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COMPARISONS OF THE PERFORMANCES OF ESTIMATORS OF A BOUNDED NORMAL MEAN UNDER SQUARED-ERROR LOSS

Authors: Yiping Dou
– Department of Statistics, University of British Columbia, Canada
`ydou@stat.ubc.ca`

Constance van Eeden
– Department of Statistics, University of British Columbia, Canada
`cve@xs4all.nl`

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Abstract:

- This paper is concerned with the estimation under squared-error loss of a normal mean θ based on $X \sim \mathcal{N}(\theta, 1)$ when $|\theta| \leq m$ for a known $m > 0$. Nine estimators are compared, namely the maximum likelihood estimator (mle), three dominators of the mle obtained from Moors, from Charras and from Charras and van Eeden, two minimax estimators from Casella and Strawderman, a Bayes estimator of Marchand and Perron, the Pitman estimator and Bickel's asymptotically-minimax estimator. The comparisons are based on analytical as well as on graphical results concerning their risk functions. In particular, we comment on their gain in accuracy from using the restriction, as well as on their robustness with respect to misspecification of m.

Key-Words:

- *admissibility; Bayes estimator; bounded Normal mean; restricted estimators; robustness; squared-error loss.*

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1. INTRODUCTION

The problem considered in this paper is the estimation under squared-error loss of a normal mean θ based on $X \sim \mathcal{N}(\theta, 1)$ when $|\theta| \leq m$ for a known $m > 0$.

This estimation problem is considered by Casella and Strawderman (1981), by Marchand and Perron (2001), by Bickel (1981) and by Gatsonis, MacGibbon and Strawderman (1987). Casella and Strawderman show that, when $0 < m \leq m_o \approx 1.056742$, there exists a unique minimax estimator of θ with respect to a symmetric two-point least-favourable prior on $\{-m, m\}$. They give an explicit expression for it and show that it dominates the maximum likelihood estimator (mle) when $m \leq 1$. They also give a class of minimax estimators for the case where $1.4 \leq m \leq 1.6$. These estimators are Bayes with respect to a symmetric three-point prior on $\{-m, 0, m\}$. Bickel gives an estimator which is asymptotically minimax as $m \to \infty$ and Gatsonis, MacGibbon and Strawderman graphically compare these estimators and the Pitman estimator for several values of m. Marchand and Perron consider the problem of estimating θ when $X \sim \mathcal{N}_k(\theta, I)$ with $\|\theta\| \leq m$ and give conditions on m, k and the prior for Bayes estimators to dominate the mle. An example of their results is that the Bayes estimator with respect to the uniform prior on the boundary of the parameter space dominates the mle when $m \leq \sqrt{k}$, generalizing the Casella–Strawderman result to $k > 1$. Dominators for the mle can also be obtained from results of Charras (1979), of Moors (1981, 1985) and of Charras and van Eeden (1991). These authors consider estimation in restricted parameter spaces in a very general setting, give conditions for inadmissibility for squared-error loss and either give methods of constructing dominators (Moors and Charras and van Eeden) or prove the existence of dominators within a given class of estimators (Charras). Their conditions are satisfied for the bounded-normal-mean problem and one of the purposes of this paper is to find explicit expressions for these dominators and compare their risk functions, analytically as well as graphically, with those of the mle, the Casella–Strawderman minimax estimators, Bickel's asymptotically minimax estimator, the Pitman estimator and one of the Marchand–Perron Bayes estimators. In these comparisons, questions of an estimator's gain in accuracy obtained from using the restriction are looked at, as well as how this gain depends on m and how robust the estimators are with respect to misspecification of m.

One of our analytical results shows that, if and only if $m \leq 1$, Moors' dominator of the mle of a bounded normal mean is the Casella–Strawderman minimax estimator, implying (by the Casella–Strawderman result for $m \leq 1$) that this Moors dominator of the mle is admissible when $m \leq 1$. Another analytical result we have is that the dominators in the Charras–van Eeden class are all inadmissible. We also show, again analytically, that the estimator $\delta_o(x) \equiv 0$ (which we call the "trivial estimator") dominates the mle if and only if $0 < m \leq m_1 \approx 0.5204372$. Marchand and Perron (2001) show, as a special case of their results for a $k \geq 1$-dimensional restricted normal mean, that (when $k = 1$) every symmetric estimator dominates the mle when $m \leq m_o \approx .4837$. Finally we find, numerically, that the Marchand–Perron Bayes estimator considered by us has a risk function which is, on the whole interval $[-m, m]$, very close to that of one of the Casella–Strawderman minimax estimators.

Explicit expressions for the estimators are presented in Section 2. Our numerical comparisons are presented in the form of graphs and discussed in Section 3. The proofs of the lemmas and theorems are given in Appendix A.

We know of only one other family of distributions for which Charras's (1979) and Moors' (1981, 1985) dominators have been obtained and compared. These results can be found in Perron (2003). He compares the mle with its Charras and its Moors dominators, as well as with the Pitman estimator and the Bayes estimator with respect to a prior proportional to $\bigl(p(1-p)\bigr)^{-1}$ for the case where $X \sim \text{Bin}(n,p)$ when $p \in [a, 1-a]$ for a given $a \in (0, 1/2)$. He gives an algorithm for finding the Charras dominator.

2. THE ESTIMATORS

The problem of estimating a bounded normal mean based on $X \sim \mathcal{N}(\theta, 1)$ is a special case of the following problem: $(\mathcal{X}, \mathcal{A})$ is a measurable space and $\mathcal{P} = \{P_\theta, \theta \in D\}$ is a family of probability measures on $(\mathcal{X}, \mathcal{A})$ where $D \subset \mathbb{R}^k$ is a subset of the set of θ for which P_θ is such a probability measure. Further, D is convex and closed. The problem is to find, for a given loss function, "good" estimators of θ based on a random vector $X \in \mathbb{R}^n$ defined on $(\mathcal{X}, \mathcal{A})$, where $\delta(X)$ is an estimator of θ if it satisfies $P_\theta\bigl(\delta(X) \in D\bigr) = 1$ for all $\theta \in D$. Many analytical results concerning admissibility and minimaxity for such models have, for various loss functions, been obtained (see e.g. van Eeden (2006)).

The present section contains explicit expressions for each of the estimators of a bounded normal mean considered in this paper. It also contains their known, as well as our, analytical properties.

The maximum likelihood estimator

The mle of θ for our problem of estimating a bounded normal mean is given by

$$\delta^{\text{mle}}(X) = \begin{cases} -m & \text{if } X \leq -m \\ X & \text{if } -m < X < m \\ m & \text{if } X \geq m\ . \end{cases}$$

It is well-known that this estimator is inadmissible for our problem.

Casella and Strawderman's minimax estimators

Casella and Strawderman (1981) give conditions for a Bayes estimator to be minimax for estimating a bounded normal mean based on $X \sim \mathcal{N}(\theta, 1)$ with squared-error loss. They show that a two-point symmetric prior on $\{-m, m\}$ is least favourable if $m \leq m_0 \approx 1.056742$, implying that the corresponding Bayes estimator is minimax. This m_0 is the solution of $R(0, \delta^{\text{cs.2}}) - R(m, \delta^{\text{cs.2}}) = 0$, where $\delta^{\text{cs.2}}$ is the Bayes estimator which is given by

$$\delta^{\text{cs.2}}(X) = m \tanh(mX) .$$

The authors show that this minimax estimator dominates the mle when $m \leq 1$. They also give a class of minimax estimators for symmetric three-point priors as follows: for a three-point prior $\pi(0) = \alpha$ and $\pi(-m) = \pi(m) = (1-\alpha)/2$, the Bayes estimator under squared-error loss is given by

$$\delta^{\text{cs.3}}(X) = \frac{(1-\alpha)\ m \tanh(mX)}{1 - \alpha + \alpha \exp(m^2/2)/\cosh(mX)} . \tag{2.1}$$

Casella and Strawderman show that, if α and m satisfy

$$(m^2 - 1)\left(m^2 - 1 + \exp(m^2/2)\right)^{-1} \leq \alpha \leq 2\left(2 + \exp(m^2/2)\right)^{-1} , \tag{2.2}$$

and α is such that $R(0, \delta^{\text{cs.3}}) - R(m, \delta^{\text{cs.3}}) = 0$, then $\delta^{\text{cs.3}}$ is minimax for estimating θ when $|\theta| \leq m$. They find numerically that these two conditions are satisfied when $1.4 \leq m \leq 1.6$.

A Bayes estimator of Marchand and Perron

Marchand and Perron (2001) consider the estimation, for squared-error loss, of θ based on $X \sim \mathcal{N}_k(\theta, I)$ when $\|\theta\| \leq m$ for a known $m > 0$. The purpose of their paper is finding dominators of the mle. One of their classes of dominators consists of Bayes estimators with respect priors of the form $\pi(\theta) = K e^{-h(\|\theta\|^2)}$, where K is a normalizing constant. Their Corollary 4 gives sufficient conditions on the triple (m, h, k) for the resulting Bayes estimator to dominate the mle. For our case where $k = 1$, taking $m > \sqrt{k} = 1$, $h(\theta^2) = -a\,\theta^2/2$ and a the unique solution to (see their Example 3 on the lines 4–16 of their page 1088)

$$\int_0^m t^2\, e^{\frac{a-1}{2} t^2}\, dt = \int_0^m e^{\frac{a-1}{2} t^2}\, dt \tag{2.3}$$

assures that the first and second conditions of their Corollary 4 are satisfied.

But, it shows that the third condition of Corollary 4 is not satisfied for this triple (m, h, k) by using Corollary 4 on the authors' page 1090 together with the fact (see their Table 1 and the Remark 2 on their page 1088) that $\Delta_E(p)$ is empty when $k = 1$. So, this Bayes estimator might not dominate the mle. In order to get some insight into this question of domination, we compare (in Section 3) this Bayes estimator with a satisfying (2.3), with our other estimators for $m = 1.5$, as well as for $m = 1.8$.

Marchand and Perron (2001) show that (2.3) has a unique solution and that the corresponding Bayes estimator is given by

$$\delta^{\mathrm{E}}(X) = \frac{X}{|X|} \frac{\displaystyle\int_0^m t^{\frac{3}{2}} I_{1/2}(t|X|)\, e^{\frac{(a-1)t^2}{2}}\, dt}{\displaystyle\int_0^m t^{\frac{1}{2}} I_{-1/2}(t|X|)\, e^{\frac{(a-1)t^2}{2}}\, dt}\,, \tag{2.4}$$

where $I_\nu(t)$ is the modified Bessel function of order ν (see e.g. Robert (1990)).

The following theorem gives an alternate expression for the estimator valid for the case when $a \in (0, 1)$. The theorem also gives an equality which is equivalent to, and easier to solve than, (2.3) when $a \in (0, 1)$.

Theorem 2.1. *When $a \in (0, 1)$, an alternate expression for the estimator is*

$$\delta^{\mathrm{E}}(X) = \frac{X}{|X|} \frac{1}{\sqrt{1-a}} \frac{\displaystyle\int_0^{m\sqrt{1-a}} u \sinh\!\left(u \frac{|X|}{\sqrt{1-a}}\right) e^{-u^2/2}\, du}{\displaystyle\int_0^{m\sqrt{1-a}} \cosh\!\left(u \frac{|X|}{\sqrt{1-a}}\right) e^{-u^2/2}\, du}\,. \tag{2.5}$$

Moreover, when $a \in (0, 1)$, (2.3) is equivalent to

$$a\left(\Phi\big(m\sqrt{1-a}\big) - \frac{1}{2}\right) = m\sqrt{1-a}\; \phi\big(m\sqrt{1-a}\big)\,, \tag{2.6}$$

where $\Phi(t)$ and $\phi(t)$ are the standard normal distribution function and density function.

Moors' dominating estimator of the mle

Moors (1981, 1985) considers the problem described in the beginning of this section and gives sufficient conditions for "boundary estimators" to be inadmissible for squared-error loss. Here, a boundary estimator is an estimator which takes values on or near the boundary of D with positive probability for some $\theta \in D$. He assumes that the problem is invariant with respect to a finite group

$G=(g_1,...,g_p)$ of measure preserving transformations from $\mathcal{X}$ to $\mathcal{X}$ and that the induced group $\tilde{G}$ is commutative and satisfies

$$\tilde{g}(ad_1+bd_2)=a\tilde{g}(d_1)+b\tilde{g}(d_2) \qquad \text{for all } \ d_1,d_2\in D, \quad \text{all } \ \tilde{g}\in\tilde{G} \ .$$

He then constructs random, closed, convex subsets D_X of D with the property that an estimator δ for which $P_\theta\big(\delta(X)\notin D_X\big)>0$ for some $\theta\in D$ is inadmissible. These sets D_X are defined as follows. Let p_θ be the density of P_θ with respect to a σ-finite measure ν defined on $(\mathcal{X},\mathcal{A})$ and let

$$\alpha\big(X,\bar{g}_j(\theta)\big)=\frac{p_{\bar{g}_j(\theta)}(X)}{S(X;\theta)} \ , \qquad j=1,...,p \ ,$$

where $S(X;\theta)=\sum_{j=1}^{p}p_{\bar{g}_j(\theta)}(X)>0$. Further, he defines

$$h_X(\theta) \ = \ \begin{cases} \displaystyle\sum_{j=1}^{p}\alpha\big(X,\bar{g}_j(\theta)\big)\,\bar{g}_j(\theta) & \text{when } \ S(X;\theta)>0 \\ \theta & \text{when } \ S(X;\theta)=0 \ . \end{cases}$$

Then D_X is the convex closure of the range of $h_X(\theta)$ for $\theta\in D$ and boundary estimators $\delta(X)$, i.e. estimators $\delta(X)$ for which $P_\theta\big(\delta(X)\notin D_X\big)>0$ for some $\theta\in D$, are inadmissible and are dominated by their projection unto D.

For the problem of estimating a bounded normal mean under squared-error loss, Moors' conditions are satisfied with $p=2$, $g_1(x)=x$ and $g_2(x)=-x$ which gives $h_X(\theta)=\theta\tanh(\theta X)$, because $p_\theta(x)=\exp\big(-(x-\theta)^2/2\big)/\sqrt{2\pi}$. So the subset D_X is given by

$$D_X= \ \big(-m\tanh(m|X|), \, m\tanh(m|X|)\big) \ ,$$

which implies by Moors that any estimator δ for which

$$P_\theta\Big(\delta(X)\notin\big(-m\tanh(m|X|), \, m\tanh(m|X|)\big)\Big) \ > \ 0 \qquad \text{for some } \ \theta\in D$$

is inadmissible and is dominated by its projection unto D. Hence, Moors' dominator of the mle is given by

$$(2.7) \qquad \delta^{\mathrm{mr}}(X) = \begin{cases} -m\tanh(m|X|) & \text{if } X\le -m\tanh(m|X|) \\ X & \text{if } \ -m\tanh(m|X|)<X<m\tanh(m|X|) \\ m\tanh(m|X|) & \text{if } X\ge m\tanh(m|X|) \ . \end{cases}$$

The following theorem shows that, for $m\le 1$, Moors' dominating estimator of the mle is Casella and Strawderman's minimax estimator. We also obtain there a more explicit expression for this dominator for the case where $m>1$. The proof of the theorem is given in Appendix A.

Theorem 2.2. *Moors' dominator of the mle can also be written as*

(i) *if* $0 < m \leq 1$ *then* $\delta^{\mathrm{mr}}(X) = m \tanh(mX)$*;*

(ii) *if* $m > 1$*, then*

$$\delta^{\mathrm{mr}}(X) \;=\; \begin{cases} m \tanh(mX) & \textit{if } \; X \geq \xi(m) \;\; \textit{or} \;\; X \leq -\xi(m) \\ X & \textit{if } \; -\xi(m) < X < \xi(m) \;, \end{cases}$$

where $\xi(m)$*,* $r(m) < \xi(m) < m$*, is the unique root of* $u(x) = x - m \tanh(mx) = 0$ *for* $x > 0$ *and* $r(m) = \frac{1}{m} \ln\bigl[m + \sqrt{m^2 - 1}\bigr]$*.*

Charras's and Charras and van Eeden's dominators of the mle

Charras (1979) considers the problem as described in the beginning of this section. He gives, for squared-error loss, conditions for boundary estimators to be non-Bayes as well as conditions for them to be inadmissible, where a boundary estimator is, for him, an estimator δ for which $P_\theta\bigl(\delta(X) \in B\bigr) > 0$ for some $\theta \in D$ and B is the boundary of D. For the case where $k = 1$ and $\theta \in [a, b]$ for known $-\infty < a < b < \infty$, he gives conditions for the existence of classes of dominators of his boundary estimators and ways to construct them.

