{\theta}}_-)$, $c(\widehat{\boldsymbol{\theta}}, \boldsymbol{z}) - c(\widehat{\boldsymbol{\theta}}_-, \boldsymbol{z})$, $g^{-1}(c(\widehat{\boldsymbol{\theta}}, \boldsymbol{z})) - g^{-1}(c(\widehat{\boldsymbol{\theta}}_-, \boldsymbol{z}))$, $\boldsymbol{s}(\widehat{\boldsymbol{\theta}}, \boldsymbol{z}) - \boldsymbol{s}(\widehat{\boldsymbol{\theta}}_-, \boldsymbol{z})$, $\mathbb{A}(\widehat{\boldsymbol{\theta}}, \boldsymbol{z}) - \mathbb{A}(\widehat{\boldsymbol{\theta}}_-, \boldsymbol{z})$, $\mathbb{A}^{-1}(\widehat{\boldsymbol{\theta}}, \boldsymbol{z}) - \mathbb{A}^{-1}(\widehat{\boldsymbol{\theta}}_-, \boldsymbol{z})$, $r_i(\widehat{\boldsymbol{\theta}}) - r_i(\widehat{\boldsymbol{\theta}}_-)$, and their parts or norms where $\widehat{\boldsymbol{\theta}}_-$ is the quantile coefficient estimate obtained by excluding the suspected observation(s) from the sample. Of course, the differences of the whole quantile cuts corresponding to $\widehat{\boldsymbol{\theta}}$ and $\widehat{\boldsymbol{\theta}}_-$ could also be investigated. And it would be wise to consult such differences even in testing various submodels where the role of $\widehat{\boldsymbol{\theta}}_-$ would be played by the optimal estimate of $\boldsymbol{\theta}$ in the restricted model.

One could also inspect various charts to check the behavior of the homogenized (pseudo) residuals. In a well-specified model, they should be (roughly) mutually independent, identically distributed, and independent of the covariates (and also of the responses if all the conditional distributions were elliptical). For example, one may plot r_i or r_i^2 on their lagged values and (the norms or components of) $\boldsymbol{Y}_i$ and $\boldsymbol{Z}_i$, $i = 1, ..., n$.

One could verify as well whether the estimated quantile cuts share their centers, axes, and hyperplanes of symmetry with the expected conditional distributions. The opposite might imply that the model assumptions were wrong, owing to Theorem 3.5.

If $c(\widehat{\boldsymbol{\theta}}, \boldsymbol{z})$ is unexpectedly negative for common regressor values, then there must be something wrong with the model specification too.

Finally, one might also validate the model by comparing the resulting quantile cuts with those obtained with another multivariate quantile regression method that requires even weaker assumptions and is still applicable to the data. Depending on the context, the benchmark or the nonparametric proposals of [26], [20], [14] or [4] could often serve the purpose quite well.

8. ILLUSTRATIONS

This section presents some pictures to support the claim that the parametric elliptical regression g-quantiles are indeed promising candidates for wide dissemination thanks to their many good properties. For the sake of simplicity, only the most often recommended natural choice $g_I(t) = t$ is considered hereinafter.

Unfortunately, the precise rules for choosing g in different situations are still to be developed. For the time being, it only seems wise to scale the data properly before their analysis and then to use g_I in the absence of outliers. The choice is also preferable from the computational point of view.

The examples below testify that the elliptical quantile regression can work well both for elliptical and non-elliptical underlying error distributions, and also for the number of observations n as low as 99 and as high as 99 999. For the sake of simplicity and ease of presentation, the colors of both data points and quantile cuts are changing in dependence of the corresponding regressor values, and only bivariate responses with scalar regressors are considered. Nevertheless, there is no intrinsic restriction on the dimension of responses or regressors involved in the empirical model provided that the number of free model parameters is low relative to the total number of observations and not too large for the computation to terminate successfully.

The elliptical regression τ-g-quantiles are parametrized by means of $\boldsymbol{s}_\tau$, $\mathbb{A}_\tau$, and c_τ. In the examples, $\mathbb{A}_\tau$ is always considered in its spectral decomposition (4.3) described by d_τ^2 and α_τ, although less complicated parametrizations of $\mathbb{A}_\tau$ should be generally preferred for models with constant $\mathbb{A}_\tau$; see Section 4 for the discussion of some possibilities.

Figure 1 is included to demonstrate that parametric elliptical g-quantile regression is suitable for both small and large data sets and for capturing various kinds of heteroscedasticity.

Figure 2 illustrates another key advantage of elliptical regression g-quantiles, namely their ability to easily incorporate many types of a priori information regarding the model parameters. Last but not least, Figure 3 indicates that the concept of parametric elliptical regression quantiles is not bound to linear regression settings and can be used even for fitting highly complicated nonlinear models.

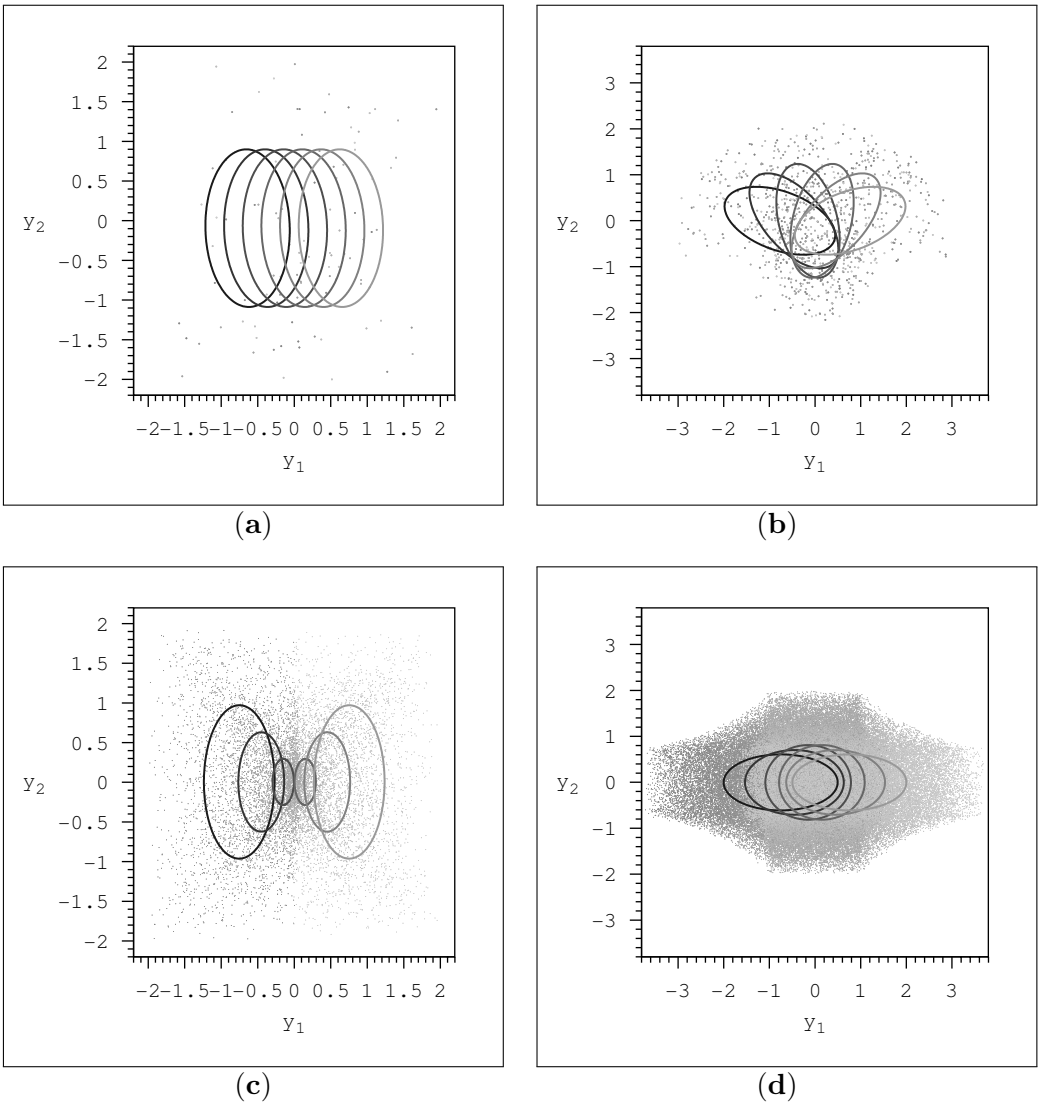

Figure 1: **Classification of heteroscedasticity in $\mathbb{R}^2$.** The plots illustrate four basic patterns of heteroscedasticity in $\mathbb{R}^2$ with elliptical regression 0.3-g_I-quantile cuts computed for six equidistant reference points $z_0 = -0.75, -0.45, ..., 0.75$ from n regression observations (Y_1, Y_2, Z) generated by the regression model $(Y_1, Y_2)' = (Z, 0)' + q(\boldsymbol{\varepsilon})$, $Z \sim U([-1,1])$ is independent of $\boldsymbol{\varepsilon} \sim U([-1,1]) \times U([-2,2])$:
(**a**) no heteroscedasticity $\big[n = 99,\ q(\boldsymbol{\varepsilon}) = \boldsymbol{\varepsilon}\big]$,
(**b**) rotational heteroscedasticity $\big[n = 999,\ q(\boldsymbol{\varepsilon}) = \boldsymbol{\varepsilon}'\mathbb{P}$ where $\mathrm{vec}(\mathbb{P})' = \big(\cos(\pi Z/2), \sin(\pi Z/2), -\sin(\pi Z/2), \cos(\pi Z/2)\big)\big]$,
(**c**) multiplicative heteroscedasticity $\big[n = 9\,999,\ q(\boldsymbol{\varepsilon}) = (0.1 + 0.9|Z|)\,\boldsymbol{\varepsilon}\big]$, and
(**d**) proportional heteroscedasticity $\big[n = 99\,999,\ q(\boldsymbol{\varepsilon}) = \boldsymbol{\varepsilon}'\mathbb{P}$ where $\mathrm{vec}(\mathbb{P})' = \big(\exp(|Z|), 0, 0, \exp(-|Z|)\big)\big]$.

The four plots in Figure 1 illustrate all the core types of heteroscedastic behavior described in Section 5 with different numbers of observations. The elliptical regression τ-g_I-quantiles, $\tau = 0.3$, were always computed from n regression observations (Y_1, Y_2, Z) generated by the regression model $(Y_1, Y_2)' = (Z, 0)' + q(\boldsymbol{\varepsilon})$ where $Z \sim U([-1,1])$, $\boldsymbol{\varepsilon} \sim U([-1,1]) \times U([-2,2])$ is independent of Z (as everywhere below), and $q(\boldsymbol{\varepsilon})$ denotes a transformation of $\boldsymbol{\varepsilon}$ specific to each case. As for their parametrization by means of $\boldsymbol{s}_\tau$, d_τ, α_τ, and c_τ, always $\boldsymbol{s}_\tau = (\beta_1 Z, \beta_2)'$ and also $d_\tau^2 = \delta_1^2$, $\alpha_\tau = \alpha_1$, and $c_\tau = \gamma_1$ up to the exceptions listed below together with other specific features unique to individual pictures (a) to (d):

(**a**) no heteroscedasticity: $n = 99$, $q(\boldsymbol{\varepsilon}) = \boldsymbol{\varepsilon}$,

(**b**) rotational heteroscedasticity: $n = 999$, $\alpha_\tau = \pi\alpha_1 Z$, $q(\boldsymbol{\varepsilon}) = \boldsymbol{\varepsilon}'\mathbb{P}$ where $\mathrm{vec}(\mathbb{P})' = \big(\cos(\pi Z/2), \sin(\pi Z/2), -\sin(\pi Z/2), \cos(\pi Z/2)\big)$,

(**c**) multiplicative heteroscedasticity: $n = 9\,999$, $c_\tau = \gamma_1 + \gamma_2|Z| + \gamma_3 Z^2$, $q(\boldsymbol{\varepsilon}) = (0.1 + 0.9|Z|)\,\boldsymbol{\varepsilon}$, and

(**d**) proportional heteroscedasticity: $n = 99\,999$, $d_\tau^2 = \exp(\delta_1 Z)$, $q(\boldsymbol{\varepsilon}) = \boldsymbol{\varepsilon}'\mathbb{P}$ where $\mathrm{vec}(\mathbb{P})' = \big(\exp(|Z|), 0, 0, \exp(-|Z|)\big)$.

The objective function defining elliptical regression τ-g-quantiles was optimized over all the scalar parameters occurring in the parametrization, as in all the following examples. In this case, it was over all $\boldsymbol{\theta} = (\beta_1, \beta_2, \delta_1, \alpha_1, \gamma_1, \gamma_2, \gamma_3)' \in \mathbb{R}^7$ in case (c) and over $\boldsymbol{\theta} = (\beta_1, \beta_2, \delta_1, \alpha_1, \gamma_1)' \in \mathbb{R}^5$ otherwise.

Figure 2 depicts elliptical regression τ-g_I-quantiles with the trend, obtained for $\tau = 0.5$ from $n = 9\,999$ observations following the regression model $(Y_1, Y_2) = (Z, Z^2) + (1 + 3|\sin(\pi Z/2)|)\,\boldsymbol{\varepsilon}$ where $Z \sim U(-2, 2)$ and $\boldsymbol{\varepsilon} \sim N(0, 1/4) \times N(0, 1/4)$. They were parametrized with $\boldsymbol{s}_\tau = (\beta_1 + \beta_2 Z + \beta_3 Z^2, \beta_4 + \beta_5 Z + \beta_6 Z^2)'$, $d_\tau^2 = \delta_1^2$, $\alpha_\tau = \alpha_1$ and

(**a**) $c_\tau = \gamma_1$ or

(**b**) $c_\tau = \gamma_1 + \gamma_2|\sin(\pi Z/2)| + \gamma_3 \sin^2(\pi Z/2)$;

compare it to Figure 5 of [20] that is based on the same data generating model. This figure reminds you that one can easily enforce homoscedasticity or numerous equality constraints on model parameters when examining various submodels. In this particular case, the knowledge of the scale period is used in advance.

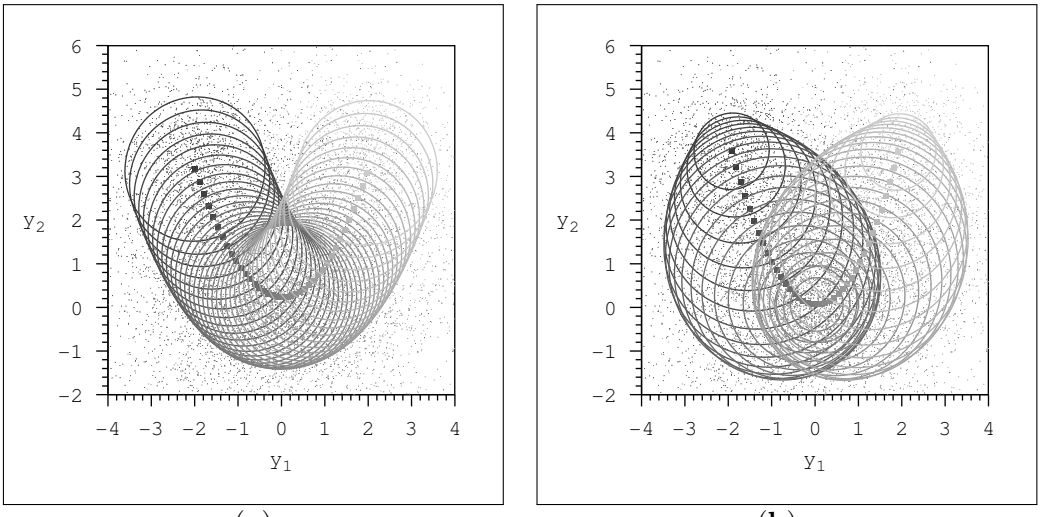

Figure 2: **Elliptical regression quantiles and a priori information.** The plots show elliptical regression τ-g_I-quantile cuts and their centers, $\tau = 0.5$, obtained for reference points $z_0 = -1.9, -1.8, ..., 1.9$ from $n = 9\,999$ observations following the regression model $(Y_1, Y_2) = (Z, Z^2) + (1 + 3|\sin(\pi Z/2)|)\,\boldsymbol{\varepsilon}$ where $Z \sim U(-2, 2)$ is independent of $\boldsymbol{\varepsilon} \sim N(0, 1/4) \times N(0, 1/4)$. They assume a general quadratic trend in each component and
(**a**) homoscedasticity or
(**b**) the right form of heteroscedasticity.
Both the quantile curves and data points lighten with increasing values of the corresponding regressor.

Figure 3 is inspired by the well known Lissajous curves and highlights the fact that the parametric elliptical regression τ-g-quantiles are especially convenient for fitting highly nonlinear models if one has an idea how to correctly describe the nonlinearity. They are computed for $\tau \in \{0.1, 0.3, 0.5, 0.7\}$ and g_I from $n = 9\,999$ observations coming from a complicated nonlinear regression model $(Y_1, Y_2)' = \big(1.5 + \sin(Z), 1.5 + \sin(2Z)\big)' + q(\boldsymbol{\varepsilon})$, $Z \sim U([-\pi, \pi])$, $\boldsymbol{\varepsilon} \sim U([-0.25, 0.25]) \times U([-0.25, 0.25])$, where

(**a**) $q(\boldsymbol{\varepsilon}) = \boldsymbol{\varepsilon}$ or

(**b**) $q(\boldsymbol{\varepsilon}) = \cos(Z)\,\boldsymbol{\varepsilon}$.

The quantile parameters were always looked for in the same form with generally τ-dependent coefficients: $\boldsymbol{s}_\tau = \big(\beta_1 + \beta_2 \sin(\beta_3 Z), \beta_4 + \beta_5 \sin(\beta_6 Z)\big)'$, $d_\tau^2 = \delta_1^2$, $\alpha_\tau = \alpha_1$, and $c_\tau = \gamma_1 + \gamma_2^2 \cos^2(\gamma_3 Z)$.

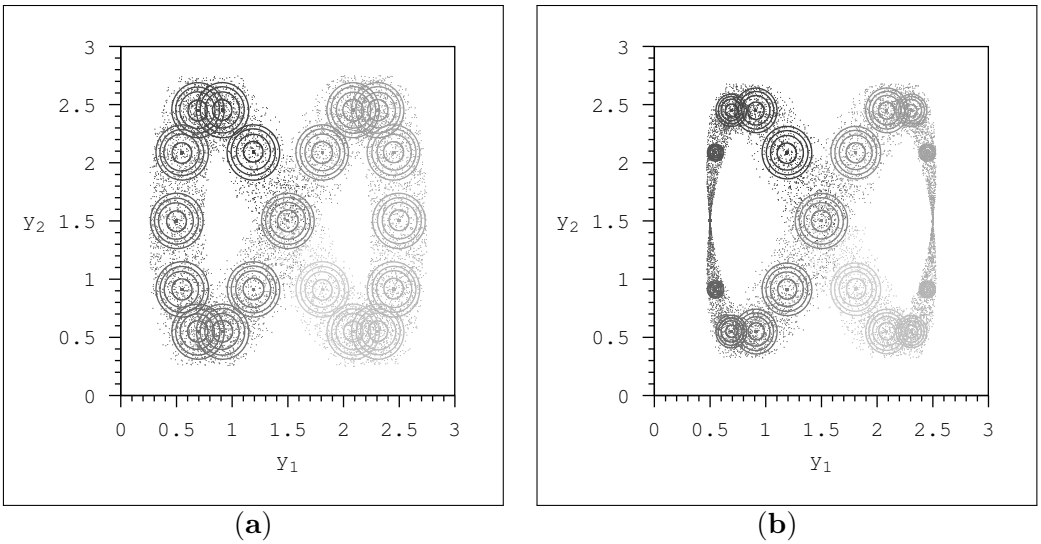

Figure 3: **Elliptical regression quantiles and nonlinearity.** The plots display elliptical regression τ-g_I-quantiles, $\tau \in \{0.1, 0.3, 0.5, 0.7\}$, for 19 equidistant reference points $z_0 = -9\pi/10, -8\pi/10, ..., 9\pi/10$, computed from $n = 9\,999$ observations coming from a complicated nonlinear regression model $(Y_1, Y_2)' = \big(1.5 + \sin(Z), 1.5 + \sin(2Z)\big)' + q(\boldsymbol{\varepsilon})$, $Z \sim U([-\pi, \pi])$ is independent of $\boldsymbol{\varepsilon} \sim U([-0.25, 0.25]) \times U([-0.25, 0.25])$, where
(**a**) $q(\boldsymbol{\varepsilon}) = \boldsymbol{\varepsilon}$ or
(**b**) $q(\boldsymbol{\varepsilon}) = \cos(Z)\,\boldsymbol{\varepsilon}$.
The quantile curves lighten with increasing z_0 and the data points get darker while the regressor values are decreasing.

The elliptical regression quantile methodology remains under investigation also in the next section where it is applied to real biometric data.

9. APPLICATION

For the sake of comparison, the parametric elliptical regression quantile methodology is tested on the same body girth measurements data of [19] as in [15], namely on $n = 260$ observations of calf maximum girth Y_1 (cm) and thigh (maximum) girth Y_2 (cm) of the physically active women whose age (years), weight (kg), height (cm) and body mass index (BMI $= 10\,000$ weight/height^2) are separately tried as the only regressor Z in the attempts to explain Y_1 and Y_2. Although the observations do not constitute a random sample from any well-defined population, they are considered suitable for illustrating various statistical concepts.

In this particular case study, the parametric elliptical regression τ-g-quantiles are computed for $g = g_I$. They are plotted only for $\tau \in \{0.1, 0.9\}$ and for $Z = z_0$ where z_0 is equal to the empirical p-th quantile of the regressor, $p \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$. The results are displayed in the same way as in Figure 7 of [15] to make the comparison as easy as possible. The only notable difference lies in the colors and quantile levels. That is to say that the pictures here are only black-and-white and, consequently, they illustrate the elliptical regression τ-g_I-quantiles only for two representative values of τ to stay legible. Note also that the quantile levels used for indexing the elliptical regression quantiles by their overall probability coverage are not related to those used by the multiple-output directional quantile regression of [15] or [29] in any predictable way.

Figure 4 adopts the parametrization $\boldsymbol{s}_\tau = (\beta_1 + \beta_2 Z, \beta_3 + \beta_4 Z)'$, $d_\tau^2 = \delta_1^2$, $\alpha_\tau = \alpha_1$, and $c_\tau = \gamma_1 + \gamma_2 Z$ (with possibly different coefficients for each τ) that allows for changes in location and scale and thus mimics the model used in [15] quite closely. Not surprisingly, it also produces similar output. Figures 4(a) and 4(c) clearly reveal certain location shift and scale increase of plotted τ-quantile cuts caused by increasing weight and BMI, respectively. Figure 4(b) indicates that age influences only the location and volume of the outer quantile cuts but not of the inner ones. Figure 4(d) suggests that increasing height shifts both the inner and outer quantile cuts in mutually orthogonal directions but only affects the volume of the outer ones. Although all of these patterns can be more or less observed in Figure 7 of [15] as well, they are more clearly articulated through the simple elliptical shapes here. See also [14] and [17] for other quantile regression fits of the same data and their explanations.

Figure 5 plots the results regarding BMI for the generalized parametrization with $d_\tau^2 = (\delta_1 + \delta_2 Z)^2$, $\alpha_\tau = \alpha_1 + \alpha_2 Z$, and the other settings left unchanged, as in Figure 4(c). The modification permits more flexible changes of the regression quantile shape and is able to detect even the slight rotation of the outer quantile cuts with increasing BMI, observed in [15].

Although the analysis above is too simplistic to establish anything certain about female legs, it clearly demonstrates that the generalized parametric elliptical quantile regression is a powerful and flexible analytical method capable of pointing out even the smallest subtleties in the data behavior.

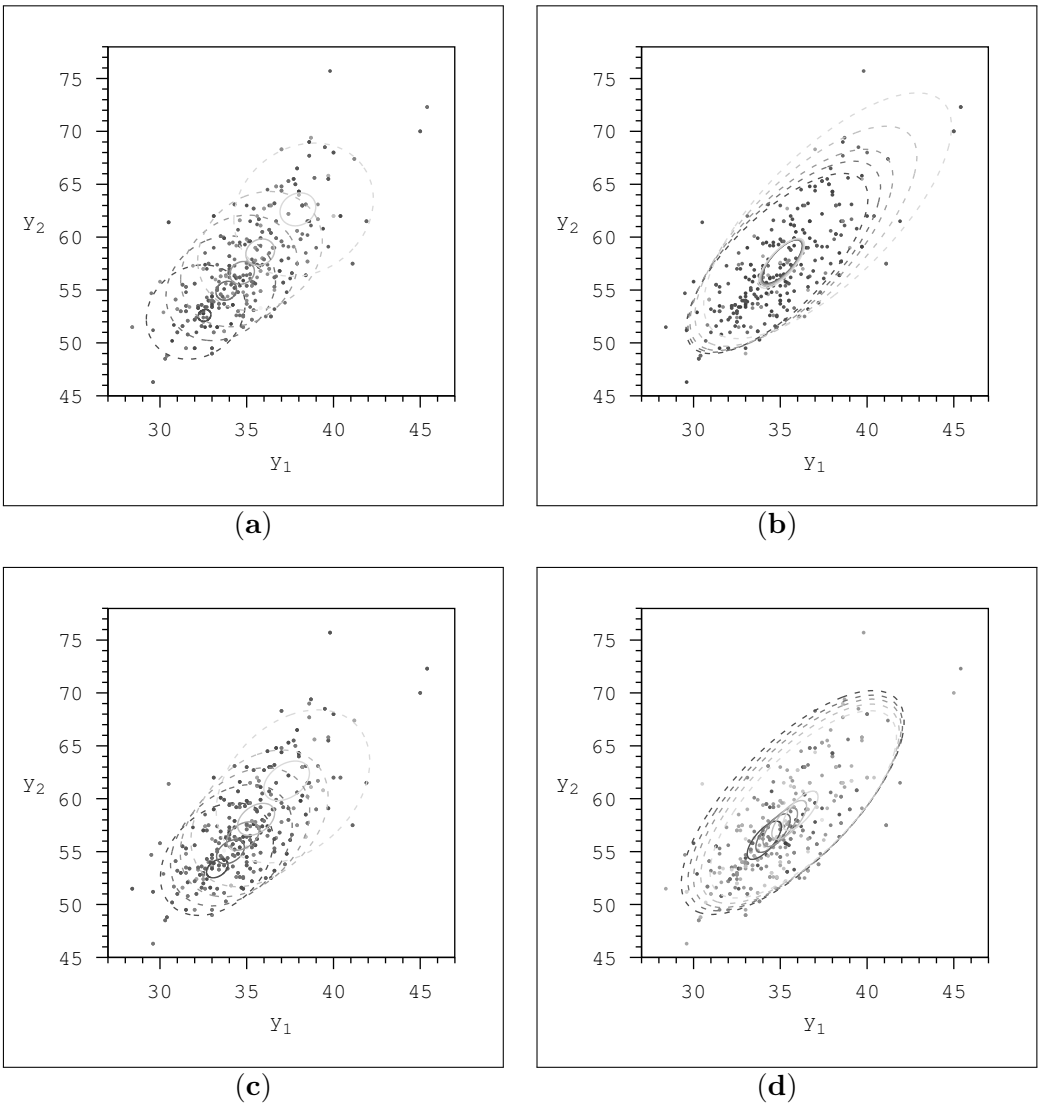

Figure 4: **Application to real data I.** The plots illustrate the dependence of female calf maximum girth (Y_1) and thigh (maximum) girth (Y_2) on
(**a**) weight,
(**b**) age,
(**c**) BMI, or
(**d**) height
by means of parametric elliptical g_I-quantile regression with a single regressor (Z), constant matrix parameter $\mathbb{A}$, linear inflation factor c, and linear trend $\boldsymbol{s}$. The elliptical regression g_I-quantiles are displayed for both $\tau = 0.1$ (solid line) and $\tau = 0.9$ (dashed line) and for regressor values z_0 equal to the empirical p-th quantile of Z, $p = 0.1, 0.3, 0.5, 0.7,$ and 0.9. The quantile curves lighten with increasing p and the data points get darker while the regressor values are decreasing.

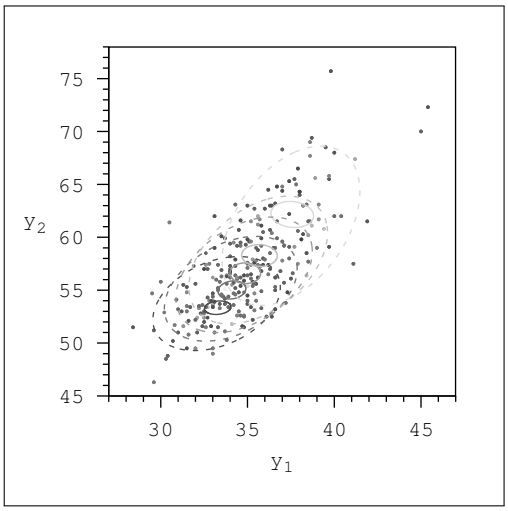

Figure 5: **Application to real data II.** The plot shows the dependence of female calf maximum girth (Y_1) and thigh (maximum) girth (Y_2) on BMI by means of parametric elliptical quantile regression assuming linear trend and a general form of heteroscedasticity. The elliptical regression g_I-quantiles are displayed for both $\tau = 0.1$ (solid line) and $\tau = 0.9$ (dashed line) and for regressor values z_0 equal to the empirical p-th quantile of the regressor, $p = 0.1, 0.3, 0.5, 0.7,$ and 0.9. The quantile curves lighten with increasing p and the data points get darker while the regressor value is decreasing.

10. CONCLUDING REMARKS

All the presented theory and pictures demonstrate that the generalized parametric elliptical quantile regression may lead to natural and reasonable fits, even when the assumption of conditional symmetry cannot be relied on, as in Section 9. That is to say that the conditional central symmetry may simplify model validation and make the results from a well parametrized model particularly easy to interpret, but it is not strictly required for the method to work.

Sections 7, 8, and 9 also tacitly assume that the sample estimators of the quantile coefficients and cuts are consistent. It still has to be proved in full generality although it is already known in some special cases; see [17].

There is always a risk that the complicated non-convex optimization behind the generalized parametric elliptical quantile regression will terminate without finding the real global minimum. Nevertheless, this threat can be fought back by using global optimization strategies and model validation tools. And this problem should not theoretically appear at all for $g(t) = t$ and well-specified or specific models [17], and it is thus not likely to be severe in very similar situations.

The dependence of generalized parametric elliptical regression quantiles on function g may rise another concern as it may seem to introduce too much arbitrariness into the model selection. However, simple fully affine equivariant parametrizations strongly ask for a power

function g, and then its selection becomes as arbitrary as the choice of $p > 0$ in the standard L_p regression. Only L_2 and L_1 regression methods are usually used because of their simplicity and easily interpretable results. And the same reasons lead to the choices $g(t) = t$ or $g(t) = \sqrt{t}$ in the generalized parametric elliptical quantile regression, though the latter seems reasonable only in certain special cases.

This article should be interpreted only as a single step on the long way to the successful elliptical quantile regression methodology. The next steps will include nonparametric generalizations, statistical inference, and a powerful and reliable software support.

It is difficult to predict if the proposed generalized parametric elliptical quantile regression withstands the test of time but, for the time being, it appears quite promising.

ACKNOWLEDGMENTS

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A COUPLE OF NON REDUCED BIAS GENERALIZED MEANS IN EXTREME VALUE THEORY: AN ASYMPTOTIC COMPARISON

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Abstract:

- *Lehmer's mean-of-order p* (L_p) generalizes the arithmetic mean, and L_p *extreme value index* (EVI)-estimators can be easily built, as a generalization of the classical Hill EVI-estimators. Apart from a reference to the asymptotic behaviour of this class of estimators, an asymptotic comparison, at optimal levels, of the members of such a class reveals that for the optimal (p, k) in the sense of minimal mean square error, with k the number of top order statistics involved in the estimation, they are able to overall outperform a recent and promising generalization of the Hill EVI-estimator, related to the power mean, also known as Hölder's mean-of-order-p. A further comparison with other 'classical' non-reduced-bias estimators still reveals the competitiveness of this class of EVI-estimators.

Key-Words:

- *heavy tails; optimal tuning parameters; semi-parametric estimation; statistical extreme value theory.*

AMS Subject Classification:

- 62G32, 62E20.

1. GENERALIZED MEANS' ESTIMATORS AND SCOPE OF THE ARTICLE

Let us consider the notation $(X_{1:n}, ..., X_{n:n})$ for the ascending order statistics associated with a random sample of size n, $(X_1, ..., X_n)$, from a *cumulative distribution function* (CDF) F. Let us further assume that there exist sequences of real constants $\{a_n > 0\}$ and $\{b_n \in \mathbb{R}\}$ such that the maximum, linearly normalized, i.e. $(X_{n:n} - b_n)/a_n$, converges in distribution to a non-degenerate *random variable* (RV). Then (Gnedenko, [24]), the limit distribution is necessarily of the type of the general *extreme value* (EV) CDF, given by

$$\text{EV}_\xi(x) := \begin{cases} \exp\left(-(1+\xi x)^{-1/\xi}\right), & 1+\xi x > 0, \quad \text{if} \quad \xi \neq 0, \\ \exp\left(-\exp(-x)\right), & x \in \mathbb{R}, \quad \text{if} \quad \xi = 0. \end{cases} \tag{1.1}$$

The CDF F is then said to belong to the *max-domain of attraction* of EV_ξ, defined in (1.1), we use the notation $F \in \mathcal{D}_{\mathcal{M}}(\text{EV}_\xi)$, and the parameter ξ is the *extreme value index* (EVI), the primary parameter of extreme events. It is well-known that the EVI measures the heaviness of the right-tail function $\overline{F}(x) := 1 - F(x)$, and the heavier the right-tail function, the larger ξ is. From a quantile point of view, with $F^{\leftarrow}(x) := \inf\{y\colon F(y) \geq x\}$ denoting the generalized inverse function of F, further consider $U(t) := F^{\leftarrow}(1 - 1/t)$, $t \geq 1$, the *reciprocal tail quantile function* (RTQF). Then, with $\mathcal{R}_a$ denoting the class of regularly varying functions at infinity, with an index of regular variation equal to $a \in \mathbb{R}$, i.e. positive measurable functions $g(\cdot)$ such that for all $x > 0$, $g(tx)/g(t) \to x^a$, as $t \to \infty$, (see Bingham *et al.*, [7], among others),

$$\begin{aligned} F \in \mathcal{D}_{\mathcal{M}}^{+} := \mathcal{D}_{\mathcal{M}}\left(\text{EV}_\xi\right)_{\xi>0} &\iff \overline{F} \in \mathcal{R}_{-1/\xi} \quad \text{(Gnedenko, [24])} \\ &\iff U \in \mathcal{R}_\xi \qquad \text{(de Haan, [39])}. \end{aligned} \tag{1.2}$$

In this article we work with a Pareto-type underlying CDF, satisfying (1.2), i.e. with an associated positive EVI for maxima. These heavy-tailed models are quite common in a large variety of fields of application, like bibliometrics, biostatistics, computer science, insurance, finance, social sciences, statistical quality control and telecommunications, among others. For Pareto-type models, the classical EVI-estimators are the *Hill* (H) estimators (Hill, [44]), which are the averages of the log-excesses, i.e.

$$\hat{\xi}^{\text{H}}(k) \equiv \text{H}(k) := \frac{1}{k}\sum_{i=1}^{k} V_{ik}, \qquad V_{ik} := \ln X_{n-i+1:n} - \ln X_{n-k:n}, \quad 1 \leq i \leq k < n. \tag{1.3}$$

One of the interesting facts concerning the H EVI-estimators is that various asymptotically equivalent versions of $\text{H}(k)$ can be derived through essentially different methods, such as the maximum likelihood method or the mean excess function approach, showing that the Hill estimator is quite natural. Details can be found in Beirlant *et al.* ([4]), among others. We merely note that from a quantile point of view, and with $U(\cdot)$ the RTQF, we can write the distributional identity $X \overset{d}{=} U(Y)$, with Y a unit Pareto RV, i.e. an RV with a CDF $F_Y(y) = 1 - 1/y$, $y \geq 1$. For the order statistics associated with a random unit Pareto sample $(Y_1, ..., Y_n)$, we have the distributional identity $Y_{n-i+1:n}/Y_{n-k:n} \overset{d}{=} Y_{k-i+1:k}$, $1 \leq i \leq k$. Moreover, $kY_{n-k:n}/n \xrightarrow[n\to\infty]{\mathbb{P}} 1$, i.e. $Y_{n-k:n} \overset{\mathbb{P}}{\sim} n/k$. Consequently, and provided that $k = k_n$, $1 \leq k < n$, is an intermediate sequence of integers, i.e. if

$$k = k_n \to \infty \qquad \text{and} \qquad k_n = o(n), \quad \text{as } n \to \infty, \tag{1.4}$$

we get

$$V_{ik} \stackrel{d}{=} \xi \ln Y_{k-i+1:k} + o_{\mathbb{P}}(1) \stackrel{d}{=} \xi E_{k-i+1:k} + o_{\mathbb{P}}(1)\,, \tag{1.5}$$

with E denoting a standard exponential RV and the $o_{\mathbb{P}}(1)$-term uniform in i, $1 \le i \le k$ (see Caeiro *et al.*, [14], among others, for further details on this uniform behaviour). The log-excesses, V_{ik}, $1 \le i \le k$, in (1.3), are thus approximately the k order statistics of a sample of size k from an exponential parent with mean value ξ, motivating the H EVI-estimators in (1.3).

Beyond the average, the p-moments of log-excesses, i.e.

$$M_{k,n}^{(p)} := \frac{1}{k} \sum_{i=1}^{k} \{\ln X_{n-i+1:n} - \ln X_{n-k:n}\}^p\,, \qquad p \ge 1\,, \tag{1.6}$$

introduced in Dekkers *et al.* ([19]) $\left[M_{k,n}^{(1)} \equiv \mathrm{H}(k)\right]$ have also played a relevant role in the EVI-estimation, and can more generally be parameterized in $p \in \mathbb{R}\backslash\{0\}$. Note next that a simple generalization of the mean is Lehmer's mean-of-order-p (see Havil, [43], p. 121). Given a set of positive numbers $\mathbf{a} = (a_1, ..., a_k)$, such a mean generalizes both the arithmetic mean ($p = 1$) and the harmonic mean ($p = 0$), being defined as

$$L_p(\mathbf{a}) := \sum_{i=1}^{k} a_i^p \Big/ \sum_{i=1}^{k} a_i^{p-1}\,, \qquad p \in \mathbb{R}\,.$$

Further note that $\lim\limits_{p\to-\infty} L_p(\mathbf{a}) = \min\limits_{1\le i\le k} a_i$ and $\lim\limits_{p\to+\infty} L_p(\mathbf{a}) = \max\limits_{1\le i\le k} a_i$.

The H EVI-estimators can thus be considered as the Lehmer mean-of-order-1 of the k log-excesses $\mathbf{V} := (V_{ik},\ 1 \le i \le k)$, in (1.3), $k < n$. We now more generally consider the Lehmer mean-of-order-p of those statistics. From (1.5), since $\mathbb{E}(E^p) = \Gamma(p+1)$ for any real $p > -1$, with $\Gamma(\cdot)$ denoting the complete Gamma function, the law of large numbers enables us to say that

$$\frac{1}{k} \sum_{i=1}^{k} V_{ik}^p \xrightarrow[n\to\infty]{\mathbb{P}} \Gamma(p+1)\, \xi^p\,.$$

Hence the reason for the class of *Lehmer mean-of-order-p* (L_p) EVI-estimators,

$$\hat{\xi}^{\mathrm{L}_p}(k) \equiv \mathrm{L}_p(k) := \frac{L_p(\mathbf{V})}{p} = \frac{1}{p} \frac{\sum\limits_{i=1}^{k} V_{ik}^p}{\sum\limits_{i=1}^{k} V_{ik}^{p-1}} = \frac{M_{k,n}^{(p)}}{p\, M_{k,n}^{(p-1)}} \qquad \left[\mathrm{L}_1(k) \equiv \mathrm{H}(k)\right], \tag{1.7}$$

consistent for all $\xi > 0$ and real $p > 0$, and where $M_{k,n}^{(p)}$ is given in (1.6).

As a possible competitive class of EVI-estimators, we further refer the one recently studied in Brilhante *et al.* ([8]), Gomes and Caeiro ([25]) and Caeiro *et al.* ([14]), among others, based on the power mean. Given a set of non-negative numbers $\mathbf{a} = (a_1, ..., a_k)$, such a mean generalizes the arithmetic mean ($p = 1$), the geometric mean ($p = 0$) and the harmonic mean ($p = -1$), being defined as

$$M_p(\mathbf{a}) := \left(\frac{1}{k} \sum_{i=1}^{k} a_i^p \right)^{1/p}\,, \qquad p \in \mathbb{R}\,.$$

Further note that $\lim_{p\to 0} M_p(\mathbf{a}) \equiv M_0(\mathbf{a}) = \left(\prod_{i=1}^k a_i\right)^{1/k}$, $\lim_{p\to-\infty} M_p(\mathbf{a}) = \min_{1\le i\le k} a_i$ and $\lim_{p\to+\infty} M_p(\mathbf{a}) = \max_{1\le i\le k} a_i$. On the basis of the fact that the Hill EVI-estimator in (1.3) is the logarithm of the *geometric mean* of

$$U_{ik} := X_{n-i+1:n}/X_{n-k:n}\,, \qquad 1\le i\le k<n\,, \tag{1.8}$$

the consideration of the power mean, also known as Hölder's *mean-of-order-p* (MO_p), of those same statistics leads to

$$\hat{\xi}^{\mathrm{H}_p}(k) \equiv \mathrm{H}_p(k) := \begin{cases} \left(1-\left(\frac{1}{k}\sum_{i=1}^k U_{ik}^p\right)^{-1}\right)\Big/p\,, & \text{if } \ p<1/\xi,\ p\neq 0\,,\\ \mathrm{H}(k)\,, & \text{if } \ p=0\,, \end{cases} \tag{1.9}$$

the so-called MO_p EVI-estimators, almost simultaneously considered, for $p\ge 0$, in Brilhante *et al.* ([8]), Paulauskas and Vaičiulis ([45]) and Beran *et al.* ([6]). As a measure of comparison, and just as in Gomes and Henriques-Rodrigues ([30]) (see also Gomes and Henriques-Rodrigues, [31]), the *Pareto probability weighted moments* (PPWM) EVI-estimators, introduced in Caeiro and Gomes ([11]), and further studied in Caeiro *et al.* ([17], [15]) will also be considered. The PPWM EVI-estimators, quite common in the areas of climatology and hydrology, are consistent only for $\xi<1$, depend on the statistics $\hat{a}_j(k) := \frac{1}{k}\sum_{i=1}^k \big((i-1)/(k-1)\big)^j X_{n-i+1:n}$, $j=0,1$, and are defined by

$$\hat{\xi}^{\mathrm{PPWM}}(k) \equiv \mathrm{PPWM}(k) := 1-\frac{\hat{a}_1(k)}{\hat{a}_0(k)-\hat{a}_1(k)}\,, \qquad 1\le k<n\,. \tag{1.10}$$

We also mention the possibly *reduced-bias* (RB) class of EVI-estimators in Caeiro and Gomes ([10]) (see also, Caeiro and Gomes, [9], [12]),

$$\hat{\xi}^{\mathrm{CG}_{p,\delta}}(k) \equiv \mathrm{CG}_{p,\delta}(k) := \frac{\Gamma(p)}{M_{k,n}^{(p-1)}}\left(\frac{M_{k,n}^{(\delta p)}}{\Gamma(\delta p+1)}\right)^{1/\delta}, \qquad \delta>0,\ p>0 \quad \big[\mathrm{CG}_{1,1}(k)\equiv \mathrm{H}(k)\big]\,. \tag{1.11}$$

For $\delta=2$ in (1.11), we obtain a class studied in Caeiro and Gomes ([9]), which generalizes the estimator $\mathrm{CG}_{1,2}(k)=\sqrt{M_{k,n}^{(2)}/2}$, studied in Gomes *et al.* ([34]), where also $\mathrm{L}_2(k) = M_{k,n}^2/\big(2M_{k,n}^{(1)}\big)$ was introduced and studied both asymptotically and for finite samples. And we can also consider the class of L_p EVI-estimators in (1.7), as a non-RB particular case of (1.11). Indeed, $\mathrm{L}_p(k)\equiv \mathrm{CG}_{p,1}(k)$.

Remark 1.1. Note that all the aforementioned EVI-estimators are scale invariant, but not location-invariant. They can however become location-invariant if we apply the *peaks over random threshold* (PORT) methodology, basing them not on the original sample, but on the excesses over a central empirical quantile and even over the minimum of the available sample whenever possible, i.e. when the underlying parent F has a finite left endpoint. For details on the topic, see, among others, Araújo Santos *et al.* ([1]), where the acronym PORT was introduced, Gomes *et al.* ([27]), and more recently, Gomes and Henriques-Rodrigues ([30]) and Gomes *et al.* ([32]).

In Section 2, after the introduction of a few technical details in the field of *extreme value theory* (EVT), we deal with the asymptotic behaviour of the L_p EVI-estimators, in (1.7).

In Section 3, it is shown that at optimal k-levels and for the optimal p, the members of such a class are able to overall outperform the optimal EVI-estimators in (1.9), which on its turn had been shown in Brilhante *et al.* ([8]) to have a similar behaviour comparatively with the optimal Hill EVI-estimators, for an adequate optimal p ($\neq 0$). We next compare them, asymptotically and at optimal levels, with the optimal PPWM EVI-estimators, in (1.10). Finally, in Section 4, we advance with an overall comparison of a wide number of EVI-estimators, drawing some concluding remarks.

2. ASYMPTOTIC BEHAVIOUR OF THE EVI-ESTIMATORS

After a reference, in Section 2.1, to the most common second-order framework for heavy-tailed models, we briefly refer, in Section 2.2, the asymptotic behaviour of the EVI-estimators defined in Section 1. A recent review on the topic of statistical univariate EVT can be found in Gomes and Guillou ([28]). See also Beirlant *et al.* ([2]) and Scarrot and MacDonald ([48]).

2.1. A few technical details in the field of EVT

In the area of statistical EVT and whenever working with large values, a model F is commonly said to be heavy-tailed whenever (1.2) holds. The second-order parameter ρ (≤ 0) rules the rate of convergence in any of the first-order conditions, in (1.2), and can be defined as the non-positive parameter appearing in the limiting relation

$$\lim_{t\to\infty} \frac{\ln U(tx) - \ln U(t) - \xi \ln x}{A(t)} = \begin{cases} \left(x^{\rho}-1\right)/\rho\,, & \text{if} \quad \rho<0\,, \\ \ln x\,, & \text{if} \quad \rho=0\,, \end{cases} \tag{2.1}$$

which is assumed to hold for every $x > 0$, and where $|A|$ must then be of regular variation with index ρ. This condition has been widely accepted as an appropriate condition to specify the right-tail of a Pareto-type distribution in a semi-parametric way. For technical simplicity, we often assume that we are working in Hall–Welsh class of models (Hall and Welsh, [42]), with an RTQF,

$$U(t) = C\, t^{\xi}\Big(1 + \xi\, \beta\, t^{\rho}/\rho + o(t^{\rho})\Big), \qquad \text{as} \quad t\to\infty\,, \tag{2.2}$$

$C > 0$, $\beta \neq 0$ and $\rho < 0$. Equivalently, we can say that, with (β, ρ) the vector of second-order parameters, the general second-order condition in (2.1) holds with $A(t) = \xi\, \beta\, t^{\rho}$, $\rho < 0$. Further details on second-order conditions can be found in Beirlant *et al.* ([4]), de Haan and Ferreira ([40]) and Fraga Alves *et al.* ([22]), among others.

2.2. Asymptotic behaviour of the EVI-estimators under consideration

Trivial adaptations of the results in de Haan and Peng ([41]), Caeiro and Gomes ([10]), Caeiro and Gomes ([11]) and Brilhante *et al.* ([8]), respectively for the H, $\mathrm{CG}_{p,\delta}$, PPWM and H_p classes of EVI-estimators, enable us to state:

Theorem 2.1. *Under the validity of the first-order condition, in* (1.2)*, and for intermediate sequences* $k = k_n$*, i.e. if* (1.4) *holds, the classes of* H_p*,* PPWM *and* $\mathrm{CG}_{p,\delta}$ *EVI-estimators, respectively defined in* (1.9)*,* (1.10)*, and* (1.11)*, generally denoted by* $\hat{\xi}^{\bullet}(k)$*, are consistent for the estimation of* $\xi > 0$*, provided that we work in* $\mathcal{S}_{\bullet}$*, where* $\mathcal{S}_{\mathrm{H}_p} = \{(\xi, p) : \xi > 0, p < 1/\xi\}$*,* $\mathcal{S}_{\mathrm{PPWM}} = \{\xi : 0 < \xi < 1\}$ *and* $\mathcal{S}_{\mathrm{CG}_{p,\delta}} = \{(\xi, p, \delta) : \xi > 0, p > 0, \delta > -1/p\}$*.*

Assume further that (2.1) *holds. Then, for* $\xi > 0$*, adequate regions of the spaces of parameters and with* $\mathcal{N}(\mu, \sigma^2)$ *standing for a normal* RV *with mean value* μ *and variance* σ^2*,*

$$\sqrt{k}\,(\hat{\xi}^{\bullet}(k) - \xi) \xrightarrow[n\to\infty]{d} \mathcal{N}(\lambda_A b_{\bullet}, \sigma^2_{\bullet}) \quad \text{if} \quad \sqrt{k}\,A(n/k) \underset{n\to\infty}{\longrightarrow} \lambda_A, \ \text{finite}. \tag{2.3}$$

Moreover

$$b_{\mathrm{H}_p} = \frac{1 - p\xi}{1 - p\xi - \rho}, \quad \sigma^2_{\mathrm{H}_p} = \frac{\xi^2 (1 - p\xi)^2}{1 - 2p\xi}, \quad \text{if} \quad p < 1/(2\xi), \tag{2.4}$$

$$b_{\mathrm{PPWM}} = \frac{(1-\xi)(2-\xi)}{(1-\xi-\rho)(2-\xi-\rho)}, \quad \sigma^2_{\mathrm{PPWM}} = \frac{\xi^2 (1-\xi)(2-\xi)^2}{(1-2\xi)(3-2\xi)}, \quad \text{if} \quad \xi < 1/2,$$

and

$$\begin{aligned} b_{\mathrm{CG}_{p,\delta}} &= \frac{(1-\rho)^{-\delta p} - \delta(1-\rho)^{-p+1} + \delta - 1}{\delta\,\rho}, \\ \sigma^2_{\mathrm{CG}_{p,\delta}} &= \frac{\xi^2}{\delta^2} \left\{ \frac{2\Gamma(2\delta p)}{\delta p \Gamma^2(\delta p)} + \frac{\delta^2 \Gamma(2p-1)}{\Gamma^2(p)} - \frac{2\Gamma\big((\delta+1)p\big)}{p\Gamma(p)\,\Gamma(\delta p)} - (\delta-1)^2 \right\}, \end{aligned} \tag{2.5}$$

$$\text{if} \quad p > 1/2, \ \delta > 0.$$

For the particular case $\delta = 1$, in (1.11), i.e. for the L_p EVI-estimators in (1.7), we can state:

Corollary 2.1. *Under the validity of the initial first-order conditions in* Theorem 2.1*, the class of* L_p EVI*-estimators, in* (1.7)*, is consistent for the estimation of* ξ*, provided that we work in* $\mathcal{S}_{\mathrm{L}_p} = \{(\xi, p) : \xi > 0, p > 0\}$*. Under the second-order conditions of* Theorem 2.1*,* (2.3) *holds, with*

$$b_{\mathrm{L}_p} = \frac{1}{(1-\rho)^p} \quad \text{and} \quad \sigma^2_{\mathrm{L}_p} = \frac{\xi^2\,\Gamma(2p-1)}{\Gamma^2(p)} \quad \text{if} \quad p > 1/2. \tag{2.6}$$

More specifically, and for all $\rho \le 0$*, one can write the asymptotic distributional representation*

$$\mathrm{L}_p(k) \overset{d}{=} \xi + \frac{\sigma_{\mathrm{L}_p} Z_k^{(p)}}{\sqrt{k}} + b_{\mathrm{L}_p} A(n/k) + o_{\mathbb{P}}\big(A(n/k)\big), \tag{2.7}$$

with $\big(b_{\mathrm{L}_p}, \sigma^2_{\mathrm{L}_p}\big)$ *given in* (2.6)*, and where* $Z_k^{(p)}$ *is an asymptotically standard normal* RV*.*

Remark 2.1. Note that regarding the L_p EVI-estimators, in (1.7), Corollary 2.1 is a particular case of Theorem 1 in Caeiro and Gomes ([10]), but generalizing now consistency for $p > 0$ and asymptotic normality for $p > 1/2$ rather than $p \ge 1$. Further note that for $\delta = 1$ there is a full agreement between (2.6) and (2.5), the result provided in Theorem 1 of Caeiro and Gomes ([10]). A detailed proof of Corollary 2.1 can be found in Penalva *et al.* ([47]).

Remark 2.2. Further note that for the MO_p EVI-estimators, denoted by H_p and defined in (1.9), a distributional representation of the type of the one in (2.7) holds for $p < 1/(2\xi)$, with $\left(b_{\mathrm{L}_p}, \sigma^2_{\mathrm{L}_p}\right)$ replaced by $\left(b_{\mathrm{H}_p}, \sigma^2_{\mathrm{H}_p}\right)$, given in (2.4).

For any $\xi > 0$, the asymptotic variance $\sigma^2_{\mathrm{L}_p}(\xi)$, in (2.6), has a minimum at $p = 1$. In Figure 1 (*left*), we present the normalized standard deviation, $\sigma_{\mathrm{L}_p}(\xi)/\xi$, independent of ξ, as a function of p. On another side, the asymptotic bias ruler, $b_{\mathrm{L}_p}(\rho)$, also in (2.6), is independent of ξ and always decreasing in p. Such a performance is shown in Figure 1 (*right*).

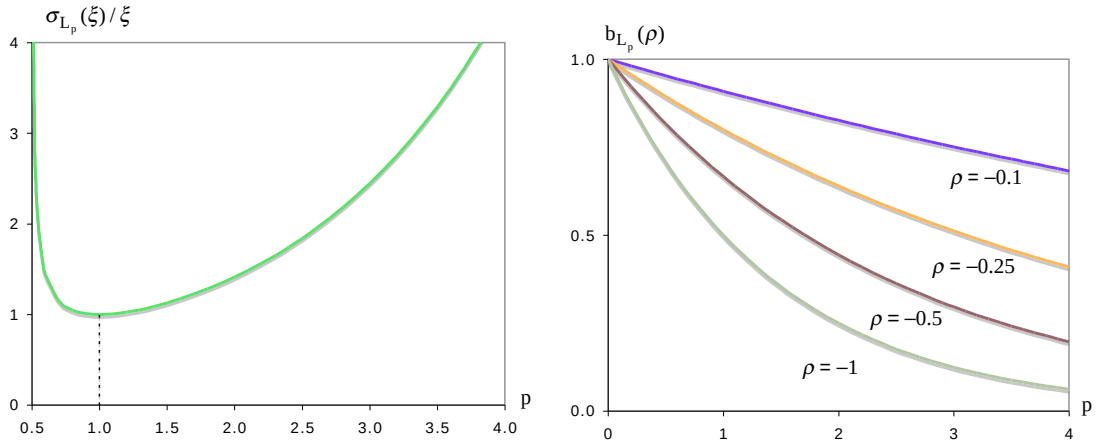


Figure 1: Graph of $\sigma_{\mathrm{L}_p}(\xi)/\xi$, as a function of $p > 1/2$ (*left*) and of the asymptotic bias ruler $b_{\mathrm{L}_p}(\rho)$, for $\rho = -0.1, -0.25, -0.5$ and -1, as a function of $p \geq 0$.

The aforementioned results claim for an asymptotic study, at optimal (k, p), of the class of EVI-estimators in (1.7), a topic to be dealt with in Section 3.

3. ASYMPTOTIC COMPARISON AT OPTIMAL LEVELS

We next proceed to the comparison of the aforementioned non-RB EVI-estimators, generally denoted by $\hat{\xi}^{\bullet}(k)$, at their optimal levels. This is again done in a way similar to the one used in several articles, among which we refer Dekkers and de Haan ([20]), de Haan and Peng ([41]), Gomes and Martins ([33]), Gomes *et al.* ([36], [37], [35], [26]), Gomes and Neves ([38]), Gomes and Henriques-Rodrigues ([29], [30]), and Brilhante *et al.* ([8]), among others. Let us assume that for any intermediate sequence of integers $k = k_n$, (2.3) holds. We write $\mathrm{Bias}_{\infty}\left(\hat{\xi}^{\bullet}(k)\right) := b_{\bullet}\, A(n/k)$ and $\mathrm{Var}_{\infty}\left(\hat{\xi}^{\bullet}(k)\right) := \sigma^2_{\bullet}/k$. The so-called *asymptotic mean square error* (AMSE) is then given by $\mathrm{AMSE}\left(\hat{\xi}^{\bullet}(k)\right) := \sigma^2_{\bullet}/k + b^2_{\bullet}\, A^2(n/k)$. Regular variation theory enabled Dekkers and de Haan ([20]) to show that, whenever $b_{\bullet} \neq 0$, there exists a function $\varphi(n) = \varphi(n, \xi, \rho)$, such that

$$\lim_{n\to\infty} \varphi(n)\ \mathrm{AMSE}\left(\hat{\xi}^{\bullet}_0\right) \;=\; \left(\sigma^2_{\bullet}\right)^{-\frac{2\rho}{1-2\rho}} \left(b^2_{\bullet}\right)^{\frac{1}{1-2\rho}} \;=:\; \mathrm{LMSE}\left(\hat{\xi}^{\bullet}_0\right), \tag{3.1}$$

where $\hat{\xi}_0^{\bullet} := \hat{\xi}^{\bullet}\big(k_{0|\bullet}(n)\big)$ and $k_{0|\bullet}(n) := \arg\min_k \mathrm{MSE}\big(\hat{\xi}^{\bullet}(k)\big)$. Moreover, if we slightly restrict the second-order condition in (2.1), assuming (2.2), we can write

$$k_{0|\bullet}(n) \;=\; \arg\min_k \mathrm{MSE}\big(\hat{\xi}^{\bullet}(k)\big) \;=\; \left(\frac{\sigma_\bullet^2\, n^{-2\rho}}{b_\bullet^2\, \xi^2\, \beta^2(-2\rho)}\right)^{1/(1-2\rho)} \big(1+o(1)\big)\,.$$

We consider the following:

Definition 3.1. Given two biased estimators $\hat{\xi}^{(1)}(k)$ and $\hat{\xi}^{(2)}(k)$, for which (2.3) holds, with constants (σ_1, b_1) and (σ_2, b_2), $b_1, b_2 \neq 0$, respectively, both computed at their optimal levels, the *asymptotic root efficiency* (AREFF) of $\hat{\xi}_0^{(1)}$ relatively to $\hat{\xi}_0^{(2)}$ is

$$\text{(3.2)} \qquad \mathrm{AREFF}_{1|2} \equiv \mathrm{AREFF}_{\hat{\xi}_0^{(1)}|\hat{\xi}_0^{(2)}} := \sqrt{\mathrm{LMSE}\big(\hat{\xi}_0^{(2)}\big)/\mathrm{LMSE}\big(\hat{\xi}_0^{(1)}\big)} = \left(\left(\frac{\sigma_2}{\sigma_1}\right)^{-2\rho} \left|\frac{b_2}{b_1}\right|\right)^{\frac{1}{1-2\rho}},$$

with LMSE defined in (3.1).

Remark 3.1. Note that the AREFF-indicator, in (3.2), has been conceived so that the highest the AREFF indicator is, the better is the estimator identified with the superscript (1).

The non-RB L_p, H_p, and PPWM EVI-estimators, respectively given in (1.7), (1.9) and (1.10), will be crucially included in the asymptotic comparison in Section 3.1.

3.1. Asymptotic comparison of EVI-estimators at optimal levels

Let us now turn back to the L_p EVI-estimators in (1.7), at optimal k-levels in the sense of minimum RMSE. We have

$$\mathrm{LMSE}(\mathrm{L}_{0|p}) \;=\; \Big(\xi^2\, \Gamma(2p-1)/\,\Gamma^2(p)\Big)^{-\frac{2\rho}{1-2\rho}} \Big((1-\rho)^{-2p}\Big)^{\frac{1}{1-2\rho}}$$

and

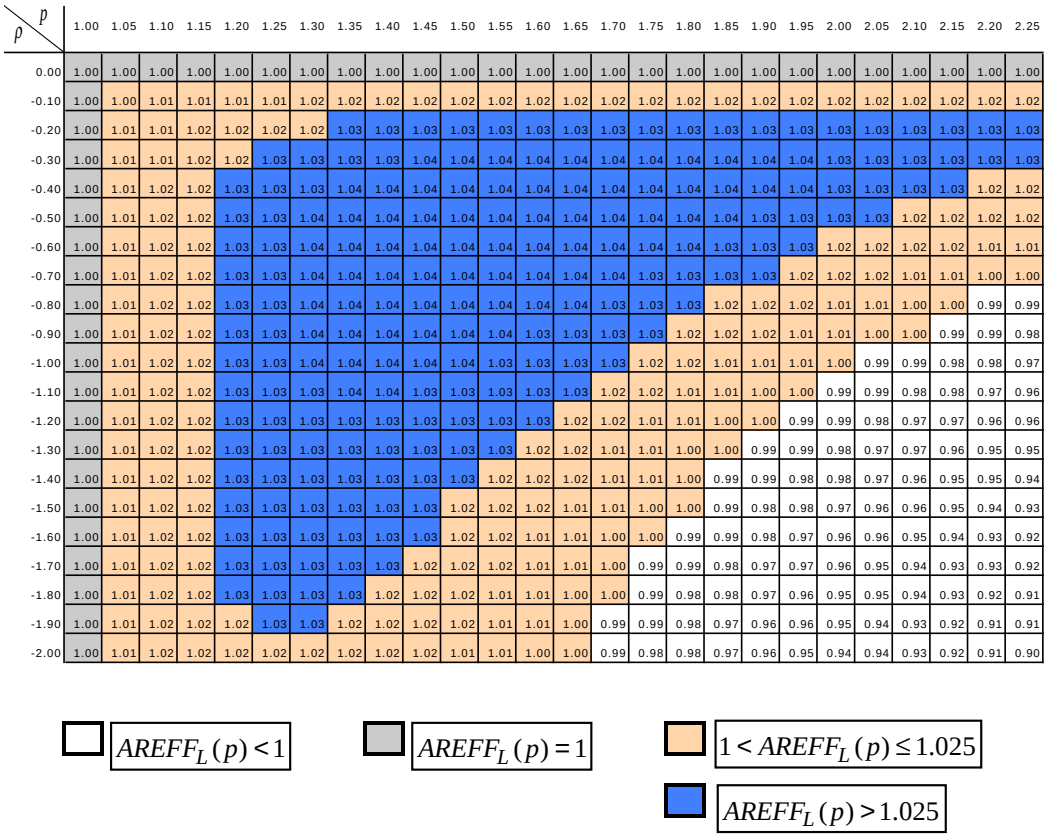
$$\text{(3.3)} \qquad \mathrm{AREFF}_{\mathrm{L}}(p) \;\equiv\; \mathrm{AREFF}_{\mathrm{L}_{0|p}|\mathrm{L}_{0|1}} \;=\; \left(\Big(\Gamma(p)/\sqrt{\Gamma(2p-1)}\Big)^{-2\rho}\, (1-\rho)^{p-1}\right)^{\frac{1}{1-2\rho}}.$$

Remark 3.2. In Gomes *et al.* ([34]) was shown that the AREFF of the optimal $\mathrm{L}_2(k)$ comparatively to the optimal $\mathrm{L}_1(k)$ is given by $[2^{\rho}(1-\rho)]^{1/(1-2\rho)}$, in agreement with (3.3). As noticed in the aforementioned article, $\mathrm{AREFF}_{\mathrm{L}}(2) > 1 \iff -1 < \rho < 0$.

To measure the performance of $\mathrm{H}_{0|p}$, with H_p the MO_p EVI-estimator in (1.9), Brilhante *et al.* ([8]) computed a similar AREFF-indicator, given by

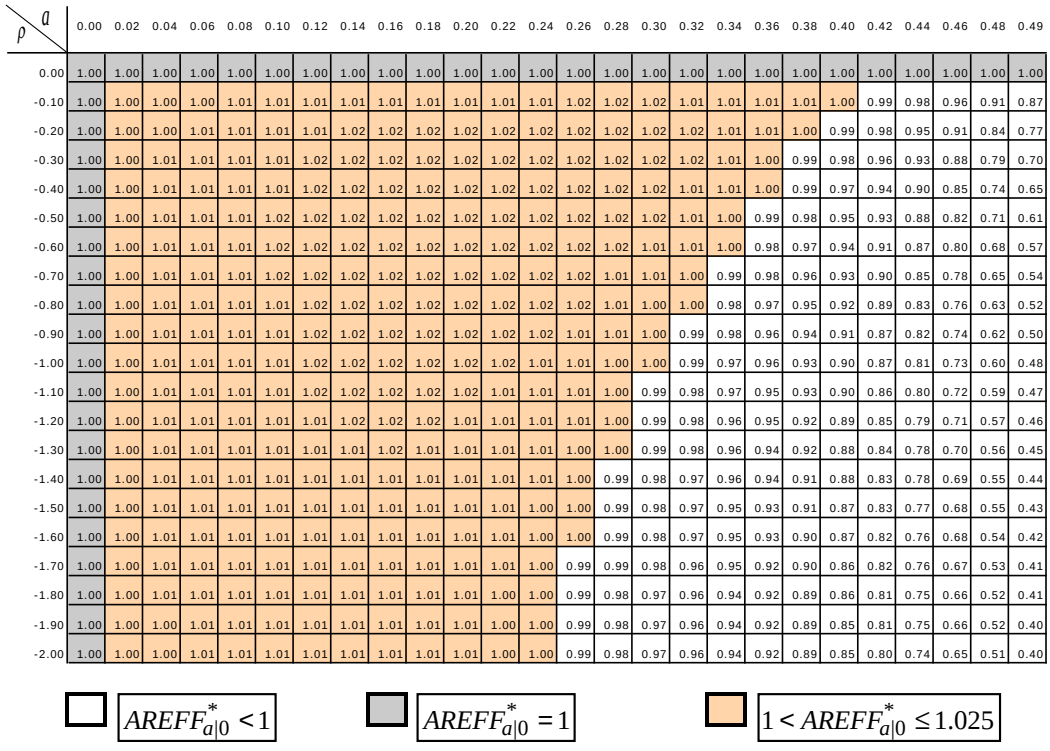
$$\text{(3.4)} \qquad \mathrm{AREFF}_{\mathrm{H}}(p) \;\equiv\; \mathrm{AREFF}_{\mathrm{H}_{0|p}|\mathrm{H}_{0|0}} \;=\; \left(\left(\frac{\sqrt{1-2p\xi}}{1-p\xi}\right)^{-2\rho} \left|\frac{1-p\xi-\rho}{(1-\rho)\,(1-p\xi)}\right|\right)^{\frac{1}{1-2\rho}},$$

reparameterized in $(\rho,\ a = p\xi < 1/2)$, and denoted by $\mathrm{AREFF}^*_{a|0}$. In Figure 2, we picture $\mathrm{AREFF}_{\mathrm{L}}(p)$ in (3.3) (*top*) and $\mathrm{AREFF}^*_{a|0}$ (*bottom*).



ρ \ p	1.00	1.05	1.10	1.15	1.20	1.25	1.30	1.35	1.40	1.45	1.50	1.55	1.60	1.65	1.70	1.75	1.80	1.85	1.90	1.95	2.00	2.05	2.10	2.15	2.20	2.25
0.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
-0.10	1.00	1.00	1.01	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02
-0.20	1.00	1.01	1.01	1.02	1.02	1.02	1.02	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03
-0.30	1.00	1.01	1.01	1.02	1.02	1.03	1.03	1.03	1.03	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.03	1.03	1.03	1.03	1.03	1.03
-0.40	1.00	1.01	1.02	1.02	1.03	1.03	1.03	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.03	1.03	1.03	1.03	1.02	1.02
-0.50	1.00	1.01	1.02	1.02	1.03	1.03	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.03	1.03	1.03	1.03	1.02	1.02	1.02	1.02
-0.60	1.00	1.01	1.02	1.02	1.03	1.03	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.03	1.03	1.03	1.02	1.02	1.02	1.02	1.01	1.01
-0.70	1.00	1.01	1.02	1.02	1.03	1.03	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.03	1.03	1.03	1.03	1.02	1.02	1.02	1.01	1.01	1.00	1.00
-0.80	1.00	1.01	1.02	1.02	1.03	1.03	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.03	1.03	1.03	1.02	1.02	1.02	1.01	1.01	1.00	1.00	0.99	0.99
-0.90	1.00	1.01	1.02	1.02	1.03	1.03	1.04	1.04	1.04	1.04	1.04	1.04	1.03	1.03	1.03	1.03	1.02	1.02	1.02	1.01	1.01	1.00	1.00	0.99	0.99	0.98
-1.00	1.00	1.01	1.02	1.02	1.03	1.03	1.04	1.04	1.04	1.04	1.04	1.03	1.03	1.03	1.03	1.02	1.02	1.01	1.01	1.01	1.00	0.99	0.99	0.98	0.98	0.97
-1.10	1.00	1.01	1.02	1.02	1.03	1.03	1.03	1.04	1.04	1.03	1.03	1.03	1.03	1.03	1.02	1.02	1.01	1.01	1.00	1.00	0.99	0.99	0.98	0.98	0.97	0.96
-1.20	1.00	1.01	1.02	1.02	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.02	1.02	1.01	1.01	1.00	1.00	0.99	0.99	0.98	0.97	0.97	0.96	0.96
-1.30	1.00	1.01	1.02	1.02	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.02	1.02	1.01	1.01	1.00	1.00	0.99	0.99	0.98	0.97	0.97	0.96	0.95	0.95
-1.40	1.00	1.01	1.02	1.02	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.02	1.02	1.02	1.01	1.01	1.00	0.99	0.99	0.98	0.98	0.97	0.96	0.95	0.95	0.94
-1.50	1.00	1.01	1.02	1.02	1.03	1.03	1.03	1.03	1.03	1.03	1.02	1.02	1.02	1.01	1.01	1.00	1.00	0.99	0.98	0.98	0.97	0.96	0.96	0.95	0.94	0.93
-1.60	1.00	1.01	1.02	1.02	1.03	1.03	1.03	1.03	1.03	1.03	1.02	1.02	1.01	1.01	1.00	1.00	0.99	0.99	0.98	0.97	0.96	0.96	0.95	0.94	0.93	0.92
-1.70	1.00	1.01	1.02	1.02	1.03	1.03	1.03	1.03	1.03	1.02	1.02	1.02	1.01	1.01	1.00	0.99	0.99	0.98	0.97	0.97	0.96	0.95	0.94	0.93	0.93	0.92
-1.80	1.00	1.01	1.02	1.02	1.03	1.03	1.03	1.03	1.02	1.02	1.02	1.01	1.01	1.00	1.00	0.99	0.98	0.98	0.97	0.96	0.95	0.95	0.94	0.93	0.92	0.91
-1.90	1.00	1.01	1.02	1.02	1.02	1.03	1.03	1.02	1.02	1.02	1.02	1.01	1.01	1.00	0.99	0.99	0.98	0.97	0.96	0.96	0.95	0.94	0.93	0.92	0.91	0.91
-2.00	1.00	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.01	1.01	1.00	1.00	0.99	0.98	0.98	0.97	0.96	0.95	0.94	0.94	0.93	0.92	0.91	0.90

$AREFF_L(p) < 1$ $AREFF_L(p) = 1$ $1 < AREFF_L(p) \le 1.025$ $AREFF_L(p) > 1.025$



ρ \ a	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14	0.16	0.18	0.20	0.22	0.24	0.26	0.28	0.30	0.32	0.34	0.36	0.38	0.40	0.42	0.44	0.46	0.48	0.49
0.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
-0.10	1.00	1.00	1.00	1.00	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.02	1.02	1.02	1.01	1.01	1.01	1.01	1.00	0.99	0.98	0.96	0.91	0.87
-0.20	1.00	1.00	1.00	1.01	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.01	1.01	1.00	0.99	0.98	0.95	0.91	0.84	0.77
-0.30	1.00	1.00	1.01	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.01	1.00	0.99	0.98	0.96	0.93	0.88	0.79	0.70
-0.40	1.00	1.00	1.01	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.01	1.01	1.00	0.99	0.97	0.94	0.90	0.85	0.74	0.65
-0.50	1.00	1.00	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.01	1.00	0.99	0.98	0.95	0.93	0.88	0.82	0.71	0.61
-0.60	1.00	1.00	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.01	1.01	1.00	0.98	0.97	0.94	0.91	0.87	0.80	0.68	0.57
-0.70	1.00	1.00	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.01	1.01	1.00	0.99	0.98	0.96	0.93	0.90	0.85	0.78	0.65	0.54
-0.80	1.00	1.00	1.01	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.01	1.00	1.00	0.98	0.97	0.95	0.92	0.89	0.83	0.76	0.63	0.52
-0.90	1.00	1.00	1.01	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.02	1.01	1.01	1.00	0.99	0.98	0.96	0.94	0.91	0.87	0.82	0.74	0.62	0.50
-1.00	1.00	1.00	1.01	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.01	1.01	1.00	1.00	0.99	0.97	0.96	0.93	0.90	0.87	0.81	0.73	0.60	0.48
-1.10	1.00	1.00	1.01	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.01	1.01	1.01	1.00	0.99	0.98	0.97	0.95	0.93	0.90	0.86	0.80	0.72	0.59	0.47
-1.20	1.00	1.00	1.01	1.01	1.01	1.01	1.01	1.02	1.02	1.02	1.01	1.01	1.01	1.01	1.00	0.99	0.98	0.96	0.95	0.92	0.89	0.85	0.79	0.71	0.57	0.46
-1.30	1.00	1.00	1.01	1.01	1.01	1.01	1.01	1.01	1.02	1.01	1.01	1.01	1.01	1.00	1.00	0.99	0.98	0.96	0.94	0.92	0.88	0.84	0.78	0.70	0.56	0.45
-1.40	1.00	1.00	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00	0.99	0.98	0.97	0.96	0.94	0.91	0.88	0.83	0.78	0.69	0.55	0.44
-1.50	1.00	1.00	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00	1.00	0.99	0.98	0.97	0.95	0.93	0.91	0.87	0.83	0.77	0.68	0.55	0.43
-1.60	1.00	1.00	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00	1.00	0.99	0.98	0.97	0.95	0.93	0.90	0.87	0.82	0.76	0.68	0.54	0.42
-1.70	1.00	1.00	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00	0.99	0.99	0.98	0.96	0.95	0.92	0.90	0.86	0.82	0.76	0.67	0.53	0.41
-1.80	1.00	1.00	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00	1.00	0.99	0.98	0.97	0.96	0.94	0.92	0.89	0.86	0.81	0.75	0.66	0.52	0.41
-1.90	1.00	1.00	1.00	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00	1.00	0.99	0.98	0.97	0.96	0.94	0.92	0.89	0.85	0.81	0.75	0.66	0.52	0.40
-2.00	1.00	1.00	1.00	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.01	1.00	1.00	0.99	0.98	0.97	0.96	0.94	0.92	0.89	0.85	0.80	0.74	0.65	0.51	0.40

$AREFF^*_{a|0} < 1$ $AREFF^*_{a|0} = 1$ $1 < AREFF^*_{a|0} \le 1.025$

Figure 2: $\mathrm{AREFF}_{\mathrm{L}}(p)$, in (3.3) (*top*) and $\mathrm{AREFF}^*_{a|0}$ (*bottom*).

The gain in efficiency is not terribly high, but, at optimal levels, there is a wide region of the (p, ρ)-plane where the new class of L_p EVI-estimators performs better than the Hill EVI-estimators, with efficiencies slightly higher than the ones associated with the comparison of H_p and the Hill, in the (a, ρ)-plane. This result together with the fact that as far as we know, the EVI-estimators in (1.9) computed at the optimal (k, p) in the sense of maximal $\text{AREFF}_{\text{H}}(p)$, with $\text{AREFF}_{\text{H}}(p)$ given in (3.4), i.e. computed at $p_{\text{M|H}} \equiv p_{\text{M|H}}(\rho) := \arg\max_p \text{AREFF}_{\text{H}}(p)$, explicitly given by

$$p_{\text{M|H}} = \varphi_\rho/\xi\,, \qquad \text{with} \quad \varphi_\rho := 1 - \rho/2 - \sqrt{\rho^2 - 4\rho + 2}\Big/2\,, \tag{3.5}$$

$b_{p_{\text{M|H}}} \neq 0$, is, as expected, a non-RB EVI-estimator which is able to beat the Hill EVI-estimator in the whole (ξ, ρ)-plane, immediately leads us to think on what happens for the optimal value of p associated with the L_p EVI-estimation. Contrarily to the explicit expression for $p_{\text{M|H}}$, in (3.5), the value of $p_{\text{M|L}} = p_{\text{M|L}}(\rho) := \arg\max_p \text{AREFF}_{\text{L}}(p)$, with $\text{AREFF}_{\text{L}}(p)$ given in (3.3), is an implicit function of ρ, easy to evaluate numerically. Some of those values are presented in Table 1.

Table 1: Values of $p_{\text{M|L}} = p_{\text{M|L}}(\rho) := \arg\max_p \text{AREFF}_{\text{L}}(p)$ for a few values of $|\rho|$.

$\lvert\rho\rvert$	0^+	0.01	0.1	0.2	0.3	0.4	0.5	0.6	0.8	1.0	1.5	2	$+\infty$
$p_{\text{M|L}}$	1	1.98	1.86	1.75	1.67	1.61	1.56	1.52	1.45	1.40	1.32	1.27	1

In Figure 3, we picture the indicator $\text{AREFF}_{\text{L}}(p)$, as a function of p for a few values of ρ.

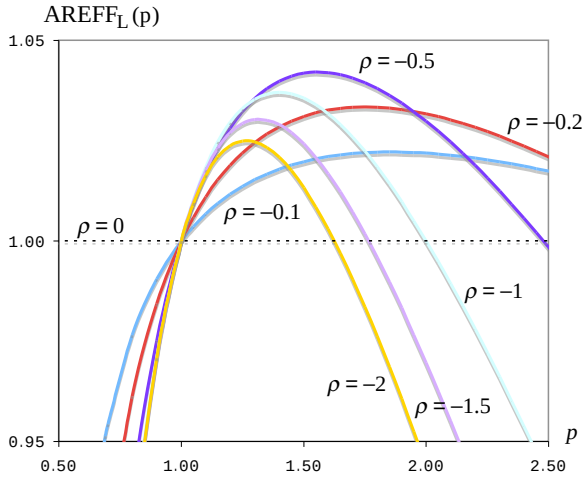


Figure 3: $\text{AREFF}_{\text{L}}(p)$, as a function of p, for $|\rho| = 0, 0.1, 0.2, 0.5(0.5)2$.

Indeed, just as $\text{AREFF}_{\text{H}}(p_{\text{M|H}}) > 1$, for any $\rho < 0$ and $\xi > 0$, also $\text{AREFF}_{\text{L}}(p_{\text{M|L}}) > 1$, for any $\rho < 0$ and $\xi > 0$. Moreover,

$$\text{AREFF}_{\text{L}}(p_{\text{M|L}}) > \text{AREFF}_{\text{H}}(p_{\text{M|H}})\,,$$

as illustrated in Figure 4.

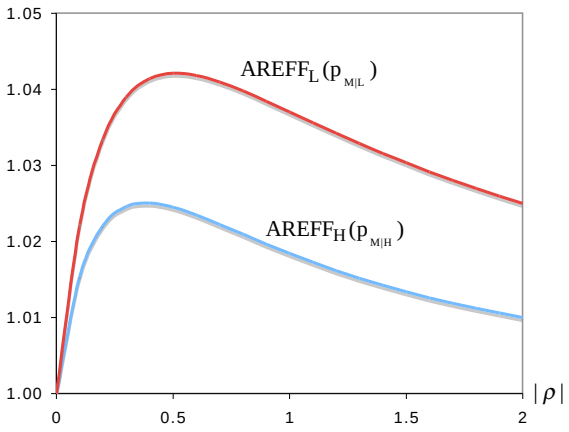


Figure 4: $\mathrm{AREFF}_{\mathrm{L}}(p_{\mathrm{M|L}})$ and $\mathrm{AREFF}_{\mathrm{H}}(p_{\mathrm{M|H}})$ as a function of $|\rho| = 0(0.1)2$.

Just as done in Gomes and Henriques-Rodrigues ([30]), and due to the competitive behaviour of the PPWM EVI-estimators, we still compare the L_p with the PPWM EVI-estimators, in (1.10), again at optimal levels. Whereas the gain in efficiency of the PPWM comparatively to the optimal H_p EVI-estimator happens in a wide region of the (ξ, ρ)-plane, $\mathrm{L}^* := \mathrm{L}_{p_{\mathrm{M|L}}}$ beats the optimal PPWM EVI-estimator (now denoted P, for sake of simplicity) in a wider region of the (ξ, ρ)-plane, as can be seen in Figure 5 (*bottom*). Indeed, in Figure 5 (*top*), we reproduce the Figure in Gomes and Henriques-Rodrigues ([31]), related to the comparative behaviour between $\mathrm{H}^* := \mathrm{H}_{p_{\mathrm{M|H}}}$ and the optimal PPWM EVI-estimator.

So far, asymptotically and for a heavy right-tail, the class of Lehmer's EVI-estimators, in (1.7), seems indeed to be the most competitive class of non-RB EVI-estimators in the literature. Note however that further classes of generalized means, among which we mention the ones studied in Paulauskas and Vaičiulis ([46]), may possibly provide even more astonishing results.

4. AN ASYMPTOTIC COMPARISON WITH OTHER EVI-ESTIMATORS AT OPTIMAL LEVELS

As mentioned above, the optimal MO_p EVI-estimator (H^*), associated with a value $p_{\mathrm{M|H}} \neq 0$, can beat the optimal Hill EVI-estimator in the whole (ξ, ρ)-plane. But it is now beaten by the optimal Lehmer EVI-estimator (L^*), also in the whole (ξ, ρ), an atypical behaviour among other classical EVI-estimators. We thus consider now sensible to compare H^* and L^* with the most common EVI-estimators in the literature, non generally RB, but possibly RB in some regions of the (ξ, ρ)-plane.

We shall take into account the *moment* (M) EVI-estimators, studied in Dekkers *et al.* ([19]), based on $\left(M_{k,n}^{(1)}, M_{k,n}^{(2)}\right)$, with $M_{k,n}^{(p)}$ defined in (1.6). They are consistent for all $\xi \in \mathbb{R}$, being given by

$$\hat{\xi}^{\mathrm{M}}(k) \equiv \mathrm{M}(k) := M_{k,n}^{(1)} + \frac{1}{2}\left\{1 - \left(M_{k,n}^{(2)} / \left(M_{k,n}^{(1)}\right)^2 - 1\right)^{-1}\right\}. \tag{4.1}$$

ρ \ ξ	0.05	0.07	0.09	0.11	0.13	0.15	0.17	0.19	0.21	0.23	0.25	0.27	0.29	0.31	0.33	0.35	0.37	0.39	0.41	0.43	0.45
0.00	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H
-0.05	P	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*
-0.07	P	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*
-0.09	P	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*
-0.11	P	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*
-0.13	P	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*
-0.15	P	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*
-0.17	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*
-0.19	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*
-0.21	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*
-0.23	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*
-0.25	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*
-0.27	P	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*
-0.29	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*	H*
-0.31	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*	H*
-0.33	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*	H*
-0.35	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*	H*
-0.37	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*	H*
-0.39	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*	H*
-0.41	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*	H*
-0.43	P	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*	H*
-0.45	P	P	P	P	P	P	P	P	P	P	P	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*

ρ \ ξ	0.05	0.07	0.09	0.11	0.13	0.15	0.17	0.19	0.21	0.23	0.25	0.27	0.29	0.31	0.33	0.35	0.37	0.39	0.41	0.43	0.45
0.00	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H	H
-0.05	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.07	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.09	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.11	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.13	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.15	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.17	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.19	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.21	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.23	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.25	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.27	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.29	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.31	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.33	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.35	L*	L*	L*	P	P	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.37	L*	L*	L*	P	P	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.39	L*	L*	P	P	P	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.41	L*	L*	P	P	P	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.43	L*	P	P	P	P	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.45	L*	P	P	P	P	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*

Figure 5: Best EVI-estimator asymptotically and at optimal levels for a choice between H* and PPWM (*top*) and between L* and PPWM (*bottom*).

We additionally consider the *generalized Hill* (GH) EVI-estimators (Beirlant *et al.*, [5]), based on the Hill estimators in (1.3) and with the functional form

$$\hat{\xi}^{\mathrm{GH}}(k) \equiv \mathrm{GH}(k) := \hat{\xi}^{\mathrm{H}}(k) + \frac{1}{k}\sum_{i=1}^{k}\left\{\ln \hat{\xi}^{\mathrm{H}}(i) - \ln \hat{\xi}^{\mathrm{H}}(k)\right\}, \tag{4.2}$$

further studied in Beirlant *et al.* ([3]). Just as in de Haan and Ferreira ([40]), we also consider, for $\xi < 1$, the *generalized Pareto* (GP) PWM (GPPWM) EVI-estimators, based on the sample of exceedances over the high random level $X_{n-k:n}$ and defined by

$$\hat{\xi}^{\mathrm{GPPWM}}(k) \equiv \mathrm{GPPWM}(k) := 1 - \frac{2\,\hat{a}_1^\star(k)}{\hat{a}_0^\star(k) - 2\,\hat{a}_1^\star(k)}, \tag{4.3}$$

with $k = 1, ..., n-1$, and

$$\hat{a}_s^\star(k) := \frac{1}{k}\sum_{i=1}^{k}\left(\frac{i-1}{k-1}\right)^s \left(X_{n-i+1:n} - X_{n-k:n}\right), \qquad s = 0, 1\,.$$

Finally, with U_{ik}, $1 \le i \le k$, given in (1.8), and the notation

$$L_{k,n}^{(j)} := \frac{1}{k}\sum_{i=1}^{k}\left(1 - U_{ik}^{-1}\right)^j, \qquad j \ge 1\,,$$

we further consider the *mixed moment* (MM) EVI-estimators (Fraga Alves *et al.*, [23]), defined by

$$\hat{\xi}^{\mathrm{MM}}(k) \equiv \mathrm{MM}(k) := \frac{\hat{\varphi}_{k,n} - 1}{1 + 2\min(\hat{\varphi}_{k,n} - 1, 0)}, \qquad \text{with} \quad \hat{\varphi}_{k,n} := \frac{M_{k,n}^{(1)} - L_{k,n}^{(1)}}{\left(L_{k,n}^{(1)}\right)^2}. \tag{4.4}$$

The estimators in (4.3) are consistent only for $0 < \xi < 1$. The estimators in (4.1), (4.2) and (4.4) are consistent for any $\xi \in \mathbb{R}$, but will be here considered only for $\xi > 0$.

Remark 4.1. Note that the MM EVI-estimators, in (4.4), are, for a wide class of models with $\xi > 0$, very close to the implicit ML EVI-estimators, based on the excesses $W_{ik} := X_{n-i+1:n} - X_{n-k:n}$, $1 \le i \le k < n$ (see Fraga Alves *et al.*, [23], for details on the topic). A comprehensive study of the asymptotic properties of the aforementioned ML EVI-estimators has been undertaken in Drees *et al.* ([21]).

Remark 4.2. Further note that all the aforementioned EVI-estimators in this section are scale invariant. The GPPWM and the ML EVI-estimators are also location invariant, and can be regarded as classes of PORT EVI-estimators. We can further consider PORT-M, GH and MM EVI-estimators.

Under the validity of the second-order condition in (2.1), and for intermediate $k = k_n$, (2.3) holds, with

$$b_{\mathrm{M}} = b_{\mathrm{GH}} = \frac{\xi - \xi\rho + \rho}{\xi(1-\rho)^2}, \qquad \sigma_{\mathrm{M}}^2 = \sigma_{\mathrm{GH}}^2 = 1 + \xi^2\,,$$

$$b_{\mathrm{MM}} = b_{\mathrm{ML}} = \frac{(1+\xi)(\xi+\rho)}{\xi(1-\rho)(1+\xi-\rho)}, \qquad \sigma_{\mathrm{MM}}^2 = \sigma_{\mathrm{ML}}^2 = (1+\xi)^2\,,$$

and for $\xi < 1/2$,

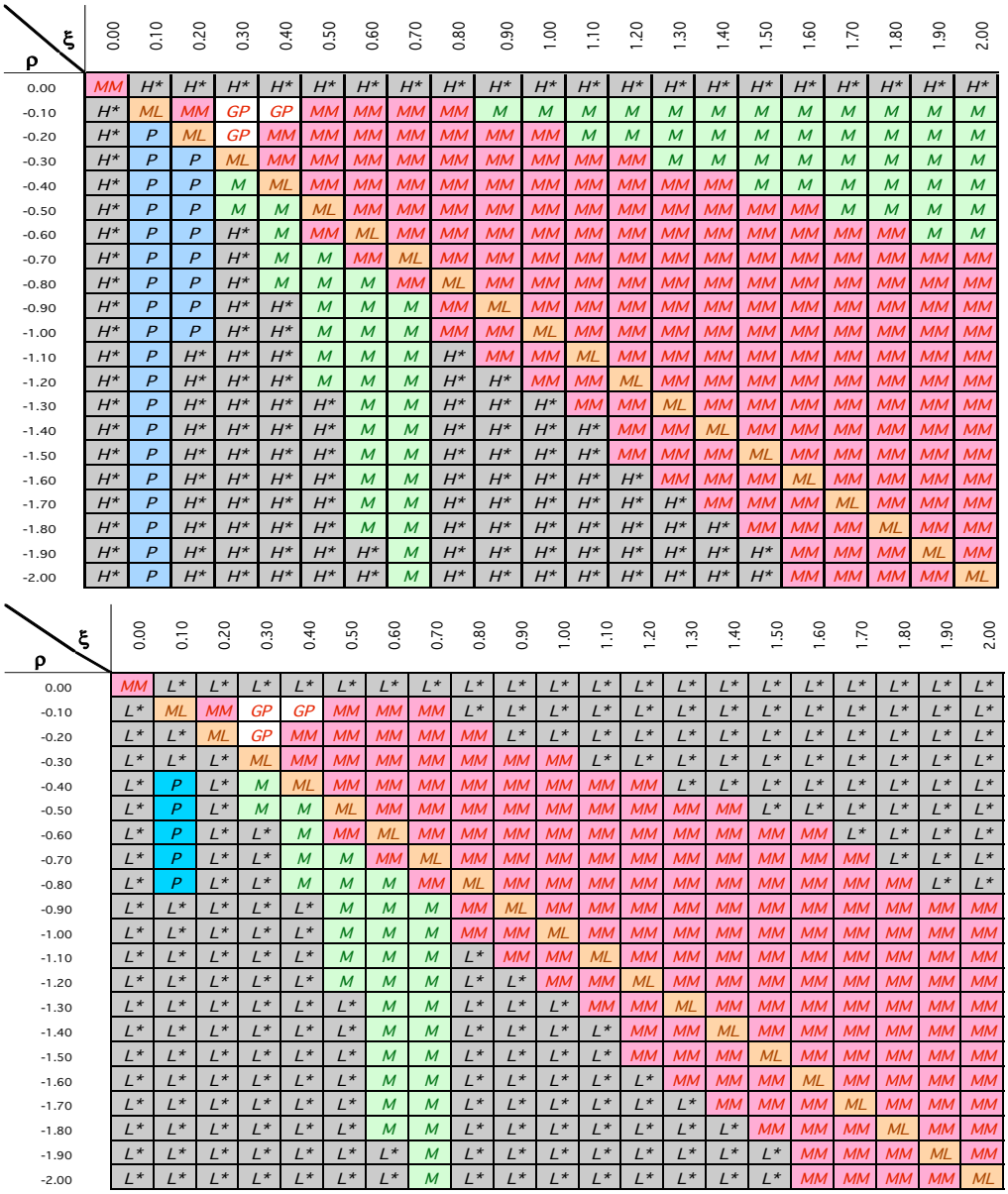
$$b_{\text{GPPWM}} = \frac{(\xi+\rho)\, b_{\text{PPWM}}}{\xi} \qquad \text{and} \qquad \sigma^2_{\text{GPPWM}} = \frac{(1-\xi+2\,\xi^2)\,(1-\xi)\,(2-\xi)^2}{(1-2\,\xi)\,(3-2\,\xi)}\,.$$

As happened before with the optimal MO_p EVI-estimator, the optimal Lehmer EVI-estimator can be beaten by the optimal M (and GH) EVI-estimator in a region close to $\xi = -\rho/(1-\rho)$, where $b_{\text{M}} = b_{\text{GH}} = 0$. The optimal MM EVI-estimator in (4.4), asymptotically equivalent to the optimal ML-estimator, unless $\xi+\rho = 0$ and $(\xi,\rho) \neq (0,0)$, outperforms the M EVI-estimator at optimal levels, in a region around $\xi+\rho = 0$, and can even outperform the optimal Lehmer EVI-estimator. The GPPWM EVI-estimator, in (4.3), is RB for $\xi+\rho = 0$, and can beat the MM EVI-estimator in a short region of the (ξ,ρ)-plane, as can be seen in Figure 6, where we exhibit the comparative behaviour of all 'classical' EVI-estimators under consideration, including both the L^* and the H^* classes (Figure 6, *bottom*), after including only the H^* class (Figure 6, *top*), as done in Brilhante *et al.* ([8]). The GPPWM and PPWM EVI-estimators are respectively denoted by GP and P. The PPWM, despite of non-RB, can beat even the optimal Lehmer for a few values of ξ around 0.1, as detected before (see also Figure 5, *bottom*).

Remark 4.3. As already mentioned in Brilhante *et al.* ([8]), note that in the region $\xi+\rho \neq 0$ and $\xi \neq -\rho/(1-\rho)$, where a further study under the third-order framework is needed, all RB EVI-estimators, like the corrected-Hill EVI-estimators in Caeiro *et al.* ([16]), overpass at optimal levels all classical and non-RB EVI-estimators available in the literature. They were thus not included in Figure 6, so that we can see the comparative behaviour of the non-RB EVI-estimators. A similar comment applies to the optimal $\text{CG}_{p,\delta}$ EVI-estimators, in (1.11).

Remark 4.4. As expected, none of the estimators can always dominate the alternatives, but the L_p EVI-estimators have a quite interesting performance, being unexpectedly able to beat the $\text{MO}_p \equiv \text{H}_p$ EVI-estimators at optimal levels in the whole (ξ,ρ)-plane.

Remark 4.5. For a final adaptive EVI-estimation, i.e. for the choice of (k,p) in (1.7), a double-bootstrap algorithm, of the type of Algorithm 4.1 in Brilhante *et al.* ([8]), now based on the asymptotic behaviour in (2.7), can be used. Such an algorithm relies on the minimization of a bootstrap estimate of the AMSE. Also, the slight modification of the semi-parametric bootstrap method in Caers *et al.* ([18]), provided in the Algorithm 4.3 of Caeiro and Gomes ([13]) is expected to provide an adequate estimation of the bootstrap MSE. Alternatively, one can use any of the available methods based on sample-path stability (see also Caeiro and Gomes, [13], among others).