The inadmissibility results of Charras (1979) are published in Charras and van Eeden (1991), but his dominators are only mentioned there. Instead, Charras and van Eeden study a different class of dominators (proposed by a referee of this Charras and van Eeden paper) of Charras' boundary estimators. The authors construct, for squared-error loss, a class of dominators δ^{cve} for boundary estimators $\delta(X)$ of θ when $\theta \in [a, b]$ with $-\infty < a < b < \infty$, where they suppose that these boundary estimators δ satisfy

$$\left.\begin{aligned} P_\theta\bigl(\delta(X) = a\bigr) \;>\; 0 \\ P_\theta\bigl(\delta(X) = b\bigr) \;>\; 0 \end{aligned}\right\} \qquad \text{for all } \;\; \theta \in [a, b] \;.$$

They further suppose that, for each $\theta_o \in D$,

$$\lim_{\theta \to \theta_o} \int_{\mathcal{X}} |p_\theta - p_{\theta_o}| \, d\nu \;=\; 0 \;, \tag{2.8}$$

where p_θ is the density of P_θ with respect to the σ-finite measure ν.

The authors then show that there exists estimators of the form

$$\delta^{\mathrm{cve}}(X) \;=\; \begin{cases} a + \varepsilon_1 & \text{if } \; \delta(X) \leq a \\ \delta(X) & \text{if } \; a < \delta(X) < b \\ b - \varepsilon_2 & \text{if } \; \delta(X) \geq b \end{cases} \tag{2.9}$$

where $\varepsilon_1 > 0$, $\varepsilon_2 > 0$ and $\varepsilon_1 + \varepsilon_2 \leq b - a$, which dominate δ.

This Charras–van Eeden result with $a = -m$ and $b = m$ clearly applies to our problem of dominating the mle of a bounded normal mean, where because of the symmetry of the problem, one can take $0 < \varepsilon_1 = \varepsilon_2 = \varepsilon \leq m$. This gives a class of dominators of the mle of a bounded normal mean for squared-error loss and using the results of Charras and van Eeden (1991) one finds that $\varepsilon \in (0, \varepsilon_o]$, where $\varepsilon_o = \min\bigl(m\bigl(8\,\Phi(-2m)/(1+2\phi(-2m))\bigr),\, m\bigr)$, gives a dominator of the mle. However, each of these dominators is inadmissible. This follows from Brown (1986)'s necessary condition for admissibility for squared-error loss in the estimation of the mean of an exponential-family distribution. He shows that an admissible estimator has to be non-decreasing and our estimator $\delta^{\mathrm{cve}}(X)$ is clearly not non-decreasing, while the $\mathcal{N}(\theta, 1)$ is an exponential-family distribution. This inadmissibility result is summarized in the following theorem:

Theorem 2.3. *Let $X \sim \mathcal{N}(\theta, 1)$ with $|\theta| \leq m$ for a known positive m. Then the Charras–van Eeden dominators (2.9) of the mle are inadmissible for squared-error loss.*

We have not been able to find dominators for these inadmissible dominators and so will not consider them any further in this paper.

We now present Charras's (1979) method of obtaining dominators for his boundary estimators and use it to find dominators of the mle in the bounded-normal-mean problem.

Let δ be a Charras boundary estimator, then Charras considers the following class of estimators

$$\delta^{\mathrm{t}}(X) = \begin{cases} a(t) & \text{if } \delta(X) \leq a(t) \\ \delta(X) & \text{if } a(t) < \delta(X) < b(t) \\ b(t) & \text{if } \delta(X) \geq b(t)\ , \end{cases} \tag{2.10}$$

where $a(t)$ and $b(t)$, $t \in [0,1]$, take values in $[a,b]$ with $a(0) = a$, $b(0) = b$, $a(1) = b(1)$, $a(t)$ is non-decreasing and $b(t)$ is non-increasing. He then gives sufficient conditions on the functions $a(t)$ and $b(t)$, on the distribution of X and of $\delta(X)$ and on the loss function, for δ^{t} to dominate δ. These conditions are given in Appendix A. Here we give this domination result for the special case of the bounded normal mean when $a(t) = -m(1-t)$ and $b(t) = m(1-t)$, $t \in [0,1]$. Obviously, Charras's conditions are satisfied in the bounded-normal-mean case and his dominator of the mle can then be written as follows:

$$\delta^{\mathrm{ch}}(X) = \begin{cases} -m(1-t) & \text{if } X \leq -m(1-t) \\ X & \text{if } -m(1-t) < X < m(1-t) \\ m(1-t) & \text{if } X \geq m(1-t)\ . \end{cases}$$

For simplicity of the proof we let $\varepsilon = mt \in [0, m]$ and rewrite this dominator as follows:

$$\delta^{\text{ch}}(X) = \begin{cases} -(m-\varepsilon) & \text{if } X \le -(m-\varepsilon) \\ X & \text{if } -(m-\varepsilon) < X < m-\varepsilon \\ m-\varepsilon & \text{if } X \ge m-\varepsilon\ . \end{cases}$$

Then the following theorem holds:

Theorem 2.4. *Let $X \sim \mathcal{N}(\theta, 1)$ with $|\theta| \le m$ for a known $m > 0$. Then, for squared-error loss, $\{\delta^{\text{ch}} \colon 0 < \varepsilon \le \varepsilon_m\}$ is a class of dominating estimators of the mle, where ε_m is the unique root to $\psi_m(x) = 0$, with $\psi_m(x) = g(2m - x) + g(x) - 2x$ and $g(x) = 2x\,\Phi(-x)$.*

The proof of this theorem is given in Appendix A. It is Charras's proof applied to our special case.

The trivial estimator

For the estimator $\delta_o(X) \equiv 0$ the following theorem holds. Its proof is in Appendix A.

Theorem 2.5. *Let m_1 be the unique positive solution to $u(2m) + 1/2 - m^2 = 0$, where $u(x) = x^2\,\Phi(-x) - \Phi(-x) - x\,\phi(x)$. Then, for squared-error loss, the estimator δ_o dominates the mle if and only if $0 < m \le m_1 \approx 0.5204372$.*

A related result can be found in Marchand and Perron (2001). They present dominators of the mle of θ when $X \sim \mathcal{N}_k(\theta, I)$ with $k \ge 1$, $\|\theta\| \le m$ and squared-error loss. One of their results says that, when $k = 1$, any symmetric estimator dominates the mle when $m \le m_o \approx .4837$.

The Pitman estimator

The Pitman estimator of θ for our problem is defined as the Bayes estimator with respect to a uniform prior on $[-m, m]$ and squared-error loss. This Bayes estimator is the posterior mean of θ given X. Since the marginal density of X is given by

$$p(X) = \int_{-m}^{m} p_\theta(X)\,\pi(\theta)\,d\theta = \frac{1}{2m}\left[\Phi(m - X) - \Phi(-m - X)\right],$$

the posterior density of θ given X is given by

$$\begin{aligned} p(\theta|X) &= \frac{p_\theta(X)\,\pi(\theta)}{p(X)} \\ &= \frac{1}{\Phi(m-X)-\Phi(-m-X)}\,\frac{1}{\sqrt{2\pi}}\,\exp\left\{-\frac{(\theta-X)^2}{2}\right\}\,1_{\{|\theta|\le m\}}\ . \end{aligned}$$

Hence the Pitman estimator of θ is given by

$$\begin{aligned} \delta^{\mathrm{p}}(X) \;=\; E(\theta|X) \;&=\; X + \frac{\displaystyle\int_{-m-X}^{m-X} z\,\phi(z)\,dz}{\Phi(m-X)-\Phi(-m-X)} \\ &= X - \frac{\phi(m-X)-\phi(m+X)}{\Phi(m-X)-\Phi(-m-X)}\ . \end{aligned}$$

Bickel's asymptotically minimax estimator

Bickel (1981) constructs, for squared-error loss, a class of asymptotically minimax estimators for estimating a bounded normal mean. He constructs this class in the following way:

Let, for $|x|<1$, $\bar\psi = \pi\tan(\frac{\pi}{2}x)$ and let

$$\psi_m(x) \;=\; \begin{cases} \bar\psi(x) & \text{if } |x| \le 1-a_m^2 \\ \Big(\bar\psi(1-a_m^2) + \bar\psi'(1-a_m^2)\big(x^2-(1-a_m^2)\big)\Big)\,\operatorname{sgn} x & \text{if } |x| > 1-a_m^2\ . \end{cases}$$

He then shows that an asymptotically minimax estimator δ^{b} is given by

$$\delta^{\mathrm{b}}(X) \;=\; X - \frac{1}{n}\,\psi_m\!\left(\frac{X}{n}\right),$$

where $n = m(1-a_m)^{-1}$, $a_m < 1$ and $ma_m \to \infty$ as $m \to \infty$. Bickel (1981) suggests taking $a_m = m^{\frac{1}{8}}$ which gives the following expression for $\psi_m(x)$:

$$\begin{cases} \pi\,\tan\!\left(\dfrac{\pi}{2}\,x\right) & \text{if } |x| \le g(m) \\ \left[\pi\,\tan\!\left(\dfrac{\pi}{2}\,g(m)\right) + \dfrac{\pi^2}{2}\,\sec^2\!\left(\dfrac{\pi}{2}\,g(m)\,\big(x-g(m)\big)\right)\right]\operatorname{sgn} x & \text{if } |x| > g(m)\ , \end{cases}$$

where $g(m) = 1-m^{-1/4}$.

Then Bickel's asymptotically minimax estimator of θ is given by

$$\delta^{\mathrm{b}}(X) \;=\; X - \frac{1-m^{\frac{1}{8}}}{m}\,\psi_m\!\left(\frac{(1-m^{-\frac{1}{8}})\,X}{m}\right)$$

and the minimax value is given by $1-\frac{\pi^2}{m^2}+o(m^2)$ as $m\to\infty$.

3. NUMERICAL COMPARISONS

Appendix B contains graphs of the risk functions for squared-error loss of the estimators $\delta^{\rm mle}$, $\delta^{\rm cs.2}$, $\delta^{\rm cs.3}$, $\delta^{\rm E}$, $\delta^{\rm mr}$, $\delta^{\rm ch}$, $\delta^{\rm p}$ and $\delta^{\rm b}$ for several values of m. For the estimator $\delta^{\rm cs.3}$ the value $\alpha = .341$ (see (2.1)) is used, while for $\delta^{\rm ch}$, $\varepsilon = \varepsilon_m$ (see Theorem 2.4) is used. For the estimator $\delta^{\rm E}$ a value of $m > 1$ is needed.

Because of their symmetries, the risk functions are plotted only on the positive part of the parameter space. Moreover to check the robustness of the estimators with respect to misspecification of m, the risk functions are plotted on a somewhat wider interval, namely the interval $[0, 5m/4]$.

Figure 1 gives the risk functions for $m = .5$, .8, 1.0 and 1.5, while Figure 2 gives them for $m = 1.8$, 3, 5 and 10. The values of ε_m for these m (needed for the estimator $\delta^{\rm ch}$) are given in Table 1, while the values of a needed for $\delta^{\rm E}$ are given in Table 2.

Table 1: Values of ε_m for $\delta^{\rm ch}$.

m	.5	.8	1.0	1.5	1.8	≥ 3
ε_m	.276	.195	.101	.008	.001	.000

Table 2: Values of a for $\delta^{\rm E}$.

m	1.5	1.8	3	5	10
a	2.02	0.82	0.03	1.48×10^{-5}	6.91×10^{-17}

From the graphs one sees that

1. For $m = .5$, .8 and 1, $\delta^{\rm mr}$ has the same risk function as Casella and Strawderman's minimax estimator $\delta^{\rm cs.2}$. This is in accordance with our Theorem 2.2 which says that, for $m \leq 1$, these estimators are the same estimator.
2. Our Theorem 2.4 says that $\delta^{\rm ch}$ dominates $\delta^{\rm mle}$. This is clearly visible in the graphs for $m = .5$, .8 and 1. For larger m there is little difference between the risk functions of these two estimators and, in fact, little difference between the risk functions of $\delta^{\rm mle}$, $\delta^{\rm mr}$ and $\delta^{\rm ch}$, verifying the intuitively obvious result that, as $m \to \infty$, the differences

between these estimators converge almost surely to zero. This asymptotic result also holds for the estimators δ^{mle}, δ^{p} and δ^{b}, but for these estimators it takes a larger m for the risk functions to be close.

3. From the graph for $m = 1.5$ it is seen that, risk-functionwise, there is very little difference between δ^{E} and $\delta^{\text{cs.3}}$. But δ^{E} is computationally more complicated — two numerical integrations are needed to find a and two more to compute the estimator, while $\delta^{\text{cs.3}}$ is easily computable from (2.1). For $m = 1.8$, no minimax estimator is available, but for this value of m, δ^{E} behaves relative to δ^{P}, as it does for $m = 1.5$ — better for the smaller values of $|\theta|$, worse for values of $|\theta|$ closer to m with a fairly constant risk function. But the computational problems with this estimator relative to the others might, for a user, well be the determining factor concerning the question of which estimator to use.

4. In each of the graphs for $m \geq 3$, each of δ^{mle}, δ^{mr}, δ^{ch} and δ^{p} are close to being minimax with a minimax value ≈ 1. This is another example of the above-mentioned asymptotic result because, for the unrestricted case, the minimax value equals 1. Further, from the graphs for $m \leq 3$ one sees that, for these estimators, the maximum value of the risk function increases with m.

5. If one does not use the information that $|\theta| \leq m$, the best estimator of θ is X. Its risk function (for squared-error loss) is constant and equal to 1. From the graphs one can observe the gain in accuracy with which one can estimate θ when the restriction on θ is used in the construction of the estimator. One also sees that this gain (of course) decreases as m increases. For $m = .5$, e.g., one can get a minimum gain (over Θ) of about 80.1%, for $m = .8$ this is about 62.6%, for $m = 1$ about 55.0%, for $m = 1.5$ about 42.4%, for $m = 1.8$ about 28.7%, and for $m = 3$ about 3.9%. For the other values of m, this minimum gain is about 0 for all the restricted estimators except the Bickle's asymptotic estimator δ^{b}. The risk function of Bickle's estimator is, for large m, parallel to the one for the unrestricted estimator, X, under the squared-error loss. For $m = 5$, the minimum gain is about 39.5% and for $m = 10$ about 9.9% for δ^{b}. So, it is "worth the trouble" to use the information that $|\theta| \leq m$ at least for values of m that are not too large. Of course this increase in accuracy also occurs in other restricted-parameter-space models, but there are not many cases where numerical results about the gain in accuracy have been obtained (see e.g. van Eeden (2006), Chapter 7, which also contains robustness results for models other than the present one).

6. The graph for $m = .5$ gives an example of our Theorem 2.5, where it is shown that, for $m \leq m_1 \approx 0.5204372$, the trivial estimator dominates δ^{mle}: in the graph the risk function of δ^{mle} is, on the whole interval $[-m, m]$, $>$ than θ^2.

7. In each of the graphs we see that δ^{p} dominates each of the other estimators, except δ^{b}, on the middle part of the parameter space, but not near the endpoints.

8. For the estimator δ^{b}, the graph of its risk function is given for $m = 5$ and for $m = 10$. For those m, it dominates all the other estimators on the middle part of the parameter space, but not near the endpoints.

9. Graphs of the risk functions of δ^{mle}, $\delta^{\mathrm{cs.2}}$, δ^{p} and $\delta^{\mathrm{cs.3}}$ for $m = .5$, .75, 1.5 and 2 can be found in Gatsonis, MacGibbon and Strawderman (1987).

10. The robustness of the domination results with respect to miss-specification of the parameter space can be observed by studying the behaviour of the risk functions for values of θ in the neighbourhood of the value of m used to construct the estimators. For δ^{mle}, δ^{mr} and δ^{ch}, for instance, one sees that, for those m for which the risk functions are not too close (i.e. for $m = .5$, .8 and 1), the domination results hold on a small interval outside the parameter space.

11. The graphs for $m = .5$, .8 and 1 seem to indicate that δ^{mr} dominates δ^{ch}. We do not know whether this holds in general.

APPENDIX

A. PROOFS OF THE RESULTS IN SECTION 2

In this section proofs are given for the results in Section 2.

A.1. Proofs for the Marchand–Perron estimator

Proof of Theorem 2.1: From Berry (1990) we have, for $\nu \geq 0$,

$$I_\nu(t) \;=\; \left(\frac{t}{2}\right)^{\nu} \sum_{k=0}^{\infty} \frac{\left(\frac{1}{2}\,t\right)^{2k}}{k!\;\Gamma(\nu+k+1)}$$

and

$$I_{1/2}(t) \;=\; \sqrt{\frac{2t}{\pi}}\;\frac{\sinh(t)}{t}\;. \tag{A.1}$$

Further,

$$I_{3/2}(t) = I_{-1/2}(t) - \frac{1}{t}\, I_{1/2}(t) \qquad \text{and} \qquad I_{3/2}(t) = -\sqrt{\frac{2t}{\pi}}\,\frac{\sinh(t)}{t^2} + \sqrt{\frac{2t}{\pi}}\,\frac{\cosh(t)}{t}$$

give

$$I_{-1/2}(t) \;=\; I_{3/2}(t) + \frac{1}{t}\, I_{1/2}(t) \;=\; \sqrt{\frac{2t}{\pi}}\,\frac{\cosh(t)}{t}\;. \tag{A.2}$$

Then, using (A.1) and (A.2) and putting, when $a \in (0,1)$, $t = u(\sqrt{1-a})^{-1}$ in (2.4), gives (2.5).