ρ \ ξ	0.00	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00	1.10	1.20	1.30	1.40	1.50	1.60	1.70	1.80	1.90	2.00
0.00	MM	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*	H*
-0.10	H*	ML	MM	GP	GP	MM	MM	MM	MM	M	M	M	M	M	M	M	M	M	M	M	M
-0.20	H*	P	ML	GP	MM	MM	MM	MM	MM	MM	MM	M	M	M	M	M	M	M	M	M	M
-0.30	H*	P	P	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	M	M	M	M	M	M	M	M
-0.40	H*	P	P	M	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	M	M	M	M	M	M
-0.50	H*	P	P	M	M	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	M	M	M	M
-0.60	H*	P	P	H*	M	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	M	M
-0.70	H*	P	P	H*	M	M	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM
-0.80	H*	P	P	H*	M	M	M	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM
-0.90	H*	P	P	H*	H*	M	M	M	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM
-1.00	H*	P	P	H*	H*	M	M	M	MM	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM
-1.10	H*	P	H*	H*	H*	M	M	M	H*	MM	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM
-1.20	H*	P	H*	H*	H*	M	M	M	H*	H*	MM	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM
-1.30	H*	P	H*	H*	H*	H*	M	M	H*	H*	H*	MM	MM	ML	MM	MM	MM	MM	MM	MM	MM
-1.40	H*	P	H*	H*	H*	H*	M	M	H*	H*	H*	H*	MM	MM	ML	MM	MM	MM	MM	MM	MM
-1.50	H*	P	H*	H*	H*	H*	M	M	H*	H*	H*	H*	MM	MM	MM	ML	MM	MM	MM	MM	MM
-1.60	H*	P	H*	H*	H*	H*	M	M	H*	H*	H*	H*	H*	MM	MM	MM	ML	MM	MM	MM	MM
-1.70	H*	P	H*	H*	H*	H*	M	M	H*	H*	H*	H*	H*	H*	MM	MM	MM	ML	MM	MM	MM
-1.80	H*	P	H*	H*	H*	H*	M	M	H*	H*	H*	H*	H*	H*	H*	MM	MM	MM	ML	MM	MM
-1.90	H*	P	H*	H*	H*	H*	H*	M	H*	H*	H*	H*	H*	H*	H*	H*	MM	MM	MM	ML	MM
-2.00	H*	P	H*	H*	H*	H*	H*	M	H*	H*	H*	H*	H*	H*	H*	H*	MM	MM	MM	MM	ML

ρ \ ξ	0.00	0.10	0.20	0.30	0.40	0.50	0.60	0.70	0.80	0.90	1.00	1.10	1.20	1.30	1.40	1.50	1.60	1.70	1.80	1.90	2.00
0.00	MM	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.10	L*	ML	MM	GP	GP	MM	MM	MM	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.20	L*	L*	ML	GP	MM	MM	MM	MM	MM	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.30	L*	L*	L*	ML	MM	MM	MM	MM	MM	MM	MM	L*	L*	L*	L*	L*	L*	L*	L*	L*	L*
-0.40	L*	P	L*	M	ML	MM	MM	MM	MM	MM	MM	MM	MM	L*	L*	L*	L*	L*	L*	L*	L*
-0.50	L*	P	L*	M	M	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	L*	L*	L*	L*	L*	L*
-0.60	L*	P	L*	L*	M	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	L*	L*	L*	L*
-0.70	L*	P	L*	L*	M	M	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	L*	L*	L*
-0.80	L*	P	L*	L*	M	M	M	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	L*	L*
-0.90	L*	L*	L*	L*	L*	M	M	M	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM
-1.00	L*	L*	L*	L*	L*	M	M	M	MM	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM	MM
-1.10	L*	L*	L*	L*	L*	M	M	M	L*	MM	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM	MM
-1.20	L*	L*	L*	L*	L*	M	M	M	L*	L*	MM	MM	ML	MM	MM	MM	MM	MM	MM	MM	MM
-1.30	L*	L*	L*	L*	L*	L*	M	M	L*	L*	L*	MM	MM	ML	MM	MM	MM	MM	MM	MM	MM
-1.40	L*	L*	L*	L*	L*	L*	M	M	L*	L*	L*	L*	MM	MM	ML	MM	MM	MM	MM	MM	MM
-1.50	L*	L*	L*	L*	L*	L*	M	M	L*	L*	L*	L*	MM	MM	MM	ML	MM	MM	MM	MM	MM
-1.60	L*	L*	L*	L*	L*	L*	M	M	L*	L*	L*	L*	L*	MM	MM	MM	ML	MM	MM	MM	MM
-1.70	L*	L*	L*	L*	L*	L*	M	M	L*	L*	L*	L*	L*	L*	MM	MM	MM	ML	MM	MM	MM
-1.80	L*	L*	L*	L*	L*	L*	M	M	L*	L*	L*	L*	L*	L*	L*	MM	MM	MM	ML	MM	MM
-1.90	L*	L*	L*	L*	L*	L*	L*	M	L*	L*	L*	L*	L*	L*	L*	L*	MM	MM	MM	ML	MM
-2.00	L*	L*	L*	L*	L*	L*	L*	M	L*	L*	L*	L*	L*	L*	L*	L*	MM	MM	MM	MM	ML

Figure 6: Comparative overall behaviour of the EVI-estimators under study, considering only the optimal H_p, denoted H^* (*top*) and including both H^* and the optimal L_p, denoted L^* (*bottom*).

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MINIMUM DISTANCE TESTS AND ESTIMATES BASED ON RANKS

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Abstract:

- It is well known that the least squares estimate in classical linear regression model is very sensitive to violation of the assumptions, in particular normality of model errors. That is why a lot of alternative estimates has been developed to overcome these shortcomings. Quite interesting class of such estimates is formed by R-estimates. They use only ranks of response variable instead of their actual value.
  The goal of this paper is to extend this class by another estimates and tests based only on ranks. First, we will introduce a new rank test in linear regression model. The test statistic is based on a certain minimum distance estimator, but unlike classical rank tests in regression it is not a simple linear rank statistic. Then, we will return back to estimates and generalize minimum distance estimates for various type of distances.
  We will show that in some situation these tests and estimates have greater power than the classical ones. Theoretical results will be accompanied by a simulation study to illustrate finite sample behavior of estimates and tests.

Key-Words:

- *minimum distance estimates; ranks; robustness; tests.*

AMS Subject Classification:

- 62G05, 62G10, 62G35.

1. INTRODUCTION

Consider the model of regression line

$$Y_i = \beta_0 + x_i\beta + e_i\,, \qquad i = 1, ..., n\,, \tag{1.1}$$

where β_0 and β are unknown parameters, $x_1, ..., x_n$ are regressors, model errors $e_1, ..., e_n$ are assumed to be i.i.d. with an unknown distribution function F and uniformly continuous density f. Our aim is to estimate the slope parameter β and test the hypothesis

$$\mathbf{H}_0\colon\ \beta = 0 \qquad \text{against} \qquad \mathbf{K}_0\colon\ \beta \neq 0\,.$$

There is a lot of methods described in the literature. Ordinary least squares estimate and the corresponding t-test which are optimal for normal model errors. Unfortunately, normality assumption is often in practice not satisfied. Its violation may cause that the estimate or test fails.

We do not put any assumptions on the shape of the distribution function F. Generally, F is unknown; therefore we should use a nonparametric approach. We will focus on rank tests and estimates that instead of original response variables Y_i's use their ranks.

Rank tests form a class of statistical procedures which have the advantage of simplicity combined with surprising power. Modern development of rank tests began in the 1930's, see e.g. [2] and [4]. Well known is also Wilcoxon [11] who introduced popular Wilcoxon test for comparing two treatments. At first, it was believed that a high price in loss of efficiency when using rank tests has to be paid. However, it turned out that efficiency of rank tests behaves quite well under the classical assumption of normality. In addition these tests remain valid and have high efficiency when the assumption of normality is not satisfied. These facts were first brought out by Pitman [8]. Recently rank tests have been still very popular and widely used, see [1] and [5].

Let us briefly show the classical approach based on linear rank statistic (see e.g. [3]). It was developed more than fifty years ago and it is still being used thanks to its simplicity and robustness. Denote

$$Q_n = \frac{1}{n}\sum_{i=1}^{n}(x_i - \overline{x})^2\,, \qquad \text{with} \quad \overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i\,.$$

Let R_i be the rank of Y_i among $Y_1, ..., Y_n$ and define linear rank statistic

$$S_n = \frac{1}{\sqrt{n}}\sum_{i=1}^{n}(x_i - \overline{x})\ \varphi\!\left(\frac{R_i}{n+1}\right)$$

for some nondecreasing, nonconstant, square integrable score function $\varphi\colon (0,1) \mapsto \mathbb{R}$. Test criterion for $\mathbf{H}_0$ is then

$$T_n^2 = \frac{S_n^2}{A^2(\varphi)\,Q_n}\,, \tag{1.2}$$

where

$$A^2(\varphi) = \int_0^1 \big(\varphi(t) - \overline{\varphi}\big)^2\,dt\,, \qquad \overline{\varphi} = \int_0^1 \varphi(t)\,dt\,.$$

T_n^2 has under $\mathbf{H}_0$ asymptotically (under very mild conditions) χ^2 distribution with 1 degree of freedom.

Remark 1.1. The choice $\varphi(u) = u$, for $0 < u < 1$, leads to Wilcoxon rank test in regression. Hájek in [3] proved that such test in locally most powerful linear rank test for logistic model errors. In this case it has even greater power than t-test.

2. EMPIRICAL PROCESSES IN SIMPLE LINEAR REGRESSION

Koul [6] considered a class of estimates in linear regression model based on minimization of certain type of distances. Let us remind his approach. Define

$$T_{g,n}(s,t) \;=\; \frac{1}{\sqrt{n}} \sum_{i=1}^{n} g(x_i)\, \mathbb{I}\big\{R_{i,t} \le ns\big\}\,, \qquad 0 \le s \le 1\,, \quad t \in \mathbb{R}\,, \tag{2.1}$$

$$K_{g,n}(t) \;=\; \int_0^1 T_{g,n}^2(s,t)\, dL(s)\,, \qquad t \in \mathbb{R}\,, \tag{2.2}$$

where $R_{i,t}$ is the rank of the residual $Y_i - x_i t$ among $Y_1 - x_1 t, ..., Y_n - x_n t$. L is a distribution function on $[0,1]$ and g a real (weight) function such that $\sum_{i=1}^n g(x_i) = 0$.

The minimum distance estimator $\widehat{\beta}_{g,n}$ is then defined as

$$\widehat{\beta}_{g,n} \;=\; \arg\min\Big\{K_{g,n}(t)\colon t \in \mathbb{R}\Big\}\,.$$

Koul [6] showed that such estimates might have in some situations greater efficiency then corresponding R-estimates and LSE respectively. He also proved their asymptotic unbiasedness and normality. We will develop his idea and introduce a class of test statistics based on these estimates. We will investigate their finite sample as well as asymptotic behavior. Finally, we will return back to the estimates, generalize them and show that some have greater efficiency then original Koul's estimates.

3. TEST IN SIMPLE LINEAR REGRESSION

Recall that we want to test whether regression is present, i.e. we test the null hypothesis

$$\mathbf{H}_0\colon\ \beta = 0 \qquad \text{against} \qquad \mathbf{K}_0\colon\ \beta \ne 0\,.$$

We put the hypothetical value $\beta = 0$ into (2.1) and (2.2) and get the test statistic

$$K_{g,n}(0) \;=\; K_{g,n}^* = \int_0^1 T_{g,n}^2(s,0)\, dL(s)\,. \tag{3.1}$$

Discuss some computation aspects of (3.1). First, have a look at the formula (3.1) for $K^*_{g,n}$. Inserting (2.1) into (2.2) for $t = 0$ we have

$$\begin{aligned} K^*_{g,n} &= \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n} g(x_i)\, g(x_j) \int_0^1 \mathbb{I}\big\{R_i \le ns\big\}\, \mathbb{I}\big\{R_j \le ns\big\}\, dL(s) \\ &= \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n} g(x_i)\, g(x_j) \int_{\max\left\{\frac{R_i}{n}, \frac{R_j}{n}\right\}}^1 1\, dL(s)\,. \end{aligned}$$

L is a distribution function, hence $L(\max\{a,b\}) = \max\{L(a), L(b)\}$, it also remains true for limits from the left

$$K^*_{g,n} = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n} g(x_i)\, g(x_j) \left(1 - \max\left\{L\Big(\frac{R_i}{n}-\Big), L\Big(\frac{R_j}{n}-\Big)\right\}\right).$$

Since $\sum_{i=1}^n g(x_i) = 0$ we get

$$K^*_{g,n} = -\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n} g(x_i)\, g(x_j)\, \max\left\{L\Big(\frac{R_i}{n}-\Big), L\Big(\frac{R_j}{n}-\Big)\right\}.$$

Using the fact

$$2\max\{a,b\} = a + b + |a-b|\,, \qquad \forall\, a, b \in \mathbb{R}\,,$$

and $\sum_{i=1}^n g(x_i) = 0$ we have

$$K^*_{g,n} = -\frac{1}{2n}\sum_{i=1}^{n}\sum_{j=1}^{n} g(x_i)\, g(x_j) \left|L\Big(\frac{R_i}{n}-\Big) - L\Big(\frac{R_j}{n}-\Big)\right|,$$

which is much more convenient for practical computations.

Since $K^*_{g,n}$ depends on Y_i's only through their ranks R_i's, it is a rank statistic. However, unlike the classical rank test statistic T_n^2 defined in (1.2), $K^*_{g,n}$ is not a linear function of the ranks. That may cause some computation issues, but we can profit from its greater power in some situations.

Under $\mathbf{H}_0$ ($\beta = 0$) model (1.1) reduces to

$$Y_i = \beta_0 + e_i\,, \qquad i = 1, ..., n\,. \tag{3.2}$$

Since distribution of model errors e_i is absolutely continuous, there can be any ties in ranks with probability 0. Thanks to invariance of ranks with respect to the location, distribution of $R_1, ..., R_n$ under null hypothesis is uniform over all $n!$ permutations of numbers $\{1, ..., n\}$. Therefore distribution of $K^*_{g,n}$ given $x_1, ..., x_n$ under $\mathbf{H}_0$ is distribution-free and may be even computed directly. To do it, we have to compute all values of the test statistic $K^*_{g,n}$ for each of $n!$ permutations of numbers $\{1, ..., n\}$. From there we can get $(1-\alpha)$-quantile or the corresponding p-value.

However, for large sample size n computation of exact (conditional) distribution may be time consuming, that is why we will investigate asymptotic distribution of $K^*_{g,n}$.

For $s \in [0,1]$ define empirical processes

$$\widehat{V}_{g,n}(s) = \frac{1}{\sqrt{n}}\sum_{i=1}^{n} g(x_i)\, \mathbb{I}\big\{e_i \le F_n^{-1}(s)\big\}\,,$$

$$V_{g,n}(s) \;=\; \frac{1}{\sqrt{n}} \sum_{i=1}^{n} g(x_i)\, \mathbb{I}\big\{e_i \le F^{-1}(s)\big\}\,,$$

where $F_n(s) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}\{e_i \le s)\}$ is empirical distribution function.

Now, state assumptions needed for proofs of asymptotic properties of $K^*_{g,n}$. Note that all limits are considered as $n \to \infty$:

(3.3) $\qquad x_1, ..., x_n$ are not all equal,

(3.4) $$\max_{i=1,...,n} \frac{(x_i - \bar{x})^2}{\sum_{j=1}^{n}(x_j - \bar{x})^2} \;\to\; 0\,,$$

(3.5) $$g(x_i) \neq 0 \quad \text{for some} \quad i = 1, ..., n\,,$$

(3.6) $$\text{there exists} \;\; \alpha_1 > 0\,, \quad \text{such that} \;\; \frac{1}{n}\sum_{i=1}^{n} g(x_i)\,(x_i - \overline{x}) \;\to\; \alpha_1\,,$$

(3.7) $$\max_{i=1,...,n} g^2(x_i) \;\to\; 0\,,$$

(3.8) $$\sup_{n\in\mathbb{N}} \max_{i=1,...,n} |g(x_i)| \le c \quad \text{for some} \;\; 0 < c < \infty\,,$$

(3.9) $$\text{there exists} \;\; \gamma^2 > 0\,, \quad \text{such that} \;\; \frac{1}{n}\sum_{i=1}^{n} g^2(x_i) \;\to\; \gamma^2\,.$$

Remark 3.1. Assumptions (3.3) and (3.4) state that the design points $x_1, ..., x_n$ are well-defined. Remaining assumptions put conditions on the g function. If there exists a limit $\lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n}(x_i - \overline{x})^2$, then the natural choice $g(x_i) = x_i - \overline{x}$ meets the above assumptions.

Lemma 3.1. *Under (3.3)–(3.6) it holds*

$$\left| K^*_{g,n} - \int \widehat{V}^2_{g,n}(s)\, dL(s) \right| \;=\; o_p(1)\,, \qquad \text{as} \quad n \to \infty\,.$$

Proof: For convenience we will drop off an index g in $K^*_{g,n}$ and $\widehat{V}_{g,n}$. Adding and subtracting $\widehat{V}_n(s)$ in the first integral, squaring and using Cauchy–Schwarz inequality we get

$$\begin{aligned}
&\left| \int T_n^2(s)\, dL(s) - \int \widehat{V}_n^2(s)\, dL(s) \right| \;= \\
&\qquad = \;\left| \int \Big[T_n(s) - \widehat{V}_n(s)\Big]^2 dL(s) \;+\; 2\int \widehat{V}_n(s)\Big(T_n(s) - \widehat{V}_n(s)\Big)\, dL(s) \right| \\
&\qquad \le \;\sup_{0\le s\le 1} \big|T_n(s) - \widehat{V}_n(s)\big|^2 + 2\sqrt{\int \widehat{V}_n^2(s)\, dL(s) \int \Big(T_n(s) - \widehat{V}_n(s)\Big)^2 dL(s)}\,.
\end{aligned}$$

The fact

$$\sup_{0\le s\le 1} \Big|T_n(s) - \widehat{V}_n(s)\Big| \;\le\; 2 \max_{i=1,...,n} \big|g(x_i)\big| \;=\; o_p(1)$$

together with $\int \widehat{V}_n^2(s)\, dL(s) = O_p(1)$ proves the Lemma. □

Lemma 3.2. *Under (3.3)–(3.6) it holds*

$$\left|K^*_{g,n} - \int V^2_{g,n}(s)\, dL(s)\right| = o_p(1)\,, \qquad as \quad n \to \infty\,.$$

Proof:

$$\begin{aligned}(3.10)\qquad &\left|\int T_n^2(s)\, dL(s) - \int V_n^2(s)\, dL(s)\right| = \\ &= \left|\int \Big[T_n(s) - V_n(s)\Big]^2 dL(s) + 2\int V_n(s)\Big(T_n(s) - V_n(s)\Big)\, dL(s)\right|.\end{aligned}$$

Using Minkowski inequality

$$\begin{aligned}(3.11)\qquad \int \Big[T_n(s) - V_n(s)\Big]^2 dL(s) &= \int \Big[T_n(s) - \widehat{V}_n(s) + \widehat{V}_n(s) - V_n(s)\Big]^2 dL(s) \\ &\le 2\int \Big[T_n(s) - \widehat{V}_n(s)\Big]^2 dL(s) + 2\int \Big[\widehat{V}_n(s) - V_n(s)\Big]^2 dL(s)\,.\end{aligned}$$

By Cauchy–Schwarz inequality

$$\begin{aligned}(3.12)\qquad \left|\int V_n(s)\Big(T_n(s) - V_n(s)\Big)\, dL(s)\right| &\le \sqrt{\int V_n^2(s)\, dL(s) \int \Big[T_n(s) - V_n(s)\Big]^2 dL(s)} \\ &= o_p(1)\,,\end{aligned}$$

because $\int V_n^2(s)\, dL(s) = O_p(1)$ and $\int \big[T_n(s) - V_n(s)\big]^2 dL(s) = o_p(1)$.

Observe that

$$V_n\big(FF_n^{-1}(s)\big) = \sum_{i=1}^n g(x_i)\, \mathbb{I}\big\{e_i \le F^{-1}FF_n^{-1}(s)\big\} = \sum_{i=1}^n g(x_i)\, \mathbb{I}\big\{e_i \le F_n^{-1}(s)\big\} = \widehat{V}_n(s)\,.$$

Therefore

$$\sup_{0\le s\le 1}\big|\widehat{V}_n(s) - V_n(s)\big| = \sup_{0\le s\le 1}\big|V_n\big(FF_n^{-1}(s)\big) - V_n(s)\big| = o_p(1)\,,$$

because

$$\begin{aligned}\sup_{0\le s\le 1}\big|FF_n^{-1}(s) - s\big| &= \sup_{0\le s\le 1}\Big|FF^{-1}(s) - F_nF_n^{-1}(s) + F_nF_n^{-1}(s) - s\Big| \\ &\le \sup_{x\in\mathbb{R}}\big|F(x) - F_n(x)\big| + \sup_{0\le s\le 1}\big|F_nF_n^{-1}(s) - s\big| = o_p(1)\,.\end{aligned}$$

Now, combining previous result, Lemma 3.1 and (3.10), (3.11) and (3.12) we have proven the Lemma. □

Remark 3.2. The previous lemma states that the asymptotic distribution of $K^*_{g,n}$ is the same as $\int V^2_{g,n}(s)\, dL(s)$ that is easier to investigate. Now, we are able to state the theorem about asymptotic null distribution of $K^*_{g,n}$.

Theorem 3.1. *Under (3.3)–(3.9) in model (1.1) under* $\mathbf{H}_0$

$$K^*_{g,n} \xrightarrow{d} \gamma^2 \cdot Y_L\,, \qquad \text{with} \quad Y_L = \int_0^1 B^2(s)\, dL(s)\,,$$

where $B(s)$ *is a Brownian bridge in* $\mathcal{C}[0,1]$.

Proof: Recall that

$$\begin{aligned} V_{g,n}(s) &= \frac{1}{\sqrt{n}} \sum_{i=1}^{n} g(x_i)\, \mathbb{I}\big\{e_i \le F^{-1}(s)\big\} \\ &= \frac{1}{\sqrt{n}} \sum_{i=1}^{n} g(x_i)\, \mathbb{I}\big\{F(e_i) \le s\big\} \\ &= \frac{1}{\sqrt{n}} \sum_{i=1}^{n} g(x_i)\, \mathbb{I}\big\{U_i \le (s)\big\}\,, \end{aligned}$$

where $U_1, ..., U_n$ are i.i.d. random variables with uniform $\mathcal{U}(0,1)$ distribution.

By [6] we have

$$V_{g,n}(s) \implies \gamma \cdot B(s) \qquad \text{in} \quad \mathcal{D}[0,1]$$

and therefore $\int V^2_{g,n}(s)\, dL(s) \xrightarrow{d} \gamma^2 \int B^2(s)\, dL(s)$. That together with Lemma 3.2 proves Theorem 3.1. □

Distribution of random variable Y_L for $L(s) = s$ was first investigated by Smirnov [9]. Values of its distribution function may be found for example in [10], some quantiles are listed in Table 1. For other choices of function L one has to use simulated values.

Table 1: Quantiles of distribution Y_L for $L(s) = s$.

α	0.90	0.95	0.99	0.999
α-quantile	0.34730	0.46136	0.74346	1.16786

In [7] we also investigated the behavior of $K^*_{g,n}$ under the local alternative

$$\mathbf{K}_{0,n}\colon\ \beta = n^{-1/2}\beta^*\,, \qquad 0 \ne \beta^* \in \mathbb{R} \ \text{ fixed}\,.$$

The resulting distribution cannot be expressed in a closed formula, that is why we omit it here. Power of the test will be illustrated later in the simulation study.

4. GENERALIZATION OF THE TEST

In the definition of the test statistic $K^*_{g,n}$ (3.1) we used second power of the L^2-norm of the empirical process $T_{g,n}(s,0)$. Instead, we may use any norm on $\mathcal{D}[0,1]$. For simplicity, we will consider only the class of L^p-norms for $p \in [1,\infty]$.

For $p \in [1, \infty)$ define

$$K_{g,n}^{(p)} = \left(\int_0^1 \left| T_{g,n}(s,0) \right|^p dL(s) \right)^{\frac{1}{p}}, \tag{4.1}$$

for $p = \infty$ define

$$K_{g,n}^{(\infty)} = \max\left\{ \left| T_{g,n}(s,0) \right| : \, s \in [0,1] \right\}. \tag{4.2}$$

Remark 4.1. Obviously, for $p = 2$ we have $\left(K_{g,n}^{(2)}\right)^2 = K_{g,n}^{*}$.

From computation point of view, formulas (4.1) and (4.2) might be simplified. Obviously, $T_{g,n}(0,0) = 0$ and $T_{g,n}(s,0)$ is piecewise constant:

$$T_{g,n}(s,0) = \frac{1}{\sqrt{n}} \sum_{i:\, R_i \le j} g(x_i)\,, \qquad \frac{j-1}{n} < s \le \frac{j}{n}\,, \quad j = 1, ..., n\,.$$

Therefore,

$$K_{g,n}^{(\infty)} = \frac{1}{\sqrt{n}} \max_{i=1,...,n} \left| \sum_{i:\, R_i \le j} g(x_i) \right|,$$

$$K_{g,n}^{(1)} = \frac{1}{n^{3/2}} \sum_{i=1}^{n} \left| \sum_{i:\, R_i \le j} g(x_i) \right|,$$

for $L(s) = s$.

Again, since $K_{g,n}^{(p)}$ depends on Y_i's only through their ranks R_i's, it is a rank statistic, but not linear like (1.2). That may cause some computation issues, but we can profit from its greater power in some situations.

Now, focus on the distribution under the null hypothesis. Under $\mathbf{H}_0$ ($\beta = 0$) model (1.1) reduces to (3.2)

$$Y_i = \beta_0 + e_i\,, \qquad i = 1, ..., n\,.$$

Thanks to the same arguments as in the previous section, the distribution of $K_{g,n}^{(p)}$ given $x_1, ..., x_n$ under the null hypothesis is distribution-free and can be easily computed directly the same way. For large sample sizes n the following asymptotic approximation might be used.

Theorem 4.1. *Under (3.3)–(3.9) in model (1.1) under* $\mathbf{H}_0$

$$K_{g,n}^{(p)} \xrightarrow{d} \gamma \cdot Y_L^{(p)}\,, \qquad \textit{with} \quad Y_L^{(p)} = \left(\int_0^1 \left| B(s) \right|^p dL(s) \right)^{\frac{1}{p}},$$

where $B(s)$ *is a Brownian bridge in* $\mathcal{C}[0,1]$.

Proof: The proof is analogous to the proof of Theorem 3.1. □

5. CHOICE OF THE PARAMETERS IN PRACTISE

In the previous section, we derived a class of minimum distance tests. In practise there arises a question how to choose optional parameters of the test.

Function g is in fact a weight function for regressors, so it can downweight outlying observations to robustify these tests against extreme values of x_i (if g is bounded for example). Anyway, if we are not afraid of leverage observations x_i, then the optimal choice of the g function is $g(x_i) = x_i - \overline{x}$. This choice leads to the test with the greatest power among all test with different g functions.

Function L has similar interpretation as score-function φ in standard rank tests theory, optimal L could be chosen based on the estimate of unknown model errors. Anyway, the simplest choice $L(s) = s$ gives very reasonable results (see the simulations).

And finally, the choice of L^p-norm depends on the model errors e_i. From computational point of view, one should consider $p = 1, 2, \infty$ for that we have a simple formula. Power comparisons are made in the simulation study.

6. GENERALIZATIONS

In [7] we investigated behavior the test in measurement error model:

$$\begin{aligned} Y_i &= \beta_0 + \beta x_i + e_i\,, \\ w_i &= x_i + v_i\,, \qquad i = 1, ..., n\,, \end{aligned}$$

where instead of actual regressors x_i we observed w_i affected by measurement errors v_i.

We showed that the test is still valid in this model, the presence of measurement errors decreases power of the test, because we do not use values of function g in optimal points $x_1, ..., x_n$ but in w_i's.

In Section 4 we showed extension of the test using various norms for the empirical process. Analogously, we may define generalization of Koul's estimate defined in Section 2.

Consider empirical process $T_{g,n}(s,t)$ defined in (2.1) and for $p \in [1, \infty)$ define

$$K_{g,n}^{(p)}(t) = \left(\int_0^1 \left| T_{g,n}(s,t) \right|^p dL(s) \right)^{\frac{1}{p}}, \qquad t \in \mathbb{R}\,,$$

and for $p = \infty$

$$K_{g,n}^{(\infty)}(t) = \max\left\{ \left| T_{g,n}(s,t) \right| :\ s \in [0,1] \right\}, \qquad t \in \mathbb{R}\,.$$

Minimum distance estimator $\widehat{\beta}_{g,n}^{(p)}$ is then defined as

$$\widehat{\beta}_{g,n}^{(p)} = \arg\min\left\{ K_{g,n}^{(p)}(t) :\ t \in \mathbb{R} \right\}.$$

In the similar way, thanks to duality of rank tests and estimates, we may show favorable properties and good performance of the estimates. Detailed analysis will be part of our future study.

7. SIMULATIONS

To support previous theoretical results we conducted a large simulation study, let us present a few interesting results. Let us start with model (1.1) for moderate sample size $n = 30$. We have compared empirical power of our test based on the test statistic $K^*_{g,n}$ with $g(x_i) = x_i - \bar{x}$ and $L(s) = s$ (call it *minimum distance test*) with Wilcoxon test for regression (based on (1.2) with $\varphi(u) = u$) and standard t-test for regression.

Regressors $x_1, ..., x_{30}$ were once generated from uniform $\mathcal{U}(-2, 10)$ distribution and then considered fixed, model errors e_i were generated from normal, logistic, Laplace and t-distribution with 6 degrees of freedom, respectively, always with 0 mean a variance 3/2. The empirical powers of the tests were computed as a percentage of rejections of $\mathbf{H}_0$ among 10 000 replications, at significance level $\alpha = 0.05$. The results are summarized in Table 2.

Table 2: Percentage of rejections of hypothesis $\mathbf{H}_0 : \beta = 0$ of minimum distance test (MD), Wilcoxon test for regression (W) and t-test for regression (t); $n = 30$, $\alpha = 0.05$.

$\beta \setminus e_i$	$\mathcal{N}\left(0, \frac{3}{2}\right)$			$\mathrm{Log}\left(0, \frac{\sqrt{2}\,\pi}{3}\right)$			$\mathrm{Lap}\left(0, \frac{\sqrt{3}}{2}\right)$			$t(6)$		
	MD	W	t	MD	W	t	MD	W	t	MD	W	t
0	4.98	4.42	5.00	5.06	4.55	5.00	5.00	4.55	5.04	5.00	4.32	4.93
0.1	28.7	28.3	31.5	32.7	31.4	32.0	42.4	39.0	33.5	34.6	33.1	32.9
−0.1	28.3	28.2	30.9	32.7	31.2	32.2	42.5	39.0	33.7	33.3	32.1	31.9
0.2	78.2	78.8	82.3	82.5	81.8	81.9	88.3	86.6	82.0	84.5	83.9	82.6
−0.2	78.3	78.7	82.9	83.3	82.7	82.9	89.2	87.5	83.1	84.0	83.4	82.5

For normal model errors t-test achieves (not surprisingly) the largest power, but the differences among the three tests are not much distinct. For distributions with heavier tails than normal our test has the largest power, even for logistic distribution (for which Wilcoxon test is locally most powerful rank test). It is caused by the slow convergence of Wilcoxon test statistic to its asymptotic distribution.

In Table 3 comparison of tests based on various norms (L^2, L^1, L^∞) is made.

Bad performance of the test based on L^∞-norm is caused by slow convergence of corresponding test statistic to its limit distribution. For large sample size n test preserves prescribed significance level α under null hypothesis and under the alternative its power is quite similar to other tests. Tests based on L^2 and L^1-norm perform very similar. Test based on L^1-norm might have slightly greater power which is caused by faster convergence of the test statistic. On the other hand, computation of the test statistic based on L^2-norm is easier than those with L^1-norm.

Table 3: Percentage of rejections of hypothesis $\mathbf{H}_0 : \beta = 0$ of minimum distance test based on L^2, L^1 and L^∞-norm; $n = 30$, $\alpha = 0.05$.

e_i	$\mathcal{N}\left(0, \frac{3}{2}\right)$			$\mathrm{Log}\left(0, \frac{3}{\sqrt{2}\,\pi}\right)$			$\mathrm{Lap}\left(0, \frac{\sqrt{3}}{2}\right)$			$t(6)$		
β	L^2	L^1	L^∞	L^2	L^1	L^∞	L^2	L^1	L^∞	L^2	L^1	L^∞
0	5.15	5.03	2.73	5.34	5.31	2.61	5.03	5.18	2.71	4.90	4.97	2.64
0.1	30.0	31.0	17.8	33.4	34.1	20.6	43.6	43.0	30.6	35.8	36.6	22.4
−0.1	29.2	30.2	17.2	34.0	34.7	21.4	44.2	43.4	30.4	35.0	35.8	21.6
0.2	81.2	82.6	62.4	84.9	85.7	68.1	90.5	90.3	78.9	87.8	88.5	72.2
−0.2	80.6	82.6	62.2	84.9	86.0	68.8	90.5	90.4	78.9	86.8	87.4	71.2

We performed more simulations for various design points x_i, sample sizes n and model errors e_i. We also compared the tests according to the choice of functions L and g. However, the corresponding results are very similar to those presented in Tables 2 and 3.

Finally, we studied the finite sample behavior of generalized estimates from Section 6. Because of the duality of rank tests and estimates corresponding results and conclusions were the same as for the tests. That is why we omit it here.

8. CONCLUSIONS

We introduced a class of new rank tests in linear regression model. Unlike the classical ones introduced by Hájek and Šidák, our tests are not linear functions of the ranks. Thanks to that they can achieve greater power. Our tests are robust, we do not need to assume normality of model errors. Anyway, under normality our tests has similar power as classical t-test; for model errors with heavy tails our test has significantly greater power.

Our test may be also robust with respect to leverage observations. The right choice of the weight function leads to the test that is not sensitive to outlying regressors. We also generalized Koul's minimum distance estimates when considering various L^p-norms instead of L^2. Corresponding estimates have the same favorable properties as the tests.

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BAYESIAN CRITERIA FOR NON-ZERO EFFECTS DETECTION UNDER SKEW-NORMAL SEARCH MODEL

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Abstract:

- Shirakura *et al.* [12] introduced search probability (SP) in order to compare search designs (SD). Afterwards, the SP-based and other related criteria were developed, all for the normal model. In the present study, we considered a general underlying skew-normal (SN) model and obtained new criteria in a simple explicit form using the Bayesian approach. These criteria are design-dependent and hence are able to rank SDs with respect to their search performance.

Key-Words:

- *Bayesian approach; Kullback–Leibler distance; search design; search linear model; skew-normal distribution.*

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1. INTRODUCTION

At the screening stage of an experiment, a main effect plan (MEP) is employed to estimate the main effects, assuming that all interactions are negligible. MEPs were introduced and implemented after World War II, for more details refer to the pioneering paper of Box and Wilson [6]. MEPs, including saturated resolution III regular and irregular designs, have been widely used in practical industrial experiments. For example, Plackett and Burman [11] introduced an irregular saturated MEP for 2^m factorial experiments, where $m = 4t - 1$, for $t \geq 3$. Nevertheless, there might exist a small number of non-zero lower order interactions, which cause bias in estimating main effects. Enhancing the resolution, i.e., upgrading to resolution IV or V, for instance through fold-over approach to overcome the problem, increases the number of runs and, in turn, the cost of the experiment.

To save the number of runs, Srivastava [14] introduced and suggested using SDs to search for and estimate k unknown non-zero interactions in addition to estimating the main effects. Such a design is known as main effect plus k plan (MEP.k). Several researchers have developed the MEP.k (see Ghosh *et al.* [8], for a thorough review). For example, Esmailzadeh *et al.* [7] and Talebi and Jalali [18] constructed MEP.1 for 2^m factorial designs respectively, for odd and even m. Consider search linear model for providing a key condition in planning a general SD and in particular MEP.k. For a vector of observations $\boldsymbol{y}(N\times 1)$, the search linear model is

$$\boldsymbol{y} = \boldsymbol{A}_1\boldsymbol{\xi}_1 + \boldsymbol{A}_2\boldsymbol{\xi}_2 + \boldsymbol{e}\,, \qquad \mathrm{Cov}(\boldsymbol{e}) = \sigma^2\boldsymbol{I}_N\,, \tag{1.1}$$

where $\boldsymbol{A}_i(N\times\nu_i)$ are known design matrices; and $\boldsymbol{\xi}_i(\nu_i\times 1)$ are vectors of effects for $i = 1, 2$; $\boldsymbol{e}(N\times 1)$ is an error vector; σ^2 is the error variance; and $\boldsymbol{I}_N$ is the identity matrix of order N. It is known for a fact that k effects in $\boldsymbol{\xi}_2$ are non-zero, but we don't know which ones. Therefore, the plan sets out to search for and identify the non-negligible effects in $\boldsymbol{\xi}_2$ and estimate them in addition to estimating the effects in $\boldsymbol{\xi}_1$. Alternatively, let S be the set of all $\binom{\nu_2}{k}$ models with only one correct model, each including a set of k possible non-zero effects from $\boldsymbol{\xi}_2$ and $\boldsymbol{\xi}_1$. The j-th model, $j = 1, 2, ..., \binom{\nu_2}{k}$, in S is expressed as follows:

$$\boldsymbol{y} = \boldsymbol{A}_1\boldsymbol{\xi}_1 + \boldsymbol{A}_{21}(\boldsymbol{\zeta}_j)\boldsymbol{\zeta}_j + \boldsymbol{e}\,, \tag{1.2}$$

where $\boldsymbol{\zeta}_j(k\times 1)$ is a vector of k effects from $\boldsymbol{\xi}_2$ and $\boldsymbol{A}_{21}(\boldsymbol{\zeta}_j)$ is the $N\times k$ submatrix of $\boldsymbol{A}_2$ whose columns are corresponding to $\boldsymbol{\zeta}_j$.

To identify the non-zero set of effects in $\boldsymbol{\xi}_2$ for noisy case ($\sigma^2 > 0$), Srivastava [14] suggested choosing the model in (1.2) with the lowest sum of square error (SSE). Moreover, Shirakura *et al.* [12] studied the stochastic properties of SSE and derived the SP in an explicit form for $k = 1$ under the normal error. SP is design-dependent and hence Shirakura *et al.* [12] suggested using it for comparing SDs with respect to their search performance. Subsequently, Ghosh and Teschmacher [9] and Talebi and Esmailzadeh [16] derived the SP-based criteria. Furthermore, Talebi and Esmailzadeh [15] conducted another design-comparison study and derived the KL (Kullback–Leibler) criterion based on Kullback–Leibler distance, which can be used for $k \geq 1$.

All of the above proposed criteria were obtained for models with normal error. However, such models may not adequately fit the data in many practical situations. For example,

Arnold and Beaver [2] described a real situation in which the observations followed a non-normal distribution. They termed this situation 'hidden truncation', for which the model is SN. Afterwards, Arnold *et al.* [3] reported observations related to the hidden truncation. Moreover, Arellano-Valle *et al.* [1] assumed the SN error to fit a mixed model to a real set of longitudinal data on cholesterol levels collected as a part of the famed Framingham heart study. The above examples revealed the abundance of phenomena with SN models in real situations. The present study was also motivated by a hidden truncation problem, i.e. candidates who want to partake in the PhD Admission Examination of Iranian Universities must have an overall above-average Master's GPA. To deal with this, distributions such as skew-t distribution or mixture of two normal distributions may be proposed. However, based on our findings, such proposed distributions may not lead to an explicit solution. We considered the rival models in (1.2) with the multivariate SN distribution for error and used a Bayesian method to propose a new approach for finding the true model. This led to criteria which will be presented in an explicit form. The Bayesian approach in developing new explicit criteria allowed us to take into account the hierarchical principle in factorial experiments, by which the lower order interactions are more important than the higher orders. It was, therefore, rational to choose an appropriate prior distributional model for the factorial effects in order to deal with this issue. Through this prior distribution, we allocated non-zero probability to the main effects and k possible low order non-zero interactions, while all other interactions came down to zero probability. In this study, which is the first Bayesian research in the context of search design, it was shown that the Bayesian approach could simplify the complexity in deriving the appropriate criteria.

In the next section some useful preliminaries are presented. The new Bayesian search criteria will be proposed in Section 3. These criteria are

1 – expected Shannon information (ESI), and

2 – Bayesian expected Kullback–Leibler (BEKL),

which enable us to compare the search performance of any given SD. The calculations are moved to the Appendix in order to enhance the readability of the article.

2. PRELIMINARIES

The primary aim of this study was to acquire criteria for model identification in the context of search linear model. This problem has long been investigated by several researchers for models with normal error. In this study, we considered models with SN error. Thus, a better understanding of the SN distribution can be helpful.

Following Azzalini [4], who introduced SN distribution, a random variable Y has an SN distribution, denoted by $Y \sim \mathrm{SN}(\mu, \sigma, \lambda)$, with location parameter μ; scale parameter σ; and shape parameter λ, if its probability density function (pdf) is

$$f(y) = \frac{2}{\sigma}\,\phi\left(\frac{y-\mu}{\sigma}\right)\Phi\left(\lambda\,\frac{y-\mu}{\sigma}\right), \qquad y \in \mathbb{R}, \tag{2.1}$$

where $\phi(\cdot)$ and $\Phi(\cdot)$ are the pdf and cumulative distribution function (cdf) of the standard normal distribution, respectively. The multivariate SN distribution has also been proposed

by some researchers. That is, an N-dimensional random vector, $\boldsymbol{Y}$, follows a multivariate SN distribution $\mathrm{SN}_N(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\lambda})$ with location vector $\boldsymbol{\mu} \in \mathbb{R}^N$; positive definite dispersion matrix $\boldsymbol{\Sigma}_{N\times N}$; and skewness vector $\boldsymbol{\lambda} \in \mathbb{R}^N$, if its pdf is

$$f(\boldsymbol{y}) \;=\; 2\,\phi_N\big(\boldsymbol{y}\,|\,\boldsymbol{\mu}, \boldsymbol{\Sigma}\big)\;\Phi_1\big(\boldsymbol{\lambda}'\boldsymbol{\Sigma}^{-\frac{1}{2}}(\boldsymbol{y}-\boldsymbol{\mu})\big)\,, \qquad \boldsymbol{y} \in \mathbb{R}^N\,, \tag{2.2}$$

where $\phi_N(\cdot)$ is the pdf of the $\mathrm{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, (Arellano-Valle *et al.* [1]). Evidently, the random vector $\boldsymbol{Y}$ follows $\mathrm{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ for $\boldsymbol{\lambda} = \boldsymbol{0}$. Following Arellano-Valle *et al.* [1], the random vector $\boldsymbol{Y} \sim \mathrm{SN}_N(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\lambda})$ can be expressed as

$$\boldsymbol{Y} \;\overset{d}{=}\; \boldsymbol{\mu} + \boldsymbol{\Sigma}^{\frac{1}{2}}\Big(\boldsymbol{\delta}\,|T_0| + \big(\boldsymbol{I}_N - \boldsymbol{\delta}\,\boldsymbol{\delta}'\big)^{\frac{1}{2}}\,\boldsymbol{T}_1\Big)\,, \tag{2.3}$$

where $\boldsymbol{\delta} = \frac{\boldsymbol{\lambda}}{\sqrt{1+\boldsymbol{\lambda}'\boldsymbol{\lambda}}}$; $T_0 \sim \mathrm{N}(0,1)$; $\boldsymbol{T}_1 \sim \mathrm{N}(\boldsymbol{0}, \boldsymbol{I}_N)$ is independent of T_0, and $\overset{d}{=}$ stands for equality in distribution. In $Z = |T_0|$, Z has a half-normal distribution. It is worth noting that model (2.3) covers bias and correlation among errors in addition to skewness. Now, for hidden truncation problem, the SN distribution is written as follows. Suppose random vector $(X, W_1, W_2, ..., W_N)'$ distributed as $\mathrm{N}_{N+1}(\boldsymbol{\theta}, \boldsymbol{\Omega})$, where $\boldsymbol{\theta} = (\mu_x, \boldsymbol{\mu}')'$ and $\boldsymbol{\Omega} = \begin{pmatrix} 1 & \boldsymbol{\delta}' \\ \boldsymbol{\delta} & \boldsymbol{I}_N \end{pmatrix}$. Let $\boldsymbol{W} = (W_1, W_2, ..., W_N)'$, then following Azzalini [5]

$$\boldsymbol{Y} \;=\; \boldsymbol{W}\,|\,X > \mu_x \;\sim\; \mathrm{SN}_N(\boldsymbol{\mu}, \boldsymbol{I}_N, \boldsymbol{\lambda})\,, \tag{2.4}$$

where $\boldsymbol{\lambda} = (1 - \boldsymbol{\delta}'\boldsymbol{\delta})^{-\frac{1}{2}}\,\boldsymbol{\delta}$. We calculated some of the existing criteria for detecting non-zero effects under the SN search model. Based on the findings, the calculation of SP for SN model has proven to be very intricate. Furthermore, the expected KL (EKL) criterion, proposed by Talebi and Esmailzadeh [15], for $\boldsymbol{Y} \sim \mathrm{SN}_N(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\lambda})$ led to the integral below:

$$\int 2\,\phi_N\big(\boldsymbol{y}\,|\,\boldsymbol{\mu}_0, \boldsymbol{\Sigma}\big)\;\Phi_1\big(\boldsymbol{\lambda}'\boldsymbol{\Sigma}^{-\frac{1}{2}}(\boldsymbol{y}-\boldsymbol{\mu}_0)\big)\,\log\left\{\frac{\phi_N\big(\boldsymbol{y}\,|\,\boldsymbol{\mu}_0, \boldsymbol{\Sigma}\big)\;\Phi_1\big(\boldsymbol{\lambda}'\boldsymbol{\Sigma}^{-\frac{1}{2}}(\boldsymbol{y}-\boldsymbol{\mu}_0)\big)}{\phi_N\big(\boldsymbol{y}\,|\,\boldsymbol{\mu}_j, \boldsymbol{\Sigma}\big)\;\Phi_1\big(\boldsymbol{\lambda}'\boldsymbol{\Sigma}^{-\frac{1}{2}}(\boldsymbol{y}-\boldsymbol{\mu}_i)\big)}\right\}\,d\boldsymbol{y}\,, \tag{2.5}$$

where for non-zero $\boldsymbol{\zeta}_0$, $\boldsymbol{\mu}_0 = \boldsymbol{A}_1\boldsymbol{\xi}_1 + \boldsymbol{A}_{21}(\boldsymbol{\zeta}_0)\boldsymbol{\zeta}_0$ and $\boldsymbol{\mu}_j = \boldsymbol{A}_1\boldsymbol{\xi}_1 + \boldsymbol{A}_{21}(\boldsymbol{\zeta}_j)\boldsymbol{\zeta}_j$. This can not be made any simpler, and thus it is hard to be satisfied with (2.5) as a criterion. The desire of finding a very simple and conceivable criterion, consequently, motivated us to look for a different approach.

Lindley [10] defined the expected information about $\boldsymbol{\theta}$ for observation vector $\boldsymbol{y}$ in an experiment E, prior function $\pi(\boldsymbol{\theta})$, and posterior pdf $\pi(\boldsymbol{\theta}|\boldsymbol{y})$ as below:

$$I^{\boldsymbol{\theta}}\big\{E, \pi(\boldsymbol{\theta})\big\} \;=\; \int f(\boldsymbol{y}) \int \pi(\boldsymbol{\theta}|\boldsymbol{y})\,\log\frac{\pi(\boldsymbol{\theta}|\boldsymbol{y})}{\pi(\boldsymbol{\theta})}\;d\boldsymbol{\theta}\,d\boldsymbol{y}\,, \tag{2.6}$$

provided that the integral exists. This is the expected KL distance between prior and posterior distributions, which measures the average overall observations information. Using Bayes' theorem, $I^{\boldsymbol{\theta}}\{E, \pi(\boldsymbol{\theta})\}$ in (2.6) can be written as follows:

$$I^{\boldsymbol{\theta}}\big\{E, \pi(\boldsymbol{\theta})\big\} \;=\; E_{\boldsymbol{\theta}}\big\{E_{\boldsymbol{Y}|\boldsymbol{\theta}}\big(\log f(\boldsymbol{y}|\boldsymbol{\theta})\big)\big\} - E_{\boldsymbol{Y}}\big\{\log f\boldsymbol{y}\big\}\,. \tag{2.7}$$

The distance in (2.7) will be used for proposing the new criteria in Section 3.