For the proof of (2.6), note that, when $a \in (0,1)$, the right-hand side of (2.3) can be written as

$$\sqrt{\frac{2\pi}{1-a}}\,\left\{\Phi\big(m\sqrt{1-a}\big) - \frac{1}{2}\right\} \tag{A.3}$$

and the left-hand side of (2.3) as

$$\frac{\sqrt{2\pi}}{(1-a)^{3/2}}\,\left\{\Phi\big(m\sqrt{1-a}\big) - \frac{1}{2} - m\sqrt{1-a}\;\phi\big(m\sqrt{1-a}\big)\right\}\;. \tag{A.4}$$

The result then follows from (A.3) and (A.4). □

A.2. Proofs for Moors' dominator δ^{mr}

The following lemma is needed for the proof of Theorem 2.2.

Lemma A.1. *Let $u(x) = x - m\tanh(mx)$ and $v(x) = x + m\tanh(mx)$. Then*

- **(a)** *For $0 < m \le 1$, $u(x)$ and $v(x)$ are increasing in x and have the same sign as x.*
- **(b)** *For $m > 1$, let $r(m) = \frac{1}{m}\ln\big[m + \sqrt{m^2-1}\big]$.*
  Then:
  - **(i)** *$u(x)$ increases in x for $x > r(m)$ and for $x < -r(m)$. It decreases for $-r(m) < x < r(m)$.*
  - **(ii)** *$0 < r(m) < m$.*
  - **(iii)** *$u\big(r(m)\big) < 0$.*
  - **(iv)** *There exists a unique $\xi(m)$, $r(m) < \xi(m) < m$ such that $u\big(-\xi(m)\big) = u\big(\xi(m)\big) = 0$.*

Proof:

(**a**) For $0 < m \leq 1$, since $u'(x) = 1 - m^2 \operatorname{sech}^2(mx)$, we have

$$u'(x) > 0 \;\Leftrightarrow\; \exp(2mx) - 2m\exp(mx) + 1 = (e^{mx} - m)^2 + 1 - m^2 > 0\,.$$

Consequently, when $0 < m < 1$, $u'(x) > 0$ for $x \in (-\infty, \infty)$ and, when $m = 1$, $u'(x) > 0$ for $x \neq 0$ and $u'(0) = 0$. So, $u(x)$ increases in x and $u(x)$ has the same sign as x because $u(0) = 0$. Since $v'(x) = 1 + m^2 \operatorname{sech}^2(mx) > 0$ for $x \in (-\infty, \infty)$, we have $v(x)$ increases in x and $v(x)$ has the same sign as x because $v(0) = 0$.

(**b**) (**i**) Since $u'(x) = 1 - m^2 \operatorname{sech}^2(mx)$, we have

$$\begin{aligned} u'(x) > 0 \;&\Leftrightarrow\; \bigl|\exp(mx) - m\bigr| \;>\; \sqrt{m^2 - 1} \\ &\Leftrightarrow\; \begin{cases} x > r(m) > 0 & \text{if } \exp(mx) > m \\ x < -r(m) < 0 & \text{if } \exp(mx) < m\,. \end{cases} \end{aligned}$$

So, $u(x)$ increases in x when $x > r(m)$ and when $x < -r(m)$. It decreases in x when $-r(m) < x < r(m)$.

(**ii**) Let $p(x) = x - \ln\bigl[x + \sqrt{x^2 - 1}\,\bigr]/x$ for $x > 1$. Then $p(m) = m - r(m)$ for $m > 1$. Further, note that

$$p(x) \;=\; \frac{1}{x}\,\ln\biggl(\frac{\exp(x^2)}{x + \sqrt{x^2 - 1}}\biggr) \;>\; \frac{1}{x}\,\ln\biggl(\frac{\exp(x^2)}{2x}\biggr) \;>\; 0\,. \tag{A.5}$$

Since $x > 1$, $x + \sqrt{x^2 - 1} < 2x$. So the first inequality in (A.5) holds. Let $q(x) = \exp(x^2) - 2x$. Because $q(1) = e - 2 > 0$ and $q'(x) = 2\bigl(x\exp(x^2) - 1\bigr) > 0$ for $x > 1$, we have $q(x) > 0$, which shows that the second inequality in (A.5) also holds for $x > 1$. Hence, $p(x) > 0$ for $x > 1$ and so $0 < r(m) < m$ for $m > 1$.

(**iii**) Since

$$\begin{aligned} u\bigl(r(m)\bigr) \;&=\; r(m) - m\tanh\bigl(m\,r(m)\bigr) \\ &=\; \frac{1}{m}\,\ln\bigl(m + \sqrt{m^2 - 1}\bigr) - \sqrt{m^2 - 1}\;, \end{aligned}$$

we have

$$\begin{aligned} u\bigl(r(m)\bigr) < 0 \;&\Leftrightarrow\; m\sqrt{m^2 - 1} \;>\; \ln\bigl(m + \sqrt{m^2 - 1}\bigr) \\ &\Leftrightarrow\; f(m) > 0\;, \end{aligned}$$

where $f(x) = x\sqrt{x^2 - 1} - \ln\bigl(x + \sqrt{x^2 - 1}\bigr)$ for $x > 1$. Since $f(1) = 0$ and

$$\begin{aligned} f'(x) \;&=\; \sqrt{x^2 - 1} + \frac{x^2}{\sqrt{x^2 - 1}} - \frac{1}{x + \sqrt{x^2 - 1}}\,\biggl(1 + \frac{x}{\sqrt{x^2 - 1}}\biggr) \\ &=\; \sqrt{x^2 - 1} + \frac{x^2}{\sqrt{x^2 - 1}} - \frac{1}{\sqrt{x^2 - 1}} \\ &=\; 2\sqrt{x^2 - 1} \;>\; 0\;, \end{aligned}$$

for $x > 1$, we have $f(x)$ increases in x and $f(x) > f(1) = 0$ for $x > 1$. That is, $u\big(r(m)\big) < 0$ for $m > 1$.

(iv) By (i), $u(x)$ increases for $x > r(m)$ and for $x < -r(m)$. It decreases for $-r(m) < x < r(m)$. Since $u\big(r(m)\big) < 0$ (by (iii)) and $u(m) > 0$ by the continuity and monotonicity of $u(x)$, there exists a unique $\xi(m)$, $r(m) < \xi(m) < m$, such that $u\big(\xi(m)\big) = 0$. □

Proof of Theorem 2.2:

(i) When $0 < m \leq 1$, it follows from Lemma A.1 that

$$x \leq -m \tanh\big(m|x|\big) \;\;\Leftrightarrow\;\; x \leq 0$$

and

$$x \geq m \tanh\big(m|x|\big) \;\;\Leftrightarrow\;\; x \geq 0$$

and this shows that, when $m \leq 1$, we can rewrite (2.7) as $\delta^{\mathrm{mr}}(x) = m \tanh(mx)$ for $x \in (-\infty, \infty)$.

(ii) When $m > 1$, let $u(x) = x - m \tanh(mx)$. By Lemma A.1, $u(x)$ increases in x when $x > r(m)$ and when $x < -r(m)$. It decreases in x when $-r(m) < x < r(m)$. Moreover, $\xi(m)$ is the unique root of $u(x) = 0$ in $[r(m), m]$. Hence, $u(0) = u\big(-\xi(m)\big) = u\big(\xi(m)\big) = 0$, $u(x) > 0$ when $-\xi(m) < x < 0$ and when $x > \xi(m)$ and $u(x) < 0$ when $x < -\xi(m)$ and when $0 < x < \xi(m)$. So, when $m > 1$,

$$|x| < m \tanh\big(m|x|\big) \qquad \text{when } \; |x| < \xi(m)$$

and

$$|x| > m \tanh\big(m|x|\big) \qquad \text{when } \; |x| > \xi(m) \;.$$

This proves the result for the case where $m > 1$. □

A.3. Proofs for the Charras dominator δ^{ch}

Charras (1979) (see also Charras and van Eeden (1991)) gives conditions for estimators of the form (2.10) to dominate a boundary estimator δ, i.e. an estimator δ satisfying

$$\left.\begin{aligned} P_\theta\big(\delta(X) = a\big) \;&>\; 0 \\ P_\theta\big(\delta(X) = b\big) \;&>\; 0 \end{aligned}\right\} \qquad \text{for all } \;\theta \in [a, b] \;. \tag{A.6}$$

Charras' conditions on $a(t)$ and $b(t)$ for (2.10) to dominate δ are

(a) $a(t)$ and $b(t)$ are continuous.

(**b**) $a(t)$ and $b(t)$ have continuous right derivatives which are bounded in absolute value on $[0,1]$.

(**c**) $a(0)=a$, $b(0)=b$ and $a(1)=b(1)$.

(**d**) For all $t\in[0,1]$, $a'_+(t)=\dfrac{da(t)}{dt+}>0$ and $b'_+<0$.

His conditions on the distributions of X and $\delta(X)$ are

(**1**) Condition (2.8) is satisfied.

(**2**) The loss function $L(\theta,d)$ has, for all θ in a neighbourhood N of $[a,b]$, a partial derivative $\partial L/\partial d$ with respect to d which is, on $N\times N$, continuous in d and in θ.
Moreover,

$$\frac{\partial L(\theta,d)}{\partial d}\begin{cases}<0 & \text{when } d<\theta\\ =0 & \text{when } d=\theta\\ >0 & \text{when } d>\theta\ .\end{cases}$$

(**3**) The estimator δ to be dominated satisfies (A.6).

(**4**) The estimator δ has, for each $\theta\in[a,b]$, a Lebesgue density on (a,b), i.e. there exists a function $f(y,\theta)$ such that, for all (α,β) with $a<\alpha<\beta<b$,

$$P_\theta\bigl(\alpha<\delta(X)<\beta\bigr)=\int_\alpha^\beta f(y,\theta)\,dy\ .$$

Moreover, that density is bounded on $(a,b)\times[a,b]$.

Clearly, these Charras conditions are satisfied for our bounded-normal-mean problem.

Remark. Charras also has results for the case where δ has a discrete distribution.

Our proof of Theorem 2.4 is a special case of Charras' proof for his general case and we need the following lemmas A.2, A.3 and A.4 for our proof. The proofs of the lemmas A.2 and A.3 are straightforward and omitted.

Lemma A.2. *Let* $u(x)=x^2\,\Phi(-x)-\Phi(-x)-x\,\phi(x)$. *Then:*

(**i**) *The risk function of* δ^{mle} *is given by*

$$R(\theta,\delta^{\text{mle}})\;=\;1+u(m+\theta)+u(m-\theta)\ . \tag{A.7}$$

(**ii**) *The risk function of* δ^{ch} *is given by*

$$R(\theta,\delta^{\text{ch}})\;=\;1+u(m-\varepsilon+\theta)+u(m-\varepsilon-\theta)\ . \tag{A.8}$$

Lemma A.3. *Let* $g(x)=u'(x)=2\,x\,\Phi(-x)$*. Then* $g'(x)=2\big(\Phi(-x)-x\,\phi(x)\big)$, $g''(x)=2(x^2-2)\,\phi(x)$ *and the following properties of these functions hold:*

- **(i)** $g''(x)\geq 0$ *if and only if* $|x|\geq\sqrt{2}$ *and* $g''(x)\to 0$ *as* $x\to\pm\infty$.
- **(ii)** $g'(x)$ *increases in* x *if and only if* $|x|>\sqrt{2}$; $g'(x)$ *attains its maximum at* $x=-\sqrt{2}$, *its minimum at* $x=\sqrt{2}$ *and* $g'(0)=1$. *There is a unique root* η_0 *of* $g'(x)=0$, $\eta_0\in(0,\sqrt{2})$, $g'(x)\to 2$ *as* $x\to-\infty$ *and* $g'(x)\to 0$ *as* $x\to\infty$.
- **(iii)** $g(x)$ *has the same sign as* x *for* $x\in(-\infty,\infty)$; $g(x)$ *increases in* x *if* $x<\eta_0$ *and decreases otherwise;* $g(x)$ *attains its maximum at* $x=\eta_0$ *and the unique root of* $g(x)=0$ *is* $x=0$; $g(x)\to-\infty$ *as* $x\to-\infty$ *and* $g(x)\to 0$ *as* $x\to\infty$.

Lemma A.4. *Let* $h(x,\theta)=g(x+\theta)+g(x-\theta)$, *where (see the lemmas A.2 and A.3)* $g(x)=u'(x)=2x\,\Phi(-x)$ *and* $u(x)=x^2\,\Phi(-x)-\phi(-x)-x\,\phi(x)$. *Then*

- **(i)** *For fixed* $\varepsilon\in(0,m)$

$$\min_{\theta\in[m-\varepsilon,m]} h(m-\varepsilon,\theta) \;=\; h(m-\varepsilon,m) \;=\; g(2m-\varepsilon)+g(\varepsilon)-2\varepsilon\ .$$

- **(ii)** *Let* $\psi_m(x)=g(2m-x)+g(x)-2x$ *for* $x\in[0,m]$. *Then* $\psi'_m(x)<0$, $\psi_m(0)>0$ *and* $\psi_m(m)<0$, *so there exists a unique root* $\varepsilon_m\in(0,m)$ *of* $\psi_m(x)=0$ *with* $\psi_m(x)>0$ *for* $0\leq x<\varepsilon_m$ *and* $\psi_m(x)<0$ *for* $\varepsilon_m<x\leq m$.

Proof:

- **(i)** Consider

$$\frac{\partial}{\partial\theta}h(m-\varepsilon,\theta) \;=\; g'(m-\varepsilon+\theta)-g'(m-\varepsilon-\theta)\ .$$

For $\theta\in(m-\varepsilon,m]$ we have $m-\varepsilon+\theta>0$ and $m-\varepsilon-\theta<0$. So (see Lemma A.3) $g'(m-\varepsilon+\theta)<g'(0)=1$ and $g'(m-\varepsilon-\theta)>g'(0)=1$. Hence $g'(m-\varepsilon+\theta)-g'(m-\varepsilon-\theta)<0$ and so $\frac{\partial}{\partial\theta}h(m-\varepsilon,\theta)<0$. In other words, $h(m-\varepsilon,\theta)$ decreases as θ increases in $(m-\varepsilon,m]$, which implies that

$$\min_{\theta\in[m-\varepsilon,m]} h(m-\varepsilon,\theta) \;=\; h(m-\varepsilon,m)\ .$$

- **(ii)** Note that $h(m-\varepsilon,m)=g(2m-\varepsilon)+g(\varepsilon)-2\varepsilon=\psi_m(\varepsilon)$. Since $\psi'_m(x)=-2-g'(2m-x)+g'(x)$, with (see Lemma A.3) $g'(2m-x)>g'(\sqrt{2})>-1$ and $g'(x)<1$, we have $\psi'_m(x)<0$ for $x\in[0,m]$. $\square$

Proof of Theorem 2.4: First of all it is clear that, for all $\varepsilon \in (0,m]$, δ^{ch} dominates δ^{mle} on $[-m+\varepsilon, m-\varepsilon]$. Further, by symmetry, it is sufficient to look at the behaviour of the risk functions on $(m-\varepsilon, m]$.

Let

$$\Delta(\theta,\varepsilon) \,=\, R(\theta,\delta^{\mathrm{mle}}) - R(\theta,\delta^{\mathrm{ch}}) \ ,$$

then, by Lemma A.2,

$$\begin{aligned}\frac{\partial}{\partial\varepsilon}\Delta(\theta,\varepsilon) \;&=\; -\frac{\partial}{\partial\varepsilon}\Big[u(m-\varepsilon+\theta) + u(m-\varepsilon-\theta)\Big] \\ &=\; u'(m-\varepsilon+\theta) + u'(m-\varepsilon-\theta) \\ &=\; g(m-\varepsilon+\theta) + g(m-\varepsilon-\theta) \\ &=\; h(m-\varepsilon,\theta) \ ,\end{aligned}$$

where $h(x,\theta)$ and $g(x)$ are defined in Lemma A.4.

Then, by Lemma A.4 (i), we have

$$\min_{\theta\in(m-\varepsilon,m]} h(m-\varepsilon,\theta) \,=\, h(m-\varepsilon,m) \,=\, \psi(\varepsilon) \,>\, 0 \ ,$$

for $\varepsilon \in (0,\varepsilon_m)$, where ε_m is given by (ii) in Lemma A.4, implying that, for $0 \le \varepsilon \le \varepsilon_m$,

$$\frac{\partial}{\partial\varepsilon}\Delta(\theta,\varepsilon) \ge h(m-\varepsilon,m) \,=\, \psi(\varepsilon) \ge 0 \ .$$

But, $\Delta(m-\varepsilon,\theta) > 0$ for all $\varepsilon \in (0,m]$, which proves the theorem. □

A.4. Proof of Theorem 2.5

By Lemma A.2

$$\Delta_o(\theta,m) \,=\, R(\theta,\delta^{\mathrm{mle}}) - R(\theta,\delta_o) \,=\, u(m+\theta) + u(m-\theta) + 1 - \theta^2 \,.$$

So, it needs to be shown that $u(2m) + 1/2 - m^2 = 0$ has a unique positive root m_1 and that

$$u(m+\theta) + u(m-\theta) + 1 - \theta^2 \begin{cases} \ge 0 & \text{for all } \ \theta \in [0,m] \\ > 0 & \text{for some } \ \theta \in [0,m] \end{cases}$$

if and only if $0 < m < m_1$.

First note that (see Lemma A.3)

$$\Delta_o(0,m) \,=\, 2\,u(m) + 1 \,>\, 0 \qquad \text{for } \ m > 0 \ .$$

Further, with $g(x) = u'(x) = 2x\,\Phi(-x)$,

$$\frac{\partial}{\partial\theta}\Delta_o(\theta, m) \;=\; g(m+\theta) - g(m-\theta) - 2\,\theta$$

and

$$\frac{\partial^2}{\partial\theta^2}\Delta_o(\theta, m) \;=\; g'(m+\theta) + g'(m-\theta) - 2\ ,$$

so that

$$\frac{\partial}{\partial\theta}\Delta_o(\theta, m)\big|_{\theta=0} = 0 \qquad \text{for all}\;\; m > 0$$

and (see Lemma A.3)

$$\frac{\partial^2}{\partial\theta^2}\Delta_o(\theta, m) < 0 \qquad \text{for all}\;\; 0 \le \theta \le m, \;\; m > 0\ ,$$

implying that $\Delta_o(\theta, m)$ is, for each $m > 0$, decreasing in $\theta \in [0, m]$.

A necessary and sufficient condition for δ_o to dominate δ^{mle} for a given $m > 0$ is therefore that $\Delta_o(m, m) \ge 0$. But

$$\Delta_o(m, m) \;=\; u(2m) + u(0) + 1 - m^2 \;=\; u(2m) + 1/2 - m^2$$

and this function has the following properties:

(**1**) $\Delta_o(0, 0) = u(0) + 1/2 = 0$;

(**2**) $\frac{d}{dm}\Delta_o(m, m) = 2\big(g(2m) - m\big) = 2m\big(4\Phi(-2m) - 1\big)$.

So

$$\frac{d}{dm}\Delta_o(m, m) \left\{\begin{matrix} > \\ = \\ < \end{matrix}\right\} 0 \iff m \left\{\begin{matrix} < \\ = \\ > \end{matrix}\right\} \frac{1}{2}\,\Phi^{-1}\Big(\frac{3}{4}\Big)\,.$$

Further, $\Delta_o(\sqrt{2}/2, \sqrt{2}/2) = u(\sqrt{2}) < 0$ and thus there exists a unique $m_1 > 0$ with

$$\Delta_o(m_1, m_1) = 0 \quad \text{and} \quad \Delta_o(m, m) > 0 \qquad \text{for} \;\; 1 < m < m_1\ ,$$

which, together with the fact that $\Delta_o(\theta, m)$ is decreasing in θ for $\theta \in [0, m]$, proves the result. Numerically we found $m_1 \approx 0.5204372$.

B. GRAPHS FOR SECTION 3

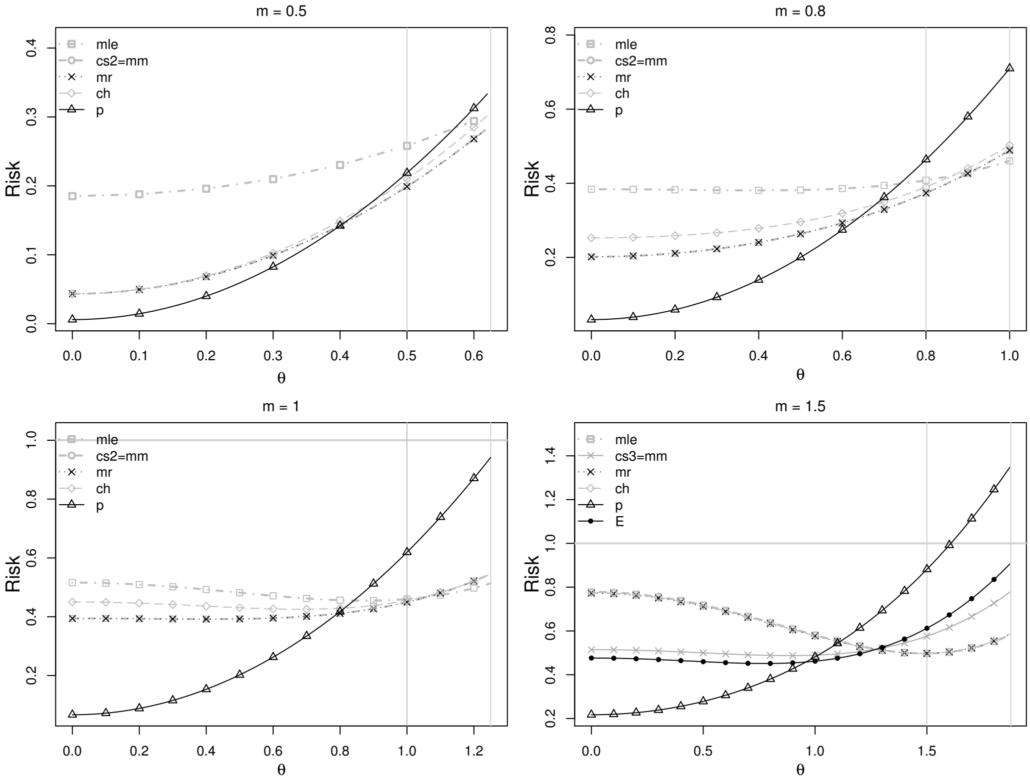

Figure 1: Risk functions of various estimators as a function of θ for $m = 0.5$, 0.8, 1.0 and 1.5.

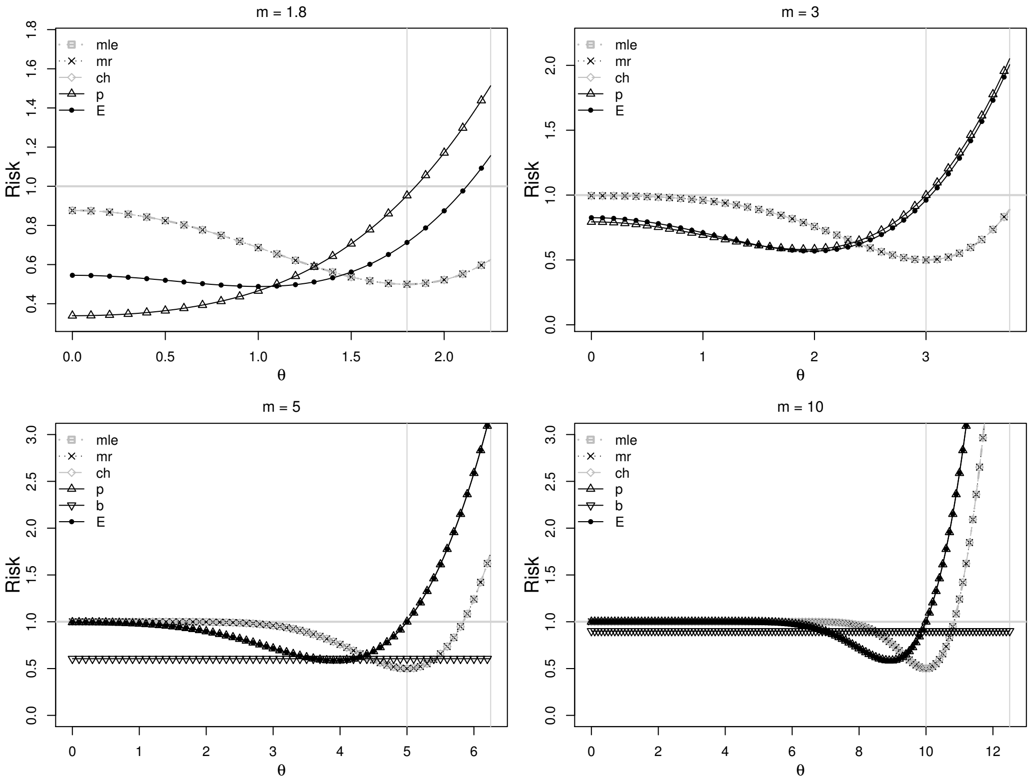

Figure 2: Risk functions of various estimators as a function of θ for $m = 1.8$, 3, 5 and 10.

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LIMIT MODEL FOR THE RELIABILITY OF A REGULAR AND HOMOGENEOUS SERIES-PARALLEL SYSTEM

Authors: Paula Reis
– CEAUL and EST, Politecnic Institut of Setúbal, Portugal
preis@est.ips.pt

Luísa Canto e Castro
– CEAUL and FCUL, University of Lisbon, Portugal
luisa.loura@fc.ul.pt

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Abstract:

- In large-scale systems the study of the exact reliability function can be an intricate problem. In these cases it is better to admit that the number of system components goes to infinity so as to find asymptotic models that give a good interpretation of the reliability. In this paper we will use some results of extreme value theory to obtain the asymptotic distribution of the reliability of a regular and homogeneous series-parallel system.

Key-Words:

- *reliability; series-parallel systems; extreme value theory; domains of atraction.*

AMS Subject Classification:

- 60K10, 60G70.

1. INTRODUCTION

When we study the reliability of some technological systems, we frequently find very complex structures due to large numbers of system components and the way the operating process uses such components. Indeed, there are situations that cannot be modelled as a simple parallel (or series) system and are best described as a series-parallel or parallel-series system. Examples of large systems with complex structures arise in transport networks of gas, oil, water and other fluids; also on telecommunication and electrical energy distribution networks and on charge and discharge networks.

The asymptotic theory of extremes, established by Gnedenko ([5]) in 1943, immediately leads to the identification of limit models for the reliability of systems with a large number of components in series or in parallel. Posterior results, such as those by Smirnov ([8]), Chernoff and Teicher ([3]) and Kolowrocki ([6] and [7]), have dealt with the same problem for homogeneous series-parallel (or parallel-series) systems. In turn, our approach will use the characterization of domains of attraction for minima for the known generalized extreme value distributions, as developed by Balkema and de Haan ([1]). In this initial work, we will restrict ourselves identifying limit laws in regular and homogeneous series-parallel systems, whenever the lifetime distribution function of each component belongs to some domain of attraction for minima.

1.1. Some basic notions of extreme value theory

Given a sequence of independent and identically distributed (i.i.d.) random variables, $\{X_i\}$, $i \geq 1$, with distribution function F, the random variable $M_n = \max(X_1, X_2, ..., X_n)$, with $n \geq 1$, has a known distribution function, given by

$$F_{M_n}(x) = \big[F(x)\big]^n \,.$$

If there exists a pair of sequences (a_n, b_n) where $a_n > 0$ and $b_n \in \mathbb{R}, \forall n \in \mathbb{N}$, and a nondegenerate distribution function G, such that, for all x where G is continuous,

$$P\big[M_n \leq a_n x + b_n\big] = \big[F(a_n x + b_n)\big]^n \underset{n\to\infty}{\longrightarrow} G(x) \,, \tag{1.1}$$

then G must be a Gumbel, a Fréchet or a Weibull distribution, whose standard forms are

$$\begin{aligned} &\text{Gumbel:} && \Lambda(x) = \exp(-e^{-x}), \quad x \in \mathbb{R} \\ &\text{Fréchet:} && \Phi_\alpha(x) = \exp(-x^{-\alpha}), \quad \alpha > 0, \;\; x \geq 0 \\ &\text{Weibull:} && \Psi_\alpha(x) = \exp\big(-(-x)^{-\alpha}\big), \quad \alpha < 0, \;\; x \leq 0 \,. \end{aligned}$$

These distributions can be represented uniquely in a parametric form, called the *von Mises–Jenkinson form* or generalized extreme value distribution (GEV),

$$(1.2) \qquad G_\gamma(x) = \begin{cases} \exp\bigl(-(1+\gamma x)^{-1/\gamma}\bigr), & 1+\gamma x \geq 0, \quad \gamma \neq 0 \\ \exp(-e^{-x}), & x \in \mathbb{R}, \qquad \gamma = 0\ . \end{cases}$$

It is easy to see that

$$G_\gamma(x) = \begin{cases} \Lambda(x), & \gamma = 0 \\ \Phi_{1/\gamma}(1+\gamma x), & \gamma > 0 \\ \Psi_{-1/\gamma}\bigl(-(1+\gamma x)\bigr), & \gamma < 0\ . \end{cases}$$

Whenever the sequences a_n and b_n exist on the above described conditions, or in other words, verifying (1.1), we will say that the distribution function F belongs to or is in the domain of attraction of G (for maxima) and we write $F \in \mathcal{D}(G)$.

The characterization of domains of attraction is closely related to the study of regular variation. Our approach about the asymptotic behaviour of the distribution function or of the reliability function for a series-parallel system, lies in known results which involve regular varying functions. We say that a real valued function, R, is regularly varying, with index ρ, at infinity and we write, $R \in \mathcal{R}_\rho$, if it is positive and measurable in $[a, +\infty[$, for some $a > 0$ and if $\forall x > 0$,

$$(1.3) \qquad \lim_{t\to\infty} \frac{R(tx)}{R(t)} = x^\rho\ ,$$

for some $\rho \in \mathbb{R}$. When $\rho = 0$, R is called a slowly varying function.

Gnedenko (1943), Balkema and de Haan (1972) established a relation between regular variation and the characterization of domains of attraction for Weibull and Fréchet laws, described in the following Theorem:

Theorem 1.1.

(1) *A distribution function F is in the domain of attraction of a Weibull law, Ψ_α, iff the right end point*[1] $x^F < \infty$ *and* $1 - F\bigl(x^F - \frac{1}{x}\bigr) \in R_{-\alpha}$, *when* $x \to \infty$. *In this case, taking δ_n such that* $n\bigl(1 - F(\delta_n)\bigr) \underset{n\to\infty}{\longrightarrow} 1$, *we will have*

$$F^n\Bigl(x^F + (x^F - \delta_n)\, x\Bigr) \longrightarrow \Psi_\alpha(x)\,, \qquad x < 0\ .$$

(2) *A distribution function F is in the domain of attraction of a Fréchet law, Φ_α, iff $1 - F \in R_{-\alpha}$. In this case*

$$F^n(a_n x) \longrightarrow \Phi_\alpha(x)\,, \qquad x > 0\ ,$$

with a_n such that $n\bigl(1 - F(a_n)\bigr) \underset{n\to\infty}{\longrightarrow} 1$.

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[1] Given a distribution function F, absolutely continuous, the right end point of its support is $x^F \equiv \sup\{x \colon F(x) < 1\}$.

It must be noted that only distribution functions with infinite right end point can be in $\mathcal{D}(\Phi_\alpha)$.

For the domain of attraction of a Gumbel law, we will use the characterization established by Balkema and de Haan ([1]):

Theorem 1.2. *A distribution function F belongs to $\mathcal{D}(\Lambda)$ iff there exist a positive function w satisfying $\lim\limits_{x\to x^F} w(x)=1$ and a differentiable, positive function g such that*

$$-\ln F(x) \;=\; w(x)\,\exp\left\{-\int_{z_0}^{x}\frac{1}{g(u)}\,du\right\},$$

for some z_0 and where we have $\lim\limits_{x\to x^F} g'(x)=0$.

The results developed for asymptotic extreme value theory for maxima are readily adapted for minima, since $m_n=\min\limits_{1\le i\le n}(X_i)=-\max\limits_{1\le i\le n}(-X_i)=-\max\limits_{1\le i\le n}(Y_i)$. If the sequence $\max\limits_{1\le i\le n}(-X_i)=\max\limits_{1\le i\le n}(Y_i)$ can be normalized, so as to admit a non degenerate limit Z, then the distribution function Z will be of the same type as G_γ, for some $\gamma\in\mathbb{R}$. Hence the limit law for minima, conveniently normalized, will verify

$$F_{-Z}(x) \;=\; P\big[-Z\le x\big] \;=\; P\big[Z\ge -x\big] \;=\; 1-G_\gamma(-x) \;=:\; H_\gamma(x)\;.$$

Therefore, we say that the distribution function F of a random variable X is in the domain of attraction for minima of H_γ, if the distribution function of $-X$ is in the domain of attraction (for maxima) of G_γ. In this case, there exists a pair of sequences (a_n,b_n) where $a_n>0$ and $b_n\in\mathbb{R}$, $\forall n\in\mathbb{N}$, such that

$$1-\big(1-F(a_nx+b_n)\big)^n \underset{n\to\infty}{\longrightarrow} H_\gamma(x)\;. \tag{1.4}$$

Remark 1.1. In most applications involving lifetimes the limit laws in (1.4) are restricted to the case $\gamma\le 0$. In fact, a lifetime T is always nonnegative, thus $-T$ is a random variable with finite right end point and can only be in the max-domain of attraction of a Weibull ($\gamma<0$) or a Gumbel ($\gamma=0$) (see Theorem 1.1 and Theorem 1.2). However, because there are systems with large durability, we will also study the case $\gamma>0$.