For the normal distribution $\mathrm{N}(\boldsymbol{0}, \sigma^2\boldsymbol{\Sigma})$ and SN distribution $\mathrm{SN}_N(\boldsymbol{0}, \sigma^2\boldsymbol{\Sigma}, \boldsymbol{\lambda})$ with unknown σ^2, let's take $\boldsymbol{y}^* = \boldsymbol{y}/\sigma$ and rewrite model (1.2) as below, which will be used throughout this article,

$$\boldsymbol{y}^* = \boldsymbol{A}(\boldsymbol{\xi}_j)\,\boldsymbol{\xi}_j^* + \boldsymbol{e}^*\,, \qquad j = 1, 2, ..., \binom{\nu_2}{k}, \tag{2.8}$$

where $\boldsymbol{\xi}_j^* = \frac{1}{\sigma}(\boldsymbol{\xi}_1', \boldsymbol{\zeta}_j')'$; $\boldsymbol{A}(\boldsymbol{\xi}_j) = [\boldsymbol{A}_1 : \boldsymbol{A}_{21}(\boldsymbol{\zeta}_j)]$; and $\boldsymbol{e}^* = \boldsymbol{e}/\sigma$. In the Bayesian framework, $\boldsymbol{\xi}_j^*$ is assumed to have the prior distribution $\mathrm{N}(\mathbf{0}, \boldsymbol{\Sigma}_0)$, where $\boldsymbol{\Sigma}_0$ is a known $(\nu_1+k)\times(\nu_1+k)$ diagonal matrix. Following Wu and Hamada [19, p. 434], by assuming large diagonal elements in $\boldsymbol{\Sigma}_0$, we are assured of the possibility of the presence of non-zero effects in $\boldsymbol{\xi}_j^*$. For a given prior, $\pi(\boldsymbol{\xi}_j^*)$, the event of observing a small interior integral in (2.6) indicates that the data support the existence of the non-negligible effects. Therefore, a small interior integral value in $I^{\boldsymbol{\theta}}\{E, \pi(\boldsymbol{\theta})\}$, presumably confirms the possibility of the presence of non-zero effects in $\boldsymbol{\xi}_j^*$. By this scenario, we suggested calculating the interior integral in (2.6) for all $\binom{\nu_2}{k}$ models in (2.8) and selecting the model with the lowest value as the true model. The following simulation study was performed as the verity performance assessment of the proposed criterion.

The search design D_1 given in the Appendix was used to generate data. Let $\boldsymbol{\xi}_1$ be the vector of the general mean and main effects and let ζ_0 be the two-factor interaction AB. Furthermore, in a hidden truncation model, assume that $\boldsymbol{\delta} = 0.2\,\mathbf{1}_{12}$, where $\mathbf{1}_{12}$ is a 12×1 vector of 1s, and $\boldsymbol{\Sigma}_0 = 100\,\boldsymbol{I}_6$. Based on these parameter values, 1 000 data set were simulated from a 12 dimensional SN distribution using "sn" package in R software. The interior integral in (2.6) was calculated for all 6 possible models with any one of the two-factor interactions. The simulation results showed that the interior integral had the lowest value for the true model with AB interaction. We also calculated SSE for all models and found that the same model had the minimum SSE. Moreover, we ran this simulation for the case $k = 2$, by assuming $\boldsymbol{\zeta}_0$ to be (AB AC) and found that the interior integral and SSE were minimal for the chosen model.

Meanwhile, for a given model, Zhang [20] used $I^{\boldsymbol{\theta}}\{E, \pi(\boldsymbol{\theta})\}$ to select the optimum design, i.e. the design which maximizes the expression in (2.6). Due to the design-independence of the prior in denominator, she concluded that maximizing $I^{\boldsymbol{\theta}}\{E, \pi(\boldsymbol{\theta})\}$ comes down to maximizing the following quantity

$$U = \int f_{\boldsymbol{y}} \left\{ \int \pi(\boldsymbol{\theta}|\boldsymbol{y}) \log \pi(\boldsymbol{\theta}|\boldsymbol{y})\, d\boldsymbol{\theta} \right\} d\boldsymbol{y}\,. \tag{2.9}$$

It is worth noting that for any given design, say D, $U(D)$ is the expected Shannon information of the posterior distribution denoted by ESI_D. Zhang [20] achieved an expression for (2.9) in the normal regression model and showed that maximization of $U(D)$ is equivalent to maximizing the determinant of inverted posterior variance of unknown parameter.

Under model uncertainty, when one is faced with a multi-model case, it is logical to calculate (2.9) for all models, opt for the model with the lowest value and then, select a design that has the maximum of such the value. In other words, let $U_i(D)$ be ESI_D in (2.9) for the i-th model, $\binom{i=1,2,\ldots,\nu_2}{k}$, then $\mathrm{MESI}_D = \min_S U_i(D)$. Evidently, in the context of search design for any given design D, the larger the value of MESI_D, the higher the performance of D in searching for non-zero effects. So, for comparing and ranking the SDs with respect to their search performance, MESI_D can be used as a criterion for design comparison. Hence, we present the following definition.

Definition 2.1. Suppose D_1 and D_2 are two SDs with N treatments, D_1 is said to be better than D_2 for identifying the set of non-zero effects if $\mathrm{MESI}_{D_1} > \mathrm{MESI}_{D_2}$.

3. MAIN RESULTS

3.1. ESI search criterion

In this section, we first introduce ESI_D as a criterion under normality assumption and then give a generalized form of the criterion using the SN model.

Consider the model in (2.8) and assume that $\boldsymbol{Y}^* \sim \mathrm{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, where $\boldsymbol{\mu} = \boldsymbol{A}(\boldsymbol{\xi}_j)\boldsymbol{\xi}_j^*$. Then for foregoing $\pi(\boldsymbol{\xi}_j^*)$, $j = 1, 2, ..., \binom{\nu_2}{k}$, the posterior distribution of $\boldsymbol{\xi}_j^*$ is proportional to $f(\boldsymbol{\xi}_j^*, \boldsymbol{y}^*)$ given in (A.1) below. After some calculations, as given in the Appendix, the interior integral in U becomes

$$E_{\boldsymbol{\xi}_j^*|\boldsymbol{y}^*}\left\{\log \pi(\boldsymbol{\xi}_j^*|\boldsymbol{y}^*)\right\} = -\frac{1}{2}\log|\boldsymbol{\Sigma}_{\boldsymbol{\xi}}| - \frac{\nu_1 + k}{2}, \tag{3.1}$$

where $\boldsymbol{\Sigma}_{\boldsymbol{\xi}}$ is a conditional posterior variance of $\boldsymbol{\xi}_j^*$ given $\boldsymbol{y}^*$. U is obtained from (3.1) by integration with respect to the marginal distribution of $\boldsymbol{Y}^*$. After removing the redundant terms, U is reduced to a simple form $\psi(D)$ for design D,

$$\psi(D) = \log|\boldsymbol{\Sigma}_{\boldsymbol{\xi}}|^{-1}. \tag{3.2}$$

Note that $|\boldsymbol{\Sigma}_{\boldsymbol{y}^*}| = |\boldsymbol{\Sigma}_{\boldsymbol{\xi}}|^{-1}|\boldsymbol{\Sigma}_0|$, hence $\psi(D)$ is proportional to $\log|\boldsymbol{\Sigma}_{\boldsymbol{y}^*}|$. It should also be noted that $\psi(D)$ is design-dependent and written in terms of the hyper parameter $\boldsymbol{\Sigma}_0$. Therefore, for any given design D, $\psi(D)$ is calculable.

Remark 3.1. In $\boldsymbol{\Sigma}_{\boldsymbol{\xi}}$, the expression $\boldsymbol{A}'(\boldsymbol{\zeta}_j)\boldsymbol{\Sigma}^{-1}\boldsymbol{A}(\boldsymbol{\zeta}_j)$ is the inverted variance of $\left(\boldsymbol{A}'(\boldsymbol{\zeta}_j)\boldsymbol{\Sigma}^{-1}\boldsymbol{A}(\boldsymbol{\zeta}_j)\right)^{-1}\boldsymbol{A}(\boldsymbol{\zeta}_j)'\boldsymbol{\Sigma}^{-1}\boldsymbol{y}^*$, and $\boldsymbol{\Sigma}_0^{-1}$ is the inverted prior variance of $\boldsymbol{\xi}_j^*$ which, in fact, combines prior information with extracted information from the data.

Now, it is assumed that vector $\boldsymbol{Y}^*$ in the model (2.8) is distributed as a multivariate SN, $\mathrm{SN}_N(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\lambda})$. Calculation of $E_{\boldsymbol{\xi}_j^*|\boldsymbol{y}^*}\left\{\log \pi(\boldsymbol{\xi}_j^*|\boldsymbol{y}^*)\right\}$ for SN distribution is not simple due to complexity of such distribution. To simplify the problem, we used expression (2.3) for $\boldsymbol{Y}^*$ and apply the conditional distribution below:

$$\boldsymbol{Y}^*|Z = z \sim \mathrm{N}\left(\boldsymbol{\mu} + z\boldsymbol{\Sigma}^{\frac{1}{2}}\boldsymbol{\delta}, \boldsymbol{G}\right), \tag{3.3}$$

where $\boldsymbol{G} = \boldsymbol{\Sigma}^{\frac{1}{2}}(\boldsymbol{I}_N - \boldsymbol{\delta}\boldsymbol{\delta}')\boldsymbol{\Sigma}^{\frac{1}{2}}$. Following Sorensen and Gianola [13], we use the distribution of $\boldsymbol{Y}^*$ condition on the latent variable Z, in writing the posterior distribution as given in (A.2). Insert the unobserved random variable Z in the parameters vector, i.e. $\boldsymbol{\theta}_j' = (\boldsymbol{\xi}_j^{*\prime}, Z)$, $j = 1, 2, ..., \binom{\nu_2}{k}$, and take the prior distributions $\mathrm{N}(\boldsymbol{0}, \boldsymbol{\Sigma}_0)$ for $\boldsymbol{\xi}_j^*$. The joint posterior distribution of $\boldsymbol{\theta}_j$ is proportional to $f(\boldsymbol{\theta}_j, \boldsymbol{y}^*)$ in (A.2).

The Shannon information criterion is

$$E_{\boldsymbol{\theta}_j|\boldsymbol{y}^*}\left\{\log \pi(\boldsymbol{\theta}_j|\boldsymbol{y}^*)\right\} = E_{Z|\boldsymbol{y}^*}\left\{E_{\boldsymbol{\xi}_j^*|z,\boldsymbol{y}^*}\left(\log \pi(\boldsymbol{\theta}_j|\boldsymbol{y}^*)\right)\right\}. \tag{3.4}$$

More calculations and details are given in the Appendix, based on which, the conditional

expectation in (3.4) is simplified to the reduced form below:

$$E_{\boldsymbol{\theta}_j|\boldsymbol{y}^*}\{\log\pi(\boldsymbol{\theta}_j|\boldsymbol{y}^*)\} = -\frac{1}{2}\log|2\pi\boldsymbol{\Sigma}_{\boldsymbol{\xi}}| - \frac{\nu_1+k}{2} - \frac{1}{2}\log(2\pi\sigma_z^2) - \frac{1}{2} + \frac{z^*\phi\left(\frac{z^*}{\sigma_z}\right)}{2\,\sigma_z\,\Phi\left(\frac{z^*}{\sigma_z}\right)} - \log\left(\Phi\left(\frac{z^*}{\sigma_z}\right)\right),$$

where $\boldsymbol{\Sigma}_{\boldsymbol{\xi}}$ and σ_z^2 are conditional posterior variance of $\boldsymbol{\xi}_j^*$ given $(z,\boldsymbol{y}^*)$ and conditional posterior variance of Z given $\boldsymbol{y}^*$, respectively. z^* is conditional posterior mean of Z given $\boldsymbol{y}^*$. More details on these can be found in the Appendix.

Meanwhile, the expected value of (2.9) is computed with respect to the marginal distribution of $\boldsymbol{Y}^*$ given in the Appendix, i.e. $\mathrm{SN}_N(\boldsymbol{0},\boldsymbol{\Sigma}_{\boldsymbol{y}^*},\boldsymbol{\gamma}_{\boldsymbol{y}^*})$. It gives

$$U = -\frac{\nu_1+k+1}{2}\log(2\pi) - \frac{\nu_1+k+1}{2} - \frac{1}{2}\log\{|\boldsymbol{\Sigma}_{\boldsymbol{\xi}}|(\sigma_z^2)\} + \frac{1}{2}E_T\left\{T\frac{\phi(T)}{\Phi(T)} - 2\log[\Phi(T)]\right\}, \tag{3.5}$$

where $T=\frac{z^*}{\sigma_z}$ with $T\sim\mathrm{SN}(0,\sigma_t^2,\sigma_t)$; $\sigma_t^2=\frac{\boldsymbol{\delta}'\boldsymbol{\Sigma}^{\frac{1}{2}}\boldsymbol{M}'\boldsymbol{\Sigma}_{\boldsymbol{y}^*}\boldsymbol{M}\boldsymbol{\Sigma}^{\frac{1}{2}}\boldsymbol{\delta}}{1+\boldsymbol{\delta}'\boldsymbol{\Sigma}^{\frac{1}{2}}\boldsymbol{M}\boldsymbol{\Sigma}^{\frac{1}{2}}\boldsymbol{\delta}}$; and $\boldsymbol{M}$ is given in the Appendix. ESI_D in (3.5) can be written as the following design-dependent criterion and then the minimum of such the criterion over all models in S be maximized over SDs to come up with the superior design

$$\psi(D,\boldsymbol{\lambda}) = \log\{|\boldsymbol{\Sigma}_{\boldsymbol{\xi}}|^{-1}(\sigma_z^2)^{-1}\} + E_T\left\{T\frac{\phi(T)}{\Phi(T)} - 2\log[\Phi(T)]\right\}. \tag{3.6}$$

It should also be noted that $|\boldsymbol{\Sigma}_{\boldsymbol{y}^*}| = |\boldsymbol{G}|\,|\boldsymbol{\Sigma}_{\boldsymbol{\xi}}|^{-1}|\boldsymbol{\Sigma}_0|(\sigma_z^2)^{-1}$, therefore

$$\psi(D,\boldsymbol{\lambda}) \propto \log|\boldsymbol{\Sigma}_{\boldsymbol{y}^*}| + E_T\left\{T\frac{\phi(T)}{\Phi(T)} - 2\log[\Phi(T)]\right\}. \tag{3.7}$$

The subsequent remarks present more details on $\psi(D,\boldsymbol{\lambda})$.

Remark 3.2. Generally, $\boldsymbol{\lambda}$ is an $N\times 1$ unknown vector. Lacking a specific knowledge on $\boldsymbol{\lambda}$ may lead one to follow the Bayesian approach for choosing a prior distribution such as uniform on a sphere.

Remark 3.3. Similar to Remark 3.1, the term $\boldsymbol{A}'(\boldsymbol{\xi}_j)\boldsymbol{G}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j)$ in $|\boldsymbol{\Sigma}_{\boldsymbol{\xi}}|^{-1}$ is the inverted variance of $\left(\boldsymbol{A}'(\boldsymbol{\xi}_j)\boldsymbol{G}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j)\right)^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j)'\,(\boldsymbol{V}\boldsymbol{G})^{-\frac{1}{2}}\,\boldsymbol{y}^*$ where $\boldsymbol{V}=\boldsymbol{\Sigma}^{\frac{1}{2}}\left(\boldsymbol{I}_N-\frac{2}{\pi}\boldsymbol{\delta}\boldsymbol{\delta}'\right)\boldsymbol{\Sigma}^{\frac{1}{2}}$.

Remark 3.4. For $\boldsymbol{\lambda}\to\boldsymbol{0}$ (Normality error case) random variable T is degenerated at zero. Therefore, the second term in (3.7) disappears and $\psi(D,\boldsymbol{\lambda})$ remains with its first term. It is similar to what is given in (3.2) for normal case. In the hidden truncation model, if for every $i=1,2,...,N$, $\delta_i\to\boldsymbol{0}$, then $\boldsymbol{Y}^*\sim\mathrm{N}(\boldsymbol{\mu},\boldsymbol{I}_N)$ and $\psi(D)$ is simplified to (3.2) with $\boldsymbol{\Sigma}=\boldsymbol{I}$.

Remark 3.5. For the special case of identical skewness, i.e. $\boldsymbol{\lambda}=\lambda\boldsymbol{1}_N$, $\lambda\in\mathbb{R}$, σ_t and $\boldsymbol{G}^{-1}=\boldsymbol{\Sigma}^{-\frac{1}{2}}(\boldsymbol{I}_N+\lambda^2\boldsymbol{1}_N\boldsymbol{1}_N')\boldsymbol{\Sigma}^{-\frac{1}{2}}$ are symmetric in λ. Therefore, $\psi(D,\lambda)$ is symmetric in λ. It should also be noted that for a hidden truncation problem with $\boldsymbol{\delta}=\delta\boldsymbol{1}_N$, $\psi(D,\delta)$ is symmetric in δ.

3.2. BEKL search criterion

In what follows, we obtain the expected KL distance, $I^{\boldsymbol{\theta}}\{E,\pi(\boldsymbol{\theta})\}$, under normal and SN distributions for error. It should be noted that by keeping the prior distribution in expected information (2.6) the results in this section will be different from the findings in Section 3.1, which were obtained from U in (2.9).

Consider model (2.8), and for more understanding, first assume that $\boldsymbol{Y}^* \sim \mathrm{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})$. Now, for $\boldsymbol{\xi}_j^* \sim \mathrm{N}(\mathbf{0},\boldsymbol{\Sigma}_0)$, $j=1,2,...,\binom{\nu_2}{k}$, compute $E_{\boldsymbol{Y}^*|\boldsymbol{\xi}_j^*}\big(\log f(\boldsymbol{y}^*|\boldsymbol{\xi}_j^*)\big)$ and $E_{\boldsymbol{Y}^*}\big\{\log f(\boldsymbol{y}^*)\big\}$ to reach $I^{\boldsymbol{\theta}_j}\big\{E,\pi(\boldsymbol{\theta}_j)\big\}$ given in (2.7). From marginal distribution of $\boldsymbol{Y}^*$, which is given in the Appendix, we have

$$E_{\boldsymbol{Y}^*}\big\{\log f(\boldsymbol{y}^*)\big\} = -\frac{N}{2}\big(\log(2\pi)+1\big) - \frac{1}{2}\log|\boldsymbol{\Sigma}_{\boldsymbol{y}^*}|\,.$$

Clearly, $E_{\boldsymbol{Y}^*|\boldsymbol{\xi}_j^*}\big(\log f(\boldsymbol{y}^*|\boldsymbol{\xi}_j^*)\big) = -\frac{N}{2}\big(\log(2\pi)+1\big)$, hence $I^{\boldsymbol{\theta}_j}\big\{E,\pi(\boldsymbol{\theta}_j)\big\}$ is

$$I^{\boldsymbol{\theta}_j}\big\{E,\pi(\boldsymbol{\theta}_j)\big\} = \frac{1}{2}\log|\boldsymbol{\Sigma}_{\boldsymbol{y}^*}|\,. \tag{3.8}$$

As can be seen in (3.8), in order to minimize $I^{\boldsymbol{\theta}_j}\big\{E,\pi(\boldsymbol{\theta}_j)\big\}$, it is enough to minimize the simple form $|\boldsymbol{\Sigma}_{\boldsymbol{y}^*}|$ over all possible $\binom{\nu_2}{k}$ models.

Now, suppose $\boldsymbol{Y}^* \sim \mathrm{SN}_N(\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\lambda})$. Let's add the unobserved random variable Z to the parameters vector to get $\boldsymbol{\theta}_j' = (\boldsymbol{\xi}_j^{*\prime}, Z)$, $j=1,2,...,\binom{\nu_2}{k}$. By assuming the prior distribution for the vector $\boldsymbol{\xi}_j^*$, as given herein, and noting that $\boldsymbol{Y}^*$ can be written as (2.3), we have

$$E_{\boldsymbol{Y}^*|\boldsymbol{\theta}_j}\big(\log f(\boldsymbol{y}^*|\boldsymbol{\theta}_j)\big) = -\frac{N}{2}\big(\log(2\pi)+1\big) - \frac{1}{2}\log|\boldsymbol{G}|\,,$$

and

$$E_{\boldsymbol{Y}^*}\big(\log f(\boldsymbol{y}^*)\big) = \log 2 - \frac{N}{2}\big(\log(2\pi)+1\big) - \frac{1}{2}\log|\boldsymbol{\Sigma}_{\boldsymbol{y}^*}| + E_T\big\{\log[\Phi(T)]\big\}\,.$$

Therefore, $I^{\boldsymbol{\theta}_j}\big\{E,\pi(\boldsymbol{\theta}_j)\big\}$ provides the following:

$$I^{\boldsymbol{\theta}_j}\big\{E,\pi(\boldsymbol{\theta}_j)\big\} = -\log 2 - \frac{1}{2}\log|\boldsymbol{G}| + \frac{1}{2}\log|\boldsymbol{\Sigma}_{\boldsymbol{y}^*}| - E_T\big\{\log[\Phi(T)]\big\}\,. \tag{3.9}$$

Evidently, minimizing $I^{\boldsymbol{\theta}_j}\big\{E,\pi(\boldsymbol{\theta}_j)\big\}$ in (3.9) is equivalent to minimizing $\Phi(D,\boldsymbol{\lambda}) = \log|\boldsymbol{\Sigma}_{\boldsymbol{y}^*}| - 2\,E_T\big\{\log\big(\Phi(T)\big)\big\}$ over the set of all possible models in S, known as the BEKL criterion. Note that the ESI in (3.7) has an extra term $E_T\big(T\frac{\phi(T)}{\Phi(T)}\big)$ in comparing to the BEKL. That is, although the prior distribution is design-independent, keeping such the prior in (2.6) leads to a simple and more flexible criterion.

The proposed BEKL measure, which is primarily proposed for model discrimination, can also be used to compare search performance of SDs. In doing so, first for each of the SDs the minimum of the BEKL (MBEKL_D) is obtained over the set of all models. Then, the design with a larger MBEKL_D is considered to be the desired one. Therefore, Definition 2.1 is valid for designs D_1 and D_2 with respect to MBEKL_D-criterion if $\mathrm{MBEKL}_{D_1} > \mathrm{MBEKL}_{D_2}$.

4. IMPLEMENTATION

In this section, we assess the performance of the two proposed Bayesian criteria through comparing and ranking rival SDs. To do so, we use MBEKL_D and MESI_D under SN distribution for error. We compare search performance of three 12-run search designs D_1, D_2 and D_3, as given in the Appendix, for a 2^4 factorial experiment. Design D_1 is a balanced array of full strength, Design D_2 is the projection of a 12-run Plackett–Burman design onto its 4 columns, and Design D_3 is a non-repeated run orthogonal main effect plan. These designs have already been compared by Ghosh and Teschmacher [9] and Talebi and Esmailzadeh [17], under normality.

Example 4.1. Let in model (1.1), $\boldsymbol{\xi}_1$ be the vector of the general mean and main effects, and $\boldsymbol{\xi}_2$ be two- and three-factor interactions, while assuming that four-factor interaction is negligible. Furthermore, it is assumed that $\boldsymbol{\xi}_2$ includes two non-zero effects at the most. D_1, D_2, and D_3 are MEP.1. They are also MEP.2 plans, when $\boldsymbol{\xi}_2$ includes only two-factor interactions, assuming higher-order interactions are all zero. We were interested in studying scores of 12 EEIU volunteers with a GPA over than mean, i.e. $\boldsymbol{Y} = \boldsymbol{W}|X > \mu_x$, where W_i's, $i = 1, 2, ..., 12$, are the scores and X is the GPA. Consider model (2.8) for the vector of observations $\boldsymbol{Y}$ and assume $(X, \boldsymbol{W}')' \sim \text{N}_{13}(\boldsymbol{\theta}, \boldsymbol{\Omega})$, where $\boldsymbol{\theta} = (\mu_x, \boldsymbol{\mu}')'$, $\boldsymbol{\mu} = \boldsymbol{A}(\boldsymbol{\xi}_j)\boldsymbol{\xi}_j^*$, and $\boldsymbol{\Omega} = \begin{pmatrix} 1 & \boldsymbol{\delta}' \\ \boldsymbol{\delta} & \boldsymbol{I}_{12} \end{pmatrix}$. In this case, $\boldsymbol{Y}$ satisfies the conditional distribution of (2.4). Data were collected through 3 possible designs D_1, D_2, and D_3. For $\boldsymbol{\delta} = \delta\,\mathbf{1}_{12}$, let $\boldsymbol{\sigma}_{D,\delta} = \left[\sigma_{t_{\zeta_1}}, \sigma_{t_{\zeta_2}}, ..., \sigma_{t_{\zeta_l}}\right]'$, where $l = \binom{\nu_2}{k}$, and $\sigma_{t_{\zeta_j}}$ denotes σ_t for the j-th model. MATLAB software was used to calculate amount of the criterion. It was learned that $\boldsymbol{\sigma}_{D,\delta} = c_\delta \mathbf{1}_l$, for D_1, D_2 and D_3, where c_δ is scalar and depends on δ for all models. It is also true that $\boldsymbol{\sigma}_{D_1,\delta} = \boldsymbol{\sigma}_{D_2,\delta} = \boldsymbol{\sigma}_{D_3,\delta}$, which means that the value of σ_t depends neither on the model nor on the design. Consequently, in order to compare designs D_1, D_2, and D_3, for a fixed value of δ, the second expression for both criteria is canceled out and, therefore, both ESI_D and BEKL_D become the same. This is true for the following design comparison and hence there is no difference in computing either of the criteria. For $k = 1$, once again we considered the prior distribution $\text{N}(\mathbf{0}, \boldsymbol{\Sigma}_0)$ for $\boldsymbol{\xi}_j^*$ in which $\boldsymbol{\Sigma}_0$ is a 6×6 diagonal matrix, with large diagonal elements of 100. The comparisons showed that D_2 is better than both D_1 and D_3, and D_1 is better than D_3. This result is the same as what was obtained using the compound criteria proposed by Talebi and Esmailzadeh [17]. For instance, when $\delta = 0.2$, values of criterion are 42.6251, 42.6738, and 42.4026 for D_1, D_2, and D_3, respectively, while the EKL values for these Designs are the same and equal to 10.667. This shows that the EKL is unable to discriminate search abilities of D_1, D_2, and D_3.

Example 4.2. In continuation of Example 4.1, let $\boldsymbol{\xi}_2$ be the vector of two-factor interactions only, and assume that three- and four-factor interactions are all zero. For $k = 1$, results showed that D_3 has the same search ability as D_1, and they are better than D_2, based on the present criteria. For example, when $\delta = 0.2$, criterion value for D_1 and D_3, is 42.6895 and for D_2 is 42.6738. For $k = 2$, assume that $\boldsymbol{\xi}_j^*$ is distributed as $\text{N}(\mathbf{0}, \boldsymbol{\Sigma}_0)$ in which $\boldsymbol{\Sigma}_0$ is a 7×7 diagonal matrix, with diagonal elements of 100. When $\delta = 0.2$, criterion value for D_1 and D_3 is 49.376, and for D_2 is 49.3115.

5. DISCUSSION

Findings in Section 4 reveal that both criteria, MESI_D and MBEKL_D increase as δ increases; this means as $\delta\,(\geq 0)$ gets larger, the capability of SD enhances in identifying the non-zero effects, which has been ignored by the former criteria. The proposed criteria are also applicable for $k > 1$. So, an important advantage of the present criteria is their flexibility with respect to distributional model and the number of non-zero effects in $\boldsymbol{\xi}_2$. This study generalizes the previously-obtained results for the normal model by utilizing the SN distribution, where normal distribution is its special case. It is notable that unlike SP, MESI_D and MBEKL_D do not depend on an unknown parameter. This allows us to come up with numerical values for the criteria. Furthermore, the results presented in Section 4 showed that MESI_D and MBEKL_D criteria have a higher discriminating power than the EKL, obtained by Talebi and Esmailzadeh [15].

A. APPENDIX

A.1. Conditional posterior distributions for normal distribution error

For $\boldsymbol{e}^* \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Sigma})$, $f(\boldsymbol{\xi}_j^*, \boldsymbol{y}^*)$ can be written as

$$\begin{aligned} f(\boldsymbol{\xi}_j^*, \boldsymbol{y}^*) &= f(\boldsymbol{y}^*|\boldsymbol{\xi}_j^*)\, \pi(\boldsymbol{\xi}_j^*) \\ &= (2\pi)^{-\frac{N+\nu_1+k}{2}}\, |\boldsymbol{\Sigma}|^{-\frac{1}{2}}\, \exp\left\{-\frac{1}{2}\left(\boldsymbol{y}^* - \boldsymbol{A}(\boldsymbol{\xi}_j)\boldsymbol{\xi}_j^*\right)' \boldsymbol{\Sigma}^{-1}\left(\boldsymbol{y}^* - \boldsymbol{A}(\boldsymbol{\xi}_j)\,\boldsymbol{\xi}_j^*\right)\right\} \\ &\quad \times\, |\boldsymbol{\Sigma}_0|^{-\frac{1}{2}}\, \exp\left\{-\frac{1}{2}\,\boldsymbol{\xi}_j^{*\prime}\,\boldsymbol{\Sigma}_0^{-1}\,\boldsymbol{\xi}_j^*\right\}, \end{aligned} \tag{A.1}$$

where $|\cdot|$ stands for determinant. Using the joint distribution in (A.1) together with some other calculations, it can be shown that the conditional posterior distributions of parameters are as follows:

$$\boldsymbol{\xi}_j^*|\boldsymbol{y}^* \sim \mathrm{N}\Big(\boldsymbol{\mu}_{\boldsymbol{\xi}_j^*},\, \left(\boldsymbol{A}'(\boldsymbol{\xi}_j)\,\boldsymbol{\Sigma}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j) + \boldsymbol{\Sigma}_0^{-1}\right)^{-1}\Big),$$

where $\boldsymbol{\mu}_{\boldsymbol{\xi}_j^*} = \left(\boldsymbol{A}'(\boldsymbol{\xi}_j)\boldsymbol{\Sigma}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j) + \boldsymbol{\Sigma}_0^{-1}\right)^{-1}\boldsymbol{A}'(\boldsymbol{\xi}_j)\boldsymbol{\Sigma}^{-1}\boldsymbol{y}^*$. The logarithm of the joint posterior distribution is

$$\begin{aligned} \log\{\pi(\boldsymbol{\xi}_j^*|\boldsymbol{y}^*)\} &= -\frac{1}{2}\,\log\Big|2\pi\left(\boldsymbol{A}'(\boldsymbol{\xi}_j)\,\boldsymbol{\Sigma}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j) + \boldsymbol{\Sigma}_0^{-1}\right)^{-1}\Big| \\ &\quad -\frac{1}{2}\,(\boldsymbol{\xi}_j^* - \boldsymbol{\mu}_{\boldsymbol{\xi}_j^*})'\left(\boldsymbol{A}'(\boldsymbol{\xi}_j)\,\boldsymbol{\Sigma}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j) + \boldsymbol{\Sigma}_0^{-1}\right)(\boldsymbol{\xi}_j^* - \boldsymbol{\mu}_{\boldsymbol{\xi}_j^*})\,. \end{aligned}$$

Note that

$$(\boldsymbol{\xi}_j^* - \boldsymbol{\mu}_{\boldsymbol{\xi}_j^*})'\left(\boldsymbol{A}'(\boldsymbol{\xi}_j)\,\boldsymbol{\Sigma}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j) + \boldsymbol{\Sigma}_0^{-1}\right)(\boldsymbol{\xi}_j^* - \boldsymbol{\mu}_{\boldsymbol{\xi}_j^*})\,\Big|\,\boldsymbol{y}^* \sim \chi^2_{\nu_1+k}\,,$$

where $\chi^2_{\nu_1+k}$ is chi-squared distribution with $\nu_1 + k$ degrees of freedom. Marginal distribution of $\boldsymbol{Y}^*$ is obtained from the joint distribution in (A.1). It can be easily shown that $\boldsymbol{Y}^*$ is distributed as $\mathrm{N}(\mathbf{0}, \boldsymbol{\Sigma}_{\boldsymbol{y}^*})$, where

$$\boldsymbol{\Sigma}_{\boldsymbol{y}^*} = \left\{\boldsymbol{\Sigma}^{-1} - \boldsymbol{\Sigma}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j)\left(\boldsymbol{A}'(\boldsymbol{\xi}_j)\,\boldsymbol{\Sigma}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j) + \boldsymbol{\Sigma}_0^{-1}\right)^{-1}\boldsymbol{A}'(\boldsymbol{\xi}_j)\,\boldsymbol{\Sigma}^{-1}\right\}^{-1}.$$

A.2. Conditional posterior distributions for SN distribution error

For $\boldsymbol{Y}^* \sim \mathrm{SN}_N(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\lambda})$, the joint density of vector $(\boldsymbol{\theta}_j, \boldsymbol{y}^*)$ is

$$\begin{aligned} f(\boldsymbol{\theta}_j, \boldsymbol{y}^*) &= f(\boldsymbol{y}^*|\boldsymbol{\theta}_j)\, f(z|\boldsymbol{\xi}_j^*)\, \pi(\boldsymbol{\xi}_j^*) \\ &= |\boldsymbol{G}|^{-\frac{1}{2}}\, \exp\left\{-\frac{1}{2}\left(\boldsymbol{y}^* - \boldsymbol{A}(\boldsymbol{\xi}_j)\boldsymbol{\xi}_j^* - z\,\boldsymbol{\Sigma}^{\frac{1}{2}}\,\boldsymbol{\delta}\right)'\boldsymbol{G}^{-1}\left(\boldsymbol{y}^* - \boldsymbol{A}(\boldsymbol{\xi}_j)\boldsymbol{\xi}_j^* - z\,\boldsymbol{\Sigma}^{\frac{1}{2}}\,\boldsymbol{\delta}\right)\right\} \\ &\quad \times\, 2\,(2\pi)^{-\frac{N+\nu_1+k+1}{2}}\, |\boldsymbol{\Sigma}_0|^{-\frac{1}{2}}\, \exp\left\{-\frac{1}{2}\left[z^2 + \boldsymbol{\xi}_j^{*\prime}\,\boldsymbol{\Sigma}_0^{-1}\,\boldsymbol{\xi}_j^*\right]\right\}. \end{aligned} \tag{A.2}$$

From (A.2), the conditional posterior distributions of unknown parameters are obtained as:

$$\boldsymbol{\xi}_j^*|z, \boldsymbol{y}^* \sim \mathrm{N}(\boldsymbol{\mu}_{\boldsymbol{\xi}_j^*}, \boldsymbol{\Sigma}_{\boldsymbol{\xi}}) \qquad \text{and} \qquad Z|\boldsymbol{y}^* \sim \mathrm{N}(z^*, \sigma_z^2)\, I(Z>0)\,,$$

in which the conditional posterior distribution of $Z|\boldsymbol{y}^*$ is truncated normal at zero with the following pdf:

$$\pi(Z|\boldsymbol{y}^*) = \phi\left(\frac{z-z^*}{\sigma_z}\right) \Big/ \left(\sigma_z\, \Phi\left(\frac{z^*}{\sigma_z}\right)\right)$$

and

$$\boldsymbol{\mu}_{\boldsymbol{\xi}_j^*} = \boldsymbol{\Sigma}_{\boldsymbol{\xi}}\, \boldsymbol{A}'(\boldsymbol{\xi}_j)\, \boldsymbol{G}^{-1}\big(\boldsymbol{y}^* - z\, \boldsymbol{\Sigma}^{\frac{1}{2}}\, \boldsymbol{\delta}\big)\,, \qquad \boldsymbol{\Sigma}_{\boldsymbol{\xi}} = \big(\boldsymbol{A}'(\boldsymbol{\xi}_j)\, \boldsymbol{G}^{-1} \boldsymbol{A}(\boldsymbol{\xi}_j) + \boldsymbol{\Sigma}_0^{-1}\big)^{-1},$$

$$z^* = \sigma_z^2\, \boldsymbol{y}^{*\prime} \boldsymbol{M}\, \boldsymbol{\Sigma}^{\frac{1}{2}}\, \boldsymbol{\delta}\,, \qquad \sigma_z^2 = \big(1 + \boldsymbol{\delta}'\, \boldsymbol{\Sigma}^{\frac{1}{2}}\, \boldsymbol{M}\, \boldsymbol{\Sigma}^{\frac{1}{2}}\, \boldsymbol{\delta}\big)^{-1},$$

$$\boldsymbol{M} = \boldsymbol{G}^{-1} + \boldsymbol{G}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j)\Big[\big(\boldsymbol{\Sigma}_{\boldsymbol{\xi}}\, \boldsymbol{A}'(\boldsymbol{\xi}_j)\, \boldsymbol{G}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j) + \boldsymbol{I}_{\nu_1+k}\big)^{-1} - \boldsymbol{I}_{\nu_1+k}\Big]\big(\boldsymbol{A}'(\boldsymbol{\xi}_j)\, \boldsymbol{G}^{-1}\boldsymbol{A}(\boldsymbol{\xi}_j)\big)^{-1}\boldsymbol{A}'(\boldsymbol{\xi}_j)\, \boldsymbol{G}^{-1}.$$

The logarithm of $\pi(\boldsymbol{\theta}_j|\boldsymbol{y}^*)$ (the joint posterior distribution of $\boldsymbol{\theta}_j$) can be written as

$$\begin{aligned}
\log \pi(\boldsymbol{\theta}_j|\boldsymbol{y}^*) \;&=\; \log\big\{\pi(\boldsymbol{\xi}_j|z, \boldsymbol{y}^*)\big\} + \log\big\{\pi(Z|\boldsymbol{y}^*)\big\} \\
&=\; -\frac{1}{2}\, \log|2\pi\, \boldsymbol{\Sigma}_{\boldsymbol{\xi}}| - \frac{1}{2}\, (\boldsymbol{\xi}_j^* - \boldsymbol{\mu}_{\boldsymbol{\xi}_j^*})'\, \boldsymbol{\Sigma}_{\boldsymbol{\xi}}^{-1} (\boldsymbol{\xi}_j^* - \boldsymbol{\mu}_{\boldsymbol{\xi}_j^*}) \\
&\quad -\frac{1}{2}\, \log(2\pi\, \sigma_z^2) - \frac{1}{2}\left(\frac{Z-z^*}{\sigma_z}\right)^2 - \log\left(\Phi\left(\frac{z^*}{\sigma_z}\right)\right),
\end{aligned}$$

It should be noted that

$$(\boldsymbol{\xi}_j^* - \boldsymbol{\mu}_{\boldsymbol{\xi}_j^*})'\, \boldsymbol{\Sigma}_{\boldsymbol{\xi}}^{-1} (\boldsymbol{\xi}_j^* - \boldsymbol{\mu}_{\boldsymbol{\xi}_j^*}) \sim \chi^2_{\nu_1+k}\,,$$

and

$$E_{Z|\boldsymbol{y}^*}(Z - z^*)^2 \;=\; \sigma_z^2 - \sigma_z\, z^* \frac{\phi(\frac{z^*}{\sigma_z})}{\Phi(\frac{z^*}{\sigma_z})}\,.$$

From (A.2) the marginal distribution of $\boldsymbol{Y}^*$ is distributed as $\mathrm{SN}_N(\boldsymbol{0}, \boldsymbol{\Sigma}_{\boldsymbol{y}^*}, \boldsymbol{\gamma}_{\boldsymbol{y}^*})$, in which $\boldsymbol{\Sigma}_{\boldsymbol{y}^*} = \big\{\boldsymbol{M} - \sigma_z^2\, \boldsymbol{M}\, \boldsymbol{\Sigma}^{\frac{1}{2}}\, \boldsymbol{\delta}\, \boldsymbol{\delta}'\, \boldsymbol{\Sigma}^{\frac{1}{2}}\, \boldsymbol{M}'\big\}^{-1}$ and $\boldsymbol{\gamma}_{\boldsymbol{y}^*} = \boldsymbol{\Sigma}_{\boldsymbol{y}^*}^{\frac{1}{2}} \frac{\boldsymbol{M}\, \boldsymbol{\Sigma}^{\frac{1}{2}}\, \boldsymbol{\delta}}{\sqrt{1+\boldsymbol{\delta}'\, \boldsymbol{\Sigma}^{\frac{1}{2}}\, \boldsymbol{M}\, \boldsymbol{\Sigma}^{\frac{1}{2}}\, \boldsymbol{\delta}}}$.

A.3. Search designs D_1, D_2 and D_3 with 12 runs and 4 factors

D_1				D_2				D_3			
A	B	C	D	A	B	C	D	A	B	C	D
+	+	+	+	+	−	+	−	+	+	+	+
-	−	−	−	+	+	−	+	+	−	+	+
−	−	−	+	−	+	+	−	−	−	+	+
−	−	+	−	+	−	+	+	−	+	−	+
−	+	−	−	+	+	−	+	+	−	−	+
+	−	−	−	+	+	+	−	−	−	−	−
−	−	+	+	−	+	+	+	−	+	+	−
−	+	−	+	−	−	+	+	+	−	+	−
+	−	−	+	−	−	−	+	−	−	+	−
−	+	+	−	+	−	−	−	+	+	−	−
+	−	+	−	−	+	−	−	+	−	−	−
+	+	−	−	−	−	−	−	−	−	−	−

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EFFICIENCY OF THE PRINCIPAL COMPONENT LIU-TYPE ESTIMATOR IN LOGISTIC REGRESSION

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Abstract:

- In this paper we propose a principal component Liu-type logistic estimator by combining the principal component logistic regression estimator and Liu-type logistic estimator to overcome the multicollinearity problem. The superiority of the new estimator over some related estimators are studied under the asymptotic mean squared error matrix. A Monte Carlo simulation experiment is designed to compare the performances of the estimators using mean squared error criterion. Finally, a conclusion section is presented.

Key-Words:

- *Liu-type estimator; logistic regression; mean squared error matrix; maximum likelihood estimator; multicollinearity.*

AMS Subject Classification:

- 62J07, 62J12.

1. INTRODUCTION

Consider the following binary logistic regression model

$$\pi_i = \frac{\exp(x_i'\beta)}{1+\exp(x_i'\beta)}, \qquad i=1,...,n, \tag{1.1}$$

where $x_i' = (1\ x_{i1} \cdots x_{iq})$ denotes the i-th row of X which is an $n \times p$ $(p = q+1)$ data matrix with q known covariate vectors, y_i shows the response variable which takes on the value either 0 or 1 with $y_i \sim \text{Bernoulli}(\pi_i)$, y_i's are supposed to be independent of one another and $\beta' = (\beta_0\ \beta_1 \cdots \beta_q)$ stands for a $p \times 1$ vector of parameters.

Usually the maximum likelihood (ML) method is used to estimate β. The corresponding log-likelihood equation of model (1.1) is given by

$$L = \sum_{i=1}^{n} y_i \log(\pi_i) + (1-y_i)\log(1-\pi_i), \tag{1.2}$$

where π_i is the i-th element of the vector π, $i = 1, 2, ..., n$.

ML estimator can be obtained by maximizing the log-likelihood equation given in (1.2). Since Equation (1.2) is non-linear in β, one should use an iterative algorithm called iteratively re-weighted least squares algorithm (IRLS) as follows (Saleh and Kibria, [18]):

$$\hat{\beta}^{t+1} = \hat{\beta}^t + \left(X'V^tX\right)^{-1}X'V^t\left(y-\hat{\pi}^t\right), \tag{1.3}$$

where π^t is the estimated values of π using $\hat{\beta}_t$ and $V^t = \text{diag}\left(\hat{\pi}_i^t(1-\hat{\pi}_i^t)\right)$ such that $\hat{\pi}_i^t$ is the i-th element of $\hat{\pi}_t$. After some algebra, Equation (1.3) can be written as follows:

$$\hat{\beta}_{\text{ML}} = \left(X'VX\right)^{-1}X'Vz, \tag{1.4}$$

where $z' = (z_1 \cdots z_n)$ with $\eta_i = x_i'\beta$ and $z_i = \eta_i + (y_i - \pi_i)\,(\partial\eta_i/\partial\pi_i)$.

In linear regression analysis, multicollinearity has been regarded as a problem in the estimation. In dealing with this problem, many ways have been introduced to deal with this problem. One approach is to study the biased estimators such as ridge estimator (Hoerl and Kennard, [7]), Liu estimator (Liu, [14]), Liu-type estimator (Huang *et al.*, [8]), modified Liu-type estimator (Alheety and Kibria, [2]) and improved ridge estimators (Yüzbaşı *et al.*, [21]). Alternatively, many authors such as Xu and Yang ([20]) and Li and Yang ([13]), have studied the estimation of linear models with additional restrictions.

As in linear regression, estimation in logistic regression is also sensitive to multicollinearity. When there is multicollinearity, columns of the matrix $X'VX$ become close to be dependent. It implies that some of the eigenvalues of $X'VX$ become close to zero. Thus, mean squared error value of MLE is inflated so that one cannot obtain stable estimations. Thus many authors have studied how to reduce the multicollinearity, such as Lesaffre and Max ([12]) discussed the multicollinearity in logistic regression, Schaefer *et al.* ([19]) proposed the ridge logistic (RL) estimator, Aguilera *et al.* ([1]) proposed the principal component logistic regression (PCLR) estimator, Månsson *et al.* ([15]) introduced the Liu logistic (LL)

estimator, by combining the principal component logistic regression estimator and ridge logistic estimator to deal with multicollinearity. Moreover, Inan and Erdoğan ([9]) proposed Liu-type logistic estimator (LTL) and Asar ([3]) studied some properties of LTL.

In this study, by combining the principal component logistic regression estimator and the Liu-type logistic estimator, the principal component Liu-type logistic estimator is introduced as an alternative to the PCLR, ML and LTL to deal with the multicollinearity.

The rest of the paper is organized as follows. In Section 2, the new estimator is proposed. Some properties of the new estimator are presented in Section 3. A Monte Carlo simulation is given in Section 4 and some concluding remarks are given in Section 5.

2. THE NEW ESTIMATOR

The logistic regression model is expressed by Aguilera *et al.* ([1]) in matrix form in terms of the logit transformation as $L = X\beta = XTT'\beta = Z\alpha$ where $T = [t_1, ..., t_p]$ shows an orthogonal matrix with $Z'VZ = T'X'VXT = \Lambda$ and $\Lambda = \text{diag}(\lambda_1, ..., \lambda_p)$, $\lambda_1 \geq \cdots \geq \lambda_p$, is the ordered eigenvalues of $X'VX$. Then T and Λ may be written as $T = (T_r \ T_{p-r})$ and $\begin{bmatrix} \Lambda_r & O \\ O & \Lambda_{p-r} \end{bmatrix}$ where $Z_r'VZ_r = T_r'X'VXT_r = \Lambda_r$ and $Z_{p-r}'VZ_{p-r} = T_{p-r}'X'VXT_{p-r} = \Lambda_{p-r}$. The Z matrix and the α vector can be partitioned as $Z = (Z_r \ Z_{p-r})$ and $\alpha = (\alpha_r' \ \alpha_{p-r}')'$. The handling of multicollinearity by means of PCLR corresponds to the transition from the model $L = X\beta = XT_rT_r'\beta + XT_{p-r}T_{p-r}'\beta = Z_r\alpha_r + Z_{p-r}\alpha_{p-r}$ to the reduced model $L = Z_r\alpha_r$. Then by Equation (1.1) and PCLR method we get the PCLR estimator.

Inan and Erdoğan ([9]) proposed Liu-type logistic estimator (LTL) as

$$\hat{\beta}(k,d) = \left(X'VX + kI\right)^{-1}\left(X'Vz - d\hat{\beta}_{\text{ML}}\right), \tag{2.1}$$

where $-\infty < d < \infty$ and $k > 0$ are biasing parameters.

The principal component logistic regression estimator (Aguilera *et al.*, [1]) is defined as

$$\hat{\beta}_r = T_r\left(T_r'X'VXT_r\right)^{-1}T_r'X'Vz\,. \tag{2.2}$$

We can write (2.2) as follows:

$$\hat{\beta}_r = T_r\left(T_r'X'VXT_r\right)^{-1}T_r'X'Vz = T_rT_r'\hat{\beta}_{\text{ML}}\,. \tag{2.3}$$

Then we can introduce a new estimator by replacing $\hat{\beta}^*(k,d)$ with $\hat{\beta}_{\text{ML}}$ in (2.3), and we get

$$\begin{aligned} \hat{\beta}_r(k,d) &= T_rT_r'\hat{\beta}(k,d) \\ &= T_r\left(T_r'X'VXT_r + kI_r\right)^{-1}\left(T_r'X'VXT_r - dI_r\right)\left(T_r'X'VXT_r\right)^{-1}T_r'X'Vz\,, \end{aligned} \tag{2.4}$$

where $-\infty < d < \infty$ and $k > 0$ are biasing parameters. We call this estimator as the principal component Liu-type logistic regression (PCLTL) estimator.

Remark 2.1. It is obvious that

$$\hat{\beta}_r(k,d) = T_r\left(T_r'X'VXT_r + kI_r\right)^{-1}\left(T_r'X'VXT_r - dI_r\right)T_r'\hat{\beta}_r\,.$$

Thus we can see the PCLTL estimator as a linear combination of the PCLR estimator.