1.2. Regular and homogeneous series-parallel system

In reliability studies, we classify a system as being *series-parallel* if it is composed by subsystems with components in series and if those subsystems are organized in parallel (see Figure 1).

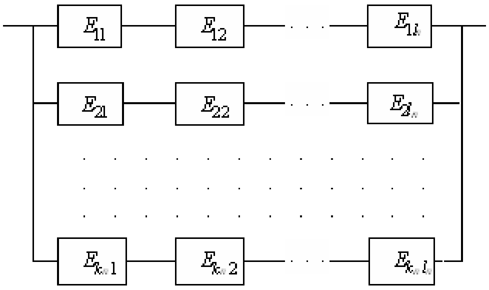

Figure 1: Scheme of a regular homogeneous series-parallel system.

Let E_{ij}, with $i = 1, 2, ..., k$ and $j = 1, 2, ..., l_i$, be the components of a *Series-Parallel System* S, formed by k subsystems in parallel of l_i components in series. Let X_{ij} be the lifetime of E_{ij}, i.e., X_{ij} represents the lifetime of the j-th component of the i-th subsystem. We will assume that all X_{ij}'s are independent. The lifetime T of the whole system is given by

$$T = \max_{1\le i\le k} \left(\min_{1\le j\le l_i} X_{ij} \right) .$$

The system S is called *regular* whenever

$$l_1 = l_2 = ... = l_k = l \ ,$$

and it is *homogeneous* whenever the components E_{ij} have the same *reliability function* $R(x) = P(X_{ij} > x) = 1 - F(x)$, with $x \in \,]-\infty, +\infty[$, i.e., if the random variables X_{ij} have the same distribution function $F(x) = P(X_{ij} \le x)$.

Suppose now that $k = k_n$ and $l = l_n$, i.e., (k_n) and (l_n) are sequences of real numbers such that at least one of them has a limit equal to infinity when n goes to infinity. Then we obtain sequences of regular systems whose families of reliability functions, in the case of an homogeneous system, are defined by (see in [6])

$$R_n(x) = 1 - \Big[1 - \big(R(x)\big)^{l_n}\Big]^{k_n}, \qquad \text{for } \ x \in \,]-\infty, +\infty[\ \text{ and each } \ n \in \mathbb{N} \ ,$$

or in terms of the sequence of distribution functions,

$$\begin{aligned} F_n(x) &= 1 - \left(1 - \Big[1 - \big(R(x)\big)^{l_n}\Big]^{k_n}\right) \\ &= \Big[1 - \big(1 - F(x)\big)^{l_n}\Big]^{k_n}, \qquad \text{for } \ x \in \,]-\infty, +\infty[\ \text{ and each } \ n \in \mathbb{N} \ . \end{aligned} \tag{1.5}$$

Assuming that F is in the domain of attraction of a law for minima, H_γ, our purpose will be to analyse the asymptotic behaviour of the functions $R_n(x)$ and $F_n(x)$ defined above. Although our goal is to treat this problem in its maximum generality, in this paper we will only treat the case where k_n goes to infinity. More precisely, we will suppose that $k_n = n$ and investigate which should be the asymptotic behaviour of l_n, so that, using a suitable normalization, we can find a nondegenerate limit for F_n.

2. CHARACTERIZATION OF THE DOMAINS OF ATTRACTION

From (1.5), it follows that $F_n(x)$ is the distribution function of the maxima of k_n i.i.d. random variables, each one with distribution function given by $H_n(x) = \big[1-\big(1-F(x)\big)^{l_n}\big]$, and we want to determine in which domain of attraction for maxima belongs $H_n(x)$. Now, assuming that F is in the domain of attraction for minima of a law $H_\gamma(x) = 1-G_\gamma(-x)$, then the asymptotic behaviour of the right tail of H_n must be similar to the right tail of the minima law H_γ. In the next paragraphs we will analyse the right tail behaviour of H_γ, for $\gamma<0$, $\gamma=0$ and $\gamma>0$, in order to identify the max-stable law to which it is attracted.

2.1. Case $\gamma < 0$ (Weibull for minima)

The function $H_\gamma(x)$ is defined, for all $x\in\mathbb{R}$, by

$$\begin{aligned}
H_\gamma(x) &= 1-G_\gamma(-x)\\
&= \begin{cases} 1-\exp\Big(-(1-\gamma x)^{-1/\gamma}\Big), & 1-\gamma x\ge 0\\ 0, & 1-\gamma x<0\end{cases} \qquad (2.1)\\
&= \begin{cases} 1-\exp\Big(-(1-\gamma x)^{-1/\gamma}\Big), & x\ge \frac{1}{\gamma}\\ 0, & x<\frac{1}{\gamma}\ .\end{cases}
\end{aligned}$$

Since the right end point is infinite, we will first check whether or not H_γ is in the Fréchet max-domain of attraction. By Theorem 1, and using (1.3) and (2.1), we have

$$\begin{aligned}
\lim_{t\to+\infty}\frac{1-H_\gamma(tx)}{1-H_\gamma(t)} &= \lim_{t\to+\infty}\frac{e^{-(1-\gamma tx)^{-1/\gamma}}}{e^{-(1-\gamma t)^{-1/\gamma}}}\\
&= \lim_{t\to+\infty}\exp\left\{\Big(-(1-\gamma\,t\,x)^{-1/\gamma}\Big)\left[1-\left(\frac{1-\gamma\,t}{1-\gamma\,t\,x}\right)^{-1/\gamma}\right]\right\}\\
&= \lim_{t\to+\infty}\exp\left\{\Big(-(1-\gamma\,t\,x)^{-1/\gamma}\Big)\left[1-\left(\frac{\frac{1}{\gamma t}-1}{\frac{1}{\gamma t}-x}\right)^{-1/\gamma}\right]\right\}\\
&= \begin{cases} 0, & x^{1/\gamma}<1\\ +\infty, & x^{1/\gamma}>1\ .\end{cases}
\end{aligned}$$

It follows that $1-H_\gamma$ is not a regularly varying function at infinity and therefore cannot belong to the Fréchet max-domain of attraction. We claim, however, that $H_\gamma\in\mathcal{D}(\Lambda)$. In fact, since

$$\ln H_\gamma(x) \;=\; \ln\Big(1-\big(1-H_\gamma(x)\big)\Big) \;\sim\; -\big(1-H_\gamma(x)\big)\ ,$$

when $x \to x^{H_\gamma}$, we get $-\frac{\ln H_\gamma(x)}{1-H_\gamma(x)} \underset{x\to x^{H_\gamma}}{\longrightarrow} 1$. Without loss of generality, let us suppose $w(x) = -\frac{\ln H_\gamma(x)}{1-H_\gamma(x)} > 0$, for all x, to get

$$\begin{aligned}
-\ln H_\gamma(x) &= \left(-\frac{\ln H_\gamma(x)}{1-H_\gamma(x)}\right)\bigl(1-H_\gamma(x)\bigr) \\
&= w(x)\exp\Bigl(-(1-\gamma x)^{-1/\gamma}\Bigr) \\
&= w(x)\exp\left\{-\int_{1/\gamma}^{x} \frac{1}{g(u)}\,du\right\},
\end{aligned}$$

for $x > \frac{1}{\gamma}$ and where $g(x) = (1-\gamma x)^{1/\gamma+1} > 0$ is such that

$$\lim_{x\to+\infty} g'(x) = \lim_{x\to+\infty}\Bigl[-(\gamma+1)\,(1-\gamma x)^{1/\gamma}\Bigr] = 0\ .$$

Consequently, by Theorem 1.2, $H_\gamma(x)$ is in the Gumbel max-domain of attraction. In this case, the attraction constants can be defined by (see [4])

$$\begin{cases} b_n\colon\ \ H_\gamma(b_n) = \exp\Bigl(-\dfrac{1}{n}\Bigr) \\ a_n\colon\ \ a_n = \dfrac{1}{k(b_n)}\ , \end{cases}$$

where

$$k(b_n) = -\frac{H'_\gamma(b_n)}{H_\gamma(b_n)\,\ln H_\gamma(b_n)}\ .$$

Now,

$$\begin{aligned}
H_\gamma(b_n) = \exp\Bigl(-\frac{1}{n}\Bigr) &\iff (1-\gamma b_n)^{-1/\gamma} = -\ln\Bigl[1-\exp\Bigl(-\frac{1}{n}\Bigr)\Bigr] \\
&\iff 1-\gamma b_n = \Bigl(-\ln\Bigl[1-\exp\Bigl(-\frac{1}{n}\Bigr)\Bigr]\Bigr)^{-\gamma} \\
&\iff b_n = \frac{1-\Bigl(-\ln\Bigl[1-\exp\bigl(-\frac{1}{n}\bigr)\Bigr]\Bigr)^{-\gamma}}{\gamma}\ .
\end{aligned}$$

On the other hand,

$$\begin{aligned}
a_n &= \frac{1}{k(b_n)} \\
&= -\frac{\exp\bigl(-\frac{1}{n}\bigr)\,\ln\Bigl(\exp\bigl(-\frac{1}{n}\bigr)\Bigr)}{(1-\gamma b_n)^{-1/\gamma-1}\Bigl(1-\exp\bigl(-\frac{1}{n}\bigr)\Bigr)} \\
&= \frac{1}{n\Bigl(\exp\bigl(\frac{1}{n}\bigr)-1\Bigr)\,(1-\gamma b_n)^{-1/\gamma-1}} \\
&= \frac{1}{n\Bigl(\exp\bigl(\frac{1}{n}\bigr)-1\Bigr)\,\Bigl(-\ln\Bigl[1-\exp\bigl(-\frac{1}{n}\bigr)\Bigr]\Bigr)^{\gamma+1}}\ .
\end{aligned}$$

It follows that

$$(2.2)\qquad \begin{cases} a_n = \dfrac{1}{n\Big(\exp\big(\frac{1}{n}\big)-1\Big)\,\Big(-\ln\Big[1-\exp\big(-\frac{1}{n}\big)\Big]\Big)^{\gamma+1}}\,, \\[2ex] b_n = \dfrac{1-\Big(-\ln\Big[1-\exp\big(-\frac{1}{n}\big)\Big]\Big)^{-\gamma}}{\gamma}\,, \qquad\qquad \gamma<0\;. \end{cases}$$

2.2. Case $\gamma > 0$ (Fréchet for minima)

Let us suppose that the distribution function of the lifetime of each component belongs to the domain of attraction of a Fréchet for minima. We have, for $x \in \mathbb{R}$,

$$\begin{aligned} H_\gamma(x) \;&=\; 1-G_\gamma(-x) \\ (2.3)\qquad &=\; \begin{cases} 1-\exp\Big(-(1-\gamma x)^{-1/\gamma}\Big)\,, & x \le \frac{1}{\gamma} \\ 1\,, & x > \frac{1}{\gamma}\;. \end{cases} \end{aligned}$$

In this case, since $x^{H_\gamma} = \frac{1}{\gamma}$, $H_\gamma(x)$ cannot be in the Fréchet domain of attraction for maxima, but it can, however, be in the max-domain of attraction of a Weibull or a Gumbel. Now,

$$\begin{aligned} 1-H_\gamma\bigg(x^{H_\gamma}-\frac{1}{x}\bigg) \;&=\; \exp\Bigg(-\bigg(1-\gamma\Big(\frac{1}{\gamma}-\frac{1}{x}\Big)\bigg)^{-1/\gamma}\Bigg) \\ &=\; \exp\Bigg(-\bigg(\frac{\gamma}{x}\bigg)^{-1/\gamma}\Bigg) \\ &=\; e^{-\gamma^{-1/\gamma}x^{1/\gamma}}\,, \qquad \gamma>0, \quad x>0\;, \end{aligned}$$

so applying Theorem 1.2 and (2.3) we get

$$\begin{aligned} \lim_{t\to\infty}\frac{e^{-\gamma^{-1/\gamma}(tx)^{1/\gamma}}}{e^{-\gamma^{-1/\gamma}t^{1/\gamma}}} \;&=\; \lim_{t\to\infty} e^{-\gamma^{-1/\gamma}t^{1/\gamma}(x^{1/\gamma}-1)} \\ &=\; \begin{cases} 0\,, & x^{1/\gamma}>1 \\ +\infty\,, & x^{1/\gamma}<1\;. \end{cases} \end{aligned}$$

We conclude therefore that the function H_γ is not in the domain of attraction for maxima of a Weibull. Following the same reasoning as in the previous case, we now prove that H_γ verifies the representation given by Theorem 1.2, and so H_γ

is in the Gumbel max-domain of attraction. In fact, with $w(x) = -\frac{\ln H_\gamma(x)}{1-H_\gamma(x)}$, we have

$$\begin{aligned} -\ln H_\gamma(x) &= w(x)\exp\Big(-(1-\gamma x)^{-1/\gamma}\Big) \\ &= w(x)\exp\left\{-\int_{-\infty}^{x}\frac{1}{g(u)}\,du\right\}, \end{aligned}$$

for $x < \frac{1}{\gamma}$ and where $g(x) = (1-\gamma x)^{1/\gamma+1} > 0$ is such that

$$\lim_{x\to\frac{1}{\gamma}} g'(x) = \lim_{x\to\frac{1}{\gamma}} \Big[-(\gamma+1)\,(1-\gamma x)^{1/\gamma}\Big] = 0 .$$

The possible attraction constants are defined by (see [4])

$$\begin{cases} b_n\colon \quad H_\gamma(b_n) = \exp\Big(-\dfrac{1}{n}\Big) \\ a_n\colon \quad a_n = \dfrac{1}{k(b_n)} \;. \end{cases}$$

Calculations similar to the case $\gamma < 0$ yield

$$(2.4) \qquad \begin{cases} a_n = \dfrac{1}{n\Big(\exp(\frac{1}{n})-1\Big)\Big(-\ln\Big[1-\exp(-\frac{1}{n})\Big]\Big)^{\gamma+1}}\,, \\[2ex] b_n = \dfrac{1-\Big(-\ln\Big[1-\exp(-\frac{1}{n})\Big]\Big)^{-\gamma}}{\gamma}\,, \qquad\qquad \gamma > 0 . \end{cases}$$

2.3. Case $\gamma = 0$ (Gumbel for minima)

Finally we analyse the case where the lifetime of the components is in the domain of attraction of a Gumbel for minima. The function $H_0(x)$ is defined, for all $x \in \mathbb{R}$, by

$$H_0(x) = 1 - G_0(-x) = 1 - \exp\big(-\exp(x)\big)\,,$$

so that

$$-\ln H_0(x) = w(x)\exp\left\{-\int_{-\infty}^{x} e^u\,du\right\},$$

with $w(x)$ defined as in the previous cases. Once again, the conditions of Theorem 1.2 are verified, considering $g(x) = e^{-x} > 0$, $\forall x \in \mathbb{R}$, and therefore the distribution function $H_0(x)$ is in the max-domain of attraction of a Gumbel law. The sequences (a_n) and (b_n) are now given by

$$(2.5) \qquad \begin{cases} a_n = \dfrac{1}{n\Big(\exp(\frac{1}{n})-1\Big)\Big(-\ln\Big[1-\exp(-\frac{1}{n})\Big]\Big)}\,, \\[2ex] b_n = \ln\Big(-\ln\Big[1-\exp(-\frac{1}{n})\Big]\Big)\,, \end{cases}$$

since

$$\begin{aligned} H_0(b_n) = \exp\left(-\frac{1}{n}\right) \quad &\Longleftrightarrow \quad \exp(-e^{b_n}) = 1 - \exp\left(-\frac{1}{n}\right) \\ &\Longleftrightarrow \quad e^{b_n} = -\ln\left[1 - \exp\left(-\frac{1}{n}\right)\right] \\ &\Longleftrightarrow \quad b_n = \ln\left(-\ln\left[1 - \exp\left(-\frac{1}{n}\right)\right]\right) \end{aligned}$$

and

$$\begin{aligned} a_n &= \frac{1}{k(b_n)} \\ &= -\frac{\Big(1 - \exp\big(-\exp(b_n)\big)\Big)\,\ln\Big(1 - \exp\big(-\exp(b_n)\big)\Big)}{\exp(b_n)\,\exp\big(-\exp(b_n)\big)} \\ &= \frac{\exp\big(-\frac{1}{n}\big)\,\ln\Big(\exp\big(-\frac{1}{n}\big)\Big)}{\ln\Big(1 - \exp\big(-\frac{1}{n}\big)\Big)\,\Big(1 - \exp\big(-\frac{1}{n}\big)\Big)} \\ &= \frac{1}{n\Big(\exp\big(\frac{1}{n}\big) - 1\Big)\,\Big(-\ln\big[1 - \exp\big(-\frac{1}{n}\big)\big]\Big)} \;. \end{aligned}$$

We can sum up the results derived in the last three paragraphs by saying that for all $\gamma \in \mathbb{R}$ there are sequences (a_n) and (b_n), with $a_n > 0$ and $b_n \in \mathbb{R}$, such that

$$H^n_\gamma(a_n x + b_n) \underset{n\to\infty}{\longrightarrow} \Lambda(x) \;, \tag{2.6}$$

i.e., all stable laws for minima are in the Gumbel max-domain of attraction.

3. LIMIT MODEL FOR THE RELIABILITY OF A REGULAR AND HOMOGENEOUS SERIES-PARALLEL SYSTEM

Using the above results it is possible to obtain the limit behaviour for the reliability of a regular series-parallel system, with a large number of components, whose lifetimes are i.i.d. and belong to the domain of attraction of a stable law for minima, which in turn allows us to establish the following result:

Theorem 3.1. *Let F be a distribution function in the domain of attraction of $H_\gamma(x)$, i.e., assume that there are sequences (a_n) and (b_n), with $a_n > 0$ and $b_n \in \mathbb{R}$, $\forall n \in \mathbb{N}$, such that*

$$1 - \big(1 - F(a_n x + b_n)\big)^n = H_\gamma(x) + \varepsilon_n(x) = 1 - G_\gamma(-x) + \varepsilon_n(x) \;, \tag{3.1}$$

with $\varepsilon_n(x) \to 0$, $\forall x \in \mathbb{R}$ *and where* $G_\gamma(x)$ *is defined in (1.2). Given a sequence of integers such that* $\frac{l_n}{n} n^{\frac{n}{l_n}} e_n = o(1)$, *with* $e_n = \sup\limits_{x\in\mathbb{R}} |\varepsilon_n(x)|$, *then for all* $\gamma \in \mathbb{R}$, *there exist* $\alpha_n > 0$ *and* $\beta_n \in \mathbb{R}$, $\forall n \in \mathbb{N}$ *such that, for the sequence of distribution functions, conveniently normalized, the following holds*

$$F_n(\alpha_n x + \beta_n) = \Big[1 - \big(1 - F(\alpha_n x + \beta_n)\big)^{l_n}\Big]^n \underset{n\to\infty}{\longrightarrow} \Lambda(x) \ , \tag{3.2}$$

for all $x \in \mathbb{R}$, *i.e., for a regular homogeneous series-parallel system, constituted by* n *parallel subsystems of* l_n *components in series, the sequence of reliability functions,conveniently normalized, verifies*

$$R_n(\alpha_n x + \beta_n) = 1 - \Big[1 - \big(1 - F(\alpha_n x + \beta_n)\big)^{l_n}\Big]^n \underset{n\to\infty}{\longrightarrow} 1 - \Lambda(x) \ ,$$

for all $x \in \mathbb{R}$. *Further we can consider* $\alpha_n = a_n a_n^*$, $\beta_n = a_n b_n^* + b_n$ *with*

$$a_n^* = \frac{1 - \gamma b_n^*}{n\Big(\exp\big(\frac{1}{n}\big) - 1\Big)\Big(-\ln\Big[1 - \exp\big(-\frac{1}{n}\big)\Big]\Big)} \tag{3.3}$$

and

$$b_n^* = \begin{cases} -\dfrac{1}{\gamma}\left[\left(\dfrac{l_n}{n\Big(-\ln\Big[1-\exp\big(-\frac{1}{n}\big)\Big]\Big)}\right)^{\gamma} - 1\right], & \gamma \neq 0 \\[3ex] -\ln\left(\dfrac{l_n}{n\Big(-\ln\Big[1-\exp\big(-\frac{1}{n}\big)\Big]\Big)}\right), & \gamma = 0 \ . \end{cases} \tag{3.4}$$

Proof: Given the sequences (a_n) and (b_n) for which (3.1) is valid and taking (α_n) and (β_n) such that $\alpha_n = a_n a_n^*$ and $\beta_n = a_n b_n^* + b_n$, we have

$$\begin{aligned} \big(1 - F(\alpha_n x + \beta_n)\big)^{l_n} &= \big(1 - F(a_n a_n^* x + a_n b_n^* + b_n)\big)^{l_n} \\ &= \Big[\Big(1 - F\big(a_n(a_n^* x + b_n^*) + b_n\big)\Big)^n\Big]^{\frac{l_n}{n}} \\ &= \Big(1 - H_\gamma(a_n^* x + b_n^*) + \varepsilon_n(a_n^* x + b_n^*)\Big)^{\frac{l_n}{n}} \\ &= \big(1 - H_\gamma(a_n^* x + b_n^*)\big)^{\frac{l_n}{n}} + \rho_n(x) \ . \end{aligned} \tag{3.5}$$

First, we will analyse the component $\big(1 - H_\gamma(a_n^* x + b_n^*)\big)^{\frac{l_n}{n}}$ and later we will prove that $n\rho_n(x) \to 0$, $\forall x \in \mathbb{R}$, where (l_n), (a_n^*) and (b_n^*) satisfy the previously mentioned conditions. Now, for $\gamma \neq 0$ we have, successively,

$$\begin{aligned} \big(1 - H_\gamma(a_n^* x + b_n^*)\big)^{\frac{l_n}{n}} &= \Big[G_\gamma\big(-(a_n^* x + b_n^*)\big)\Big]^{\frac{l_n}{n}} \\ &= \exp\left\{-\left(\left(\frac{l_n}{n}\right)^{-\gamma} - \gamma\left(\left(\frac{l_n}{n}\right)^{-\gamma} a_n^* x + \left(\frac{l_n}{n}\right)^{-\gamma} b_n^*\right)\right)^{-1/\gamma}\right\} \\ &= \exp\Big\{-\big(1 - \gamma(\alpha_n^* x + \beta_n^*)\big)^{-1/\gamma}\Big\} \;=\; 1 - H_\gamma(\alpha_n^* x + \beta_n^*) \ , \end{aligned} \tag{3.6}$$

with

$$\text{(3.7)}\qquad \begin{cases} \alpha_n^* = \left(\dfrac{l_n}{n}\right)^{-\gamma} a_n^* \\ \beta_n^* = \left(\dfrac{l_n}{n}\right)^{-\gamma} \left(\dfrac{\gamma b_n^* - 1}{\gamma}\right) + \dfrac{1}{\gamma} \; . \end{cases}$$

Hence for $\alpha_n = a_n a_n^*$, $\beta_n = a_n b_n^* + b_n$ and for α_n^* and β_n^* given by (3.7), we can write

$$\text{(3.8)}\qquad \bigl(1 - F(\alpha_n x + \beta_n)\bigr)^{l_n} = 1 - H_\gamma(\alpha_n^* x + \beta_n^*) + \rho_n(x) \; .$$

Using (3.3), (3.4) and (3.7) the sequence α_n^* verifies

$$\begin{aligned} \alpha_n^* &= \left(\frac{l_n}{n}\right)^{-\gamma} a_n^* \\ &= \left(\frac{l_n}{n}\right)^{-\gamma} \left(\frac{1 + \left(\frac{l_n}{n\left(-\ln\left[1-\exp\left(-\frac{1}{n}\right)\right]\right)}\right)^{\gamma} - 1}{n\Bigl(\exp\bigl(\frac{1}{n}\bigr) - 1\Bigr) \Bigl(-\ln\Bigl[1 - \exp\bigl(-\frac{1}{n}\bigr)\Bigr]\Bigr)}\right) \\ &= \left(\frac{l_n}{n}\right)^{-\gamma} \left(\frac{\bigl(\frac{l_n}{n}\bigr)^{\gamma}}{n\Bigl(\exp\bigl(\frac{1}{n}\bigr) - 1\Bigr) \Bigl(-\ln\Bigl[1 - \exp\bigl(-\frac{1}{n}\bigr)\Bigr]\Bigr) \Bigl(-\ln\Bigl[1 - \exp\bigl(-\frac{1}{n}\bigr)\Bigr]\Bigr)^{\gamma}}\right) \\ &= \frac{1}{n\Bigl(\exp\bigl(\frac{1}{n}\bigr) - 1\Bigr) \Bigl(-\ln\Bigl[1 - \exp\bigl(-\frac{1}{n}\bigr)\Bigr]\Bigr)^{\gamma+1}} \; . \end{aligned}$$

Moreover, given (3.4) for $\gamma \neq 0$, $l_n = n\bigl(-\ln\bigl[1 - \exp\bigl(-\frac{1}{n}\bigr)\bigr]\bigr)\,(1 - \gamma b_n^*)^{1/\gamma}$ and it follows that

$$\begin{aligned} \beta_n^* &= \left(\frac{l_n}{n}\right)^{-\gamma} \left(\frac{\gamma b_n^* - 1}{\gamma}\right) + \frac{1}{\gamma} \\ &= \frac{n^{-\gamma}\Bigl(-\ln\Bigl[1 - \exp\bigl(-\frac{1}{n}\bigr)\Bigr]\Bigr)^{-\gamma} (1 - \gamma b_n^*)^{-1}\,(\gamma b_n^* - 1)}{\gamma\, n^{-\gamma}} + \frac{1}{\gamma} \\ &= -\frac{\Bigl(-\ln\Bigl[1 - \exp\bigl(-\frac{1}{n}\bigr)\Bigr]\Bigr)^{-\gamma} (1 - \gamma b_n^*)^{-1}\,(1 - \gamma b_n^*)}{\gamma} + \frac{1}{\gamma} \\ &= \frac{1 - \Bigl(-\ln\Bigl[1 - \exp\bigl(-\frac{1}{n}\bigr)\Bigr]\Bigr)^{-\gamma}}{\gamma} \; . \end{aligned}$$

This means that (α_n^*) and (β_n^*) verify (2.2) and (2.4) and consequently are a suitable choice of sequences for the convergence of H_γ^n to the Gumbel law. To prove that $\rho(x)$ in (3.8) is such that $n\,\rho(x)$ goes to zero, we start by observing that since $n\bigl(\exp\bigl(\frac{1}{n}\bigr) - 1\bigr) \sim 1$ and $-\ln\bigl(1 - \exp\bigl(-\frac{1}{n}\bigr)\bigr) \sim \ln n$, as $n \to \infty$, the constants (α_n^*) and (β_n^*) are asymptotically given by

$$\alpha_n^* \sim \frac{1}{(\ln n)^{\gamma+1}} \qquad \text{and} \qquad \beta_n^* \sim \frac{1 - (\ln n)^{-\gamma}}{\gamma} \; ,$$

and so using (3.7) we get,

$$\begin{aligned} a_n^* x + b_n^* \; &= \; \Big(\frac{l_n}{n}\Big)^{\gamma} \alpha_n^* x + \Big(\frac{l_n}{n}\Big)^{\gamma} \Big(\frac{\gamma\beta_n^* - 1}{\gamma}\Big) + \frac{1}{\gamma} \\ &\sim \; \Big(\frac{l_n}{n \ln n}\Big)^{\gamma} \Big(\frac{x}{\ln n} - \frac{1}{\gamma}\Big) + \frac{1}{\gamma} \; . \end{aligned} \tag{3.9}$$

Moreover, from (3.6), (3.7) and (3.9) we obtain

$$\begin{aligned} \big(1 - H_\gamma(a_n^* x + b_n^*)\big)^{\frac{l_n}{n}-1} \; &\sim \; \frac{\exp\Big\{-\Big(1 - \gamma\Big(\frac{1}{(\ln n)^{\gamma+1}}\, x + \frac{1-(\ln n)^{-\gamma}}{\gamma}\Big)\Big)^{-1/\gamma}\Big\}}{\exp\Big\{-\Big(1 - \gamma\Big(\big(\frac{l_n}{n \ln n}\big)^{\gamma} \big(\frac{x}{\ln n} - \frac{1}{\gamma}\big) + \frac{1}{\gamma}\Big)\Big)^{-1/\gamma}\Big\}} \\ &\sim \; \frac{\exp\Big\{-\ln n \big(1 - \gamma \frac{x}{\ln n}\big)^{-1/\gamma}\Big\}}{\exp\Big\{-\frac{n \ln n}{l_n} \big(1 - \gamma \frac{x}{\ln n}\big)^{-1/\gamma}\Big\}} \\ &\sim \; \exp\Big\{\Big(\frac{n}{l_n} - 1\Big) \ln n \Big(1 - \frac{\gamma}{\ln n}\, x\Big)^{-1/\gamma}\Big\} \\ &\sim \; n^{\frac{n}{l_n}-1} \; , \end{aligned} \tag{3.10}$$

when $n \to \infty$ and $\forall x \in \mathbb{R}$. Now, since H_γ is a continuous distribution function on $\mathbb{R}$, the convergence of $\varepsilon_n(x)$ in (3.1) is naturally the uniform convergence and we can write $\lim\limits_{n\to\infty} e_n = \lim\limits_{n\to\infty} \big[\sup\limits_{x\in\mathbb{R}} |\varepsilon_n(x)|\big] = 0$. Furthermore, taking into account that $a_n^* x + b_n^*$ converges to x^{H_γ}, we also have $\varepsilon_n(a_n^* x + b_n^*) \to 0$, uniformly in $\mathbb{R}$, when $n \to \infty$. These results, together with (3.10) and $\frac{l_n}{n}\, n^{\frac{n}{l_n}} e_n \to 0$, when $n \to \infty$, allow us to obtain the following approximation for $\rho_n(x)$ in (3.5),

$$\begin{aligned} \rho_n(x) \; &= \; \frac{l_n}{n}\, \varepsilon_n(a_n^* x + b_n^*) \big(1 - H_\gamma(a_n^* x + b_n^*)\big)^{\frac{l_n}{n}-1} + o(\xi_n) \\ &\sim \; \frac{l_n}{n^2}\, \varepsilon_n(a_n^* x + b_n^*)\, n^{\frac{n}{l_n}} + o(\xi_n) \; , \end{aligned}$$

with $\xi_n = \frac{l_n}{n^2}\, n^{\frac{n}{l_n}} e_n$, so that $n\,\rho_n(x) \to 0$. To derive the main result in (3.2) for $\gamma \neq 0$, observe that, using (3.8), we have

$$\begin{aligned} &\Big[1 - \big(1 - F(\alpha_n x + \beta_n)\big)^{l_n}\Big]^n = \\ &\qquad = \; \big[H_\gamma(\alpha_n^* x + \beta_n^*) + \rho_n(x)\big]^n \\ &\qquad = \; \big[H_\gamma(\alpha_n^* x + \beta_n^*)\big]^n \Big[1 + \frac{\rho_n(x)}{H_\gamma(\alpha_n^* x + \beta_n^*)}\Big]^n \\ &\qquad = \; \big[H_\gamma(\alpha_n^* x + \beta_n^*)\big]^n \Big[1 + \frac{n\,\rho_n(x)}{H_\gamma(\alpha_n^* x + \beta_n^*)} + o\Big(\frac{n\,\rho_n(x)}{H_\gamma(\alpha_n^* x + \beta_n^*)}\Big)\Big] , \end{aligned}$$

where (α_n^*) and (β_n^*) are normalizing sequences for the convergence of $\big[H_\gamma(\alpha_n^* x + \beta_n^*)\big]^n$ to $\Lambda(x)$. So since $H_\gamma(\alpha_n^* x+\beta_n^*) \to 1$, when n goes to infinity, we finally obtain

$$F_n(\alpha_n x+\beta_n) \,=\, \Big[1-\big(1-F(\alpha_n x+\beta_n)\big)^{l_n}\Big]^n \underset{n\to\infty}{\longrightarrow} \Lambda(x) \ ,$$

or in other words,

$$R_n(\alpha_n x+\beta_n) \,=\, 1-\Big[1-\big(1-F(\alpha_n x+\beta_n)\big)^{l_n}\Big]^n \underset{n\to\infty}{\longrightarrow} 1-\Lambda(x) \ .$$

In the case $\gamma = 0$, we can also write

$$\big[1-H_0(a_n^* x+b_n^*)\big]^{\frac{l_n}{n}} \,=\, 1-H_0(\alpha_n^* x+\beta_n^*) \ , \tag{3.11}$$

where

$$\begin{cases} \alpha_n^* \,=\, a_n^* \\ \beta_n^* \,=\, b_n^* + \ln\!\left(\dfrac{l_n}{n}\right) . \end{cases} \tag{3.12}$$

Using (3.3), (3.4) and (3.12) it now follows that

$$\alpha_n^* \,=\, \frac{1}{n\Big(\exp\big(\frac{1}{n}\big)-1\Big)\,\Big(-\ln\Big[1-\exp\big(-\frac{1}{n}\big)\Big]\Big)} \ ,$$

and moreover

$$\begin{aligned} \beta_n^* \,&=\, b_n^* + \ln\!\left(\frac{l_n}{n}\right) \\ &=\, -\ln\!\left(\frac{l_n}{n\Big(-\ln\Big[1-\exp\big(-\frac{1}{n}\big)\Big]\Big)}\right) + \ln\!\left(\frac{l_n}{n}\right) \\ &=\, \ln\!\left(\frac{\frac{l_n}{n}}{\frac{l_n}{n\left(-\ln\left[1-\exp\left(-\frac{1}{n}\right)\right]\right)}}\right) \,=\, \ln\!\left(-\ln\!\left[1-\exp\!\left(-\frac{1}{n}\right)\right]\right) . \end{aligned}$$

This means that the sequences (α_n^*) and (β_n^*) verify (2.5) and therefore are a suitable choice of sequences for the convergence of H_0^n to the Gumbel law. Given that $\alpha_n^* \sim \frac{1}{\ln n}$ and $\beta_n^* \sim \ln(\ln n)$ and given (3.12), we have the approximation

$$\begin{aligned} a_n^* x + b_n^* \,&=\, \alpha_n^* x + \left(\beta_n^* - \ln\!\left(\frac{l_n}{n}\right)\right) \\ &\sim\, \frac{x}{\ln n} + \ln\!\left(\frac{n\ln n}{l_n}\right) . \end{aligned}$$

Once again we can show that $\big(1-H_0(a_n^* x+b_n^*)\big)^{\frac{l_n}{n}} \sim n^{\frac{n}{l_n}}$ and $n\rho_n(x)\to 0$, when $n\to\infty$, $\forall x\in\mathbb{R}$, yielding

$$F_n(\alpha_n x+\beta_n) \,=\, \Big[1-\big(1-F(\alpha_n x+\beta_n)\big)^{l_n}\Big]^n \underset{n\to\infty}{\longrightarrow} \Lambda(x) \ ,$$

i.e.,

$$R_n(\alpha_n x+\beta_n) \underset{n\to\infty}{\longrightarrow} 1-\Lambda(x) \ ,$$

which proves the result. □

Example 3.1. Let be $X \curvearrowright \operatorname{Exp}(1)$.