Remark 2.2. It is easy to obtain the followings:

(**a**) $\hat{\beta}_r(0,0) = \hat{\beta}_r = T_r\left(T_r'X'VXT_r\right)^{-1}T_r'X'Vz$, PCLR estimator;

(**b**) $\hat{\beta}_p(0,0) = \hat{\beta}_{\mathrm{ML}} = \left(X'VX\right)^{-1}X'Vz$, ML estimator;

(**c**) $\hat{\beta}_p(k,d) = \hat{\beta}(k,d) = \left(X'VX + kI\right)^{-1}\left(X'Vz - d\hat{\beta}_{\mathrm{ML}}\right)$, LTL estimator.

Thus, the new estimator in (2.4) includes the PCLR, ML and LTL estimators as its special cases.

In the next section, we will study the properties of the new estimator.

3. THE PROPERTIES OF NEW ESTIMATOR

For the sake of convenience, we present some lemmas which are needed in the following discussions.

Lemma 3.1 (Farebrother, [6]; Rao and Tountenburg, [17]). *Suppose that M is a positive definite matrix, namely $M > 0$, α is some vector, then $M - \alpha\alpha' \geq 0$ if and only if $\alpha' M^{-1}\alpha \leq 1$.*

Lemma 3.2 (Baksalary and Trenkler, [5]). *Let $C_{n\times p}$ be the set of complex matrices and $H_{n\times n}$ be the Hermitian matrices. Further, given $L \in C_{n\times p}$, L^*, $R(L)$ and $\kappa(L)$ denote the conjugate transpose, the range and the set of all generalized inverses, respectively of L. Let $A \in H_{n\times n}$, $a_1 \in C_{n\times 1}$ and $a_2 \in C_{n\times 1}$ be linearly independent, $f_{ij} = a_i'A^{-}a_j$, $i,j = 1,2$ and $A \in \kappa(L)$, $a_1 \notin R(A)$. Let*

$$s = \left[a_1'\left(I - AA^{-}\right)'\left(I - AA^{-}\right)a_2\right] \Big/ \left[a_1'\left(I - AA^{-}\right)'\left(I - AA^{-}\right)a_1\right].$$

Then $A + a_1a_1' - a_2a_2' \geq 0$ if and only if one of the following sets of conditions holds:

(**a**) $A \geq 0$, $a_i \in R(A)$, $i = 1,2$, $(f_{11}+1)(f_{22}-1) \leq |f_{12}|^2$,

(**b**) $A \geq 0$, $a_1 \notin R(A)$, $a_2 \in R(A : a_1)$, $(a_2 - sa_1)'A^{-}(a_2 - sa_1) \leq 1 - |s|^2$,

(**c**) $A = U\Delta U' - \lambda vv'$, $a_i \in R(A)$, $i = 1,2$, $v'a_1 \neq 0$, $f_{11}+1 \leq 0$, $f_{22}-1 \leq 0$, $(f_{11}+1)(f_{22}-1) \geq |f_{12}|^2$,

where $(U : v)$ shows a sub-unitary matrix, λ is a positive scalar and Δ is a positive definite diagonal matrix. Further, the conditions (a), (b) and (c) denote all independent of the choice of A^{-}, A^{-} stands for the generalized inverse of A.

To compare the estimators, we use the mean squared error matrix (MSEM) criterion which is defined for an estimator $\check{\beta}$ as follows:

$$\mathrm{MSEM}\big(\check{\beta}\big) \;=\; \mathrm{Cov}\big(\check{\beta}\big) + \mathrm{Bias}\big(\check{\beta}\big)\,\mathrm{Bias}\big(\check{\beta}\big)',$$

where $\mathrm{Cov}\big(\check{\beta}\big)$ is the covariance matrix of $\check{\beta}$, and $\mathrm{Bias}\big(\check{\beta}\big)$ is the bias vector of $\check{\beta}$. Moreover, scalar mean squared error (SMSE) of an estimator $\check{\beta}$ is also given as

$$\mathrm{SMSE}\big(\check{\beta}\big) \;=\; \mathrm{tr}\big\{\mathrm{MSEM}\big(\check{\beta}\big)\big\}\,.$$

3.1. Comparison of the new estimator (PCLTL) to the ML estimator

From (2.4), we can compute the asymptotic variance of the new estimator as follows:

$$\mathrm{Cov}\big(\hat{\beta}_r(k,d)\big) \;=\; T_r\,S_r(k)^{-1}\,\Lambda_r^{-1}S_r(d)\;\Lambda_r\,S_r(d)\;\Lambda_r^{-1}S_r(k)^{-1}\,T_r'\,, \tag{3.1}$$

where $S_r(k) = \Lambda_r + k\,I_r,\;\; S_r(d) = \Lambda_r - d\,I_r$.

Using (2.4), we get:

$$E\big(\hat{\beta}_r(k,d)\big) \;=\; T_r\,S_r(k)^{-1}\,\Lambda_r^{-1}S_r(d)\;\Lambda_r T_r'\beta\,. \tag{3.2}$$

By

$$T_r\,S_r(k)^{-1}\,\Lambda_r T_r' - I_p \;=\; -\Big(T_{p-r}\,T_{p-r}' + k\,T_r\,S_r(k)^{-1}\,T_r'\Big)\,, \tag{3.3}$$

then we get the asymptotic bias of the new estimator as follows:

$$\mathrm{Bias}\big(\hat{\beta}_r(k,d)\big) \;=\; \Big(-T_{p-r}\,T_{p-r}' - (d+k)\,T_r\,S_r(k)^{-1}\,T_r'\Big)\,\beta\,.$$

Now, we can get the asymptotic mean squared error matrix of the new estimator as follows:

$$\begin{aligned}\mathrm{MSEM}\big(\hat{\beta}_r(k,d)\big) \;=\;& T_r\,S_r(k)^{-1}\,\Lambda_r^{-1}S_r(d)\;\Lambda_r\,S_r(d)\;\Lambda_r^{-1}S_r(k)^{-1}\,T_r' \\ &+ \Big(-T_{p-r}\,T_{p-r}' - (d+k)\,T_r\,S_r(k)^{-1}\,T_r'\Big)\,\beta \\ &\times\,\beta'\Big(-T_{p-r}\,T_{p-r}' - (d+k)\,T_r\,S_r(k)^{-1}\,T_r'\Big)\,.\end{aligned} \tag{3.4}$$

Theorem 3.1. *Assume that $d < k$ and $d + k > 0$ then the new estimator is superior to the ML estimator under the asymptotic mean squared error matrix criterion if and only if*

$$\beta' T_r(k+d)^2\Big[2(k+d)\,I_r + (k^2-d^2)\,\Lambda_r^{-1}\Big]^{-1}T_r'\beta + \beta' T_{p-r}\,\Lambda_{p-r}\,T_{p-r}'\beta \;\le\; 1\,.$$

Proof: The asymptotic mean squared error matrix of MLE is given by

$$\mathrm{MSEM}\big(\hat{\beta}\big) = \big(X'VX\big)^{-1}. \tag{3.5}$$

By $\Lambda = \begin{pmatrix} \Lambda_r & O \\ O & \Lambda_{p-r} \end{pmatrix}$ and $T = (T_r, T_{p-r})$, we may obtain

$$\left(X'VX\right)^{-1} = T\Lambda^{-1}T' = T_r\Lambda_r^{-1}T_r' + T_{p-r}\Lambda_{p-r}^{-1}T_{p-r}'.$$

Let us consider the difference $\Delta_1 = \mathrm{MSEM}\left(\hat{\beta}\right) - \mathrm{MSEM}\left(\hat{\beta}_r(k,d)\right)$ such that

$$\begin{aligned} \Delta_1 \;=\; & T_r S_r(k)^{-1}\left[2(k+d)I_r + (k^2-d^2)\Lambda_r^{-1}\right] S_r(k)^{-1}T_r' \\ & + T_{p-r}\left[\Lambda_{p-r} - T_{p-r}'\beta\beta'T_{p-r}\right]T_{p-r}' - (k+d)^2\, T_r S_r(k)^{-1} \\ & \times T_r'\beta\beta' S_r(k)^{-1}T_r' + (k+d)\, T_r S_r(k)^{-1}T_r'\beta\beta'T_{p-r}T_{p-r}' \\ & + (k+d)\, T_{p-r}T_{p-r}'\beta\beta'T_r S_r(k)^{-1}T_r'. \end{aligned} \tag{3.6}$$

Let

$$S^* = \begin{pmatrix} \frac{S_r(k)}{k+d} & 0 \\ 0 & \Lambda_{p-r} \end{pmatrix}$$

and

$$(\Lambda^*)^{-1} = \begin{pmatrix} \frac{2(k+d)I_r + (k^2-d^2)\Lambda_r^{-1}}{(k+d)^2} & 0 \\ 0 & \Lambda_{p-r} \end{pmatrix}. \tag{3.7}$$

Now we can write (3.6) as

$$\Delta_1 \;=\; T(S^*)^{-1}\left[(\Lambda^*)^{-1} - T'\beta\beta'T\right](S^*)^{-1}T'. \tag{3.8}$$

Thus Δ_1 is a nonnegative definite matrix if and only if $(\Lambda^*)^{-1} - T'\beta\beta'T$ is a nonnegative definite matrix. Using Lemma 3.1, $(\Lambda^*)^{-1} - T'\beta\beta'T$ is a nonnegative definite matrix if and only if $\beta'T\Lambda^*T'\beta \le 1$. Invoking the notation of Λ^* in (3.7), we can prove Theorem 3.1. □

3.2. Comparison of the new estimator (PCLTL) to the PCLR estimator

Theorem 3.2. *Suppose that $d < k$ and $d + k > 0$ then the new estimator is better than the PCLR estimator under the asymptotic mean squared error matrix criterion if and only if $T_r'\beta = 0$.*

Proof: Suppose that $k = d$ in Equation (3.4), then we get

$$\mathrm{MSEM}\left(\hat{\beta}_r\right) \;=\; T_r\Lambda_r^{-1}T_r' + \left(T_rT_r' - I_p\right)\beta\beta'\left(T_rT_r' - I_p\right). \tag{3.9}$$

Now let us consider the difference $\Delta_2 = \mathrm{MSEM}\left(\hat{\beta}_r\right) - \mathrm{MSEM}\left(\hat{\beta}_r(k,d)\right)$ such that

$$\begin{aligned} \Delta_2 \;=\; & T_r S_r(k)^{-1}\left[2(k+d)I_r + (k^2-d^2)\Lambda_r^{-1}\right] S_r(k)^{-1}T_r' \\ & + \left(T_rT_r' - I_p\right)\beta\beta'\left(T_rT_r' - I_p\right) \\ & + \left(-T_{p-r}T_{p-r}' - (d+k)\, T_r S_r(k)^{-1}T_r'\right)\beta \\ & \times \beta'\left(-T_{p-r}T_{p-r}' - (d+k)\, T_r S_r(k)^{-1}T_r'\right). \end{aligned} \tag{3.10}$$

To apply Lemma 3.2, let $A = T_r B T_r'$, where

$$B = S_r(k)^{-1}\left[2(k+d)I_r + (k^2-d^2)\Lambda_r^{-1}\right]S_r(k)^{-1}$$

and $a_1 = \left(T_r T_r' - I_p\right)\beta$, $a_2 = \left(-T_{p-r}T_{p-r}' - (d+k)T_r S_r(k)^{-1}T_r'\right)\beta$.

When $d < k$ and $d + k > 0$, B is a positive definite matrix. Then we get the Moore–Penrose inverses of A which is $A^+ = T_r B^{-1} T_r'$, and $AA^+ = T_r T_r'$. Thus $a_1 \in R(A)$ if and only if $a_1 = 0$. Since $a_1 \neq 0$, we cannot use part (a) and (c) of Lemma 3.2, we can only apply part (b) of Lemma 3.2. Using the definition of s, we may obtain that $s = 1$. On the other hand, $a_2 - a_1 = A\eta$, where

$$\eta = (d+k)T_r S_r(k)\left[2(k+d)I_r + (k^2-d^2)\Lambda_r^{-1}\right]^{-1}T_r'\beta\,.$$

Thus, we can easily obtain $a_2 \in R(A : a_1)$. Then Using Lemma 3.2, we can get that the new estimator is superior to the PCLR estimator under the asymptotic mean squared error matrix criterion if and only if $(a_2 - a_1)A^-(a_2 - a_1) \leq 0$ or $\eta' A\eta \leq 0$. In fact, $(a_2 - a_1)A^-(a_2 - a_1) \geq 0$, so the new estimator is better than the PCLR estimator under the asymptotic mean squared error matrix criterion if and only if $\eta' A\eta = 0$, that is

$$\beta' T_r\left[2(k+d)I_r + (k^2-d^2)\Lambda_r^{-1}\right]^{-1}T_r'\beta = 0$$

and $\beta' T_r\left[2(k+d)I_r + (k^2-d^2)\Lambda_r^{-1}\right]^{-1}T_r'\beta = 0$ if and only if $T_r'\beta = 0$. Thus, the proof is finished. □

3.3. Comparison of the new estimator (PCLTL) to the Liu-type logistic estimator

Theorem 3.3. *The new estimator is superior to the Liu-type logistic estimator under the asymptotic mean squared error matrix criterion if and only if* $T_{p-r}'\beta = 0$.

Proof: Putting $r = p$ into (3.4), we get

$$\begin{aligned}\mathrm{MSEM}\left(\hat{\beta}(k,d)\right) &= TS(k)^{-1}S(d)\,\Lambda^{-1}S(d)\,S(k)^{-1}T' \\ &\quad + (k+d)^2\,TS(k)^{-1}T'\beta\beta'TS(k)^{-1}T',\end{aligned} \tag{3.11}$$

where $S(k) = \Lambda + kI_p$ and $S(d) = \Lambda - dI_p$. Now we study the following difference $\Delta_3 = \mathrm{MSEM}\left(\hat{\beta}(k,d)\right) - \mathrm{MSEM}\left(\hat{\beta}_r(k,d)\right)$ where

$$\begin{aligned}\Delta_3 &= TS(k)^{-1}S(d)\,\Lambda^{-1}S(d)\,S(k)^{-1}T' \\ &\quad - T_r S_r(k)^{-1}\Lambda_r^{-1}S_r(d)\,\Lambda_r\,S_r(d)\,\Lambda_r^{-1}S_r(k)^{-1}T_r' \\ &\quad + (k+d)^2\,TS(k)^{-1}T'\beta\beta'TS(k) \\ &\quad - \left(-T_{p-r}T_{p-r}' - (d+k)\,T_r S_r(k)^{-1}T_r'\right)\beta \\ &\quad \times \beta'\left(-T_{p-r}T_{p-r}' - (d+k)\,T_r S_r(k)^{-1}T_r'\right).\end{aligned}$$

Suppose that $C = T_{p-r} D T'_{p-r}$, where

$$D = S_{p-r}(k)^{-1} S_{p-r}(d)\, \Lambda_{p-r}^{-1} S_{p-r}(d)\, S_{p-r}(k)^{-1}$$

and $a_3 = (d+k)\, TS(k)^{-1} T'\beta$, $a_2 = \left(-T_{p-r} T'_{p-r} - (d+k)\, T_r S_r(k)^{-1} T'_r\right)\beta$. We can apply part (b) of Lemma 3.2. The Moore–Penrose inverse of C is $C^+ = T_{p-r} D^{-1} T'_{p-r}$, and $CC^+ = T_{p-r} T'_{p-r}$. So $a_3 \notin R(C)$, $a_2 \in R(C : a_3)$, $s = 1$ and $a_2 - a_3 = C\eta_1$, where

$$\eta_1 = -T_{p-r} S_{p-r}(k)^{-1} S_{p-r}(d)\, \Lambda_{p-r}^{-1} T'_{p-r} \beta\,.$$

Then by Lemma 3.2, we obtain that the new estimator is superior to the Liu-type logistic estimator under the asymptotic mean squared error matrix criterion if and only if $(a_2 - a_3)\, C^-(a_2 - a_3) \le 0$ or $\eta_1' C \eta_1 \le 0$. In fact, $(a_2 - a_3)\, C^-(a_2 - a_3) \ge 0$, so the new estimator is better than the Liu-type logistic estimator under the asymptotic mean squared error matrix criterion if and only if $\eta_1' C \eta_1 = 0$, that is $\beta' T_{p-r} \Lambda_{p-r} T'_{p-r} \beta = 0$. □

4. A MONTE CARLO SIMULATION STUDY

In this simulation study, we study the logistic regression model. In this section, we present the details and the results of the Monte Carlo simulation which is conducted to evaluate the performances of the MLE, PCLR, LTL and PCLTL estimators. There are several papers studying the performance of different estimators in the binary logistic regression. Therefore, we follow the idea of Lee and Silvapulle ([11]), Månsson *et al.* ([15]), Asar ([3]) and Asar and Genç ([4]) generating explanatory variables as follows:

$$x_{ij} = \left(1 - \rho^2\right)^{1/2} z_{ij} + \rho\, z_{iq}\,, \tag{4.1}$$

where $i = 1, 2, ..., n$, $j = 1, 2, ..., q$ and z_{ij}'s are random numbers generated from standard normal distribution. Effective factors in designing the experiment are the number of explanatory variables q, the degree of the correlation among the independent variables ρ^2 and the sample size n.

Four different values of the correlation ρ corresponding to 0.8, 0.9, 0.99 and 0.999 are considered. Moreover, four different values of the number of explanatory variables consisting of $q = 6$, 8 and 12 are considered in the design of the experiment. The sample size varies as 50, 100, 200, 500 and 1000. Moreover, we choose the number of principal components using the method of percentage of the total variability which is defined as

$$\text{PTV} = \frac{\sum_{j=1}^{r} \lambda_j}{\sum_{j=1}^{p} \lambda_j} \times 100\,.$$

In the simulation, PTV is chosen as 0.75 for $q = 8$ and 12 and 0.83 for $q = 6$ (see Aguilera *et al.* ([1])).

The coefficient vector is chosen due to Newhouse and Oman ([16]) such that $\beta'\beta = 1$ which is a commonly used restriction, for example see Kibria ([10]). We generate the n observations of the dependent variable using the Bernoulli distribution $\text{Be}(\pi_i)$ where $\pi_i = \frac{e^{x_i\beta}}{1+e^{x_i\beta}}$ such that x_i is the i-th row of the data matrix X.

The simulation is repeated for 10 000 times. To compute the simulated MSEs of the estimators, the following equation is used respectively:

$$\mathrm{MSE}\big(\tilde{\beta}\big) = \frac{\sum_{c=1}^{10000}\big(\tilde{\beta}_c - \beta\big)'\big(\tilde{\beta}_c - \beta\big)}{10000}, \tag{4.2}$$

where $\widetilde{\beta}_c$ is MLE, PCLR, LTL, and PCLTL in the c-th replication. The convergence tolerance is taken to be 10^{-6} in the IRLS algorithm.

We choose the biasing parameter as follows:

1. LTL: We refer to Asar ([3]) and choose $d_{\mathrm{LTL}} = \frac{1}{2}\min\left\{\frac{\lambda_j}{\lambda_j+1}\right\}_{j=1}^{p}$ where min is the minimum function and $k_{\mathrm{AM}} = \frac{1}{p}\sum_{j=1}^{p}\frac{\lambda_j - d\big(1+\lambda_j\hat{\alpha}_j^2\big)}{\lambda_j\hat{\alpha}_j^2}$.

2. PCLTL: We propose to use the modifications of the methods given above as follows:

$$d_{\mathrm{PCLTL}} = \frac{1}{2}\min\left\{\frac{\lambda_j}{\lambda_j+1}\right\}_{j=1}^{r}$$

and

$$k_{\mathrm{PCLTL}} = \frac{1}{r}\sum_{j=1}^{r}\frac{\lambda_j - d_{\mathrm{PCLTL}}\big(1+\lambda_j\,\hat{\alpha}_j^2\big)}{\lambda_j\,\hat{\alpha}_j^2}.$$

Table 1: Simulated MSE values of the estimators when $q = 6$.

n	Estimator	ρ			
		0.8	0.9	0.99	0.999
50	MLE	0.9942	0.8060	4.8571	41.7598
	LTL	0.8645	0.7561	2.2694	14.5135
	PCLR	0.9441	0.7780	1.9253	10.1568
	PCLTL	**0.8619**	**0.7480**	**0.9481**	**2.2783**
100	MLE	0.7050	0.7478	4.1961	38.1615
	LTL	0.7328	0.7613	2.6520	15.3411
	PCLR	**0.6913**	**0.7342**	1.6385	14.3406
	PCLTL	0.7169	0.7460	**1.0849**	**2.5414**
200	MLE	0.7286	0.8308	1.2978	5.8428
	LTL	0.7784	**0.7862**	**0.8506**	**1.6886**
	PCLR	**0.7221**	0.8223	1.1428	4.2635
	PCLTL	0.7668	0.7879	0.8571	1.7816
500	MLE	0.7428	0.7620	1.3640	4.0893
	LTL	0.8043	0.7665	1.0366	1.7055
	PCLR	**0.7417**	**0.7551**	0.9309	2.3118
	PCLTL	0.7895	0.7595	**0.8193**	**1.2168**
1000	MLE	0.7325	0.7512	0.9295	1.3950
	LTL	0.7550	0.7930	0.8030	0.8265
	PCLR	**0.7317**	**0.7463**	0.8421	1.1389
	PCLTL	0.7449	0.7878	**0.7766**	**0.8130**

Table 2: Simulated MSE values of the estimators when $q = 8$.

n	Estimator	ρ			
		0.8	0.9	0.99	0.999
50	MLE	0.9148	1.2089	3.8258	54.7686
	LTL	0.8065	0.9414	1.2265	16.7926
	PCLR	0.7669	0.8948	2.3655	12.4373
	PCLTL	**0.7237**	**0.8477**	**1.1400**	**3.2686**
100	MLE	0.7917	0.8182	2.2287	35.6674
	LTL	0.8264	0.7728	1.0472	14.5687
	PCLR	**0.7512**	0.7857	1.5575	17.9893
	PCLTL	0.8204	**0.7573**	**1.0189**	**9.3816**
200	MLE	0.7891	0.8598	1.7860	17.1105
	LTL	0.8293	0.8094	1.0451	6.3030
	PCLR	**0.7710**	0.7962	1.3309	7.4095
	PCLTL	0.8150	**0.7893**	**0.9678**	**3.2204**
500	MLE	0.7359	0.8031	1.2199	3.9098
	LTL	0.7612	0.8043	0.9003	1.4233
	PCLR	**0.7244**	**0.7608**	1.0378	2.4107
	PCLTL	0.7511	0.7959	**0.8712**	**1.2120**
1000	MLE	0.7502	0.7889	0.8576	5.0227
	LTL	0.7873	0.7933	0.7935	2.6289
	PCLR	**0.7462**	0.7516	0.8086	1.8239
	PCLTL	0.7781	**0.7800**	**0.7861**	**1.1132**

Table 3: Simulated MSE values of the estimators when $q = 12$.

n	Estimator	ρ			
		0.8	0.9	0.99	0.999
50	MLE	1.1407	1.2743	11.0452	81.6076
	LTL	0.8948	0.9622	3.4314	15.0524
	PCLR	0.8437	0.9409	3.7290	12.2146
	PCLTL	**0.8157**	**0.8961**	**1.8368**	**2.0556**
100	MLE	0.9247	1.4041	4.8286	22.7269
	LTL	0.8618	1.0687	2.0033	3.4810
	PCLR	**0.7999**	**0.8438**	1.3798	10.3112
	PCLTL	0.8152	0.8585	**0.8643**	**2.7653**
200	MLE	0.8238	1.0956	1.9228	15.8403
	LTL	0.8111	0.9612	0.9866	4.2617
	PCLR	0.7959	**0.8369**	1.4330	5.6484
	PCLTL	**0.7940**	0.8518	**0.9760**	**1.9115**
500	MLE	0.8009	0.8173	3.3133	11.2533
	LTL	0.8387	0.8357	2.3419	4.4671
	PCLR	**0.7809**	**0.8042**	1.0087	6.5955
	PCLTL	0.8331	0.8150	**0.8581**	**3.7834**
1000	MLE	0.7798	0.8081	1.0899	4.4119
	LTL	0.8205	0.8286	**0.8784**	1.7929
	PCLR	**0.7733**	**0.7965**	1.0258	1.7815
	PCLTL	0.8089	0.8212	0.9056	**1.0085**

According to Tables 1–3, the following results are obtained:

1. MSE of the MLE is inflated when the degree of correlation is increased and the sample size is low. On the other hand, the performance of MLE becomes quite well when the sample size is high enough.
2. Similarly, if we consider PCLR and LTL, the MSE values are also inflated for increasing values of the degree of correlation especially when $n = 50$.
3. MLE, PCLR and LTL produce high MSE values when the sample size is low and the degree of correlation is high. However, PCLTL seems to be robust to this situation in most of the cases.
4. Increasing the sample size makes a positive effect on the estimators in most of the situations. However, there is a degeneracy in this property.
5. When the degree of correlation is low, there is no estimator beating all others.
6. Overall, the new estimator PCLTL has the lowest MSE value in most of the situations considered in the simulation.

5. CONCLUSION

In this paper, we develop a new principal component Liu-type logistic estimator as a combination of the principal component logistic regression estimator and Liu-type logistic estimator to overcome the multicollinearity problem. We have proved some theorems showing the superiority of the new estimator over the other estimators by studying their asymptotic mean squared error matrix criterion. Finally, a Monte Carlo simulation study is presented in order to show the performance of the new estimator. According to the results, it seems that PCLTL is a better alternative in multicollinear situations in the binary logistic regression model.

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ON KERNEL HAZARD RATE FUNCTION ESTIMATE FOR ASSOCIATED AND LEFT TRUNCATED DATA

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Abstract:

- Let $\{X_N,\, N \geq 1\}$ be a sequence of strictly stationary associated random variables of interest, and $\{T_N,\, N \geq 1\}$ be a sequence of random truncating variables assumed to be independent from $\{X_N,\, N \geq 1\}$. In this paper, we establish the strong uniform consistency with a rate of a kernel hazard rate function estimator, when the variable of interest is subject to random left truncation under association condition. Simulation results are also provided to evaluate the finite-sample performances of the proposed estimator.

Key-Words:

- *associated data; hazard rate function; Lynden-Bell estimator; random left truncation; strong uniform consistency rate.*

AMS Subject Classification:

- 62G05, 62G07, 62G20.

1. INTRODUCTION AND MOTIVATION

First of all, let us recall that a set of random variables (rv's) $(X_1, X_2, ..., X_N)$ is said to be associated if for every pair of functions $g_1(\cdot)$ and $g_2(\cdot)$ from $\mathbb{R}^N$ to $\mathbb{R}$, which are non decreasing component-wise, $\mathrm{cov}(g_1(\mathbf{X}), g_2(\mathbf{X})) \geq 0$, whenever the covariance is defined, where $\mathbf{X} = (X_1, X_2, ..., X_N)$. An infinite sequence $\{X_N,\, N \geq 1\}$ of rv's is said to be associated if every finite subset is associated. This definition was introduced by Esary *et al.* ([9]), mainly for the sake of applications. For instance, association occurs often in certain reliability theory problems, as well as in some important models employed in statistical mechanics. It is of interest to note that association and mixing define two distinct but not disjoint classes of processes (see, e.g. Doukhan and Louhichi ([7]), for examples of sequences that are associated but not mixing, associated and mixing, and mixing but not associated ones).

Let us now recall that a strong mixing condition refers more to σ-algebra than to rv's. On the one hand, a main inconvenience of mixing conditions is the difficulty of checking them. On the other hand, an important property of associated random rv's is that zero correlation implies independence. Also, large classes of examples of associated processes are deduced from the fact that any independent sequence is associated and that monotonic functions of independent sequences remain associated. So, the main advantage of the concept of association compared to mixing is that the conditions of limit theorems are easier to verify since, a covariance is much easier to compute than a mixing coefficient.

As examples of associated rv's, we recall that most often in reliability studies, the rv's which are generally lifetimes of components, are not independent but are associated. In fact, as an example, there are structures in which the components share the load so that failure of one component results in increased load on each of the remaining components. Thus, failure of one component will adversely effect the performance of all the minimal path structures containing it. In such a model, the random variables of interest are not independent but are associated. In addition, let $\{X_i,\, i \geq 1\}$ be independent and identically distributed (iid) rv's and Y be independent of $\{X_i,\, i \geq 1\}$. Then $\{Z_i = X_i + Y,\, i \geq 1\}$ are associated. Thus, if independent components of a system are subject to the same stress, then their lifetimes are associated. A variety of relevant examples and ample bibliographical references can be found in (Bulinski and Shashkin ([3])). In that book, the reader can find a number of new results and examples related to associated random sequences and random fields. For completeness on the subject in the complete data case we refer the reader to the monographs by Oliveira ([17]) and Prakasa Rao ([20]).

Survival analysis is the part of statistics, in which the variable of interest (lifetime) may often be interpreted as the time elapsed between two events and then, one may not be able to observe completely the variable under study. Such variables typically appear in a medical or an engineering life test studies. Among the different forms in which incomplete data appear, censoring and truncation are two common ones.

Left truncation in studies of developmental processes is not just of theoretical interest: It can cause substantial bias if ignored. An important example of such a model arises in the analysis of survival data of patients infected by the AIDS virus from contaminated blood transfusions (Chen *et al.* ([6])). Other examples in which a large fraction of potential observations are left truncated are rate of spontaneous abortion (Meister and Schaefer ([16])) and age at menopause transition stages (Harlow *et al.* ([12])).

Let $\{X_N,\, N \geq 1\}$ be a sequence of strictly stationary associated rv's of interest defined on a probability space $(\Omega, \mathscr{F}, \mathbb{P})$ with an unknown probability density function (pdf) $f = dF$. Let $\{T_N,\, N \geq 1\}$ be a sequence of stationary associated rv's of truncation with an unknown Lipschitz distribution function (df) G. In this paper we follow the same sampling scheme as that of (Woodroofe ([25])) whose observable sample of size n is a subset of N pairs $\{(X_1, T_1), ..., (X_N, Y_N)\}$, where N is deterministic but unknown while n is random. As it was pointed out by the reviewer, one may consider another approach in which the sample size n is a non-random known value, and the observations are drawn from an infinite sequence of random vectors. In fact, such an approach was used by (He and Yang ([14])). However, our main motivation in following the first approach is computational since, in our simulation studies we use the ratio $\frac{n}{N}$ to estimate different values of the parameter α.

Under random left truncation scheme, only those pairs (X_i, T_i) satisfying $X_i \geq T_i$ are observed. In the sequel we assume that $\{X_N,\, N \geq 1\}$ is independent from $\{T_N,\, N \geq 1\}$ and $(X_1, T_1), ..., (X_n, T_n)$ denotes the sequence which one actually observes within a sample (X_i, T_i); $1 \leq i \leq N$. Obviously the observed sequence remains associated since any subset of associated rv's are associated (see Esary *et al.* ([9]), Property $\mathscr{P}_1$)). As a consequence of truncation, the sample size $n = \sum_{i=1}^{N} 1_{\{X_i \geq T_i\}}$ is random, and from the strong law of large numbers, $n/N \to \alpha := \mathbb{P}(X_i \geq T_i)$, almost surely (a.s.), as $N \to \infty$. Without further mention, we shall assume that $\alpha > 0$ because, otherwise, no data will be available.

Throughout this study, all probability statements are to be interpreted as conditional probability statements, that is $\mathbf{P}(\cdot) = \mathbb{P}(\cdot \,|\, X \geq T)$. Likewise $\mathbf{E}$ and $\mathbb{E}$ will denote the expectation operators related to $\mathbf{P}$ and $\mathbb{P}$, respectively. Then conditionally on n, estimation results are stated considering $n \to \infty$ which hold true with respect to the probability $\mathbb{P}$ since $n \leq N$.

In what follows, the star notation (*) relates to any characteristic of the actually observed data (conditionally on n). So, following Stute ([21]), the df's of X and T become

$$F^\star(x) := \alpha^{-1} \int_{-\infty}^{x} G(z)\, dF(z) \qquad \text{and} \qquad G^\star(x) := \alpha^{-1} \int_{-\infty}^{\infty} G(x \wedge z)\, dF(z)\,,$$

where $t \wedge z := \min(x, z)$. Then, for any df W, let us define $a_W = \inf\{u \colon W(u) > 0\}$ and $b_W = \sup\{u \colon W(u) < 1\}$, as the endpoints of the W support. As pointed out in Woodroofe ([25]), the df's F and G can be completely estimated only if $a_G \leq a_F$, $b_G \leq b_F$ and $\int_{a_F}^{\infty} (G)^{-1} dF < \infty$.

Let $C(\cdot)$ be a function defined by

$$\begin{aligned} C(x) &:= \mathbf{P}\big(T \leq x \leq X\big) \\ &= G^\star(x) - F^\star(x) \\ &= \alpha^{-1} G(x) \big[1 - F(x)\big]\,, \qquad a_G < x < b_F\,. \end{aligned} \tag{1.1}$$

It is easily seen that $F^\star$, $G^\star$ and C are readily estimable through

$$F_n^\star(x) = n^{-1} \sum_{i=1}^{n} 1_{\{X_i \leq x\}}\,, \quad G_n^\star(t) = n^{-1} \sum_{i=1}^{n} 1_{\{T_i \leq t\}} \quad \text{and} \quad C_n(x) = G_n^\star(x) - F_n^\star(x)\,.$$

The well-known estimates of F and G proposed by Lynden-Bell ([15]) are

$$F_n(x) = 1 - \prod_{X_i \leq x} \left[\frac{n\, C_n(X_i) - 1}{n\, C_n(X_i)}\right] \quad \text{and} \quad G_n(t) = \prod_{T_i > t} \left[\frac{n\, C_n(T_i) - 1}{n\, C_n(T_i)}\right], \tag{1.2}$$

respectively, assuming no ties among the rv's. Note that Stute and Wang ([22]) showed how to break ties without destroying the product limit structure. Therefore, throughout we shall assume without loss of generality that there are no ties.

For technical reasons, we need to introduce a pseudo-kernel estimate of f, which will be of a great importance later, defined by

$$\tilde{f}_n(x) := \frac{\alpha}{nh_n} \sum_{i=1}^{n} \frac{1}{G(X_i)} K\left(\frac{x - X_i}{h_n}\right), \tag{1.3}$$

where K is a smooth probability kernel and $h_n =: h$ is a sequence of bandwidths tending to 0 at appropriate rates. For an interesting overview of nonparametric curve estimation, we refer the reader to Cao *et al.* ([5]) and the references therein.

Note that in a real data situation or in simulation studies we shall, however, not dwell on (1.3) since G is unknown. And, as the original sample size N is unknown (although deterministic), the classical estimator $\hat{\alpha}_n = n/N$ for the rate of no truncation α cannot be used, and then, another estimator derived from (1.1) is required, namely

$$\alpha_n := \frac{G_n(x)\left[1 - F_n(x)\right]}{C_n(x)},$$

for any x such that $C_n(x) > 0$. This estimator was proposed and studied in the iid case in (He and Yang ([13]) Theorem 2.2, p. 1014). These authors proved that α_n does not depend upon the argument x and its value can then be obtained for any x such that $C_n(x) \neq 0$. Furthermore, they showed (Corollary 2.5) that $\alpha_n \to \alpha$, a.s., as $n \to \infty$. Then, by plug-in method we can construct a feasible kernel estimate of f. Thus

$$\hat{f}_n(x) := \frac{\alpha_n}{nh} \sum_{i=1}^{n} \frac{1}{G_n(X_i)} K\left(\frac{x - X_i}{h}\right). \tag{1.4}$$

From now on, the sum in the latter formula is taken over the i's such that $G_n(X_i) \neq 0$. Recall that asymptotic results for (1.4), in both iid and strong mixing condition cases have been stated in (Ould Saïd and Tatachak ([18], [19]), Benrabah *et al.* ([2])).

It is well known that the cumulative hazard function $\Lambda(y) = -\log(1-F(x))$, for any x such that $F(x) < 1$, and its corresponding hazard rate function $\lambda(x) := \Lambda'(x) = f(x)/(1-F(x))$, are important in several fields of applied statistics (medicine, reliability, ...) for the assessment of risks in survival studies. Recall that the nonparametric hazard rate estimation was introduced in statistical literature by Watson and Leadbetter ([24]). Now, using (1.2) and (1.4), an estimate for $\lambda(x)$ for an n-sample, at risk of being truncated from the left, is defined by

$$\hat{\lambda}_n(x) = \frac{\hat{f}_n(x)}{1 - F_n(x)}. \tag{1.5}$$

As far as we know, in truncation and dependence setting, the only existing result dealing with hazard rate estimation is that of Sun and Zhou ([23]) stated under strong mixing condition, while in the complete associated data case (no truncation), Bagai and Prakasa Rao ([1]) stated strong uniform consistencies (with no rates) for kernel-type density and failure rate estimates. Hence, in this paper, we intend to extend the existing results to truncated and associated data.

The paper is organized as follows: In Section 2, an asymptotic analysis is presented together with the list of the assumptions under which the main results are stated. To support the main results, a simulation study illustrates the behaviour of the estimators as shown in Section 3. Proofs and some auxiliary results with their proofs are relegated to Section 4.

2. ASYMPTOTIC ANALYSIS

In the sequel, $\mathscr{D} := [a, b]$ such that $a_G \leq a_F < a < b < b_F$ will denote a compact set and the letter c is used indiscriminately as a generic positive constant. To state our asymptotic analysis, the following conditions are assumed:

A1. $\displaystyle\int \frac{dF(z)}{G^2(z)} < +\infty\,;$

A2. The covariance term satisfies: $\rho(s) := \sup_{j:|\ell-j|\geq s} \operatorname{cov}(X_j, X_\ell)$ for all $\ell \geq 1$ and $s > 0$, where $\rho(s) \leq \gamma_0\, e^{-\gamma s}$ for some positive constants γ_0 and $\gamma\,;$

A3. K is a Lipschitz continuous pdf, compactly supported and $\displaystyle\int u\, K(u)\, du = 0\,;$

A4. f is twice continuously differentiable on $\mathscr{D}$ such that $\displaystyle\sup_{x\in\mathscr{D}} \left|f^{(2)}(x)\right| < +\infty\,;$

A5. The joint pdf $f^{\star}_{1,j}(\cdot,\cdot)$ of (X_1, X_{1+j}) satisfies: $\displaystyle\sup_{j>1}\sup_{u,v\in\mathscr{D}} \left|f^{\star}_{1,j}(u,v)\right| \leq c\,;$

A6. h satisfies: $h \to 0$ and $nh^{1+\delta} \to +\infty$ along with n, for any $0 < \delta < 1$.

Remark 2.1. Assumptions A1–A2 satisfy conditions H1–H3 in (Guessoum *et al.* ([11])). Furthermore, Assumption A1 was used in (Stute ([21])) and Assumption A2 quantifies a progressive tendency to asymptotic independence of "past" and "future". This latter condition was used in (Doukhan and Neumann ([8])) in order to state an exponential inequality which is needed to prove Proposition 2.1 hereinafter. Assumptions A3–A4 are frequently used in studying uniform consistency of estimates. Assumption A5 is often assumed in kernel estimation studies under dependence structure and allows to bound the covariance term. Finally, Assumption A6 is standard in nonparametric density estimation.

Proposition 2.1. *Under assumptions A1–A6, for large enough n we have*

$$\sup_{x\in\mathscr{D}} \left|\tilde{f}_n(x) - \mathbf{E}\big(\tilde{f}_n(x)\big)\right| = O\left(\sqrt{\frac{\log n}{nh}}\right) \quad a.s.$$

Theorem 2.1. *If assumptions A1–A6 hold true, then for large enough n we have*

$$\sup_{x\in\mathscr{D}} \left|\hat{f}_n(x) - f(x)\right| = O\left\{\sqrt{\frac{\log n}{nh}} + \left(\frac{\log\log n}{n}\right)^{\theta} + h^2\right\} \quad a.s.\,,$$

where $0 < \theta < \gamma/(2\gamma+\beta+9)$ for any real $\beta > 0$ and γ is that in A2.

Theorem 2.2. *Under assumptions A1–A6, for large enough n we have*

$$\sup_{x\in\mathscr{D}} \left|\hat{\lambda}_n(x) - \lambda(x)\right| = O\left\{\sqrt{\frac{\log n}{nh}} + \left(\frac{\log\log n}{n}\right)^{\theta} + h^2\right\} \quad a.s.$$

Remark 2.2. The rates in Theorem 2.1 and Theorem 2.2 are still slower than those stated for complete data in the iid and mixing cases (see Estévez and Quintela ([10])), or under left truncation model (see Ould Saïd and Tatachak ([18], [19]), Sun and Zhou ([23])). Our rates depend upon the parameter θ which controls the covariance's decaying under association dependence as stated in (Cai and Roussas ([4])), whereas the iterated logarithm form is related to the truncation effect. Note that by setting $\gamma = 3(r-2)/2$, $r > 2$, we recognize the θ appearing in (Guessoum *et al.* ([11]), Theorem 3.1). Finally, we point out that for γ large enough, our rates approach the classical optimal ones as θ grows to its upper bound ($\theta = 1/2$).

3. SOME SIMULATION RESULTS

To examine the behaviour over finite samples of the estimators given in statements (1.4) and (1.5), respectively, we have conducted a numerical study via simulation. The log-normal distribution has been selected because of the shape of its hazard function which is flatter around of its maximum. In the computation of the estimators, we used the bi-weight kernel $\big(K(x) = \big(1-|x|^2\big)^2 1_{|x|\leq 1}\big)$ which verifies our conditions in stating our main results. We also used optimal global and local bandwidths, that minimized the global mean square error (GMSE) and the simple mean square error (MSE) criteria, respectively. These bandwidths were selected in the grid of values $\mathscr{H} = \big\{h_k = 10^{-1} + 5(k-1)10^{-2},\ k = 1, 2, ..., 19\big\}$.

3.1. Models and procedure

- *Step 1.* The sequence $\big\{(X_k, T_k),\ k = 1, ..., n\big\}$ is generated as follows:
  For $i = 1, 2, ..., N$, we first generate $Z_i = (W_{i-1} + W_{i-2}/2)$, where $\{W_r,\ r = -1, 0, ..., N-1\}$ are iid rv's drawn from $\mathscr{N}(0,1)$ and put $X_i = \exp(Z_i)$, $i = 1, ..., N$. Hence, the sequence $\{X_k,\ k = 1, 2, ..., N\}$ is associated and follows a $\log\big(\mathscr{N}\big(0, \sqrt{1/2}\,\big)\big)$ distribution. At each iteration the X_i's are compared to the T_i's generated from $\exp(\mu)$ in order to keep only the pairs (X_i, T_i) satisfying $X_i \geq T_i$. The parameter μ is adjusted to get $\mathbb{P}(X \geq T) \approx \alpha$. Hence, a truncation sequence $\big\{(X_i, T_i),\ i = 1, ..., n\big\}$ is generated and the estimator $\lambda_n(\cdot)$ is computed using the bi-weight kernel and bandwidths $h \in \mathscr{H}$.

- *Step 2.* We repeat B simulation runs as described in *Step 1* for every fixed combination of size n and truncating rate (TR) $1-\alpha$.
  For a given functional g and its estimate $\hat{g}_{n,h}$, the GMSE computed along $B = 200$ Monte Carlo trials and a grid of bandwidths $h \in \mathscr{H}$ is defined as

$$\mathrm{GMSE}(h) = \frac{1}{Bm} \sum_{k=1}^{B} \sum_{\ell=1}^{m} \big(\hat{g}_{n,h,k}(x_\ell) - g(x_\ell)\big)^2,$$

  where m is a number of equidistant points x_ℓ belonging to the range $]0, 4]$ and $\hat{g}_{n,h,k}(x_\ell)$ is the value of $\hat{g}_{n,h}(x_\ell)$ computed at iteration k. In computing the GMSE's, optimal global bandwidths (ogb) were used for both density and hazard rate function estimation. The values $\mathrm{GMSE} := \min_{h\in\mathscr{H}} \mathrm{GMSE}(h)$ and the corresponding global bandwidths $h_{\mathrm{opt}} := \arg\min_{h\in\mathscr{H}} \mathrm{GMSE}(h)$ are reported in Table 1 and Table 2.

The MSE's reported in Table 3 were evaluated by using optimal local bandwidths (olb) for hazard rate estimation. Furthermore, to display the quality of fit of the estimators, we first plotted the target density f together with its average and median estimates as illustrated in Figure 1 and Figure 2. Then, we plotted the target hazard rate λ with its average and median estimates for both global optimal bandwidths and local optimal ones as shown in Figure 3, Figure 4 and Figure 5.

Table 1: Density function with optimal global bandwidths.

$1-\alpha$ (TR)	n					
	50		100		200	
	h_{opt}	GMSE	h_{opt}	GMSE	h_{opt}	GMSE
0.05	0.575	0.0073	0.475	0.0048	0.375	0.0029
0.15	0.600	0.0090	0.475	0.0079	0.400	0.0073
0.25	0.575	0.0155	0.475	0.0122	0.400	0.0096

Table 2: Hazard rate function with optimal global bandwidths.

TR	n					
	50		100		200	
	h_{opt}	GMSE	h_{opt}	GMSE	h_{opt}	GMSE
0.05	0.825	0.2052	0.675	0.1404	0.600	0.0743
0.15	0.800	0.2574	0.725	0.1732	0.640	0.0908
0.25	0.750	0.2676	0.750	0.1800	0.650	0.1145

Table 3: Hazard rate function with optimal local bandwidths.

TR	n		
	30	50	100
	MSE	MSE	MSE
0.05	0.2247	0.1949	0.1286
0.15	0.2632	0.2104	0.1500
0.25	0.3384	0.2848	0.1848

3.2. Comments on the simulation results

As it can be seen from the tables and figures, the higher the sample size and smaller the TR, the better the quality of fit. This means that the errors tend to be negligible in each case when n increases. Likewise, the quality of fit deteriorates slightly for sufficiently high TR value but, it increases along with n and becomes better in any cases. Note also that, in particular, the estimation of the hazard rate function suffers from the well-known boundary effects that occur in nonparametric functional estimation. If the target functional has a support on $[0, \infty)$, the use of classical estimation methods with symmetric kernels yield a large bias on the zero boundary and leads to a bad quality of the estimates. This is the case here and is due to the fact that symmetric kernel estimators assign non-zero weight at the interval $(-\infty, 0]$.

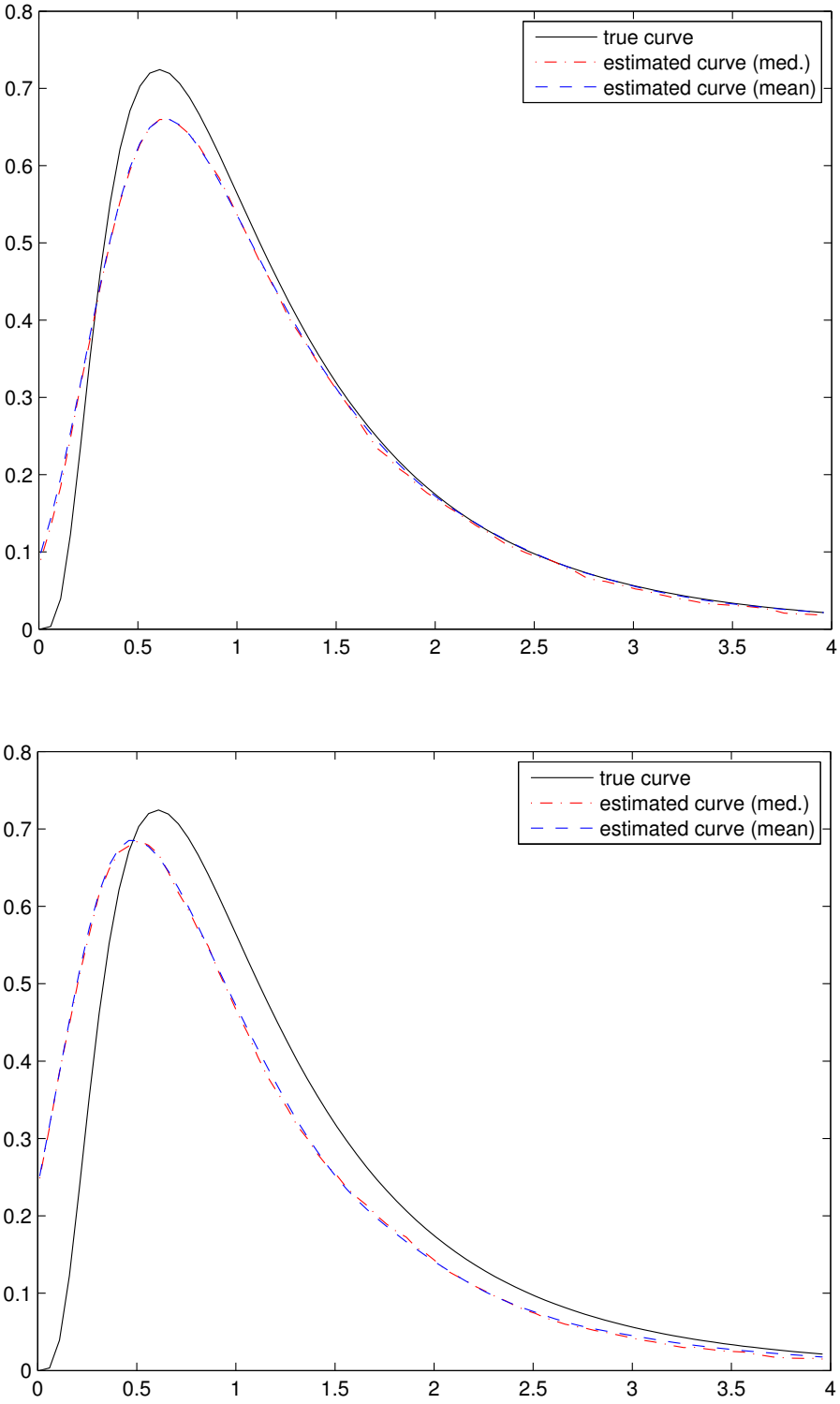

Figure 1: Density estimation (ogb): $n = 100$ and TR $\approx 0.05, 0.25$.