Observe that

$$\left(1-F\left(\frac{x}{n}\right)\right)^n = \left(e^{-\frac{x}{n}}\right)^n = e^{-x} = \Psi_1(-x) = 1-H_{-1}(x) \ .$$

The conditions of theorem 3 are satisfied, setting $a_n=\frac{1}{n}$, $b_n=0$ and $\varepsilon_n(x)=0$, $\forall x\in\mathbb{R}$. For any sequence l_n, by now considering

$$\begin{cases} a_n^* = \dfrac{1+b_n^*}{n\Big(\exp\big(\frac{1}{n}\big)-1\Big)\Big(-\ln\Big[1-\exp\big(-\frac{1}{n}\big)\Big]\Big)} \\[2ex] b_n^* = \left(\dfrac{l_n}{n\Big(-\ln\Big[1-\exp\big(-\frac{1}{n}\big)\Big]\Big)}\right)^{-1} - 1 \end{cases}$$

and

$$\begin{cases} \alpha_n = \dfrac{1+b_n^*}{n^2\Big(\exp\big(\frac{1}{n}\big)-1\Big)\Big(-\ln\Big[1-\exp\big(-\frac{1}{n}\big)\Big]\Big)} \\[2ex] \beta_n = \dfrac{\Big(-\ln\Big[1-\exp\big(-\frac{1}{n}\big)\Big]\Big)}{l_n} - \dfrac{1}{n} \ , \end{cases}$$

we obtain

$$F_n(x) = \Big[1-\big(1-F(\alpha_n x+\beta_n)\big)^{l_n}\Big]^n \underset{n\to\infty}{\longrightarrow} \Lambda(x) \ ,$$

i.e.,

$$R_n(x) = 1-\Big[1-\big(1-F(\alpha_n x+\beta_n)\big)^{l_n}\Big]^n \underset{n\to\infty}{\longrightarrow} 1-\Lambda(x) \ .$$

Remark 3.1. Note that if the sequence (l_n) is constant and (k_n) goes to infinity then the limit models for the reliability of the system are the usual models for maxima.

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HIGH QUANTILE ESTIMATION AND THE PORT METHODOLOGY

Authors: Lígia Henriques-Rodrigues
– Instituto Politécnico de Tomar and CEAUL, Portugal
Ligia.Rodrigues@aim.estt.ipt.pt

M. Ivette Gomes
– Universidade de Lisboa, F.C.U.L. (D.E.I.O.) and C.E.A.U.L., Portugal
ivette.gomes@fc.ul.pt

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Abstract:

- In many areas of application, a typical requirement is to estimate a *high quantile* χ_{1-p} of probability $1-p$, a value, high enough, so that the chance of an exceedance of that value is equal to p, small. The semi-parametric estimation of high quantiles depends not only on the estimation of the tail index γ, the primary parameter of extreme events, but also on an adequate estimation of a scale first order parameter. The great majority of semi-parametric quantile estimators, in the literature, do not enjoy the adequate behaviour, in the sense that they do not suffer the appropriate linear shift in the presence of linear transformations of the data. Recently, and for heavy tails ($\gamma > 0$), a new class of quantile estimators was introduced with such a behaviour. They were named PORT-quantile estimators, with PORT standing for *peaks over random threshold.* In this paper, also for heavy tails, we introduce a new class of PORT-quantile estimators with the above mentioned behaviour, using the PORT methodology and incorporating Hill and moment PORT-classes of *tail index* estimators in one of the most recent classes of quantile estimators suggested in the literature. Under convenient restrictions on the underlying model, these classes of estimators are consistent and asymptotically normal for adequate k, the number of top order statistics used in the semi-parametric estimation of χ_{1-p}.

Key-Words:

- *statistics of extremes; heavy tails; high quantiles; semi-parametric estimation; PORT methodology; asymptotic behaviour.*

AMS Subject Classification:

- 62G32, 62E20.

1. INTRODUCTION

A model F is said to have a heavy right-tail whenever the right *tail function*, $\overline{F} := 1 - F$, is a regularly varying function with a negative index of regular variation $\alpha = -1/\gamma$, i.e., for every $x > 0$, $\lim_{t\to\infty} \overline{F}(tx)/\overline{F}(t) = x^{-1/\gamma}$. Then we are in the domain of attraction for maxima of an *extreme value* (EV) distribution function (d.f.),

$$EV_\gamma(x) = \exp\bigl(-(1+\gamma x)^{-1/\gamma}\bigr)\,, \qquad x > -1/\gamma, \quad \gamma > 0\;,$$

and we write $F \in \mathcal{D}_{\mathcal{M}}(EV_{\gamma>0})$. The parameter γ is the *tail index*, one of the primary parameters of rare events.

In a context of heavy tails, and with the notation $U(t) := F^{\leftarrow}(1-1/t)$, $t \geq 1$, $F^{\leftarrow}(y) := \inf\{x\colon F(x) \geq y\}$ the generalized inverse function of the underlying model F, the first order parameter (or tail index) γ (> 0) appears, for every $x > 0$, as the limiting value, as $t \to \infty$, of the quotient $\bigl(\ln U(tx) - \ln U(t)\bigr)/\ln x$ (de Haan, 1970). Indeed, with the usual notation RV_α for the class of regularly varying functions with an index of regularly variation α, i.e., positive measurable functions g such that $g(tx)/g(t) \to x^\alpha$, as $t \to \infty$ and for all $x > 0$, we can further say

$$F \in \mathcal{D}_{\mathcal{M}}(EV_{\gamma>0}) \quad \text{iff} \quad U \in RV_\gamma \quad \text{iff} \quad 1-F \in RV_{-1/\gamma} \quad \text{(Gnedenko, 1943)}. \tag{1.1}$$

Heavy-tailed distributions have recently been accepted as realistic models for various phenomena in economics, ecology, bibliometrics and biometry, among others. See, for instance, the recent books on the topic by Markovich (2007) and Resnick (2007).

For small values of p, we want to extrapolate beyond the sample, estimating a typical parameter in many areas of application, a high quantile χ_{1-p}, i.e., a value such that $F(\chi_{1-p}) = 1 - p$, or equivalently,

$$\chi_{1-p} = U(1/p)\,, \qquad p = p_n \to 0, \quad np_n \to K \;\text{ as }\; n \to \infty, \quad K \in [0,1]\;. \tag{1.2}$$

We are going to base inference on the largest $k+1$ order statistics, and as usual in semi-parametric estimation of parameters of extreme events, we shall assume that k is an *intermediate* sequence of integers in $[1, n[$, i.e.,

$$k = k_n \to \infty, \quad k/n \to 0\,, \qquad \text{as }\; n \to \infty\;. \tag{1.3}$$

In order to derive the asymptotic non-degenerate behaviour of semi-parametric estimators of parameters of extreme events, we need more than the first-order condition, $U \in RV_\gamma$, provided in (1.1). A convenient condition is the following second-order condition, which guarantees that

$$\lim_{t\to\infty} \frac{\ln U(tx) - \ln U(t) - \gamma \ln x}{A(t)} = \frac{x^\rho - 1}{\rho}\;, \tag{1.4}$$

which we assume to hold for every $x > 0$, being $\rho \le 0$ the "shape" or, more properly, the generalized shape second order parameter. The limit function in (1.4) is necessarily of this given form and $|A| \in RV_\rho$ (Geluk and de Haan, 1987). Sometimes, only for the sake of simplicity, we shall assume to be working in a sub-class of Hall-Welsh class of models (Hall and Welsh, 1985), where there exist $\gamma > 0$, $\rho < 0$, $C > 0$ and $\beta \neq 0$, such that, as $t \to \infty$,

$$U(t) = C\, t^{\gamma}\left(1 + \frac{A(t)}{\rho}\bigl(1 + o(1)\bigr)\right), \qquad \text{with } \ A(t) = \gamma\beta t^{\rho}\,. \tag{1.5}$$

Typical heavy-tailed models, such as the Fréchet, the Generalized Pareto and the Student-t_ν belong to such a class. Then, the second-order condition in equation (1.4) holds, with $A(t) = \gamma\beta t^{\rho}$, $\beta \neq 0$, $\rho < 0$. The parameters β and ρ are the so-called generalized scale and shape second-order parameters, respectively.

If condition (1.5) holds, $U(t) \sim Ct^{\gamma}$, as $t \to \infty$, and from (1.2), we have

$$\chi_{1-p} = U(1/p) \ \sim \ Cp^{-\gamma}, \qquad \text{as} \ \ p \to 0\ .$$

An obvious estimator of χ_{1-p} is thus $\widehat{C}p^{-\hat{\gamma}}$, with $\widehat{C}$ and $\hat{\gamma}$ any consistent estimators of C and γ, respectively.

Given a sample $(X_1, X_2, ..., X_n)$, let us denote $(X_{1:n} \le X_{2:n} \le \cdots \le X_{n:n})$ the set of associated ascending order statistics. Denoting Y a standard Pareto model, i.e., a model such that $F_Y(y) = 1 - 1/y$, $y > 1$, the universal uniform transformation and the fact that $Y_{n-k:n} \overset{p}{\sim} (n/k)$ for intermediate k, enables us to write $X_{n-k:n} \overset{p}{\sim} C(n/k)^{\gamma}$, as $n \to \infty$, where the notation $X_n \overset{p}{\sim} Y_n$ means that X_n/Y_n converges in probability to one, as $n \to \infty$. Consequently, an obvious estimator of C, proposed in Hall (1982), is

$$\widehat{C} \equiv C_{k,n,\hat{\gamma}} := X_{n-k:n}(k/n)^{\hat{\gamma}}$$

and

$$Q_{k,p_n,\hat{\gamma}} = \widehat{C}\, p_n^{-\hat{\gamma}} = X_{n-k:n}(k/np_n)^{\hat{\gamma}}$$

is the obvious quantile-estimator at the level p (Weissman, 1978). The semi-parametric estimation of high quantiles depends thus strongly on the estimation of the tail index γ, the primary parameter of extreme events.

In the classical approach, we often consider for $\hat{\gamma}$ either the Hill estimator (Hill, 1975) or the moment estimator (Dekkers *et al.*, 1989), both based on the $k+1$ top order statistics, denoted $\underline{X}_k := (X_{n-k:n}, \cdots, X_{n:n})$. The Hill estimator is the average of the log-excesses,

$$H_{k,n} \equiv H_n(\underline{X}_k) \equiv \widehat{\gamma}_{k,n,H} := \frac{1}{k}\sum_{i=1}^{k}\left(\ln X_{n-i+1:n} - \ln X_{n-k:n}\right), \tag{1.6}$$

and the moment estimator has the functional expression,

$$(1.7)\qquad M_{k,n} \equiv M_n(\underline{X}_k) \equiv \widehat{\gamma}_{k,n,M} := M_{k,n}^{(1)} + 1 - \frac{1}{2}\left\{1 - \left(M_{k,n}^{(1)}\right)^2 / M_{k,n}^{(2)}\right\}^{-1},$$

with $M_{k,n}^{(\alpha)}$ defined by

$$(1.8)\qquad M_{k,n}^{(\alpha)} \equiv M_n^{(\alpha)}(\underline{X}_k) := \frac{1}{k}\sum_{i=1}^{k}\left(\ln X_{n-i+1:n} - \ln X_{n-k:n}\right)^{\alpha}, \qquad \alpha = 1, 2\ .$$

Under the second order framework in (1.4) and for any intermediate sequence k, i.e. whenever (1.3) holds, we have for the Hill estimator H, in (1.6), and for the moment estimator M, in (1.7), generally denoted by T, the validity of the following asymptotic distributional representation,

$$(1.9)\qquad \widehat{\gamma}_{k,n,T} \stackrel{d}{=} \gamma + \frac{\sigma_T\, P_{k,T}}{\sqrt{k}} + b_T\, A(n/k)\big(1 + o_p(1)\big)\ ,$$

where $P_{k,T}$ is asymptotically standard normal and

$$(1.10)\qquad \sigma_H^2 := \gamma^2, \quad b_H := \frac{1}{1-\rho}, \quad \sigma_M^2 := 1 + \gamma^2 \quad \text{and} \quad b_M := \frac{\gamma(1-\rho) + \rho}{\gamma(1-\rho)^2}\ .$$

Most of the semi-parametric quantile estimators in the literature, like the ones in Gomes and Figueiredo (2006), Gomes and Pestana (2007), Beirlant *et al.* (2008), Caeiro and Gomes (2008), as well as in other papers on semi-parametric quantile estimation prior to 2005 (see also, de Haan and Ferreira, 2006), do not enjoy the adequate behaviour in the presence of linear transformations of the data, a behaviour related with the fact that for any quantile χ_{1-p} we have

$$(1.11)\qquad \chi_{1-p}(s + \delta X) = s + \delta\, \chi_{1-p}(X)$$

for any model X, real s and positive δ.

Recently, and for $\gamma > 0$, Araújo Santos *et al.* (2006) provided quantile estimators with the linear property in (1.11), based upon a sample of excesses over a random threshold $X_{n_q:n}$, denoted

$$(1.12)\qquad \underline{X}^{(q)} := \big(X_{n:n} - X_{n_q:n}, \cdots, X_{n_q+1:n} - X_{n_q:n}\big), \qquad n_q := [nq] + 1\ ,$$

where $[x]$ denotes, as usual, the integer part of x, with:

- $0 < q < 1$, for distributions with a left endpoint, $x_F := \inf\{x\colon F(x) > 0\}$, finite or infinite (*the random threshold* $X_{n_q:n}$ *is an empirical quantile*);
- $q = 0$, for distributions with a finite left endpoint x_F (*the random threshold is the minimum,* $X_{1:n}$).

Such estimators were named PORT-quantile estimators, with PORT standing for *peaks over random threshold*, and are based on the PORT-Hill and PORT-moment estimators, generically denoted $T(q) \equiv T_{k,n}(q) := T_n(\underline{X}^{(q)})$ for $T = H$

or M, $k < n - n_q$, and with $H_n(\underline{X}_k)$ and $M_n(\underline{X}_k)$ provided in (1.6) and (1.7), respectively. They are given by

$$Q_{k,p_n,T(q)} := \big(X_{n-k:n} - X_{n_q:n}\big) \left(\frac{k}{np_n}\right)^{T(q)} + X_{n_q:n} \ , \tag{1.13}$$

where $T(q)$ can more generally be any consistent estimator of the tail index γ, made location/scale invariant by using any of the transformed samples $\underline{X}^{(q)}$, in (1.12). The PORT-Hill and the PORT-moment estimators have been studied by simulation in Gomes *et al.* (2008a).

The class of estimators suggested here is also a function of the sample of the excesses $\underline{X}^{(q)}$ in (1.12). We use the PORT methodology and incorporate Hill and moment PORT-classes of *tail index* estimators in one of the classes of quantile estimators suggested in Caeiro and Gomes (2008), slightly modified in order to satisfy the linear property in (1.11). More specifically, we shall consider quantile estimators of the type,

$$\widetilde{Q}_{k,p_n,T(q)} := \frac{X_{n-[k/2]:n} - X_{n-k:n}}{2^{T(q)} - 1} \left(\frac{k}{np_n}\right)^{T(q)} + X_{n_q:n} \ . \tag{1.14}$$

Under convenient restrictions on the underlying model, these classes of estimators are consistent and asymptotically normal for adequate k, the number of top order statistics used in the semi-parametric estimation of χ_{1-p}.