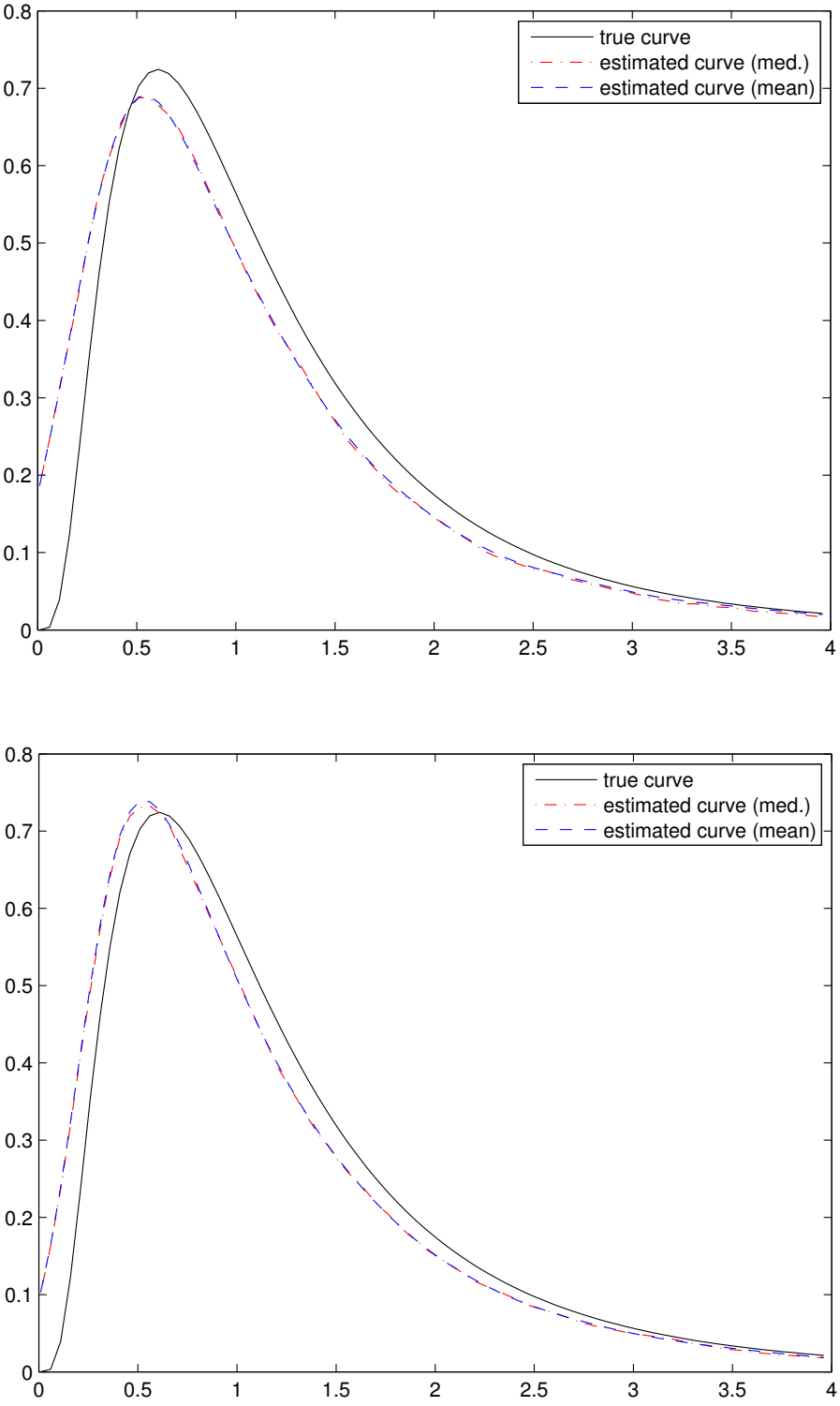

Figure 2: Density estimation (ogb): $n = 100, 500$ and TR ≈ 0.15.

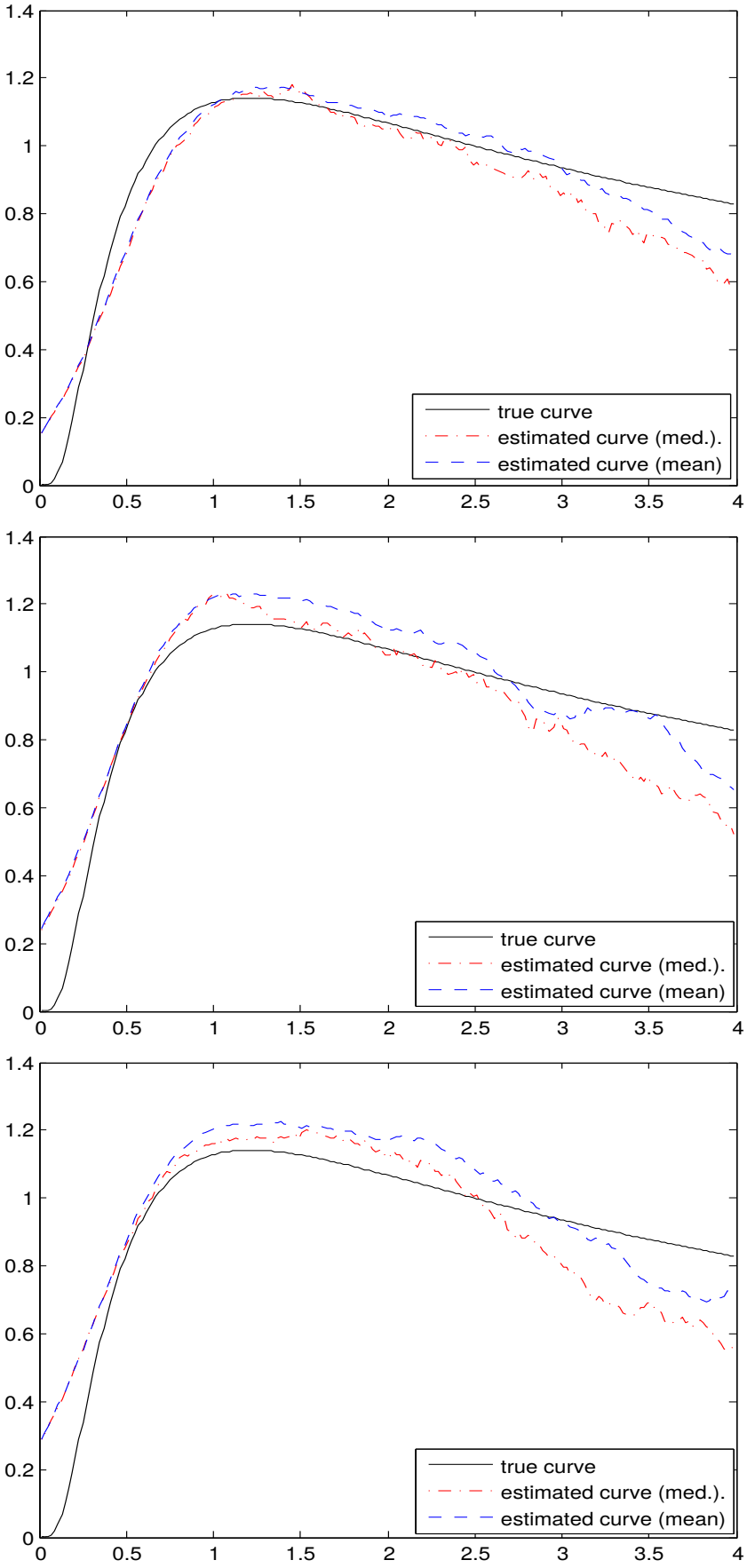

Figure 3: Hazard rate (ogb): $n = 100$ and TR $\approx 0.05, 0.15, 0.25$.

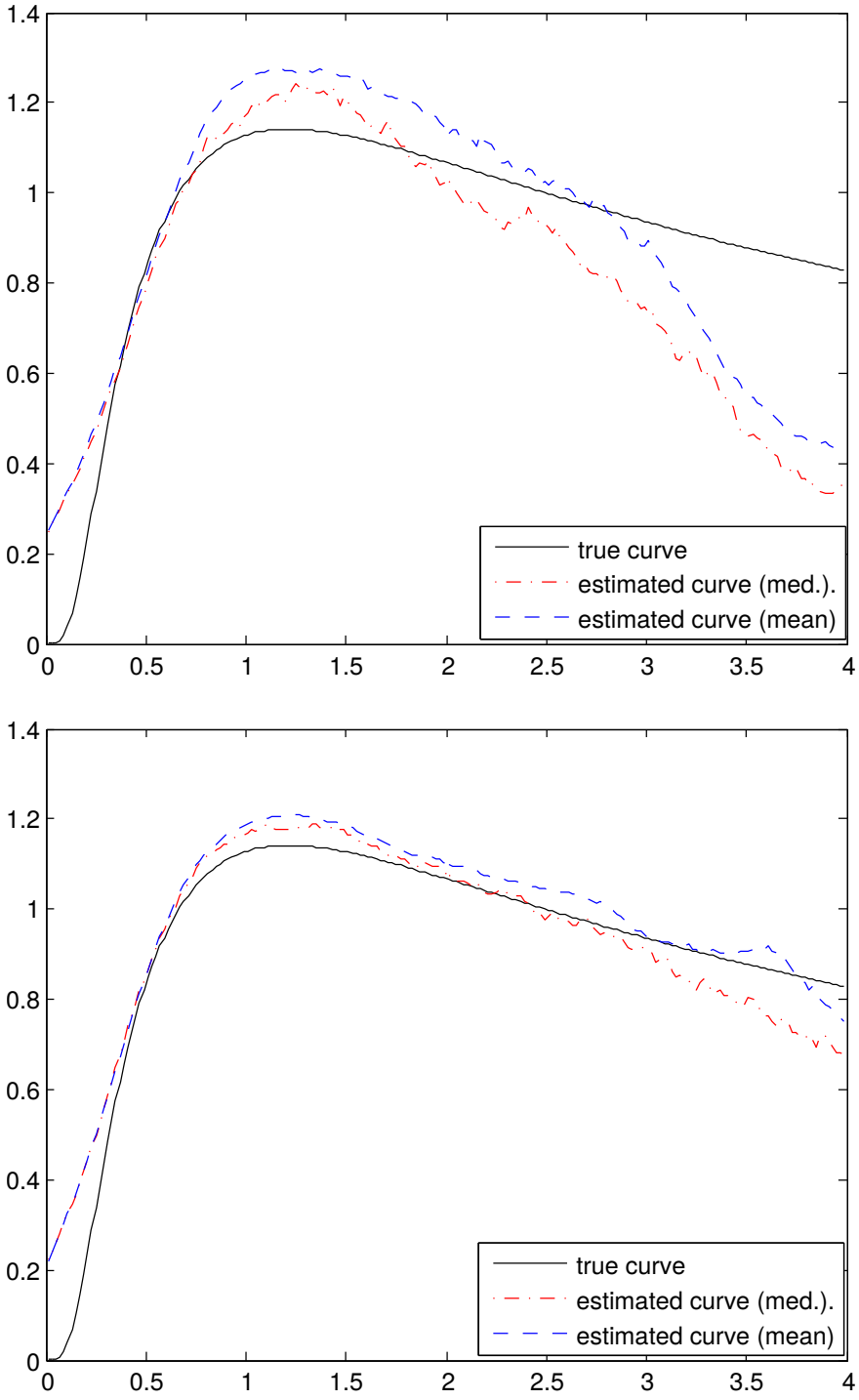

Figure 4: Hazard rate (ogb): TR ≈ 0.15 and $n = 50, 200$.

The graphs reveal this phenomenon when using optimal global bandwidths but, the bias effect is subsequently reduced and tends to disappear when optimal local bandwidths are used as shown in Figure 5. We point out that one may also select another approach to deal with the boundary bias effect which consists in using an asymmetric kernel as the Gamma kernel since it is non-negative and changes its shape depending on the position on the semi-axis. The inverse Gaussian kernel is also an interesting alternative.

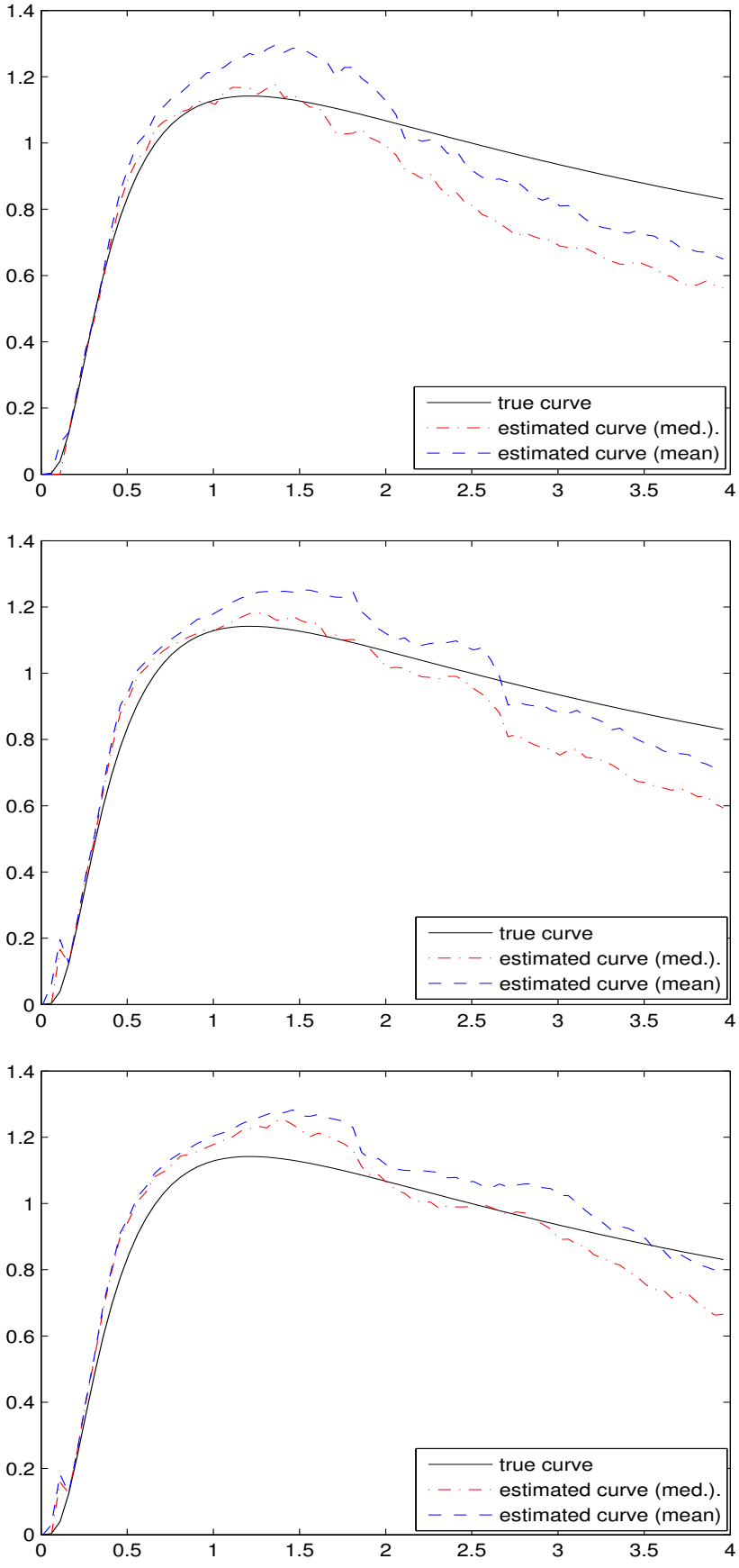

Figure 5: Hazard rate (olb): TR ≈ 0.15 and $n = 30, 50, 100$.

4. AUXILIARY RESULTS AND PROOFS

Before proving the main results, we briefly discuss the tools used here.

Remark 4.1. As it was mentioned above, there are processes which are associated but not mixing. In such cases, it would be interesting to have at disposal similar results as stated here.

It is noteworthy that for the proof of our results we use similar tools used in the α-mixing frameworks. The main difference here is that functional of associated rv's are not associated in general, which is the case when dealing with nonparametric kernel estimation. This is due to the fact that the random functions $K\big(\frac{x-X_i}{h}\big)$ are, in general not associated but remain α-mixing if the X_i's are, since K is a measurable function in general. To keep the association, we should apply only monotone transformations to the original variables, which is not the case with a general kernel. To overcome this problem, one may assume that the kernel K is of bounded variation. This condition permits to write $K = K_1 - K_2$, with K_1 and K_2 monotone functions. In this paper, we do not follow this procedure but we use results stated for weakly dependent models in the sense of Doukhan and Louhichi ([7]), since associated models are κ-weakly dependent. Note also that to treat the fluctuation part in Proposition 2.1, we use bounds for covariances in applying an exponential inequality stated by Doukhan and Neumann ([8]) for weakly dependent rv's. To this end, we use Theorem 5.3 in (Bulinski and Shashkin ([3])), and Proposition 8 in (Doukhan and Neumann ([8])).

Indeed, for any $x \in \mathscr{D}$, set $U_i(x,h) := \frac{\alpha}{G(X_i)} K\big(\frac{x-X_i}{h}\big) - \mathbf{E}\big(\frac{\alpha}{G(X_i)} K\big(\frac{x-X_i}{h}\big)\big)$. So, it follows that

$$\tilde{f}_n(x) - \mathbf{E}\big(\tilde{f}_n(x)\big) = \frac{1}{nh} \sum_{i=1}^{n} U_i(x,h)\,. \tag{4.1}$$

The proof of Proposition 2.1 is based on Lemma 4.1 and Lemma 4.2 hereafter.

Lemma 4.1. *Under the assumptions of Proposition 2.1, for all u-tuples $(s_1, ..., s_u)$ and all v-tuples $(w_1, ..., w_v)$ with $1 \le s_1 \le \cdots \le s_u \le w_1 \le \cdots \le w_v \le n$, we have*

$$\textbf{(i)} \quad \operatorname{cov}\left(\prod_{i=s_1}^{s_u} U_i(x,h)\,, \prod_{j=w_1}^{w_v} U_j(x,h) \right) =: \operatorname{cov}_1 \le c^{u+v} h^{-2}\, u\, v\, \rho(w_1 - s_u)\,,$$

$$\textbf{(ii)} \quad \operatorname{cov}\left(\prod_{i=s_1}^{s_u} U_i(x,h)\,, \prod_{j=w_1}^{w_v} U_j(x,h) \right) =: \operatorname{cov}_2 \le c^{u+v} h^{2}\,.$$

Proof of Lemma 4.1: Let $\mathrm{Lip}(\Phi)$ denote the Lipschitz modulus of continuity of Φ, that is

$$\mathrm{Lip}(\Phi) = \sup_{x \neq y} \frac{\big|\Phi(x) - \Phi(y)\big|}{|x-y|_1}\,, \qquad \text{where} \quad \big|(z_1, ..., z_d)\big|_1 = |z_1| + \cdots + |z_d|\,.$$

To prove item (i), we use a result in (Bulinski and Shashkin ([3]), Theorem 5.3, p. 89) and then we have

$$\mathrm{cov}_1 \le \mathrm{Lip}\left(\prod_{i=s_1}^{s_u} U_i(x,h)\right) \mathrm{Lip}\left(\prod_{j=w_1}^{w_v} U_j(x,h)\right) \sum_{i=s_1}^{s_u}\sum_{j=w_1}^{w_v} \mathrm{cov}(X_i,X_j)\,.$$

Now since

$$\mathrm{Lip}\left(\prod_{i=1}^{k} U_i(x,h)\right) \le \frac{c}{h}\left(\frac{2}{G(a)}\right)^k \|K\|_\infty^{k-1}\,,$$

where $\|K\|_\infty := \sup_u K(u)$. Then by stationarity and Assumption A2, we get

$$\mathrm{cov}_1 \le \frac{c^2\, 2^{u+v}}{h^2 G^{u+v}(a)}\, \|K\|_\infty^{u+v-2}\, u\, v\, \rho(w_1 - s_u)\,.$$

Thus result (i) holds. The result (ii) follows by simple algebra using assumptions A3–A5. The proof is finished. □

Lemma 4.2. *There exist constants $M, L_1, L_2 < +\infty$, $\mu, \lambda \ge 0$ and a non-increasing sequence of real numbers $\big(\phi(n)\big)_{n\ge 1}$ such that*

(**a**) $$\mathrm{cov}\left(\prod_{i=s_1}^{s_u} U_i(x,h)\,,\, \prod_{j=w_1}^{w_v} U_j(x,h)\right) =: \mathrm{cov} \le c^{u+v} h\, u\, v\, \phi(w_1 - s_u)\,,$$

(**b**) $$\sum_{t\ge 0} (t+1)^{k_0}\phi(t) \le L_1 L_2^{k_0} \big(k_0!\big)^{\mu}, \quad \forall\, k_0 \ge 0\,,$$

(**c**) $$\mathbf{E}\Big(\big|U_i(x,h)\big|^{k_0}\Big) \le \big(k_0!\big)^{\lambda} M^{k_0}\,.$$

The items in Lemma 4.2 are nearly the conditions of Theorem 1 in (Doukhan and Neumann ([8])). This latter will allow us to use their exponential inequality in proving Proposition 2.1.

Proof of Lemma 4.2: To prove item (a) we apply Lemma 4.1 by taking $\phi(\cdot) = \rho^{1/4}(\cdot)$ and writing $\mathrm{cov} = \mathrm{cov}_1^{1/4}\, \mathrm{cov}_2^{3/4}$. The proofs for (b) and (c) are similar to those in (Doukhan and Neumann ([8]), Proposition 8) by choosing $\lambda = 0$, $\mu = 1$ and $L_1 = L_2 = \frac{1}{1-e^{-\gamma/4}}$, and then we omit them. □

Proof of Proposition 2.1: The main tool used here to bound the fluctuation term in (4.1), is an exponential inequality due to Doukhan and Neumann ([8]), that is

$$\mathbf{P}\left(\sum_{i=1}^{n} U_i(x,h) \ge \varepsilon\right) \le \exp\left(-\frac{\varepsilon^2/2}{A_n + B_n^{1/(\mu+\lambda+2)}\, \varepsilon^{(2\mu+2\lambda+3)/(\mu+\lambda+2)}}\right), \tag{4.2}$$

where A_n can be chosen such that $A_n \le \sigma_n^2$ with

$$\sigma_n^2 := \mathrm{Var}\left(\sum_{i=1}^{n} U_i(x,h)\right),$$

and

$$B_n = 2\,cL_2\left(\frac{2^{4+\mu+\lambda}\,c\,nh\,L_1}{A_n} \vee 1\right).$$

For this purpose, let us calculate $\sigma_n^2 = (nh)^2\,\mathrm{Var}\big(\tilde{f}_n(x)\big)$. We have

$$\begin{aligned}(nh)^2\,\mathrm{Var}\big(\tilde{f}_n(x)\big) &= n\left\{\mathbf{E}\left[\frac{\alpha^2}{G^2(X_1)}\,K^2\left(\frac{x-X_1}{h}\right)\right] - \mathbf{E}^2\left[\frac{\alpha}{G(X_1)}\,K\left(\frac{x-X_1}{h}\right)\right]\right\}\\ &\quad + \sum_{i=1}^{n}\sum_{j\neq i,j=1}^{n}\mathrm{cov}\left(\frac{\alpha}{G(X_i)}\,K\left(\frac{x-X_i}{h}\right),\ \frac{\alpha}{G(X_j)}\,K\left(\frac{x-X_j}{h}\right)\right)\\ &=: V_1 + V_2\,.\end{aligned}$$

On the one hand, by assumptions A3–A4, a change of variable and the Dominated Convergence Theorem, we obtain $V_1 = O(nh)$.
On the other hand, from Lemma 4.1, we can write

$$\mathrm{cov}\left(\frac{\alpha}{G(X_i)}\,K\left(\frac{x-X_i}{h}\right),\ \frac{\alpha}{G(X_j)}\,K\left(\frac{x-X_j}{h}\right)\right) = O\big(h^2\big)\,. \tag{4.3}$$

And, let

$$\mathcal{B}_1 = \Big\{(i,j)/\ 1 \le |i-j| \le \eta_n\Big\} \quad \text{and} \quad \mathcal{B}_2 = \Big\{(i,j)/\ \eta_n+1 \le |i-j| \le n-1\Big\},$$

where $\eta_n = o(n)$. Then

$$\begin{aligned}V_2 &= \sum_{i=1}^{n}\sum_{j\in\mathcal{B}_1}\mathrm{cov}\left(\frac{\alpha}{G(X_i)}\,K\left(\frac{x-X_i}{h}\right),\ \frac{\alpha}{G(X_j)}\,K\left(\frac{x-X_j}{h}\right)\right)\\ &\quad + \sum_{i=1}^{n}\sum_{j\in\mathcal{B}_2}\mathrm{cov}\left(\frac{\alpha}{G(X_i)}\,K\left(\frac{x-X_i}{h}\right),\ \frac{\alpha}{G(X_j)}\,K\left(\frac{x-X_j}{h}\right)\right)\\ &=: V_{21} + V_{22}\,.\end{aligned}$$

From (4.3) we have

$$V_{21} = O\big(\eta_n\,nh^2\big)\,, \tag{4.4}$$

then by Assumption A2 and Lemma 4.2 (a) we obtain

$$\frac{V_{22}}{nh} \le \frac{c}{nh}\sum_{i=1}^{n}\sum_{j\in\mathcal{B}_2} h\,e^{-\frac{\gamma|i-j|}{4}} \le c\int_{\eta_n}^{n} e^{-\frac{\gamma u}{4}}\,du = O\Big(e^{-\frac{\gamma\eta_n}{4}}\Big)\,. \tag{4.5}$$

Choosing $\eta_n = O\big(h^{\delta-1}\big)$ with $0<\delta<1$ (δ may be the same as that in A6), the statements (4.4) and (4.5) give $V_{21} = o(nh)$ and $\frac{V_{22}}{nh} = o(1)$. Consequently

$$\sigma_n^2 = O\big(nh\big)\,.$$

Thus we choose $A_n = O(nh)$ and $B_n = O(1)$.
At this step we are able to apply (4.2). To end the proof of Proposition 2.1, we use a covering of the compact $\mathscr{D}$ by a finite number ℓ_n of intervals $\mathscr{D}_1, ..., \mathscr{D}_{\ell_n}$ of equal length

$a_n = O\big(n^{-1/2}h^{3/2}\big)$ and centered at points $x_1, ..., x_{\ell_n}$, respectively. Note that as $\mathscr{D}$ is bounded, there exists a constant $M_0 > 0$ such that $\ell_n \leq M_0\, a_n^{-1}$. Then observe that

$$\begin{aligned}\sup_{x\in\mathscr{D}}\Big|\tilde{f}_n(x) - \mathbf{E}\big(\tilde{f}_n(x)\big)\Big| &= \sup_{x\in\mathscr{D}}\frac{1}{nh}\left|\sum_{i=1}^{n}U_i(x,h)\right| \\ &\leq \max_{k=1,\ldots,\ell_n}\sup_{x\in\mathscr{D}_k}\frac{1}{nh}\sum_{i=1}^{n}\big|U_i(x,h) - U_i(x_k,h)\big| \\ &\quad + \max_{k=1,\ldots,\ell_n}\frac{1}{nh}\left|\sum_{i=1}^{n}U_i(x_k,h)\right|.\end{aligned}$$

First, since K is Lipschitz we have

$$\begin{aligned}\frac{1}{nh}\sum_{i=1}^{n}\big|U_i(x,h) - U_i(x_k,h)\big| &\leq \frac{1}{nh}\sum_{i=1}^{n}\frac{\alpha}{G(X_i)}\left|K\left(\frac{x-X_i}{h}\right) - K\left(\frac{x_k-X_i}{h}\right)\right| \\ &\quad + \frac{1}{h}\,\mathbf{E}\left(\frac{\alpha}{G(X_i)}\left|K\left(\frac{x-X_i}{h}\right) - K\left(\frac{x_k-X_i}{h}\right)\right|\right) \\ &\leq \frac{1}{h}\,\frac{2}{G(a)}\left|\frac{x-x_k}{h}\right| \\ &\leq \frac{c}{G(a)\sqrt{nh}} = O\left(\frac{1}{\sqrt{nh}}\right). \qquad (4.6)\end{aligned}$$

Next, by Assumption A6, if we replace ε by $\varepsilon_0\sqrt{nh\,\log n} =: \varepsilon_n$ in (4.2), we then get

$$\begin{aligned}\mathbf{P}\left(\max_{k=1,\ldots,\ell_n}\frac{1}{nh}\left|\sum_{i=1}^{n}U_i(x_k,h)\right| > \varepsilon_0\sqrt{\frac{\log n}{nh}}\right) &\leq \sum_{k=1}^{\ell_n}\mathbf{P}\left(\left|\sum_{i=1}^{n}U_i(x_k,h)\right| > \varepsilon_n\right) \\ &\leq c\,a_n^{-1}\exp\left(\frac{-\left(\varepsilon_0^2\,\log n\right)/2}{c + \varepsilon_0^{5/3}\left(\frac{\log^5 n}{nh}\right)^{1/6}}\right) \\ &\leq \frac{c}{\left(nh^{1+\delta}\right)^{\frac{3}{2(1+\delta)}}}\; n^{-c\varepsilon_0^2 + \frac{4+\delta}{2(1+\delta)}}. \qquad (4.7)\end{aligned}$$

For a suitable choice of ε_0, the right hand side term in (4.7) becomes the general term of a convergent series. Then Borel–Cantelli's lemma gives

$$\max_{k=1,\ldots,\ell_n}\frac{1}{nh}\left|\sum_{i=1}^{n}U_i(x_k,h)\right| = O\left(\sqrt{\frac{\log n}{nh}}\right).$$

This latter jointly with (4.6) allow us to conclude the desired result, that is

$$\sup_{x\in\mathscr{D}}\frac{1}{nh}\left|\sum_{i=1}^{n}U_i(x,h)\right| = O\left(\sqrt{\frac{\log n}{nh}}\right) = \sup_{x\in\mathscr{D}}\Big|\tilde{f}_n(x) - \mathbf{E}\big(\tilde{f}_n(x)\big)\Big|,$$

which ends the proof of Proposition 2.1. □

Now the proof of Theorem 2.1 is immediately established once the following lemmas (Lemma 4.3 and Lemma 4.4) are stated.

Lemma 4.3. *Under assumptions A1–A2, for n sufficiently large we have*

$$\sup_{x\in\mathscr{D}}\left|G_n(x)-G(x)\right| \;=\; O\left[\left(\frac{\log\log n}{n}\right)^{\theta}\right] \quad \text{a.s.}\,, \tag{4.8}$$

$$\left|\alpha_n-\alpha\right| \;=\; O\left[\left(\frac{\log\log n}{n}\right)^{\theta}\right] \quad \text{a.s.} \tag{4.9}$$

Proof of Lemma 4.3: To prove (4.8), it suffices to follow step by step the proof in (Guessoum *et al.* ([11]), Theorem 3.2). The result (4.9) ensues using the following decomposition

$$\begin{aligned}\left|\alpha_n-\alpha\right| \;=\; \frac{1}{C_n(x)\,C(x)}\Big|&C(x)\Big(G_n(x)-G(x)\Big)\big(1-F_n(x)\big)\\ &+C(x)\,G(x)\Big(F(x)-F_n(x)\Big)+G(x)\Big(C_n(x)-C(x)\Big)\big(F(x)-1\big)\Big|.\end{aligned}$$

Thus the result holds using (4.8) jointly with Theorem 3.2 and Lemma 4.2 in (Guessoum *et al.* ([11])). □

Lemma 4.4. *Under the hypotheses of Theorem 2.1, for large n enough we have*

$$\sup_{x\in\mathscr{D}}\left|\Big(\hat{f}_n(x)-\tilde{f}_n(x)\Big)\right| \;=\; O\left[\left(\frac{\log\log n}{n}\right)^{\theta}\right] \quad \text{a.s.}\,, \tag{4.10}$$

$$\sup_{x\in\mathscr{D}}\left|\Big(\mathbf{E}\big(\tilde{f}_n(x)\big)-f(x)\Big)\right| \;=\; O\big(h^2\big) \quad \text{a.s.} \tag{4.11}$$

Proof of Lemma 4.4: To get (4.10), remark that

$$\left|\hat{f}_n(x)-\tilde{f}_n(x)\right| \;=\; \frac{1}{nh}\sum_{i=1}^{n}\left|\frac{\alpha_n\Big(G(X_i)-G_n(X_i)\Big)+(\alpha_n-\alpha)\,G_n(X_i)}{G_n(X_i)\,G(X_i)}\right| K\left(\frac{x-X_i}{h}\right).$$

Then, Lemma 4.3 gives the result. For the bias term in statement (4.11), the result is obtained by using classical tools under assumptions A3 and A4. □

Proof of Theorem 2.1: The result holds by writing

$$\hat{f}_n(x)-f(x) \;=\; \Big(\hat{f}_n(x)-\tilde{f}_n(x)\Big)+\Big(\tilde{f}_n(x)-\mathbf{E}\big(\tilde{f}_n(x)\big)\Big)+\Big(\mathbf{E}\big(\tilde{f}_n(x)\big)-f(x)\Big)$$

and using Proposition 2.1 together with Lemma 4.4. □

Proof of Theorem 2.2: Let us consider the following decomposition

$$\hat{\lambda}_n(x)-\lambda(x) \;=\; \frac{\big(1-F(x)\big)^{-1}}{\big(1-F_n(x)\big)}\Big(\big(1-F(x)\big)\Big(\hat{f}_n(x)-f(x)\Big)-f(x)\Big(F(x)-F_n(x)\Big)\Big).$$

Then the proof follows from Theorem 3.2 in (Guessoum *et al.* ([11])) and Theorem 2.1. □

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INDEPENDENCE CHARACTERIZATION FOR WISHART AND KUMMER RANDOM MATRICES

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Abstract:

- We generalize the following univariate characterization of the Kummer and Gamma distributions to the cone of symmetric positive definite matrices: let X and Y be independent, non-degenerate random variables valued in $(0,\infty)$, then $U = Y/(1+X)$ and $V = X(1+U)$ are independent if and only if X follows the Kummer distribution and Y follows the the Gamma distribution with appropriate parameters. We solve a related functional equation in the cone of symmetric positive definite matrices, which is our first main result and apply its solution to prove the characterization of Wishart and matrix-Kummer distributions, which is our second main result.

Key-Words:

- *Wishart distribution; matrix-Kummer distribution; random matrices; independence characterization; functional equations.*

AMS Subject Classification:

- 62E10, 60E05, 39B42.

1. INTRODUCTION

In 1940s Bernstein noticed that if X and Y are independent, then $X-Y$ and $X+Y$ are independent if and only if X and Y are Gaussian, [3]. This observation suggested that independence can mean more than one could think. Many other examples of so-called independence characterizations have been identified through the years. One of the highlights in this area is Lukacs' (1955) characterization of the Gamma distribution by the independence of $X+Y$ and $X/(X+Y)$, [21]. In 1996 Casalis and Letac wrote, that independence characterizations of distributions *give insight into the laws of nature and may reveal quite beautiful mathematics*, [6]. In the cited paper they showed a new way, compared to Olkin and Rubin, [28], to generalize the Lukacs' theorem to symmetric positive definite matrices.

Another celebrated characterization origins from the Matsumoto–Yor (MY) property, see [24], [25], which says that for independent X and Y having GIG and Gamma distributions, random variables $1/(X+Y)$ and $1/X - 1/(X+Y)$ are also independent. First characterization of GIG and Gamma distributions through this property was given in [20]. It has been widely generalized and modified: symmetric cones [14], free probability [31] and others [5], [22], [23]. In 2012 a whole family of independence properties of a MY type was given by Koudou and Vallois [18]. The latter paper presents all possible distributions of independent X and Y for which there exists a (very regular, see [18]) function f such that $f(X+Y)$ and $f(X)-f(X+Y)$ are also independent. The Lukacs property corresponds to $f(x)=\log x$ and the MY property to $f(x)=1/x$. Another important case identified in [18] was $f(x)=\ln(1+1/x)$. That one concerns Kummer and Gamma distributions and can be formulated as follows: Let X has the Kummer distribution $\mathcal{K}(a,b,c)$ with density

$$f_X(x) \propto x^{a-1}(1+x)^{-(a+b)}e^{-cx}I_{(0,\infty)}(x) \tag{1.1}$$

and Y has the Gamma distribution $\mathcal{G}(b,c)$ with density

$$f_Y(y) \propto y^{b-1}e^{-cy}I_{(0,\infty)}(y)\,,$$

where $a,b,c>0$. Suppose that X and Y are independent and let

$$U = X+Y \qquad \text{and} \qquad V = \frac{1+1/(X+Y)}{1+1/X}\,. \tag{1.2}$$

Then U and V are also independent.

To derive related characterization, however, the authors needed to impose technical conditions of differentiability ([18]) or local integrability ([17]) of logarithms of strictly positive densities. Recently a regression version of this characterization under natural integrability assumption (and with no assumptions concerning densities) was given in [33]. In [30] even the integrability assumption was cleared out through the change of measure technique. In the last-mentioned paper also another independence property and a related characterization concerning Kummer and Gamma distributions were considered. The property was formulated by Hamza and Vallois in [8] and we will call it HV property in the sequel. It says that if $X\sim\mathcal{K}(a,b-a,c)$ (which means that X has Kummer distribution with parameters a, $b-a$ and c) and $Y\sim\mathcal{G}(b,c)$, $a,b,c>0$ are independent random variables and if

$$T_0(x,y) = \Big(y/(1+x),\, x\big(1+y/(1+x)\big)\Big)\,, \tag{1.3}$$

then the random vector $(U,V) = T_0(X,Y)$ has independent components, $U \sim \mathcal{K}(b, a-b, c)$ and $V \sim \mathcal{G}(a,c)$. Note that this is not a MY type property: there is no function f such that $U = f(X+Y)$ and $V = f(X) - f(X+Y)$. Further, in [29] the converse was proved:

Theorem 1.1. *Let X and Y be two independent positive random variables with positive densities on $(0,\infty)$ such that its logarithms are locally integrable. Let $(U,V) = T_0(X,Y)$. Suppose that U and V are independent. Then there exist constants $a,b,c>0$, such that $X \sim \mathcal{K}(a, b-a, c)$, $Y \sim \mathcal{G}(b,c)$ or, equivalently, $U \sim \mathcal{K}(b, a-b, c)$ and $V \sim \mathcal{G}(a,c)$.*

The proof was based on solving an associated functional equation. Completely different methods were used in [30], where a regression version of this characterization was proven. First, under integrability assumptions the recurrences for moments of X and Y were derived and solved. Then the integrability assumptions were eliminated through the change of measure technique and so Theorem 1.1 holds without any assumptions on densities, even their existence. Note also that [30] contains many references on Kummer distribution including its origins, motivations and various applications.

In this paper we consider the HV property and the related characterization of Kummer and Gamma distributions in the cone of positive definite, symmetric matrices. An analogue of Theorem 1.1 is proven in Section 5. Before that, in Section 2, we introduce matrix-Kummer and Wishart distributions. Then, in Section 3, HV property is adapted to the matrix setting. Section 4 is devoted to analysis of related functional equations and some technicalities. We also prove the first main result there, i.e. we solve functional equation (4.10). These results are applied in Section 5 to prove the main probabilistic result, i.e. the characterization of matrix-Kummer and Wishart distributions. Possible areas of impact and open questions are presented in Section 6.

2. THE MATRIX KUMMER DISTRIBUTION

Let $r \geq 1$ be an integer. Denote by Ω the linear space of real $r \times r$ symmetric matrices endowed with the inner product $\langle x, y\rangle = \mathrm{tr}(xy)$ for any $x, y \in \Omega$. Let $\Omega_+ \subset \Omega$ be the cone of positive-definite symmetric real $r \times r$ matrices. We denote by $\mathbf{e}$ the identity matrix.

For $\Sigma \in \Omega_+$ the Wishart distribution $\mathcal{W}(b,\Sigma)$ can be defined for $b \in \{0, 1/2, 1, 3/2, ..., (r-1)/2\} \cup \big((r-1)/2, \infty\big)$ as the law of a random variable Y valued in the closure of Ω_+ with Laplace transform

$$\mathbb{E}\Big(e^{\langle \sigma, Y\rangle}\Big) = \left(\frac{\det \Sigma}{\det(\Sigma - \sigma)}\right)^b, \qquad \text{for } \sigma \text{ such that } \quad \Sigma - \sigma \in \Omega_+ .$$

If $b > \frac{r-1}{2}$, then Y has density of the form:

$$\mathcal{W}(b,\Sigma)\,(dy) \;=\; \frac{(\det \Sigma)^b}{\Gamma_r(b)}\; (\det y)^{b-(r+1)/2}\, \exp\big(-\langle \Sigma, y\rangle\big)\, I_{\Omega_+}(y)\, dy\,,$$

where Γ_r is the multivariate Gamma function (see [26]) defined for any complex number z

with $\Re(z) > (r-1)/2$ by

$$\Gamma_r(z) = \pi^{r(r-1)/4} \prod_{j=1}^{r} \Gamma\left(z - \frac{j-1}{2}\right).$$

We will define matrix version of Kummer distribution following [16]. We say that random variable X valued in Ω_+ has *matrix-Kummer* distribution with parameters $a > \frac{r-1}{2}$, $b \in \mathbb{R}$, $\Sigma \in \Omega_+$, denote $X \sim \mathcal{MK}(a, b, \Sigma)$, if it has the following density

$$\mathcal{MK}(a, b, \Sigma)(dx) = C (\det x)^{a-\frac{r+1}{2}} \big(\det(\mathbf{e} + x)\big)^{-(a+b)} \exp\big(-\langle \Sigma, x\rangle\big)\, I_{\Omega_+}(x)\, dx\,,$$

where the normalizing constant C equals to $\big(\Gamma_r(a)\, \Psi(a, \frac{r+1}{2} - b; \Sigma)\big)^{-1}$ and Ψ is a confluent hypergeometric function of the second kind with matrix argument (see [9], formula (2)). In the literature this distribution is sometimes called the *Kummer-gamma distribution* or the *Kummer distribution of type II* (see e.g. [7], [27]). It also appeared recently as a member of the family named weighted-type II Wishart distribution, [2].

3. HV PROPERTY FOR POSITIVE DEFINITE MATRICES

In [16] Koudou showed that matrix-Kummer and Wishart distributions have the following property: if $X \sim \mathcal{MK}(a, b, \Sigma)$ and $Y \sim \mathcal{W}(b-a, \Sigma)$ are independent, then

$$U = \mathbb{P}\Big(\mathbf{e} + (X+Y)^{-1}\Big)^{1/2} \big(\mathbf{e} + X^{-1}\big)^{-1} \qquad \text{and} \qquad V = X + Y$$

are independent, where $\mathbb{P}(y)$ is endomorphism defined on Ω and for any $y \in \Omega_+$:

$$\mathbb{P}(y)(x) = yxy\,, \qquad x \in \Omega\,.$$

This is a generalization of the independence property of real-valued random variables related to transformation (1.2). This property is in the family of Matsumoto–Yor type independence properties defined in [17, 18]. Recently, Kołodziejek showed that this property characterizes matrix-Kummer and Wishart distributions, [15]. In this section we establish a new independence property of Wishart and matrix-Kummer random matrices, which is not of Matsumoto–Yor type. A related characterization is given in Section 5.

We want to find transformation that generalizes T_0 defined in (1.3) onto Ω_+ and that preserves the independence property for matrix-Kummer and Wishart distributions.

Let $T\colon \Omega_+^2 \to \Omega_+^2$ be defined as:

$$T(x, y) = \left(\mathbb{P}\Big[(\mathbf{e}+x)^{-\frac{1}{2}}\Big] y,\ \mathbb{P}\left[\left(\mathbf{e} + \mathbb{P}\Big[(\mathbf{e}+x)^{-\frac{1}{2}}\Big] y\right)^{\frac{1}{2}}\right] x\right). \tag{3.1}$$

Note that T is involutive (as in one-dimensional case).

To derive the Jacobian of transformation T, which is done in Proposition 3.1, we need the fact that

$$\operatorname{Det}\big(\mathbb{P}(x)\big) = (\det x)^{r+1}\,, \tag{3.2}$$

where Det is the determinant in the space of endomorphisms on Ω (see e.g. [20] or [26], Theorem 2.1.7).

Proposition 3.1. *Let u and v be in the cone of symmetric positive definite matrices. Denote by T^{-1} the inverse of T defined in (3.1). Then the Jacobian of T^{-1} is equal to*

$$\mathrm{J}_{T^{-1}}(u,v) = \big(\det[\mathbf{e}+u]\big)^{-(r+1)}\big(\det[\mathbf{e}+v+u]\big)^{\frac{r-1}{2}}. \tag{3.3}$$

Moreover, since T is an involution, the Jacobian of T is equal to $\mathrm{J}_{T^{-1}}$.

The proof of Proposition 3.1 is standard. The same technique was, for instance, used in [23] for the MY property and in [16] for the other independence property of Wishart and Kummer matrices.

Proof: Let x and y be in Ω_+. Then

$$u := \mathbb{P}\Big([\mathbf{e}+x]^{-\frac12}\Big)y \in \Omega_+, \qquad v := \mathbb{P}\Big([\mathbf{e}+u]^{\frac12}\Big)x \in \Omega_+. \tag{3.4}$$

Let $T_1, T_2 \colon \Omega_+^2 \to \Omega_+^2$ be defined by

$$T_1(x,y) = (w,z) := \Big(x, \mathbb{P}\Big([\mathbf{e}+x]^{-\frac12}\Big)y\Big)$$

and

$$T_2(w,z) = (u,v) := \Big(z, \mathbb{P}\Big([\mathbf{e}+z]^{\frac12}\Big)w\Big).$$

Then $T = T_2 \circ T_1$ and we have

$$(x,y) = T_1^{-1}(w,z) = \Big(w, \mathbb{P}\Big([\mathbf{e}+w]^{\frac12}\Big)z\Big), \tag{3.5}$$

$$(w,z) = T_2^{-1}(u,v) = \Big(\mathbb{P}\Big([\mathbf{e}+u]^{-\frac12}\Big)v, u\Big). \tag{3.6}$$

Let us note that the Jacobian J_2 of T_2^{-1} equals

$$\mathrm{Det}\begin{pmatrix} * & E \\ \mathbf{e} & 0 \end{pmatrix},$$

where $*$ does not need to be computed and E is the differential of the function $v \mapsto [e+u]^{-\frac12}\, v[e+u]^{-\frac12}$ (u is fixed) and equals $\mathbb{P}\big([\mathbf{e}+u]^{-\frac12}\big)$. Hence, by (3.2) we get

$$\mathrm{J}_2(u,v) = \mathrm{Det}\, E = \big(\det[\mathbf{e}+u]^{-\frac12}\big)^{r+1} = \big(\det[\mathbf{e}+u]\big)^{-\frac{r+1}{2}}.$$

The Jacobian J_1 of T_1^{-1} can be computed in the same way:

$$\mathrm{J}_1(w,z) = \mathrm{Det}\begin{pmatrix} \mathbf{e} & 0 \\ * & F \end{pmatrix},$$

where F is the differential of the mapping $z \mapsto \mathbb{P}\big([\mathbf{e}+w]^{\frac12}\big)z$. Then

$$\mathrm{J}_1(w,z) = \mathrm{Det}\, F = \big(\det[\mathbf{e}+w]\big)^{\frac{r+1}{2}} = \det(\mathbf{e}+u)^{-1}\det(\mathbf{e}+u+v),$$

where the last equality follows from definition of w given in (3.6) and elementary properties of determinant.

Finally, we obtain

$$\mathrm{J}(u,v) = \mathrm{J}_1(w,z)\,\mathrm{J}_2(u,v) = \big(\det(\mathbf{e}+u+v)\big)^{\frac{r+1}{2}}\big(\det[\mathbf{e}+u]\big)^{-(r+1)}. \qquad \square$$

Theorem 3.1. *Let X and Y be two independent random matrices valued in Ω_+. Assume that X has matrix-Kummer distribution $\mathcal{MK}(a, b, c\mathbf{e})$ and Y the Wishart distribution $\mathcal{W}(a+b, c\mathbf{e})$, where $a > \frac{r-1}{2}$, $b > \frac{r-1}{2} - a$, $c > 0$.*

Then the random matrices

$$U := \mathbb{P}\Big([\mathbf{e}+X]^{-\frac{1}{2}}\Big)\,Y\,, \qquad V := \mathbb{P}\Big([\mathbf{e}+U]^{\frac{1}{2}}\Big)\,X$$

are independent. Furthermore, $U \sim \mathcal{MK}(a+b, -b, c\mathbf{e})$ and $V \sim \mathcal{W}(a, c\mathbf{e})$.

Proof: Denote densities of X, Y and (U, V) by f_X, f_Y and $f_{(U,V)}$, respectively. Since X and Y are independent, we have

$$f_{(U,V)}(u,v) \;=\; |\mathrm{J}(u,v)|\, f_X(x)\, f_Y(y)\, I_{\Omega_+}(u)\, I_{\Omega_+}(v)\,,$$

where $(x, y) = T^{-1}(u, v) = \Big(\mathbb{P}\big([\mathbf{e}+u]^{-\frac{1}{2}}\big)\,v,\, \mathbb{P}\big([\mathbf{e}+x]^{\frac{1}{2}}\big)\,u\Big)$ and J is the Jacobian of T^{-1} from Proposition 3.1. Elementary properties of trace and determinant give

$$\begin{aligned}
\det(\mathbf{e}+x) \;&=\; \det\Big[\mathbb{P}\big([\mathbf{e}+u]^{-\frac{1}{2}}\big)\,\big((e+u)+v\big)\Big] \;=\; \det(\mathbf{e}+u)^{-1}\det(\mathbf{e}+u+v)\,,\\
\det(y) \;&=\; \det\Big[\mathbb{P}\big([\mathbf{e}+x]^{\frac{1}{2}}\big)\,u\Big] \;=\; \det(\mathbf{e}+x)\,\det u\,,\\
\det x \;&=\; \det v\,\det(\mathbf{e}+u)^{-1}\,,\\
\langle c\mathbf{e}, y\rangle \;&=\; c\,\big\langle \mathbf{e}, \mathbb{P}(\mathbf{e}+x)^{1/2}u\big\rangle \;=\; c\,\big\langle \mathbf{e}, (\mathbf{e}+x)\,u\big\rangle\,,\\
\langle c\mathbf{e}, x+y\rangle \;&=\; c\,\big\langle \mathbf{e}, (\mathbf{e}+u)\,x+u\big\rangle \;=\; c\langle \mathbf{e}, u\rangle + c\,\big\langle \mathbf{e}, \mathbb{P}(\mathbf{e}+u)^{1/2}x\big\rangle \;=\; \langle c\mathbf{e}, u\rangle + \langle c\mathbf{e}, v\rangle\,.
\end{aligned}$$

Hence we have

$$\begin{aligned}
f_{(U,V)}(u,v) \;&=\; C\,\det(\mathbf{e}+u)^{-(r+1)}\,\det(\mathbf{e}+u+v)^{\frac{r+1}{2}}\,(\det x)^{a-\frac{r+1}{2}}\,\det(\mathbf{e}+x)^{-b-a}\\
&\quad\cdot\,(\det y)^{a+b-\frac{r+1}{2}}\,\exp\big(-c\,\langle \mathbf{e}, x+y\rangle\big)\,I_{\Omega_+}(u)\,I_{\Omega_+}(v)\\
&=\; C\,\det(\mathbf{e}+u)^{-a}\,\det u^{a+b-\frac{r+1}{2}}\,e^{-\langle c,u\rangle}\,\det v^{a-\frac{r+1}{2}}\,e^{-\langle c,v\rangle}\,I_{\Omega_+}(u)\,I_{\Omega_+}(v)\,. \qquad \square
\end{aligned} \tag{3.7}$$

Remark 3.1. Constant C in (3.7) equals

$$C \;=\; \frac{c^{r(b+a)}}{\Gamma_r(a+b)}\;\frac{1}{\Gamma_r(a)\,\psi\big(a, \frac{r+1}{2}-b, c\mathbf{e}\big)}\,.$$

On the other hand, since $f_{(U,V)}$ is the density of $\mathcal{MK}(a+b, -b, c\mathbf{e}) \otimes \mathcal{W}(a, c\mathbf{e})$, then

$$C \;=\; \frac{c^{ra}}{\Gamma_r(a)}\;\frac{1}{\Gamma_r(a+b)\,\psi\big(a+b, \frac{r+1}{2}+b, c\mathbf{e}\big)}\,.$$

So we obtain

$$\psi\big(a+b, \tfrac{r+1}{2}+b, c\mathbf{e}\big)\,c^{rb} \;=\; \psi\big(a, \tfrac{r+1}{2}-b, c\mathbf{e}\big)\,.$$

For $r = 1$ it is a well known identity, see formula 13.1.29 in [1].

Notice that X and Y in Theorem 3.1 have very special scale parameter: the identity matrix multiplied by a positive constant c. We will show, in Section 5, that no other parameter is possible there.

4. FUNCTIONAL EQUATIONS

The main result of this section is the general solution of the functional equation

$$A(x)+B(y) \;=\; C\Big(\mathbb{P}(\mathbf{e}+x)^{-1/2}\,y\Big)+D\Big(\mathbb{P}\big[\mathbf{e}+\mathbb{P}(\mathbf{e}+x)^{-1/2}\,y\big]^{1/2}x\Big)\,, \tag{4.1}$$

where $A,B,C,D\colon \Omega_+\to\mathbb{R}$ are continuous functions. We use techniques first developed in [4] to solve equation of the form

$$a(x)+b(y) \;=\; c\big(\mathbb{P}(y)\,x\big)+d\big(\mathbb{P}(y)\,(\mathbf{e}-x)\big)\,,\qquad y\in\Omega_+\,,\quad x\in\mathcal{D}\,,$$

where $\mathcal{D}=\big\{z\in\Omega_+\colon\,\mathbf{e}-z\in\Omega_+\big\}$. This equation was concerned to prove characterization of Wishart distribution (valued in Ω_+). In [4] authors assumed that densities of considered random variables are strictly positive and twice differentiable. Earlier similar results, but under different assumptions, were obtained by Olkin and Rubin, [28], Casalis and Letac, [6], Letac and Massam, [19]. Starting from 2013 methods from [4] were improved by Kołodziejek, who:

- Generalized Lukacs' theorem to all non-octonion symmetric cones of rank greater than 2 and the Lorentz cone assuming only strict positivity and continuity of densities, [10], [12].
- Generalized independence characterization of Beta distribution to the symmetric cone setting, [13]. Functional equation, which played a crucial role there, was as follows:
$$a(x)+b\big(g(\mathbf{e}-x)\,y\big) \;=\; c(y)+d\big(g(\mathbf{e}-y)\,x\big)\,,$$
where $x,y\in\mathcal{D}$, a,b,c,d are continuous functions and g is a division algorithm.
- Solved the following equation
$$a(x)+b(y) \;=\; c(x+y)+d\big(x^{-1}-(x+y)^{-1}\big)$$
for continuous a,b,c,d defined on the symmetric cone, [14]. As a consequence he got a converse of Matsumoto–Yor theorem for random variables valued in symmetric cone, i.e. for Wishart and GIG distributions. Earlier results were obtained only for the cone Ω_+ and under stronger assumptions, [20, 32].
- Proved a new characterization of Wishart and matrix-Kummer, [15].

In the proofs in this section we try to adapt the methods developed in papers cited above in order to solve (4.1). First, we recall Lemma 3.2 from [10]. It is formulated for any symmetric cone, but we will restrict it to our setting, i.e. the cone Ω_+.

Lemma 4.1 (Additive Cauchy equation)**.** *Let $f\colon\Omega_+\mapsto\mathbb{R}$ be a measurable function such that $f(x)+f(y)=f(x+y)$ for all $(x,y)\in\Omega_+^2$. Then there exists $c\in\Omega$ such that $f(x)=\langle c,x\rangle$ for any $x\in\Omega_+$.*

Next, we give solution of slightly modified logarithmic Pexider equation for functions defined on $\Omega_+ + \mathbf{e} := \big\{x\in\Omega_+\colon x-\mathbf{e}\in\Omega_+\big\}$.

Proposition 4.1. *Let $f_1, f_2, f_3 \colon \Omega_+ + \mathbf{e} \to \mathbb{R}$ be continuous functions such that*

$$f_1(x) + f_2(y) = f_3\Big(\mathbb{P}\big(x^{1/2}\big)\, y\Big) \qquad \text{for all} \quad x, y \in \Omega_+ + \mathbf{e}\,. \tag{4.2}$$

Then there exist constants $q, \gamma_1, \gamma_2 \in \mathbb{R}$ such that for $x \in \Omega_+ + \mathbf{e}$

$$\begin{aligned} f_1(x) &= f_0(x) + \gamma_1\,, \\ f_2(x) &= f_0(x) + \gamma_2\,, \\ f_3(x) &= f_0(x) + \gamma_1 + \gamma_2\,, \end{aligned} \tag{4.3}$$

where $f_0(x) = q \log\det x$.

Proof: Let $x = \alpha\,\mathbf{e}$, $\alpha > 1$ and $\alpha \to 1^+$. Given Eq. (4.2), we have

$$f_2(y) = f_3(y) - \lim_{\alpha\to 1^+} f_1(\alpha\,\mathbf{e}) = f_3(y) - \gamma_1\,.$$

Similarly we obtain

$$f_1(x) = f_3(x) - \lim_{\alpha\to 1^+} f_1(\alpha\,\mathbf{e}) = f_3(x) - \gamma_2\,.$$

So Eq. (4.2) is equivalent to

$$f(x) + f(y) = f\Big(\mathbb{P}\big(x^{1/2}\big)\, y\Big) \qquad \text{for all} \quad x, y \in \Omega_+ + \mathbf{e}\,, \tag{4.4}$$

where $f(x) = f_3(x) - \gamma_1 - \gamma_2$.

Following the proof of Lemma 3.2 in [10], we define an extension $\bar f$ of f for all $x \in \Omega_+$:

$$\bar f(x) = \begin{cases} f(x)\,, & x \in \Omega_+ + \mathbf{e}\,, \\ f(t_x\, x) - f(t_x\,\mathbf{e})\,, & x \notin \Omega_+ + \mathbf{e}\,, \end{cases} \tag{4.5}$$

where $t_x = \frac{2}{\min_i \lambda_i}$, λ_i being the i-th eigenvalue of x. Also $t_{\mathbb{P}(x^{1/2})\,y}$ will be denoted by t_{xy}. Note that all eigenvalues of matrix $t_x\, x$ are greater than 1 for any $x \in \Omega_+$, so $t_x\, x \in \Omega_+ + \mathbf{e}$. Now, we will show that

$$\bar f(x) + \bar f(y) = \bar f\Big(\mathbb{P}\big(x^{1/2}\big)\, y\Big) \qquad \text{for all} \quad x, y \in \Omega_+\,. \tag{4.6}$$

Case 1: $x \in \Omega_+ + \mathbf{e}$, $y \notin \Omega_+ + \mathbf{e}$ and $\mathbb{P}\big(x^{1/2}\big)\, y \in \Omega_+ + \mathbf{e}$. Then, by definition (4.5) and Eq. (4.4)

$$\bar f(x) + \bar f(y) = f(x) + f(t_y\, y) - f(t_y\,\mathbf{e}) = f\Big(t_y\, \mathbb{P}\big(x^{1/2}\big)\, y\Big) - f(t_y\,\mathbf{e}) = \bar f\Big(\mathbb{P}\big(x^{1/2}\big)\, y\Big)\,.$$

Case 2: $x \in \Omega_+ + \mathbf{e}$, $y \notin \Omega_+ + \mathbf{e}$ and $\mathbb{P}\big(x^{1/2}\big)\, y \notin \Omega_+ + \mathbf{e}$. These imply that minimal eigenvalue of $\mathbb{P}\big(x^{1/2}\big)\, y$ is not greater than 1. Then

$$\begin{aligned} \bar f(x) + \bar f(y) = f(x) + f(t_y\, y) - f(t_y\,\mathbf{e}) &= f\left(\frac{t_y}{t_{xy}}\, \mathbb{P}\big(x^{1/2}\big)\, y\, t_{xy}\right) - f(t_y\,\mathbf{e}) \\ &= f\Big(\mathbb{P}\big(x^{1/2}\big)\, y\, t_{xy}\Big) - \left[f(t_y\,\mathbf{e}) - f\left(\frac{t_y}{t_{xy}}\,\mathbf{e}\right)\right] \\ &= f\Big(\mathbb{P}\big(x^{1/2}\big)\, y\, t_{xy}\Big) - f(t_{xy}\,\mathbf{e}) = \bar f\Big(\mathbb{P}\big(x^{1/2}\big)\, y\Big)\,. \end{aligned}$$

Here, besides (4.5) and (4.4), we have used the fact that every eigenvalue of $\mathbb{P}\big(x^{1/2}\big)\, y$ is not less than the product of the smallest eigenvalues of x and y. Indeed, when λ_1 is the smallest eigenvalue of $\mathbb{P}\big(x^{1/2}\big)\, y$, then from the min–max theorem we have

$$\lambda_1 \,=\, \min_{z\in\mathbb{R}^n\setminus\{0\}} \frac{\big(x^{1/2}\, y\, x^{1/2}\, z,\, z\big)}{(z,z)} \,=\, \min_{z\in\mathbb{R}^n\setminus\{0\}} \frac{\big(y\, x^{1/2}\, z,\, x^{1/2}\, z\big)}{\big(x^{1/2}\, z,\, x^{1/2}\, z\big)}\, \frac{\big(x^{1/2}\, z,\, x^{1/2}\, z\big)}{(z,z)} \,\geq\, \lambda_x\, \lambda_y \,>\, \lambda_y\,,$$

where λ_x and λ_y are the smallest eigenvalues of x and y, respectively. The last inequality follows from the fact that $x \in \Omega_+ + \mathbf{e}$.

Other cases can be easily verified in a similar way.

Since Eq. (4.6) holds for every $x, y \in \Omega_+$ then by Lemma 4.2 (Logarithmic Pexider Equation) from [11]

$$\bar{f}(x) \,=\, q \log\det x \qquad \text{on} \quad \Omega_+\,.$$

From definition $f(x) = \bar{f}(x) = f_0(x)$ for $x \in \Omega_+ + \mathbf{e}$ and the proof is complete. □

We will also need two new lemmas.

Lemma 4.2. *Let $c \in \Omega_+$. Assume that $\big\langle c, \mathbb{P}(u)\, v^2\big\rangle = \big\langle c, \mathbb{P}(v)\, u^2\big\rangle$ for all $u, v \in \Omega_+$. Then $c = \lambda\mathbf{e}$ for some $\lambda > 0$.*

Proof: For $v = c^{1/2}$ the equality $\big\langle c, \mathbb{P}(u)\, v^2\big\rangle = \big\langle c, \mathbb{P}(v)\, u^2\big\rangle$ results in

$$\begin{aligned}
\big\langle c, \mathbb{P}(u)\, c\big\rangle &= \big\langle c, \mathbb{P}(c^{1/2})\, u^2\big\rangle\,,\\
\big\langle c, \mathbb{P}(u)\, c\big\rangle &= \big\langle c^2, u^2\big\rangle\\
\big\langle \mathbf{e}, c\cdot \mathbb{P}(u)\, c\big\rangle &= \big\langle \mathbf{e}, c^2\, u^2\big\rangle\\
0 &= \big\langle \mathbf{e}, c\cdot \mathbb{P}(u)\, c - c^2\, u^2\big\rangle\,.
\end{aligned}$$

On the other hand the last equality can be written as

$$0 \,=\, \big\langle \mathbf{e}, ucuc - u^2c^2\big\rangle\,.$$

Adding last two equalities we arrive at

$$\begin{aligned}
0 &= \big\langle \mathbf{e}, ucuc + cucu - c^2u^2 - u^2c^2\big\rangle\\
&= -\big\langle \mathbf{e}, (uc-cu)(uc-cu)\big\rangle\\
&= -\big\langle (uc-cu)^{\mathsf{T}}, (uc-cu)\big\rangle\,.
\end{aligned}$$

Thus $\|uc - cu\| = 0$ and so $cu = uc$ for all $u \in \Omega_+$. We conclude (see, e.g., proof of Proposition 5.2 in [20]), that $c = \lambda\mathbf{e}$ for some $\lambda > 0$. □

Lemma 4.3. *Let $u, z \in \Omega_+$, $\alpha > 0$ and*

$$x_\alpha \,=\, \left[\mathbb{P}\left(u + \frac{1}{\alpha}\,\mathbf{e}\right)^{-1/2} \tilde{x}\right]^2 - \mathbf{e}\,, \tag{4.7}$$

where $\tilde{x} = \big(\mathbb{P}(u + \mathbf{e}/\alpha)^{1/2}\,(z + u + \mathbf{e}/\alpha)\big)^{1/2}$. Then $\lim\limits_{\alpha\to 0} \dfrac{1}{\alpha}\, x_\alpha = z$.

Proof: We have

$$\begin{aligned}\frac{x_\alpha}{\alpha} &= \frac{1}{\alpha}\left\{\left[\mathbb{P}\Big(u+\frac{\mathbf{e}}{\alpha}\Big)^{-1/2}\tilde{x}\right]^2-\mathbf{e}\right\}\\ &= \frac{1}{\alpha}\left[\mathbb{P}\Big(u+\frac{\mathbf{e}}{\alpha}\Big)^{-1/2}\mathbb{P}(\tilde{x})\Big(u+\frac{\mathbf{e}}{\alpha}\Big)^{-1}-\mathbf{e}\right]\\ &= \mathbb{P}\big(\alpha u+\mathbf{e}\big)^{-1/2}\left[\frac{1}{\alpha}\,\mathbb{P}\big(\alpha\tilde{x}\big)\big(\alpha u+\mathbf{e}\big)^{-1}-u-\frac{\mathbf{e}}{\alpha}\right].\end{aligned} \tag{4.8}$$

Note that

$$\big(\alpha u+\mathbf{e}\big)^{-1} = \mathbf{e}-\Big(\mathbf{e}+\frac{u^{-1}}{\alpha}\Big)^{-1} = \mathbf{e}-\alpha\big(\alpha\mathbf{e}+u^{-1}\big)^{-1}.$$

Indeed,

$$\big(\alpha u+\mathbf{e}\big)\Big(\mathbf{e}-\big(\mathbf{e}+(\alpha u)^{-1}\big)^{-1}\Big) = \alpha u+\mathbf{e}-\alpha u\big(\mathbf{e}+(\alpha u)^{-1}\big)\big(\mathbf{e}+(\alpha u)^{-1}\big)^{-1} = \mathbf{e}$$

and

$$\Big(\mathbf{e}-\big(\mathbf{e}+(\alpha u)^{-1}\big)^{-1}\Big)\big(\alpha u+\mathbf{e}\big) = \mathbf{e}\,.$$

We continue Eq. (4.8):

$$\begin{aligned}\frac{x_\alpha}{\alpha} &= \mathbb{P}\big(\alpha u+\mathbf{e}\big)^{-1/2}\left[\frac{1}{\alpha}\,\mathbb{P}\big(\alpha\tilde{x}\big)\Big(\mathbf{e}-\alpha\big(\alpha\mathbf{e}+u^{-1}\big)^{-1}\Big)-u-\frac{\mathbf{e}}{\alpha}\right]\\ &= \mathbb{P}\big(\alpha u+\mathbf{e}\big)^{-1/2}\left[\frac{1}{\alpha}\big(\alpha^2\tilde{x}^2-\mathbf{e}\big)-u-\mathbb{P}\big(\alpha\tilde{x}\big)\big(u^{-1}+\alpha\mathbf{e}\big)^{-1}\right].\end{aligned}$$

Recall that $\tilde{x}=\frac{1}{\alpha}\Big(\mathbb{P}\big(\alpha u+\mathbf{e}\big)\big(\alpha(z+u)+\mathbf{e}\big)\Big)^{1/2}$. Thus

$$\begin{aligned}\frac{1}{\alpha}\big((\alpha\tilde{x})^2-\mathbf{e}\big) &= \frac{1}{\alpha}\Big(\mathbb{P}\big(\alpha u+\mathbf{e}\big)^{1/2}\big(\alpha(z+u)\big)+\alpha u+\mathbf{e}-\mathbf{e}\Big)\\ &= u+\mathbb{P}\big(\alpha u+\mathbf{e}\big)^{1/2}(z+u) \;\longrightarrow\; 2u+z, \text{ when } \alpha\to 0\,.\end{aligned}$$

Note that the latter calculation also implies that $\alpha\tilde{x}\to\mathbf{e}$ when $\alpha\to 0$. With these observations we may eventually write that

$$\frac{1}{\alpha}\,x_\alpha \;\longrightarrow\; 2u+z-u-u = z\in\Omega_+\,. \qquad \square$$

The following Lemma is a simple corollary of Theorem 1 from [29].

Lemma 4.4. *Let a, b, c and d be continuous functions on $(0,\infty)$. Suppose that*

$$a(x)+b(y) = c\big(y/(1+x)\big)+d\Big(x\big(1+y/(1+x)\big)\Big) \tag{4.9}$$

then there exist constants $a, b, c\in\mathbb{R}$ and $c_1+c_2=c_3+c_4$ such that

$$\begin{aligned}a(x) &= b\log x-cx-a\log(1+x)+c_1\,,\\ b(x) &= a\log x-dx+c_2\,,\\ c(x) &= a\log x-dx-b\log(1+x)+c_3\,,\\ d(x) &= b\log x-cx+c_4\,.\end{aligned}$$

In next proposition we solve matrix-variate version of Eq. (4.9), which is our first main result. The solution will be used in the proof of the probabilistic main result of this paper — Theorem 5.1, Section 5.

Proposition 4.2. *Let $A, B, C, D\colon \Omega_+ \to \mathbb{R}$ be continuous functions, such that*

$$A(u) + B(v) \;=\; C\Big(\mathbb{P}\big(\mathbf{e}+u\big)^{-1/2} v\Big) + D\Big(\mathbb{P}\big[\mathbf{e}+\mathbb{P}\big(\mathbf{e}+u\big)^{-1/2} v\big]^{1/2} u\Big) \tag{4.10}$$

for any $u, v \in \Omega_+$. Then there exist constants $a, b, c_1, c_2, d \in \mathbb{R}$ and $\lambda > 0$ such that

$$\begin{aligned} A(x) &= a \log\det x - b \log\det(\mathbf{e}+x) + c_1 + \lambda \operatorname{tr} x\,, \\ B(x) &= b \log\det x + c_2 + d + \lambda \operatorname{tr} x\,, \\ C(x) &= b \log\det x - a \log\det(\mathbf{e}+x) + c_2 + \lambda \operatorname{tr} x\,, \\ D(x) &= a \log\det x + c_1 + d + \lambda \operatorname{tr} x\,. \end{aligned} \tag{4.11}$$

Proof: The proof is divided into three steps.

Step 1. Plugging $u = \alpha\,\mathbf{e}$, $v = \beta\,\mathbf{e}$, $\alpha, \beta > 0$, into Eq. (4.10), we have

$$\widetilde{A}(\alpha) + \widetilde{B}(\beta) \;=\; \widetilde{C}\Big(\frac{\beta}{1+\alpha}\Big) + \widetilde{D}\Big(\alpha\Big(1+\frac{\beta}{1+\alpha}\Big)\Big)\,, \tag{4.12}$$

where

$$\widetilde{A}(\alpha) := A(\alpha\,\mathbf{e})\,, \quad \widetilde{B}(\alpha) := B(\alpha\,\mathbf{e})\,, \quad \widetilde{C}(\alpha) := C(\alpha\,\mathbf{e})\,, \quad \widetilde{D}(\alpha) := D(\alpha\,\mathbf{e})\,.$$

Since we assume that functions A, B, C, D are continuous, then we can use Lemma 4.4 and obtain, *inter alia*, that

$$\widetilde{A}(x) \;=\; a \log x - b \log(1+x) - c\,x + c_1\,, \tag{4.13}$$

where constants a, b, c, c_1 are positive. This observation will be used in Step 3.

Step 2. Set $v = \mathbb{P}\big(\mathbf{e}+\alpha\,\tilde{u}\big)^{1/2} x$ and $u = \alpha\,\tilde{u}$, $x, \tilde{u} \in \Omega_+$, $\alpha > 0$, in (4.10) to get:

$$A(\alpha\,\tilde{u}) + B\Big(\mathbb{P}\big(\mathbf{e}+\alpha\,\tilde{u}\big)^{1/2} x\Big) \;=\; C(x) + D\Big(\alpha\,\mathbb{P}\big(\mathbf{e}+x\big)^{1/2}\,\tilde{u}\Big)\,. \tag{4.14}$$

When $\alpha \to 0$ we have

$$H(\mathbf{e}+x) \;:=\; B(x) - C(x) \;=\; \lim_{\alpha\to 0}\Big\{D\Big(\alpha\,\mathbb{P}(\mathbf{e}+x)^{1/2}\,\tilde{u}\Big) - A(\alpha\,\tilde{u})\Big\}\,.$$

Note that the limit on the right-hand side does not depend on $\tilde{u} \in \Omega_+$. Therefore, for $\tilde{u} = \mathbb{P}(\mathbf{e}+x)^{-1/2}\,(\mathbf{e}+y)$, $y \in \Omega_+$, we get:

$$\begin{aligned} H(\mathbf{e}+x) &= \lim_{\alpha\to 0}\Big\{D\big(\alpha(\mathbf{e}+y)\big) - A\Big(\alpha\,\mathbb{P}\big(\mathbf{e}+x\big)^{-1/2}\,(\mathbf{e}+y)\Big)\Big\} \\ &= \lim_{\alpha\to 0}\Big\{D\big(\alpha(\mathbf{e}+y)\big) - A(\alpha\,\mathbf{e}) + A(\alpha\,\mathbf{e}) - A\Big(\alpha\,\mathbb{P}\big(\mathbf{e}+x\big)^{-1/2}\,(\mathbf{e}+y)\Big)\Big\} \\ &= H(\mathbf{e}+y) + \lim_{\alpha\to 0}\Big\{A(\alpha\,\mathbf{e}) - A\Big(\alpha\,\mathbb{P}\big(\mathbf{e}+x\big)^{-1/2}\,(\mathbf{e}+y)\Big)\Big\}\,. \end{aligned}$$

Denoting

$$G\Big(\mathbb{P}\big(\mathbf{e}+x\big)^{-1/2}(\mathbf{e}+y)\Big) \;=\; -\lim_{\alpha\to 0}\Big\{A(\alpha\,\mathbf{e}) - A\Big(\alpha\,\mathbb{P}\big(\mathbf{e}+x\big)^{-1/2}(\mathbf{e}+y)\Big)\Big\},$$

we have:

$$H(\mathbf{e}+y) \;=\; H(\mathbf{e}+x) + G\Big(P\big(\mathbf{e}+x\big)^{-1/2}(\mathbf{e}+y)\Big) \qquad \text{for any} \quad x,y\in\Omega_+\,,$$

which by Proposition 4.1 gives

$$B(y) - C(y) \;=\; H(\mathbf{e}+y) \;=\; a\log\det(\mathbf{e}+y) + d_1$$

for any $y\in\Omega_+$, where $a, d_1\in\mathbb{R}$.

Notice that Eq. (4.10) can be equivalently written as

$$A\Big(\mathbb{P}\big(\mathbf{e}+u\big)^{-1/2}v\Big) + B\Big(\mathbb{P}\big[\mathbf{e}+\mathbb{P}\big(\mathbf{e}+u\big)^{-1/2}v\big]^{1/2}u\Big) \;=\; C(u)+D(v)\,.$$

Thus, if we repeat the procedure from Step 2 starting with this equation instead of (4.10), then we get

$$D(y) - A(y) \;=\; b\log\det(\mathbf{e}+y) + d_2\,, \qquad b, d_2\in\mathbb{R}\,.$$

From the solution of one-dimensional Eq. (4.12) it follows that $d_1 = d_2 = d\in\mathbb{R}$.

Step 3. The results of Step 2 allow us to define functions $f, g\colon \Omega_+\mapsto\mathbb{R}$ such that for $x\in\Omega_+$

$$\begin{aligned} A(x) \;&=\; a\log\det x - b\log\det(\mathbf{e}+x) + c_1 + f(x)\,,\\ B(x) \;&=\; b\log\det x + c_2 + d + g(x)\,,\\ C(x) \;&=\; b\log\det x - a\log\det(\mathbf{e}+x) + c_2 + g(x)\,,\\ D(x) \;&=\; a\log\det x + c_1 + d + f(x)\,, \end{aligned} \tag{4.15}$$

and due to (4.14), f and g satisfy

$$f(x) + g\Big(\mathbb{P}\big(\mathbf{e}+x\big)^{1/2}y\Big) \;=\; g(y) + f\Big(\mathbb{P}\big(\mathbf{e}+y\big)^{1/2}x\Big)\,. \tag{4.16}$$

Let $x=\alpha\,z_\alpha$, where $\alpha>0$, $z_\alpha\in\Omega_+$ and z_α converges to $z\in\Omega_+$ when α tends to 0. Also set $y = y_\alpha = \beta\,z_\alpha^{-1} - \mathbf{e}$ where $\beta>0$ is large enough for y_α to be in Ω_+ for any $\alpha>0$ and also for the limit $\lim\limits_{\alpha\to 0} y_\alpha\in\Omega_+$ (which is possible since $z_\alpha\to z\in\Omega_+$). Notice that $\mathbb{P}\big(\mathbf{e}+y_\alpha\big)^{1/2}z_\alpha = \beta\,\mathbf{e}$. These observations and Eq. (4.16) allow us to write

$$0 \;=\; \lim_{\alpha\to 0}\big\{f(\alpha\,z_\alpha) - f(\alpha\beta\,\mathbf{e})\big\}\,.$$

From Step 1, Eq. (4.13), we know that $\lim\limits_{\alpha\to 0} f(\alpha\beta\,\mathbf{e}) = 0$. Then

$$\lim_{\alpha\to 0} f(\alpha\,z_\alpha) = 0 \tag{4.17}$$

for any $z_\alpha\in\Omega_+$ such that $z_\alpha\to z\in\Omega_+$.

We will show that f is additive. Firstly, we set $y = u + \mathbf{e}/\alpha$, $u \in \Omega_+$, and $x = x_\alpha$ defined in (4.7). Note that z used in definition (4.7) is an arbitrary element from Ω_+. From Lemma 4.3 we know that x_α/α converges to $z \in \Omega_+$, when $\alpha \to 0$. Thus, for α small enough x_α is inside the cone Ω_+. Given (4.17), we also have $f(x_\alpha) = f(\alpha\, x_\alpha/\alpha) \overset{\alpha\to 0}{\longrightarrow} 0$. Note that $\mathbb{P}\big(\mathbf{e} + x_\alpha\big)^{\frac{1}{2}}\,(u + \mathbf{e}/\alpha) = z + u + \mathbf{e}/\alpha$. We rewrite Eq. (4.16) with those special x and y. After taking the limit as $\alpha \to 0$ we obtain

$$f(z) \;=\; \lim_{\alpha\to 0}\left\{ g\Big(z + u + \frac{1}{\alpha}\,\mathbf{e}\Big) - g\Big(u + \frac{1}{\alpha}\,\mathbf{e}\Big)\right\}. \tag{4.18}$$

On the other hand, if we plug $x = \alpha\, u$ and $y = \mathbf{e}/\alpha$ in Eq. (4.16) and take the limit as $\alpha \to 0$, we obtain $\lim\limits_{\alpha\to 0}\big\{g(u + \mathbf{e}/\alpha) - g(\mathbf{e}/\alpha)\big\} = f(u)$. Combining this result with Eq. (4.18) we have

$$\begin{aligned} f(u) + f(z) \;&=\; \lim_{\alpha\to 0}\left\{ g\Big(u + \frac{1}{\alpha}\,\mathbf{e}\Big) - g\Big(\frac{1}{\alpha}\,\mathbf{e}\Big) + g\Big(z + u + \frac{1}{\alpha}\,\mathbf{e}\Big) - g\Big(u + \frac{1}{\alpha}\,\mathbf{e}\Big)\right\} \\ &=\; \lim_{\alpha\to 0}\left\{ g\Big(z + u + \frac{1}{\alpha}\,\mathbf{e}\Big) - g\Big(\frac{1}{\alpha}\,\mathbf{e}\Big)\right\} \\ &=\; f(z + u)\,. \end{aligned}$$

Note that this equation, $f(u) + f(z) = f(u + z)$, holds for all $u, z \in \Omega_+$. By Lemma 4.1 we conclude that $f(x) = \langle c, x\rangle$ where $c \in \Omega_+$. Similarly, due to symmetry in (4.16), we show that $g(x) = \langle \tilde{c}, x\rangle$. Eq. (4.16) with $x = \alpha\, u$, $y = \mathbf{e}/\alpha$ implies $\tilde{c} = c$.

The last step of the proof is to show that $c = \lambda\,\mathbf{e}$ for real and positive λ. We will use Lemma 4.2 to do that. For f and g identified above, Eq. (4.16) assumes the form

$$\Big\langle c,\; \alpha^2\,\mathbb{P}\big(\mathbf{e} + x\big)^{1/2}\,(\mathbf{e} + y)\Big\rangle \;=\; \Big\langle c,\; \alpha^2\,\mathbb{P}\big(\mathbf{e} + y\big)^{1/2}\,(\mathbf{e} + x)\Big\rangle$$

for any $\alpha > 0$. Note that for any $u, v \in \Omega_+$ there exist $\alpha > 0$, $x, y \in \Omega_+$ such that $\alpha(\mathbf{e} + x) = u^2$ and $\alpha(\mathbf{e} + y) = v^2$. Thus, we can use Lemma 4.2 to conclude that $c = \lambda\,\mathbf{e}$, where $\lambda > 0$. Consequently, we have

$$\begin{aligned} A(x) \;&=\; a\,\log\det x - b\,\log\det(\mathbf{e} + x) + c_1 + \lambda\,\operatorname{tr} x\,, \\ B(x) \;&=\; b\,\log\det x + c_2 + d + \lambda\,\operatorname{tr} x\,, \\ C(x) \;&=\; b\,\log\det x - a\,\log\det(\mathbf{e} + x) + c_2 + \lambda\,\operatorname{tr} x\,, \\ D(x) \;&=\; a\,\log\det x + c_1 + d + \lambda\,\operatorname{tr} x\,. \end{aligned} \tag{4.19}$$

□

5. CHARACTERIZATION OF MATRIX-KUMMER AND WISHART DISTRIBUTIONS

In this section we prove the converse to the independence property from Theorem 3.1, that is a new characterization of the matrix-Kummer and the Wishart distributions. Similarly to the one-dimensional case considered in [29], we need to impose some regularity conditions on densities.

Theorem 5.1. *Let X and Y be independent random variables valued in Ω_+ with positive and continuous densities. Assume that random matrices*

$$U = \mathbb{P}\big[(\mathbf{e}+X)^{-1/2}\big]\, Y \qquad \text{and} \qquad V = \mathbb{P}\big[(\mathbf{e}+U)^{1/2}\big]\, X$$

are also independent.

Then there exist $a > (r-1)/2$, $b > (r-1)/2 - a$ and $\lambda > 0$ such that $X \sim \mathcal{MK}(a, b, \lambda\mathbf{e})$ and $Y \sim \mathcal{W}(a+b, \lambda\mathbf{e})$.

Proof: Recall that

$$T(x,y) = \left(\mathbb{P}\Big[(\mathbf{e}+x)^{-\frac{1}{2}}\Big]\, y,\ \mathbb{P}\left[\left(\mathbf{e}+\mathbb{P}\Big[(\mathbf{e}+x)^{-\frac{1}{2}}\Big]\, y\right)^{\frac{1}{2}}\right] x \right).$$

Then $(U,V) = T(X,Y)$ and $(X,Y) = T(U,V)$.

Independence of random variables together with continuity of their densities imply

$$f_U(u)\, f_V(v) = |\mathrm{J}(u,v)|\, f_X(x)\, f_Y(y) \qquad \text{for all} \quad u, v \in \Omega_+\,, \tag{5.1}$$

where $(x,y) = T(u,v)$ and the Jacobian J of T^{-1} is given in Proposition 3.1. Taking logarithms of both sides in (5.1) and defining functions $A, B, C, D\colon \Omega_+ \to \mathbb{R}$ as

$$\begin{aligned}
A(u) &= \log f_U(u) + \frac{r+1}{2} \log\det u\,,\\
B(u) &= \log f_V(u) + \frac{r+1}{2} \log\det u\,,\\
C(u) &= \log f_X(u) + \frac{r+1}{2} \log\det u\,,\\
D(u) &= \log f_Y(u) + \frac{r+1}{2} \log\det u\,,
\end{aligned}$$

we can rewrite Eq. (5.1) in the following way:

$$A(u) + B(v) = C\Big(\mathbb{P}\big(\mathbf{e}+u\big)^{-1/2} v\Big) + D\left(\mathbb{P}\left(\mathbf{e}+\mathbb{P}\big(\mathbf{e}+u\big)^{-1/2} v\right)^{1/2} u\right), \qquad u, v \in \Omega_+\,. \tag{5.2}$$

From Proposition 4.2 it follows:

$$\begin{aligned}
A(x) &= a \log\det x - b \log\det(\mathbf{e}+x) + c_1 + \lambda\, \mathrm{tr}\, x\,,\\
B(x) &= b \log\det x + c_2 + d + \lambda\, \mathrm{tr}\, x\,,\\
C(x) &= b \log\det x - a \log\det(\mathbf{e}+x) + c_2 + \lambda\, \mathrm{tr}\, x\,,\\
D(x) &= a \log\det x + c_1 + d + \lambda\, \mathrm{tr}\, x\,.
\end{aligned} \tag{5.3}$$

The latter and the fact, that functions A, B, C and D represent logarithms of densities of random variables, imply $X \sim \mathcal{MK}(a, b, \lambda\mathbf{e})$ and $Y \sim \mathcal{W}(a+b, \lambda\mathbf{e})$. □

6. CONCLUDING REMARKS

Recently P. Vallois indicated[1] that one can define a transformation which generalizes T_0 for random matrices, is different from (3.1) and also preserves independence of Wishart and matrix-Kummer random matrices. Namely, let

$$T(x,y) \;=\; \Big(\mathbb{P}\big(\mathbf{e}+x+y\big)\,(\mathbf{e}+x)^{-1}-\mathbf{e}\,,\;\; x+y-\Big[\mathbb{P}\big(\mathbf{e}+x+y\big)\,(\mathbf{e}+x)^{-1}-\mathbf{e}\Big]\Big)\,.$$

Vallois says, and this can be checked in standard way, that if $X\sim\mathcal{MK}(a,b,\Sigma)$ and $Y\sim\mathcal{W}(a+b,\Sigma)$ are independent, then $(U,V)=T(X,Y)$ are also independent. Note that since $U+V=X+Y$ here, then Σ can be any positive definite matrix, which was not true in our case. If the converse theorem holds, remains an open question.

We hope that the probabilistic results of this paper can help to state and prove an analogous property in free (non-commutative) probability. Let us recall that in the case of the Matsumoto–Yor property, its analogue in free probability was accomplished through an appropriate matrix independence property, [31]. This problem is currently being under study.

In [29] authors formulated multivariate characterization of a product of $p-1$ Kummer random variables and one Gamma random variable, $p\geq 2$. There, Kummer is a marginal distribution of a certain p-dimensional distribution, called tree-Kummer distribution in the paper, see Section 3 in [29]. For instance, when $p=2$, then this density is of the form

$$f(x_1,x_2)\;\propto\; x_1^{a_1-1}\,x_2^{a_2-1}\exp\Big\{-c\big(x_1+x_2+x_1x_2\big)\,I_{(0,\infty)^2}(x_1,x_2)\Big\}\,.$$

Similarly, matrix-Kummer distribution appears naturally as a marginal distribution of the following generalization of bi-Wishart distribution

$$f_{(X,Y)}(x,y)\;\propto\;(\det x)^{p-\frac{r+1}{2}}\,(\det y)^{q-\frac{r+1}{2}}\,\exp\big(-\big\langle c,\,x+y+xy\big\rangle\big)\,I_{\Omega_+\times\Omega_+}(x,y)\,,\qquad c>0\,.$$

Then the conditional distribution of X given Y is Wishart $\mathcal{W}\big(p,c(\mathbf{e}+y)\big)$, while its marginal distribution is matrix-Kummer $\mathcal{MK}(p,q-p,c)$. Also a question arises if a multivariate version of our independence characterization holds in a matrix setting?

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BOOTSTRAP PREDICTION INTERVAL FOR ARMA MODELS WITH UNKNOWN ORDERS

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Abstract:

- This paper aims to investigate the construction of the prediction intervals for ARMA (p, q) models with unknown orders. We present the bootstrap algorithms for the prediction intervals based on the bootstrap distribution of orders (p, q). The asymptotic properties of the intervals are also discussed. The Monte Carlo simulation studies show that the proposed algorithm significantly improves the coverage accuracy of the prediction interval compared to the methods using pre-estimated values of orders, especially when the sample size is small and the true model order is low.

Key-Words:

- *ARMA model; asymptotic properties; bootstrap; prediction interval.*

AMS Subject Classification:

- 62M10, 62F40.

1. INTRODUCTION

As indicated in [13], the construction of prediction intervals for time series models is both important and intriguing, see also, e.g., [1, 2, 4, 6, 7], [10], [12] and [15, 17, 18]. The prediction intervals can show explicitly the uncertainty underlying the estimation procedure and measure the accuracy with the point predictors.

An early review article by [12] covered several methods of construction of prediction intervals for linear regression models under normal assumption. [15] proposed an asymptotically valid prediction interval for linear models based on normal approximations. It is known that Gaussian-based prediction intervals produce poor coverages when the distributional assumptions are violated. As a remedy, some form of resampling, for example the residual-based bootstrap, is necessary.

The literature on predictive intervals for time series is not large. In order to construct prediction intervals without the assumption of Gaussianity, [11] developed a coherent bootstrap algorithm of constructing prediction intervals for time series that can be modeled as linear, nonlinear or nonparametric autoregression AR(p) with known order p. Their bootstrap intervals are able to capture the predictor variability due to the innovation errors as well as the estimation errors.

For other time series models, [3] presented a bootstrap approach called The Boot.EXPOS to forecast time series through combining the use of exponential smoothing methods with the bootstrap methodology. [14] developed a bootstrap prediction interval procedure by using a pre-estimated order of the AR approximation for FARIMA processes. [9] provided a bootstrap method for estimating the parameters of ARMA (p, q) models. [13] derived model-free prediction intervals based on a new model-free prediction principle and bootstrapping, which can be applied to nonparametric time series models with known orders.

To the best of our knowledge, the construction of bootstrap prediction intervals based on the bootstrap distribution of the orders for ARMA (p, q) models with unknown orders remain essentially unexplored. This is the issue we intend to address in the current paper.

Section 2 presents the algorithms for the construction of bootstrap prediction intervals for ARMA (p, q) models with known orders and unknown orders, respectively. The asymptotic validity and asymptotic pertinence of the intervals are addressed in Section 3. The paper is concluded with simulation studies comparing the finite sample performance of the proposed method with other methods in terms of coverage level and length of interval in Section 4. The proofs of the theorems are given in the Appendix.

2. BOOTSTRAP PREDICTION INTERVALS FOR ARMA MODELS

Consider the strictly stationary, causal ARMA (p, q) model defined by the recursion

$$X_t = \sum_{j=1}^{p} a_j X_{t-j} + \sum_{j=0}^{q} b_j \varepsilon_{t-j}, \qquad t \in \mathbb{Z}, \quad b_0 = 1, \tag{2.1}$$

with $\{\varepsilon_t\}$ being i.i.d. with mean zero, variance σ^2, where $1-\sum_{j=1}^{p} a_j z^j \neq 0$ and $\sum_{j=0}^{q} b_j z^j \neq 0$ for $|z| \leq 1$, and $1-\sum_{j=1}^{p} a_j z^j$ and $\sum_{j=0}^{q} b_j z^j$ have no zeros in common.

Suppose that we have the observations $\{X_t,\, t=1,2,...,n\}$ and denote by $\hat{X}_{n+1}$ the point predictor of X_{n+1} based on the data $X_1,...,X_n$. Let $\theta = (a_1,...,a_p,b_1,...,b_q)^{\mathsf{T}}$. [8] defined an M-estimator $\hat{\theta}^M$ of θ for model (2.1), where $\hat{\theta}^M = (\hat{a}^M_{1,n},...,\hat{a}^M_{p,n},\hat{b}^M_{1,n},...,\hat{b}^M_{q,n})^{\mathsf{T}}$ is the solution of the equation

$$\Psi_n(\theta) \;=\; \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \psi\big(\varepsilon_j(\theta)\big)\, Z(j-1;\theta) \;=\; 0$$

for some suitably chosen score function ψ, where

$$\varepsilon_j(\theta) \;=\; \sum_{k=0}^{j-1} \beta_k(\theta) \left(X_{j-k} - \sum_{i=1}^{p} a_i\, X_{j-k-i} \right), \qquad j=1,...,n\,,$$

and

$$Z(j-1;\theta) \;=\; \sum_{k=0}^{j-1} \beta_k(\theta) \Big(X\big(j-1-k\big)^{\mathsf{T}},\, E\big(j-1-k;\theta\big)^{\mathsf{T}} \Big)^{\mathsf{T}}, \qquad j=1,...,n\,,$$

where $\beta_k(\theta)$ satisfies

$$\sum_{k=0}^{\infty} \beta_k(\theta)\, z^k \;=\; \left(1 + \sum_{j=1}^{q} b_j\, z^j \right)^{-1}, \qquad |z| \leq 1\,,$$

and $X(j-1) = \big(X_{j-1},...,X_{j-p}\big)^{\mathsf{T}}$, $E(j-1;\theta) = \big(\varepsilon_{j-1}(\theta),...,\varepsilon_{j-q}(\theta)\big)^{\mathsf{T}}$, $X_j = 0$ and $\varepsilon_j(\theta) = 0$ for $j \leq 0$.

Theorem 3.1 of [8] showed that, under some mild conditions, $\sqrt{n}\,\big(\hat{\theta}^M - \theta\big)$ is asymptotically normally distributed. Therefore, we define $\hat{X}_{n+1}$ as

$$\hat{X}_{n+1} \;=\; \sum_{k=1}^{p} \hat{a}^M_{k,n}\, X_{n+1-k} + \sum_{k=1}^{q} \hat{b}^M_{k,n}\, \hat{\varepsilon}_{n+1-k,n}\big(\hat{\theta}^M\big)\,, \tag{2.2}$$

where

$$\hat{\varepsilon}_{j,n}\big(\hat{\theta}^M\big) \;=\; \sum_{k=0}^{j-1} \beta_k\big(\hat{\theta}^M\big) \left(X_{j-k} - \sum_{i=1}^{p} \hat{a}^M_{i,n}\, X_{j-k-i} \right), \qquad j=1,...,n\,. \tag{2.3}$$

2.1. Bootstrap prediction intervals for ARMA models with known orders

In this subsection we assume that the orders p and q of the ARMA (p,q) model are known. Inspired by the algorithms discussed in [11], we provide the following bootstrap algorithm of the prediction interval for X_{n+1} based on (2.2). Let the one-step ahead predictive root be defined as $X_{n+1} - \hat{X}_{n+1}$. The algorithm actually uses the distribution of the bootstrap predictive root to estimate the distribution of the true predictive root.

B-ARMARoots Algorithm:

1. Use observations $X_1, ..., X_n$ to obtain M-estimator $\hat{\theta}^M$ for model (2.1).

2. Compute the fitted residuals $\hat{\varepsilon}_{j,n}(\hat{\theta}^M)$ from (2.3), denote by $\hat{\varepsilon}_{\cdot,n}$ the mean of the fitted residuals, center the fitted residuals, and compute the empirical distribution $\hat{F}_n$ of $\hat{\varepsilon}_{j,n} - \hat{\varepsilon}_{\cdot,n}$

$$\hat{F}_n(x) = \frac{1}{n}\sum_{j=1}^{n} \mathbf{1}_{[\hat{\varepsilon}_{j,n}-\hat{\varepsilon}_{\cdot,n},\infty)}(x)\,, \qquad x \in \mathbb{R}\,,$$

where $\mathbf{1}_A$ is the indicator function of set A.

3. Compute the predicted future value $\hat{X}_{n+1}$ using (2.2).

4. Draw bootstrap pseudo residuals $\{\varepsilon_j^*\}$ from $\hat{F}_n$, calculate the pseudo-data $\{X_j^*\}$ by

$$X_j^* = \sum_{k=1}^{p} \hat{a}_{k,n}^M X_{j-k}^* + \sum_{k=1}^{q} \hat{b}_{k,n}^M \varepsilon_{j-k}^* + \varepsilon_j^*\,.$$

5. Use the pseudo-data $X_1^*, ..., X_n^*$ to obtain M-estimator $\hat{\theta}^{M,*}$. Then compute the residuals

$$\hat{\varepsilon}_{j,n}^*(\hat{\theta}^{M,*}) = \sum_{k=0}^{j-1} \beta_k(\hat{\theta}^{M,*}) \left(X_{j-k} - \sum_{i=1}^{p} \hat{a}_{i,n}^{M,*} X_{j-k-i} \right), \qquad j = 1, ..., n\,.$$

6. Compute the bootstrap predicted future value

$$\hat{X}_{n+1}^* = \sum_{k=1}^{p} \hat{a}_{k,n}^{M,*} X_{n+1-k} + \sum_{k=1}^{q} \hat{b}_{k,n}^{M,*} \hat{\varepsilon}_{n+1-k,n}^*(\hat{\theta}^{M,*})\,.$$

7. Compute the future bootstrap observation X_{n+1}^*

$$X_{n+1}^* = \sum_{k=1}^{p} \hat{a}_{k,n}^M X_{n+1-k} + \sum_{k=1}^{q} \hat{b}_{k,n}^M \hat{\varepsilon}_{n+1-k,n}(\hat{\theta}^M) + \varepsilon_{n+1}^*\,.$$

Then compute the one-step ahead predictive root $X_{n+1}^* - \hat{X}_{n+1}^*$.

8. Repeat Steps 4–7 above B times, compute the empirical distribution of $X_{n+1}^* - \hat{X}_{n+1}^*$ whose $\alpha/2$-quantile is denoted by $q(\alpha/2)$. Construct the $(1-\alpha)100\%$ equal-tailed prediction interval for X_{n+1} as

$$\left[\hat{X}_{n+1} + q(\alpha/2)\,,\ \hat{X}_{n+1} + q(1-\alpha/2)\right]. \tag{2.4}$$

In Step 4, to ensure the stationarity of the bootstrap series, one usually generates $n+m$ pseudo residuals from $\hat{F}_n$ for some large positive m to compute the pseudo-data $\{X_j^*\}$, and then discard the first m data.

2.2. Bootstrap prediction intervals for ARMA models with unknown orders

In practice, the orders of ARMA models are usually unknown. In this subsection we introduce the bootstrap prediction interval under this case.

Given observations $X_1, ..., X_n$ from ARMA (p, q) model (2.1), to construct the prediction interval for X_{n+1}, an intuitive method one may consider is the following

OB-ARMARoots Algorithm:

1. Determine the orders p_0, q_0 using, e.g., AIC criteria.

2. Apply B-ARMARoots Algorithm to construct the prediction interval for ARMA (p_0, q_0) model.

Since AIC is biased when the sample size is small, [5] presented a bootstrap version of AIC, denoted AIC*, which generally outperforms the original AIC. AIC* is obtained by bootstrapping both the likelihood and the bias term of AIC. That is,

$$\text{AIC}^* \;=\; -2\,\log\big(L(\hat{\theta}^*|x^*)\big) + (2K)^*, \qquad K = p + q\,,$$

with K the number of parameters and $L(\cdot)$ the log likelihood function. In the case of ARMA models, $L(\cdot)$ can be computed by using the estimated variance of the residuals.

Applying the procedure in [5], we can obtain the bootstrap distribution of the orders (p, q). Next we propose the bootstrap algorithm of the prediction interval based on the bootstrap distribution of the orders.

CB-ARMARoots Algorithm:

1. Determine a pair of maximum orders for ARMA model, say (P, Q).

2. Approximate an $\text{AR}\big(p(n)\big)$ model to $X_1, ..., X_n$. The order $p(n)$ can be selected by using the AIC criteria. Then construct the estimators of the autoregressive coefficients $\hat{\varphi}_{1,n}, ..., \hat{\varphi}_{p(n),n}$ using Yule–Walker method, compute the residuals

$$\hat{\varepsilon}_{t,n} \;=\; X_t - \sum_{j=1}^{p(n)} \hat{\varphi}_{j,n}\, X_{t-j}\,.$$

3. Center the residuals, $\tilde{\varepsilon}_{t,n} = \hat{\varepsilon}_{t,n} - \big(n - p(n)\big)^{-1} \sum_{j=p(n)+1}^{n} \hat{\varepsilon}_{j,n}$, and compute the empirical distribution of $\{\tilde{\varepsilon}_{t,n}\}$

$$\hat{F}_{\varepsilon,n}(x) \;=\; \big(n - p(n)\big)^{-1} \sum_{t=p(n)+1}^{n} \mathbf{1}_{[\tilde{\varepsilon}_{t,n} \le x]}\,.$$

4. Draw bootstrap pseudo residuals $\{\varepsilon_t^*\}$ from $\hat{F}_{\varepsilon,n}$, generate bootstrap sample $\{X_t^*\}$ by the recursion

$$X_t^* \;=\; \sum_{j=1}^{p(n)} \hat{\varphi}_{j,n}\, X_{t-j}^* + \varepsilon_t^*\,.$$

5. For bootstrap sample $\{X_t^*\}$, fit an exhaustive set of size $(P+1)*(Q+1)$ of tentative ARMA (p, q), compute AIC* for all the candidate pairs (p, q). Then $(\hat{p}^*, \hat{q}^*)$ is identified according to

$$(\hat{p}^*, \hat{q}^*) \;=\; \arg \min_{p \le P,\, q \le Q} \text{AIC}^*(p, q)\,.$$

6. Repeat Steps 4–5 B_1 times, denote the number of the pairs (p,q) out of the group of the B_1 pairs as $b_{p,q}$.

7. For any pair (p,q) in Step 6, Steps 1–7 in B-ARMARoots Algorithm are repeated $B_2 \times b_{p,q}$ times to obtain $B_2 \times b_{p,q}$ values of $X^*_{n+1} - \hat{X}^*_{n+1}$.

8. Repeat Step 7 to obtain $B_1 \times B_2$ values of $X^*_{n+1} - \hat{X}^*_{n+1}$. Then compute the empirical distribution of $X^*_{n+1} - \hat{X}^*_{n+1}$ whose $\alpha/2$-quantile is denoted by $q(\alpha/2)$. Construct the $(1-\alpha)100\%$ equal-tailed prediction interval for X_{n+1} as

$$\left[\hat{X}_{n+1} + q(\alpha/2),\ \hat{X}_{n+1} + q(1-\alpha/2)\right]. \tag{2.5}$$

In Step 1, the choice of the maximum order (P,Q) is *a priori* and arbitrary. For computational reasons and from a practical point of view, (P,Q) should not be too large. For example, economic time series can usually be modeled as ARMA processes with orders not greater than 3. Therefore, in the simulation studies in Section 4, we set $P = Q = 5$.

In Step 2, we use the AIC criteria to determine the order $p(n)$, because, as discussed in [16], the order selected from the AIC criteria is asymptotically efficient for the infinite order autoregressive models. In the simulation studies we select $p(n)$ that minimizes the AIC evaluated over a range of $[1, 10\log_{10}(n)]$. Moreover, we can also select the order $p(n)$ by iterative estimate of the spectral density on the residuals coming from the fitting procedure of tentative autoregressive models until closeness to a constant is reached. That is, starting from $\tilde{p} = 1$, we fit an AR($\tilde{p}$) model to $X_1, ..., X_n$ using e.g. Yule–Walker method and then estimate the spectral density of the residuals. If the estimated spectral density is close to a constant, stop and set $p(n) = \tilde{p}$. Otherwise, let $\tilde{p} = \tilde{p} + 1$, repeat the previous procedure until the estimator of the spectral density is almost a constant.

In Step 6, $b_{p,q}$ stands for the number of (p,q) appeared among all the B_1 pairs obtained by Step 5. For example, let $B_1 = 1000$, after Steps 4–5 are repeated 1000 times, we obtain 1000 pairs of orders $(\hat{p}^*, \hat{q}^*)$ from Step 5. If, among all these pairs, $(1,1)$ appears 10 times, then $b_{1,1} = 10$.

Again in Step 4, to ensure the stationarity of the bootstrap series, we use the techniques mentioned at the end of Section 2.1.

3. ASYMPTOTIC PROPERTIES OF BOOTSTRAP PREDICTION INTERVALS

In this section we investigate the asymptotic properties of bootstrap prediction intervals proposed in the previous section. Using the notations in [11], we define the asymptotic validity and the asymptotic pertinence of bootstrap prediction intervals for ARMA (p,q) models.

Definition 3.1 (Asymptotic validity of bootstrap prediction interval)**.** Let L_n, U_n be the functions of $X_1, ..., X_n$. The interval $[L_n, U_n]$ is called a $(1-\alpha)100\%$ asymptotically valid prediction interval for X_{n+1} if

$$P\big(L_n \le X_{n+1} \le U_n\big) \to 1-\alpha \qquad \text{as} \quad n \to \infty\,.$$

Let

$$
\begin{aligned}
A_n &= \sum_{j=1}^{p} a_j X_{n+1-j} - \sum_{j=1}^{p} \hat{a}_{j,n}^{M} X_{n+1-j}\,, \\
B_n &= \sum_{j=1}^{q} b_j \varepsilon_{n+1-j} - \sum_{j=1}^{q} \hat{b}_{j,n}^{M} \hat{\varepsilon}_{n+1-j,n}\big(\hat{\theta}^{M}\big)\,, \\
A_n^* &= \sum_{j=1}^{p} \hat{a}_{j,n}^{M} X_{n+1-j} - \sum_{j=1}^{p} \hat{a}_{j,n}^{M,*} X_{n+1-j} \\
\text{and} \\
B_n^* &= \sum_{j=1}^{q} \hat{b}_{j,n}^{M} \hat{\varepsilon}_{n+1-j,n}\big(\hat{\theta}^{M}\big) - \sum_{j=1}^{q} \hat{b}_{j,n}^{M,*} \hat{\varepsilon}_{n+1-j,n}^{*}\big(\hat{\theta}^{M,*}\big)\,.
\end{aligned}
$$

Then, the predictive root and the bootstrap predictive root can be written as

$$
\begin{aligned}
X_{n+1} - \hat{X}_{n+1} &= \varepsilon_{n+1} + A_n + B_n \\
\text{and} \\
X_{n+1}^* - \hat{X}_{n+1}^* &= \varepsilon_{n+1}^* + A_n^* + B_n^*\,.
\end{aligned}
$$

Definition 3.2 (Asymptotic pertinence of bootstrap prediction interval)**.** A bootstrap prediction interval is called asymptotically pertinent provided the bootstrap satisfies the following four conditions

- (**i**) $\sup_x \big|P\big(\varepsilon_{n+1} \le x\big) - P\big(\varepsilon_{n+1}^* \le x\big)\big| \to^p 0$ as $n \to \infty$, where $\to^p$ stands for convergence in probability.
- (**ii**) $A_n + B_n \to^p 0$ and $A_n^* + B_n^* \to^p 0$ as $n \to \infty$.
- (**iii**) $\big|P\big(a_n A_n \le x\big) - P\big(a_n A_n^* \le x\big)\big| \to^p 0$ for some sequence $a_n \to \infty$, for all points x where $P\big(a_n A_n \le x\big)$ is continuous.
- (**iv**) ε_{n+1}^* and A_n^* are independent.

The following two theorems address the asymptotic validity and the stronger property of asymptotic pertinence of the prediction interval (2.4) using B-ARMA Roots Algorithm.

Theorem 3.1. *For ARMA model (2.1) with known orders p and q, the prediction interval (2.4) is asymptotically valid.*

Theorem 3.2. *For ARMA model (2.1) with known orders p and q, the prediction interval (2.4) is asymptotically pertinent.*

The next theorem gives the asymptotic validity and the asymptotic pertinence of the prediction interval (2.5) using CB-ARMARoots Algorithm.

Theorem 3.3. *For ARMA model (2.1) with unknown orders p an q, the prediction interval (2.5) is asymptotically valid and asymptotically pertinent.*

4. MONTE CARLO SIMULATIONS

In this section, we evaluate and compare the performance of the proposed CB-ARMA algorithm based on the bootstrap distribution of the orders and the OB-ARMA algorithm with pre-estimated fixed orders, as well as two types of bootstrap prediction intervals via predictive roots and percentile methods, respectively.

In contrast to the predictive root methods adopted in this paper, the percentile method uses the bootstrap distribution of X^*_{n+1} to estimate the distribution of the future value X_{n+1} instead of using the distribution of the bootstrap predictive root to estimate the distribution of the true predictive root, where

$$X^*_{n+1} = \sum_{k=1}^{p} \hat{a}^{M,*}_{k,n} X_{n+1-k} + \sum_{k=1}^{q} \hat{b}^{M,*}_{k,n} \hat{\varepsilon}^*_{n+1-k,n}\big(\hat{\theta}^{M,*}\big) + \varepsilon^*_{n+1}\,.$$

Data are generated from the following eight models with sample sizes $n = 25, 50, 75, 100, 200$ and 400 for each model.

(**1**) ARMA(1,1) model:

$$X_{t+1} = 0.5\,X_t + 0.5\,\varepsilon_t + \varepsilon_{t+1}\,,$$

where errors $\{\varepsilon_t\}$ are from N(0,1);

(**2**) ARMA(1,1) model:

$$X_{t+1} = 0.5\,X_t + 0.5\,\varepsilon_t + \varepsilon_{t+1}\,,$$

where errors $\{\varepsilon_t\}$ are from Laplace distribution with mean 0 and variance 1;

(**3**) ARMA(1,2) model:

$$X_{t+1} = 0.5\,X_t + 0.4\,\varepsilon_t + 0.2\,\varepsilon_{t-1} + \varepsilon_{t+1}\,,$$

where errors $\{\varepsilon_t\}$ are from N(0,1);

(**4**) ARMA(1,2) model:

$$X_{t+1} = 0.5\,X_t + 0.4\,\varepsilon_t + 0.2\,\varepsilon_{t-1} + \varepsilon_{t+1}\,,$$

where errors $\{\varepsilon_t\}$ are from Laplace distribution with mean 0 and variance 1;

(**5**) ARMA(2,2) model:

$$X_{t+1} = -0.5\,X_t + 0.4\,X_{t-1} + 0.4\,\varepsilon_t + 0.2\,\varepsilon_{t-1} + \varepsilon_{t+1}\,,$$

where errors $\{\varepsilon_t\}$ are from N(0,1);

(**6**) ARMA(2,2) model:

$$X_{t+1} = -0.5\,X_t + 0.4\,X_{t-1} + 0.4\,\varepsilon_t + 0.2\,\varepsilon_{t-1} + \varepsilon_{t+1}\,,$$

where errors $\{\varepsilon_t\}$ are from Laplace distribution with mean 0 and variance 1.

(**7**) ARMA(3,1) model:

$$X_{t+1} = -0.5\,X_t + 0.2\,X_{t-1} + 0.2\,X_{t-2} + 0.4\,\varepsilon_t + \varepsilon_{t+1}\,,$$

where errors $\{\varepsilon_t\}$ are from N(0,1);

(**8**) ARMA(3,1) model:

$$X_{t+1} = -0.5\,X_t + 0.2\,X_{t-1} + 0.2\,X_{t-2} + 0.4\,\varepsilon_t + \varepsilon_{t+1}\,,$$

where errors $\{\varepsilon_t\}$ are from Laplace distribution with mean 0 and variance 1.

We use four bootstrap methods to create $B = 1000$ bootstrap pseudo-series, respectively, and construct the prediction intervals $[L, U]$ with nominal coverage levels of 95% and 90%. For CB-ARMA algorithm, we choose $B_1 = B_2 = 1000$. To assess the corresponding empirical coverage level (CVR) and average length (LEN) of the constructed interval, we also generate 1000 one-step ahead future values $X_{n+1,j} = \sum_{k=1}^{p} \hat{a}_{k,n}^{M} X_{n+1-k} + \sum_{k=1}^{q} \hat{b}_{k,n}^{M}\, \hat{\varepsilon}_{n+1-k,n}\big(\hat{\theta}^{M}\big) + \varepsilon_j^*$. Then, CVR and LEN are given by

$$\mathrm{CVR} = \frac{1}{1000} \sum_{j=1}^{1000} \mathbf{1}_{[L,U]}\big(X_{n+1,j}\big)\,, \qquad \mathrm{LEN} = U - L\,.$$

Tables 1–8 report the simulation results for eight models using four bootstrap methods. Generally speaking, the CB-ARMA algorithm based on the bootstrap distribution of the orders is generally superior to OB-ARMA algorithm. The bootstrap prediction intervals using CB-ARMARoots method proposed in this paper uniformly improve CVRs as compared to the other three methods, while in most cases the interval length is increased as a price to pay for using CB-ARMA algorithm. But there are some exceptions that the LEN of CB-ARMA intervals is smaller than the LEN of OB-ARMA intervals when $n = 200$ or $n = 400$ in Tables 2, 3, 5 and 8.

Comparing Tables 1–4 with Tables 5–8, we see that, when the true order of the ARMA model is lower, the OB-ARMA algorithm performs worse with respect to the coverage level. Because the AIC criterion tends to select higher order which results in overfitting.

From Tables 1–2 it is clear that, when the sample size is small ($n \leq 200$) and the order selected from AIC criterion is larger than the true model order, CB-ARMA algorithm compares favorably with OB-ARMA algorithm. When the sample size is large ($n = 400$), CB-ARMA algorithm still outperforms OB-ARMA algorithm in terms of coverage in most cases, but the improvement is not as big as that for the case of small sample sizes. Table 8 implies that, for large sample size and high model order, CB-ARMA and OB-ARMA have similar coverage level but OB-ARMA is slightly superior to CB-ARMA in some cases.

Moreover, ARMARoots algorithm generally offers improvements in the coverage accuracy comparing to ARMAPercentile algorithm, but using CB-ARMARoots method generally increases the length of the intervals. However, when the errors have Laplace distribution, there are several cases where CB-ARMARoots intervals have smaller length compared to CB-ARMAPercentile method.

Table 1: CVR and LEN for ARMA(1,1) with Normal innovations.

Normal	Nominal coverage 95%		Nominal coverage 90%	
	CVR	LEN	CVR	LEN
$n=25$				
CB-ARMARoots	98.7%	6.51	95.9%	4.99
CB-ARMAPercentile	97.4%	5.65	94.2%	4.77
OB-ARMARoots	91.9%	4.55	84.7%	3.91
OB-ARMAPercentile	92.7%	4.59	88.8%	3.97
$n=50$				
CB-ARMARoots	96.6%	4.47	91.4%	3.62
CB-ARMAPercentile	95.0%	4.37	89.8%	3.54
OB-ARMARoots	90.4%	3.96	88.6%	3.21
OB-ARMAPercentile	90.5%	3.84	88.2%	3.15
$n=75$				
CB-ARMARoots	97.3%	5.61	95.0%	4.75
CB-ARMAPercentile	95.8%	5.23	92.5%	4.27
OB-ARMARoots	92.1%	4.23	90.3%	3.93
OB-ARMAPercentile	92.1%	4.22	90.5%	3.95
$n=100$				
CB-ARMARoots	97.4%	4.45	92.9%	3.62
CB-ARMAPercentile	96.2%	4.31	92.0%	3.61
OB-ARMARoots	93.0%	3.65	90.6%	3.38
OB-ARMAPercentile	93.5%	3.68	90.6%	3.38
$n=200$				
CB-ARMARoots	97.2%	5.59	93.2%	4.55
CB-ARMAPercentile	92.7%	5.39	85.8%	4.42
OB-ARMARoots	93.0%	4.99	85.9%	4.15
OB-ARMAPercentile	86.4%	5.01	76.6%	4.18
$n=400$				
CB-ARMARoots	97.8%	4.62	94.6%	3.86
CB-ARMAPercentile	97.7%	4.60	94.5%	3.86
OB-ARMARoots	97.0%	4.36	93.5%	3.71
OB-ARMAPercentile	96.7%	4.20	93.3%	3.67

Table 2: CVR and LEN for ARMA(1,1) with Laplace innovations.

Laplace	Nominal coverage 95%		Nominal coverage 90%	
	CVR	LEN	CVR	LEN
$n=25$				
CB-ARMARoots	93.4%	3.26	80.8%	2.27
CB-ARMAPercentile	89.0%	3.04	79.0%	2.26
OB-ARMARoots	87.0%	2.89	68.3%	1.73
OB-ARMAPercentile	86.9%	2.89	68.7%	1.72
$n=50$				
CB-ARMARoots	97.5%	5.20	94.7%	4.14
CB-ARMAPercentile	97.1%	5.23	92.0%	3.89
OB-ARMARoots	93.7%	5.14	91.8%	4.12
OB-ARMAPercentile	93.8%	5.13	91.4%	4.09
$n=75$				
CB-ARMARoots	97.9%	5.55	94.9%	4.32
CB-ARMAPercentile	96.3%	5.25	91.6%	4.17
OB-ARMARoots	93.8%	4.51	87.9%	3.01
OB-ARMAPercentile	94.2%	4.84	87.2%	2.96
$n=100$				
CB-ARMARoots	96.6%	4.70	93.8%	3.90
CB-ARMAPercentile	96.3%	4.67	93.7%	3.93
OB-ARMARoots	93.3%	4.21	89.0%	3.05
OB-ARMAPercentile	93.4%	4.24	89.7%	3.09
$n=200$				
CB-ARMARoots	95.6%	4.66	91.3%	3.67
CB-ARMAPercentile	96.8%	4.88	92.0%	3.68
OB-ARMARoots	95.5%	4.83	90.8%	3.80
OB-ARMAPercentile	96.1%	4.80	91.8%	3.72
$n=400$				
CB-ARMARoots	95.1%	4.71	90.5%	3.69
CB-ARMAPercentile	93.7%	4.69	88.5%	3.72
OB-ARMARoots	94.5%	4.67	89.3%	3.66
OB-ARMAPercentile	93.6%	4.65	88.3%	3.69

Table 3: CVR and LEN for ARMA(1,2) with Normal innovations.

Normal	Nominal coverage 95%		Nominal coverage 90%	
	CVR	LEN	CVR	LEN
$n=25$				
CB-ARMARoots	97.2%	5.59	93.2%	4.55
CB-ARMAPercentile	92.7%	5.39	85.8%	4.42
OB-ARMARoots	93.0%	4.99	85.9%	4.15
OB-ARMAPercentile	86.4%	5.01	76.6%	4.18
$n=50$				
CB-ARMARoots	97.1%	5.31	95.1%	4.48
CB-ARMAPercentile	93.0%	5.51	88.4%	4.62
OB-ARMARoots	96.0%	4.94	93.5%	4.20
OB-ARMAPercentile	92.5%	4.95	87.5%	4.24
$n=75$				
CB-ARMARoots	97.6%	4.89	94.8%	4.04
CB-ARMAPercentile	93.8%	4.87	90.0%	4.12
OB-ARMARoots	94.4%	4.65	90.8%	3.91
OB-ARMAPercentile	92.0%	4.65	89.1%	3.91
$n=100$				
CB-ARMARoots	96.6%	4.51	92.1%	3.67
CB-ARMAPercentile	95.0%	4.42	90.1%	3.67
OB-ARMARoots	95.2%	4.00	90.0%	3.33
OB-ARMAPercentile	93.6%	4.00	88.2%	3.37
$n=200$				
CB-ARMARoots	94.7%	3.82	91.3%	3.41
CB-ARMAPercentile	94.5%	3.79	90.6%	3.31
OB-ARMARoots	92.0%	3.54	88.7%	3.20
OB-ARMAPercentile	92.2%	3.57	88.5%	3.19
$n=400$				
CB-ARMARoots	97.5%	4.46	93.8%	3.70
CB-ARMAPercentile	97.4%	4.46	93.7%	3.69
OB-ARMARoots	96.1%	4.51	94.1%	3.76
OB-ARMAPercentile	96.8%	4.49	93.8%	3.73

Table 4: CVR and LEN for ARMA(1,2) with Laplace innovations.

Laplace	Nominal coverage 95%		Nominal coverage 90%	
	CVR	LEN	CVR	LEN
$n=25$				
CB-ARMARoots	97.1%	5.17	93.0%	3.97
CB-ARMAPercentile	94.6%	5.97	89.9%	4.27
OB-ARMARoots	93.0%	4.06	88.2%	3.39
OB-ARMAPercentile	91.7%	4.06	84.5%	3.36
$n=50$				
CB-ARMARoots	96.1%	4.68	93.6%	4.01
CB-ARMAPercentile	96.0%	4.66	93.9%	4.03
OB-ARMARoots	94.9%	4.16	92.4%	3.58
OB-ARMAPercentile	94.6%	4.08	91.6%	3.47
$n=75$				
CB-ARMARoots	96.3%	4.90	92.6%	3.96
CB-ARMAPercentile	96.8%	4.84	93.5%	3.89
OB-ARMARoots	94.2%	4.80	90.2%	3.85
OB-ARMAPercentile	95.5%	4.77	92.3%	3.85
$n=100$				
CB-ARMARoots	97.8%	5.46	92.9%	3.87
CB-ARMAPercentile	96.6%	5.19	92.2%	3.87
OB-ARMARoots	96.6%	4.87	87.7%	3.28
OB-ARMAPercentile	93.7%	4.72	88.4%	3.32
$n=200$				
CB-ARMARoots	98.0%	5.62	94.4%	4.29
CB-ARMAPercentile	94.7%	5.80	89.5%	4.49
OB-ARMARoots	96.5%	4.67	91.5%	3.48
OB-ARMAPercentile	92.2%	4.62	84.6%	3.47
$n=400$				
CB-ARMARoots	97.6%	5.88	94.8%	4.67
CB-ARMAPercentile	98.0%	6.06	95.6%	4.85
OB-ARMARoots	96.6%	5.44	93.4%	4.34
OB-ARMAPercentile	96.1%	5.32	91.6%	4.26

Table 5: CVR and LEN for ARMA(2,2) with Normal innovations.

Normal	Nominal coverage 95%		Nominal coverage 90%	
	CVR	LEN	CVR	LEN
$n=25$				
CB-ARMARoots	96.0%	4.51	93.0%	3.76
CB-ARMAPercentile	94.9%	4.46	90.8%	3.65
OB-ARMARoots	93.8%	4.49	91.0%	3.70
OB-ARMAPercentile	93.3%	4.49	90.3%	3.73
$n=50$				
CB-ARMARoots	97.0%	4.34	90.5%	3.51
CB-ARMAPercentile	92.7%	3.94	88.4%	3.49
OB-ARMARoots	92.8%	3.77	89.2%	3.43
OB-ARMAPercentile	91.4%	3.76	87.1%	3.38
$n=75$				
CB-ARMARoots	98.0%	5.26	94.6%	4.29
CB-ARMAPercentile	95.9%	5.29	91.9%	4.39
OB-ARMARoots	96.5%	4.27	92.4%	3.58
OB-ARMAPercentile	95.5%	4.29	91.5%	3.60
$n=100$				
CB-ARMARoots	96.5%	5.51	93.5%	4.44
CB-ARMAPercentile	96.0%	5.96	92.4%	4.64
OB-ARMARoots	93.8%	4.31	89.5%	3.73
OB-ARMAPercentile	93.7%	4.25	89.1%	3.69
$n=200$				
CB-ARMARoots	96.5%	4.36	92.6%	3.67
CB-ARMAPercentile	97.1%	4.37	93.2%	3.66
OB-ARMARoots	96.7%	4.31	92.9%	3.63
OB-ARMAPercentile	96.5%	4.19	92.6%	3.55
$n=400$				
CB-ARMARoots	96.0%	4.07	91.3%	3.38
CB-ARMAPercentile	96.0%	4.08	91.2%	3.39
OB-ARMARoots	95.4%	4.05	91.0%	3.44
OB-ARMAPercentile	95.2%	4.03	89.9%	3.35

Table 6: CVR and LEN for ARMA(2,2) with Laplace innovations.

Laplace	Nominal coverage 95%		Nominal coverage 90%	
	CVR	LEN	CVR	LEN
$n=25$				
CB-ARMARoots	94.5%	4.05	87.6%	3.00
CB-ARMAPercentile	94.0%	3.99	86.6%	2.88
OB-ARMARoots	93.7%	3.96	80.0%	2.27
OB-ARMAPercentile	93.8%	3.98	78.5%	2.28
$n=50$				
CB-ARMARoots	98.8%	6.56	96.9%	4.97
CB-ARMAPercentile	98.9%	6.59	97.5%	5.33
OB-ARMARoots	98.0%	5.79	96.4%	4.68
OB-ARMAPercentile	98.0%	5.79	96.5%	4.69
$n=75$				
CB-ARMARoots	91.9%	3.73	88.7%	3.15
CB-ARMAPercentile	92.3%	3.75	89.2%	3.18
OB-ARMARoots	91.6%	3.69	88.4%	3.13
OB-ARMAPercentile	91.8%	3.69	88.8%	3.14
$n=100$				
CB-ARMARoots	95.6%	4.43	90.8%	3.42
CB-ARMAPercentile	95.5%	4.43	90.7%	3.39
OB-ARMARoots	94.9%	4.36	90.1%	3.35
OB-ARMAPercentile	94.7%	4.32	90.1%	3.36
$n=200$				
CB-ARMARoots	95.5%	4.44	91.2%	3.44
CB-ARMAPercentile	95.3%	4.38	91.2%	3.45
OB-ARMARoots	94.9%	4.44	90.0%	3.31
OB-ARMAPercentile	95.3%	4.43	90.5%	3.32
$n=400$				
CB-ARMARoots	94.8%	4.32	90.1%	3.42
CB-ARMAPercentile	94.1%	4.25	88.6%	3.31
OB-ARMARoots	91.6%	4.12	84.8%	3.25
OB-ARMAPercentile	93.6%	4.10	88.6%	3.24

Table 7: CVR and LEN for ARMA(3,1) with Normal innovations.

Normal	Nominal coverage 95%		Nominal coverage 90%	
	CVR	LEN	CVR	LEN
$n=25$				
CB-ARMARoots	97.2%	4.44	93.6%	3.76
CB-ARMAPercentile	95.4%	5.44	88.5%	4.19
OB-ARMARoots	96.2%	4.12	92.1%	3.54
OB-ARMAPercentile	94.7%	4.35	87.3%	3.56
$n=50$				
CB-ARMARoots	97.5%	4.38	92.7%	3.54
CB-ARMAPercentile	97.0%	4.29	91.2%	3.40
OB-ARMARoots	96.6%	4.23	89.6%	3.30
OB-ARMAPercentile	96.0%	4.16	89.6%	3.29
$n=75$				
CB-ARMARoots	95%	4.01	90.8%	3.39
CB-ARMAPercentile	96.2%	4.16	89.2%	3.27
OB-ARMARoots	94.2%	3.79	89.3%	3.22
OB-ARMAPercentile	94.0%	3.76	88.2%	3.15
$n=100$				
CB-ARMARoots	92.4%	3.57	86.0%	2.98
CB-ARMAPercentile	92.3%	3.56	86.2%	3.00
OB-ARMARoots	92.0%	3.45	86.0%	2.92
OB-ARMAPercentile	91.0%	3.38	86.4%	2.93
$n=200$				
CB-ARMARoots	90.9%	3.77	84.4%	3.07
CB-ARMAPercentile	90.8%	3.76	84.2%	3.06
OB-ARMARoots	89.8%	3.69	83.4%	3.00
OB-ARMAPercentile	89.8%	3.68	83.3%	2.99
$n=400$				
CB-ARMARoots	97.2%	4.39	90.1%	3.43
CB-ARMAPercentile	96.6%	4.37	88.0%	3.42
OB-ARMARoots	95.9%	4.11	88.4%	3.19
OB-ARMAPercentile	95.9%	4.15	87.2%	3.16

Table 8: CVR and LEN for ARMA(3,1) with Laplace innovations.

Laplace	Nominal coverage 95%		Nominal coverage 90%	
	CVR	LEN	CVR	LEN
$n=25$				
CB-ARMARoots	90.9%	3.30	84.2%	2.76
CB-ARMAPercentile	84.7%	2.94	83.3%	2.72
OB-ARMARoots	84.2%	2.94	82.8%	2.72
OB-ARMAPercentile	84.2%	2.94	82.6%	2.72
$n=50$				
CB-ARMARoots	94.0%	4.55	88.2%	3.65
CB-ARMAPercentile	92.4%	4.43	86.2%	3.61
OB-ARMARoots	92.7%	4.36	86.6%	3.48
OB-ARMAPercentile	91.7%	4.31	84.0%	3.40
$n=75$				
CB-ARMARoots	97.0%	5.14	91.6%	3.44
CB-ARMAPercentile	96.9%	5.04	91.5%	3.43
OB-ARMARoots	96.9%	5.13	91.2%	3.41
OB-ARMAPercentile	97.0%	5.18	91.5%	3.44
$n=100$				
CB-ARMARoots	97.7%	5.40	94.2%	4.11
CB-ARMAPercentile	97.7%	5.38	93.8%	3.99
OB-ARMARoots	97.5%	5.44	91.8%	3.95
OB-ARMAPercentile	97.1%	5.28	93.4%	3.93
$n=200$				
CB-ARMARoots	95.0%	4.40	90.3%	3.36
CB-ARMAPercentile	93.8%	4.27	89.5%	3.38
OB-ARMARoots	94.5%	4.09	90.6%	3.43
OB-ARMAPercentile	94.2%	4.11	89.9%	3.36
$n=400$				
CB-ARMARoots	96.2%	4.59	91.9%	3.47
CB-ARMAPercentile	96.1%	4.56	92.0%	3.49
OB-ARMARoots	96.4%	4.65	92.4%	3.50
OB-ARMAPercentile	96.4%	4.61	92.5%	3.48

5. CONCLUSIONS

In this paper we introduce the bootstrap algorithms for constructing the prediction intervals of ARMA (p, q) models with unknown orders based on the bootstrap distribution of orders. The asymptotic validity and asymptotic pertinence of the bootstrap prediction intervals are shown to hold true. We conduct simulations for several ARMA models using four bootstrap methods, i.e., CB-ARMARoots, CB-ARMAPercentile, OB-ARMARoots and OB-ARMAPercentile. From the simulation results we see that the proposed CB-ARMARoots algorithm outperforms the OB-ARMA methods using pre-estimated orders in terms of the coverage accuracy of the prediction intervals, especially when the true order of the ARMA model is low or when the sample size is small.

A. APPENDIX

Proof of Theorem 3.1: Note that if one can show that, as $n \to \infty$,

$$\sup_x \left| P\big(X_{n+1} - \hat{X}_{n+1} \le x\big) - P\big(X^*_{n+1} - \hat{X}^*_{n+1} \le x\big) \right| \ \to^p \ 0\,,$$

then standard results imply that the quantiles of the distribution of $X^*_{n+1} - \hat{X}^*_{n+1}$ can be used to consistently estimate the quantiles of the distribution of $X_{n+1} - \hat{X}_{n+1}$. This leads to the asymptotic validity of the prediction interval (2.4).

Let $Y_n = (X_n, ..., X_{n-p+1})$, $E_n = \big(\varepsilon_n, ..., \varepsilon_{n-q+1}\big)$. From Steps 6 and 7 of B-ARMARoots Algorithm, we obtain

$$\begin{aligned}
X_{n+1} &= \big(Y_n, E_n\big)\,\theta + \varepsilon_{n+1}\,,\\
\hat{X}_{n+1} &= \big(Y_n, \hat{E}_n(\hat{\theta}^M)\big)\,\hat{\theta}^M\,,\\
X^*_{n+1} &= \big(Y_n, \hat{E}_n(\hat{\theta}^M)\big)\,\hat{\theta}^M + \varepsilon^*_{n+1}\,,\\
\hat{X}^*_{n+1} &= \big(Y_n, \hat{E}^*_n(\hat{\theta}^{M,*})\big)\,\hat{\theta}^{M,*}\,.
\end{aligned}$$

Thus

$$\begin{aligned}
X_{n+1} - \hat{X}_{n+1} &= \big(Y_n, E_n\big)\,\theta - \big(Y_n, \hat{E}_n(\hat{\theta}^M)\big)\,\hat{\theta}^M + \varepsilon_{n+1}\\
&= \big(Y_n, E_n\big)\,\theta - \big(Y_n, E_n\big)\,\hat{\theta}^M + \big(Y_n, E_n\big)\,\hat{\theta}^M - \big(Y_n, \hat{E}_n(\hat{\theta}^M)\big)\,\hat{\theta}^M + \varepsilon_{n+1}\\
&:= I_1 + I_2 + \varepsilon_{n+1}\,.
\end{aligned}$$

Since $\theta - \hat{\theta}^M = O_p\big(1/\sqrt{n}\big)$, $I_1 \to^p 0$ as $n \to \infty$.

By Lemma 2.1 of [9],

$$\varepsilon_j(\theta) - \hat{\varepsilon}_{j,n}\big(\hat{\theta}^M\big) \ = \ -Z'\big(j-1; \theta, \hat{\theta}^M\big)^{\mathsf{T}}\,\big(\theta - \hat{\theta}^M\big)$$

for any $1 \le j \le n$, where $Z'\big(j-1; \theta, \hat{\theta}^M\big)$ is uniformly bounded. Thus the $\sqrt{n}$-consistency of the M-estimator implies that

$$\varepsilon_j(\theta) - \hat{\varepsilon}_{j,n}\big(\hat{\theta}^M\big) \ = \ O_p\big(1/\sqrt{n}\big)\,. \tag{A.1}$$

From (2.9) of [9],

$$\varepsilon_j(\theta) = \varepsilon_j + (1+C)^{-j} O_p(1)\,,$$

where C is a positive constant. For $n-q+1 \le j \le n$, $(1+C)^{-j} O_p(1) = O_p\big((1+C)^{-n}\big) = o_p\big(1/\sqrt{n}\big)$. Then

$$\varepsilon_j(\theta) = \varepsilon_j + o_p\big(1/\sqrt{n}\big)\,. \tag{A.2}$$

(A.1) and (A.2) yield

$$\varepsilon_j - \hat{\varepsilon}_{j,n}\big(\hat{\theta}^M\big) = O_p\big(1/\sqrt{n}\big)$$

for $n-q+1 \le j \le n$. This implies that $E_n - \hat{E}_n\big(\hat{\theta}^M\big) = O_p\big(1/\sqrt{n}\big)$ and hence $I_2 \to^p 0$ as $n \to \infty$. That is

$$X_{n+1} - \hat{X}_{n+1} = \varepsilon_{n+1} + o_p(1)\,.$$

Moreover, it follows from Theorems 3.1 and 4.1 of [9] that, as $n \to \infty$,

$$\sup_x \big|P\big(\varepsilon_{n+1} \le x\big) - P\big(\varepsilon^*_{n+1} \le x\big)\big| \to^p 0\,, \tag{A.3}$$

and

$$\hat{\theta}^{M,*} - \hat{\theta}^M \to^p 0\,.$$

Thus we obtain

$$X^*_{n+1} - \hat{X}^*_{n+1} = \varepsilon^*_{n+1} + o_p(1)\,.$$

Now Slutsky's Lemma together with (A.3) concludes the proof Theorem 3.1. □

Proof of Theorem 3.2: By (A.3), Condition (i) in Definition 3.2 holds true. In view of the proof of Theorem 3.1, Condition (ii) also holds true. Moreover, Theorem 4.1 of [9] shows that $\sqrt{n}\,A_n$ and $\sqrt{n}\,A^*_n$ have the same asymptotic distribution. This implies Condition (iii). Finally, Condition (iv) follows from the causality of Model (2.1). This completes the proof of Theorem 3.2. □

Proof of Theorem 3.3: Let F_{n+1} be the distribution of X_{n+1} given $X_1, ..., X_n$, and F^*_{n+1} be the bootstrap distribution derived from CB-ARMARoots Algorithm. To prove the asymptotic validity, it suffices to show that

$$\sup_x \big|F^*_{n+1}(x) - F_{n+1}(x)\big| \to^p 0\,.$$

Note that

$$F_{n+1}(x) = \sum_{p_0,q_0} F_{n+1}\big(x \,|\, p_0, q_0\big)\, P\big(p = p_0,\, q = q_0\big)\,,$$

$$F^*_{n+1}(x) = \sum_{p_0,q_0} F^*_{n+1}\big(x \,|\, p_0, q_0\big)\, P^*\big(p = p_0,\, q = q_0\big)\,.$$

For any $\varepsilon > 0$, there exists (P, Q) such that

$$\sum_{p_0>P} \sum_{q_0} P\big(p = p_0,\, q = q_0\big) < \varepsilon\,, \qquad \sum_{p_0} \sum_{q_0>Q} P\big(p = p_0,\, q = q_0\big) < \varepsilon\,.$$

Obviously,

$$\sum_{p_0>P,\ q_0\le Q} P\big(p=p_0,\ q=q_0\big) < \varepsilon\,, \qquad \sum_{p_0\le P,\ q_0>Q} P\big(p=p_0,\ q=q_0\big) < \varepsilon$$

and

$$\sum_{p_0>P,\ q_0>Q} P\big(p=p_0,\ q=q_0\big) < \varepsilon\,.$$

Similarly, there exists such (P^*, Q^*) for $P^*\big(p=p_0,\ q=q_0\big)$. Let $(P_0, Q_0) = \big(\max(P, P^*),\ \max(Q, Q^*)\big)$. Thus

$$\begin{aligned}
&\sup_x\big|F_{n+1}(x) - F^*_{n+1}(x)\big| \ = \\
&\quad = \ \sup_x\left|\sum_{p_0,q_0}\Big\{F_{n+1}\big(x\,|\,p_0,q_0\big)\ P\big(p=p_0,\ q=q_0\big) - F^*_{n+1}\big(x\,|\,p_0,q_0\big)\ P^*\big(p=p_0,\ q=q_0\big)\Big\}\right| \le \\
&\le \ \sup_x\left|\sum_{p_0\le P_0,\ q_0\le Q_0}\Big\{F_{n+1}\big(x\,|\,p_0,q_0\big)\ P\big(p=p_0,\ q=q_0\big) - F^*_{n+1}\big(x\,|\,p_0,q_0\big)\ P^*\big(p=p_0,\ q=q_0\big)\Big\}\right| \\
&\quad + \ \sup_x\left|\sum_{p_0\le P_0,\ q_0>Q_0}\Big\{F_{n+1}\big(x\,|\,p_0,q_0\big)\ P\big(p=p_0,\ q=q_0\big) - F^*_{n+1}\big(x\,|\,p_0,q_0\big)\ P^*\big(p=p_0,\ q=q_0\big)\Big\}\right| \\
&\quad + \ \sup_x\left|\sum_{p_0>P_0,\ q_0\le Q_0}\Big\{F_{n+1}\big(x\,|\,p_0,q_0\big)\ P\big(p=p_0,\ q=q_0\big) - F^*_{n+1}\big(x\,|\,p_0,q_0\big)\ P^*\big(p=p_0,\ q=q_0\big)\Big\}\right| \\
&\quad + \ \sup_x\left|\sum_{p_0>P_0,\ q_0>Q_0}\Big\{F_{n+1}\big(x\,|\,p_0,q_0\big)\ P\big(p=p_0,\ q=q_0\big) - F^*_{n+1}\big(x\,|\,p_0,q_0\big)\ P^*\big(p=p_0,\ q=q_0\big)\Big\}\right|.
\end{aligned}$$

Observe that

$$\begin{aligned}
&\sup_x\left|\sum_{p_0\le P_0,\ q_0\le Q_0}\Big\{F_{n+1}\big(x\,|\,p_0,q_0\big)\ P\big(p=p_0,\ q=q_0\big) - F^*_{n+1}\big(x\,|\,p_0,q_0\big)\ P^*\big(p=p_0,\ q=q_0\big)\Big\}\right| \le \\
&\qquad \le \ \sup_x\left|\sum_{p_0\le P_0,\ q_0\le Q_0} F_{n+1}\big(x\,|\,p_0,q_0\big)\ \Big(P\big(p=p_0,\ q=q_0\big) - P^*\big(p=p_0,\ q=q_0\big)\Big)\right| \\
&\qquad\quad + \ \sup_x\left|\sum_{p_0\le P_0,\ q_0\le Q_0}\Big(F_{n+1}\big(x\,|\,p_0,q_0\big) - F^*_{n+1}\big(x\,|\,p_0,q_0\big)\Big)\ P^*\big(p=p_0,\ q=q_0\big)\right| \\
&\qquad \le \ \sum_{p_0\le P_0,\ q_0\le Q_0}\Big|P\big(p=p_0,\ q=q_0\big) - P^*\big(p=p_0,\ q=q_0\big)\Big| \\
&\qquad\quad + \ \sum_{p_0\le P_0,\ q_0\le Q_0}\sup_x\Big|F_{n+1}\big(x\,|\,p_0,q_0\big) - F^*_{n+1}\big(x\,|\,p_0,q_0\big)\Big|\,.
\end{aligned}$$

Hence we obtain

$$
\begin{aligned}
\sup_x \left|F_{n+1}(x) - F^*_{n+1}(x)\right| \le & \sum_{p_0\le P_0,\, q_0\le Q_0} \left|P\big(p=p_0,\, q=q_0\big) - P^*\big(p=p_0,\, q=q_0\big)\right| \\
& + \sum_{p_0\le P_0,\, q_0\le Q_0} \sup_x \left|F_{n+1}\big(x\,|p_0,q_0\big) - F^*_{n+1}\big(x\,|p_0,q_0\big)\right| \\
& + \sum_{p_0\le P_0,\, q_0> Q_0} P\big(p=p_0,\, q=q_0\big) \;+ \sum_{p_0> P_0,\, q_0\le Q_0} P\big(p=p_0,\, q=q_0\big) \\
& + \sum_{p_0\le P_0,\, q_0> Q_0} P^*\big(p=p_0,\, q=q_0\big) \;+ \sum_{p_0> P_0,\, q_0\le Q_0} P^*\big(p=p_0,\, q=q_0\big) \\
& + \sum_{p_0> P_0,\, q_0> Q_0} P\big(p=p_0,\, q=q_0\big) \;+ \sum_{p_0> P_0,\, q_0> Q_0} P^*\big(p=p_0,\, q=q_0\big) \\
\le & \sum_{p_0\le P_0,\, q_0\le Q_0} \left|P\big(p=p_0,\, q=q_0\big) - P^*\big(p=p_0,\, q=q_0\big)\right| \\
& + \sum_{p_0\le P_0,\, q_0\le Q_0} \sup_x \left|F_{n+1}\big(x\,|p_0,q_0\big) - F^*_{n+1}\big(x\,|p_0,q_0\big)\right| + 6\,\varepsilon\,.
\end{aligned}
\tag{A.4}
$$

[5] showed that

$$
\left|P\big(p=p_0,\, q=q_0\big) - P^*\big(p=p_0,\, q=q_0\big)\right| \to^p 0\,,
$$

and Theorem 3.1 implies that

$$
\sup_x \left|F_{n+1}\big(x\,|p_0,q_0\big) - F^*_{n+1}\big(x\,|p_0,q_0\big)\right| \to^p 0\,.
$$

These, together with (A.4) and the arbitrariness of ε, yield that

$$
\sup_x \left|F_{n+1}(x) - F^*_{n+1}(x)\right| \to^p 0\,.
$$

Along similar lines of the proof of Theorem 3.2, the asymptotic pertinence of the prediction interval (2.5) also holds true. □

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