In Section 2 of this paper, we shall present a few introductory technical details and asymptotic preliminary results associated with the PORT methodology. The asymptotic behaviour of the PORT-classes of *tail index* estimators under study, together with the asymptotic comparison of the PORT-Hill and the PORT-moment estimators at optimal levels, will be derived in Section 3. In Section 4, we derive the asymptotic behaviour of the new classes of PORT-quantile estimators. Finally, in Section 5, we draw some overall conclusions.

2. TECHNICAL DETAILS RELATED WITH THE PORT METHODOLOGY

2.1. The second order framework for heavy-tailed models under a real shift

If we introduce a deterministic shift, i.e. a new location, $s \neq 0$, in the underlying model X, with quantile function $U_X(t)$, the transformed random variable (r.v.) $Y = X + s$ has an associated quantile function given by $U_s(t) \equiv U_Y(t) = U_X(t) + s$

and condition (1.4) can be rewritten as

$$\lim_{t\to\infty} \frac{\ln U_s(tx) - \ln U_s(t) - \gamma \ln x}{A_s(t)} = \frac{x^{\rho_s}-1}{\rho_s} \;, \tag{2.1}$$

for all $x > 0$, with $|A_s| \in RV_{\rho_s}$.

Let F be a model with quantile function $U(t) \equiv U_X(t)$, given in (1.5). Then

$$U_Y(t) = C\, t^{\gamma}\left(1 + \frac{A(t)}{\rho} + s\, C^{-1} t^{-\gamma} + o(t^{\rho})\right), \qquad \text{as} \quad t \to \infty \;.$$

Therefore both $U_s(t) = U_Y(t)$ and $U(t) = U_X(t)$ are asymptotically equivalent to $C\, t^{\gamma}$, but

$$\rho_s = \begin{cases} \rho & \text{if } \rho > -\gamma \\ -\gamma & \text{if } \rho \le -\gamma \,. \end{cases}$$

The function $A_s(t)$ in (2.1) can be chosen as

$$A_s(t) := \begin{cases} -\dfrac{\gamma s}{U(t)}, & \text{if } \rho < -\gamma \\ A(t) - \dfrac{\gamma s}{U(t)}, & \text{if } \rho = -\gamma \\ A(t), & \text{if } \rho > -\gamma \,. \end{cases}$$

2.2. Asymptotic preliminary results in the PORT methodology

In this subsection we begin with the presentation of the asymptotic results for the statistics $M_{k,n}^{(\alpha,q)} \equiv M_n^{(\alpha)}\big(\underline{X}^{(q)}\big)$, $k < n - n_q$, based on the sample of excesses $\underline{X}^{(q)}$, $0 \le q < 1$, in (1.12) and with $M_n^{(\alpha)}(\underline{X}_k)$ provided in (1.8).

In the following, χ_q denotes the q-quantile of F: $F(\chi_q) = q$ (by convention $\chi_0 = x_F$, whenever finite) so that,

$$X_{n_q:n} \xrightarrow[n\to\infty]{p} \chi_q \qquad \text{for} \quad 0 \le q < 1 \;. \tag{2.2}$$

We present, without proof, the following Lemma:

Lemma 2.1 (Araújo Santos *et al.*, 2006)**.** *If the second order condition (1.4) holds, if $k = k_n$ is an intermediate sequence, i.e. (1.3) holds, then, for any real q, $0 \le q < 1$, with $F(\chi_q) = q$ ($\chi_0 = x_F$, whenever finite), and for $\alpha = 1, 2$,*

$$M_{k,n}^{(\alpha,q)} - \frac{1}{k}\sum_{i=1}^{k}\left(\ln\frac{X_{n-i+1:n} - \chi_q}{X_{n-k:n} - \chi_q}\right)^{\alpha} = o_p\!\left(\frac{1}{U(n/k)}\right).$$

Remark 2.1. Note that if $q \in (0,1)$, $X_{n_q:n} - \chi_q = O_p\big(1/\sqrt{n}\big)$ and we can assure that $\sqrt{k}\,\Big(M_{k,n}^{(\alpha,q)} - \frac{1}{k}\sum_{i=1}^{k}\big(\ln(X_{n-i+1:n} - \chi_q) - \ln(X_{n-k:n} - \chi_q)\big)^{\alpha}\Big) = O_p\big(\sqrt{k/n}/U(n/k)\big) = o_p(1)$, for $\alpha = 1, 2$.

Proposition 2.1. *If the second order condition* (1.4) *holds and* $k = k_n$ *is an intermediate sequence, i.e.* (1.3) *holds, the statistics* $M_{k,n}^{(\alpha,q)} = M_n^{(\alpha)}(\underline{X}^{(q)})$, *with* $k < n - n_q$, $M_n^{(\alpha)}(\underline{X}_k)$ *given in* (1.8) *and* $\underline{X}^{(q)}$ *given in* (1.12), *satisfy for* $\alpha = 1, 2$,

$$M_{k,n}^{(1,q)} \overset{d}{=} M_{k,n}^{(1)} + \frac{\gamma\,\chi_q}{(1+\gamma)\,U(n/k)}\,\big(1 + o_p(1)\big)\,, \tag{2.3}$$

$$M_{k,n}^{(2,q)} \overset{d}{=} M_{k,n}^{(2)} + \frac{2\,\gamma^2\,(2+\gamma)\,\chi_q}{(1+\gamma)^2\,U(n/k)}\,\big(1 + o_p(1)\big)\,. \tag{2.4}$$

Proof: The first moment of the log-excesses can be rewritten as

$$M_{k,n}^{(1,q)} = \frac{1}{k}\sum_{i=1}^{k}\ln\!\left(\frac{X_{n-i+1:n} - X_{n_q:n}}{X_{n-k:n} - X_{n_q:n}}\right) = M_{k,n}^{(1)} + \frac{1}{k}\sum_{i=1}^{k}\ln\!\left(\frac{1 - \frac{X_{n_q:n}}{X_{n-i+1:n}}}{1 - \frac{X_{n_q:n}}{X_{n-k:n}}}\right).$$

Since $\ln(1+x) \sim x$, as $x \to 0$,

$$\begin{aligned}\frac{1}{k}\sum_{i=1}^{k}\ln\!\left(\frac{1 - \frac{X_{n_q:n}}{X_{n-i+1:n}}}{1 - \frac{X_{n_q:n}}{X_{n-k:n}}}\right) &\overset{p}{\sim} \frac{1}{k}\sum_{i=1}^{k}\left(\frac{X_{n_q:n}}{X_{n-k:n}} - \frac{X_{n_q:n}}{X_{n-i+1:n}}\right)\\ &= \left(\frac{X_{n_q:n}}{X_{n-k:n}}\right)\frac{1}{k}\sum_{i=1}^{k}\left(1 - \frac{X_{n-k:n}}{X_{n-i+1:n}}\right).\end{aligned}$$

If $k = k_n$ is intermediate, i.e. (1.3) holds, and $\{Y_i\}_{i=1,\ldots,k}$ is a sequence of independent and identically distributed (i.i.d.) standard Pareto r.v.'s, then $Y_{n-k:n} \overset{p}{\sim} (n/k)$ and

$$\begin{aligned}M_{k,n}^{(1,q)} &= M_{k,n}^{(1)} + \frac{\chi_q}{U(n/k)}\,\frac{1}{k}\sum_{i=1}^{k}\left(1 - \frac{X_{n-k:n}}{X_{n-i+1:n}}\right)\\ &\overset{d}{=} M_{k,n}^{(1)} + \frac{\chi_q}{U(n/k)}\,\frac{1}{k}\sum_{i=1}^{k}\big(1 - Y_i^{-\gamma}\big)\,\big(1 + o_p(1)\big)\,.\end{aligned}$$

Given that $\mathbb{E}(Y^{-\gamma}) = 1/(1+\gamma)$ and by the weak law of large numbers we get (2.3).

For $\alpha = 2$ and using similar developments, we have

$$\begin{aligned}
M_{k,n}^{(2,q)} &\overset{d}{=} \frac{1}{k}\sum_{i=1}^{k}\left(\ln\frac{X_{n-i+1:n}}{X_{n-k:n}} + \frac{\chi_q}{U(n/k)}\left(1-Y_i^{-\gamma}\right)\left(1+o_p(1)\right)\right)^2\\
&\overset{d}{=} M_{k,n}^{(2)} + \frac{2\,\chi_q}{U(n/k)}\,\frac{1}{k}\sum_{i=1}^{k}\left(\ln\frac{X_{n-i+1:n}}{X_{n-k:n}}\right)\left(1-Y_i^{-\gamma}\right)\left(1+o_p(1)\right)\\
&\overset{d}{=} M_{k,n}^{(2)} + \frac{2\,\chi_q}{U(n/k)}\left(M_{k,n}^{(1)} - \frac{1}{k}\sum_{i=1}^{k}\left(\gamma\,\ln Y_i\,Y_i^{-\gamma}\right)\left(1+o_p(1)\right)\right).
\end{aligned}$$

Since $\mathbb{E}(\ln Y\,Y^{-\gamma}) = 1/(1+\gamma)^2$ and by the weak law of large numbers we get (2.4). □

Remark 2.2. It has been proved in Gomes and Martins (2001) that, under the second order framework, in (1.4), and for levels k such that (1.3) holds, we get for $M_{k,n}^{(\alpha)} = M_n^{(\alpha)}(\underline{X}_k)$, in (1.8), an asymptotic distributional representation of the type

$$\begin{aligned}
M_{k,n}^{(1)} &\overset{d}{=} \gamma + \frac{\gamma\,Z_k^{(1)}}{\sqrt{k}} + \frac{A(n/k)}{1-\rho}\left(1+o_p(1)\right),\\
M_{k,n}^{(2)} &\overset{d}{=} 2\,\gamma^2 + \frac{2\sqrt{5}\;\gamma^2 Z_k^{(2)}}{\sqrt{k}} + \frac{2\,\gamma\left(1-(1-\rho)^2\right)}{\rho(1-\rho)^2}\,A(n/k)\left(1+o_p(1)\right),
\end{aligned}$$

where, with $\{E_i\}_{i\geq 1}$ a sequence of i.i.d. standard exponential r.v.'s,

$$Z_k^{(\alpha)} = \frac{\sqrt{k}}{\sqrt{\Gamma(2\alpha+1)-\Gamma^2(\alpha+1)}}\left(\frac{1}{k}\sum_{i=1}^{k}E_i^{\alpha} - \Gamma(\alpha+1)\right), \qquad \alpha = 1, 2\ ,$$

is asymptotically standard normal. Moreover, the covariance structure of $Z_k^{(\alpha)}$ is given by

$$\mathbb{C}\mathrm{ov}\left(Z_k^{\alpha}, Z_k^{\beta}\right) = \frac{\Gamma(\alpha+\beta+1) - \Gamma(\alpha+1)\,\Gamma(\beta+1)}{\sqrt{\Gamma(2\alpha+1)-\Gamma^2(\alpha+1)}\,\sqrt{\Gamma(2\beta+1)-\Gamma^2(\beta+1)}}\ .$$

3. ASYMPTOTIC BEHAVIOUR OF THE PORT-CLASSES OF TAIL INDEX ESTIMATORS

In this section we present, under the validity of the second order condition in (1.4), the asymptotic distributional representations of the PORT-Hill estimators, $H_{k,n}(q) := H_n(\underline{X}^{(q)})$, and the PORT-moment estimators, $M_{k,n}(q) := M_n(\underline{X}^{(q)})$, with functional expressions given by

$$H_{k,n}(q) \equiv \hat{\gamma}_{k,n,H(q)} = \frac{1}{k}\sum_{i=1}^{k}\ln\left(\frac{X_{n-i+1:n}-X_{n_q:n}}{X_{n-k:n}-X_{n_q:n}}\right)$$

and

$$M_{k,n}(q) \equiv \hat{\gamma}_{k,n,M(q)} = M_{k,n}^{(1,q)} + 1 - \frac{1}{2}\left\{1-\left(M_{k,n}^{(1,q)}\right)^2/M_{k,n}^{(2,q)}\right\}^{-1},$$

respectively, $k < n - n_q$, $M_{k,n}^{(\alpha,q)} = M_n^{(\alpha)}\big(\underline{X}^{(q)}\big)$, $M_n^{(\alpha)}(\underline{X}_k)$ and $\underline{X}^{(q)}$ provided in (1.8) and (1.12), respectively.

The following theorem has been proved in Araújo Santos *et al.* (2006).

Theorem 3.1 (Araújo Santos *et al.*, 2006)**.** *If the second order condition* (1.4) *holds, $k = k_n$ is an intermediate sequence of positive integers, i.e.* (1.3) *holds, and for any real q, $0 \le q < 1$, we have for $T_{k,n}(q)$, with T denoting either H or M, an asymptotic distributional representation of the type*

$$T(q) \equiv T_{k,n}(q) \overset{d}{=} \gamma + \frac{\sigma_T P_{k,T}}{\sqrt{k}} + \left(b_T A(n/k) + c_T \frac{\chi_q}{U(n/k)}\right)\big(1+o_p(1)\big)\ , \tag{3.1}$$

where $P_{k,T}$, given in (1.9)*, is asymptotically standard normal, σ_T^2 and b_T are provided in* (1.10)*,*

$$c_H := \frac{\gamma}{1+\gamma} \qquad \text{and} \qquad c_M := \frac{\gamma^2}{(1+\gamma)^2}\ . \tag{3.2}$$

For simplicity of notation, let us now distinguish the following regions:

- $\mathcal{R}_1 := \gamma+\rho < 0\ \wedge\ \chi_q \ne 0.$
- $\mathcal{R}_2 := \gamma+\rho > 0\ \vee\ (\gamma+\rho \le 0 \wedge \chi_q = 0).$
- $\mathcal{R}_3 := \gamma+\rho = 0\ \wedge\ \chi_q \ne 0.$

Corollary 3.1 (Araújo Santos *et al.*, 2006)**.** *Under the conditions of Theorem 3.1, the following results hold:*

- *In $\mathcal{R}_1$, $T_{k,n}(q) \overset{d}{=} \gamma + \sigma_T P_{k,T}/\sqrt{k} + c_T\chi_q\big(1+o_p(1)\big)/U(n/k)$. Consequently, if $\sqrt{k}/U(n/k) \to \lambda_1$ finite, then*

$$\sqrt{k}\left(T_{k,n}(q)-\gamma\right) \underset{n\to\infty}{\xrightarrow{d}} \text{Normal}\big(\lambda_1 c_T \chi_q, \sigma_T^2\big)\ .$$

- *In $\mathcal{R}_2$, $T_{k,n}(q) \overset{d}{=} \gamma + \sigma_T P_{k,T}/\sqrt{k} + b_T A(n/k)\big(1+o_p(1)\big)$. Consequently, if $\sqrt{k}\,A(n/k) \to \lambda_2$ finite, then*

$$\sqrt{k}\left(T_{k,n}(q)-\gamma\right) \underset{n\to\infty}{\xrightarrow{d}} \text{Normal}\big(\lambda_2 b_T, \sigma_T^2\big)\ .$$

- *In* $\mathcal{R}_3$, $T_{k,n}(q) \overset{d}{=} \gamma + \sigma_T P_{k,T}/\sqrt{k} + \big(b_T A(n/k) + c_T \chi_q/U(n/k)\big)\big(1+o_p(1)\big)$. *Consequently, if* $\sqrt{k}/U(n/k) \to \lambda_1$ *and* $\sqrt{k}\, A(n/k) \to \lambda_2$, *with* λ_1 *and* λ_2 *both finite, then*

$$\sqrt{k}\,\big(T_{k,n}(q) - \gamma\big) \ \underset{n\to\infty}{\xrightarrow{d}} \ \text{Normal}\big(\lambda_1 c_T \chi_q + \lambda_2 b_T, \sigma_T^2\big)\ .$$

3.1. Asymptotic comparison at optimal levels

We now proceed to an asymptotic comparison of the estimators at their optimal levels in the lines of de Haan and Peng (1998), Gomes and Martins (2001), Gomes *et al.* (2005, 2007b) and Gomes and Neves (2008). Suppose that $\widehat{\gamma}_{k,n,\bullet(q)}$, now denoted $\widehat{\gamma}_{\bullet(q)}(k)$, is a general semi-parametric PORT-tail index estimator, with distributional representation,

$$\widehat{\gamma}_{\bullet(q)}(k) \;=\; \gamma + \frac{\sigma_\bullet}{\sqrt{k}}\, P_{k,\bullet} + \left(b_\bullet A(n/k) + c_\bullet \frac{\chi_q}{U(n/k)}\right)\big(1 + o_p(1)\big)\ , \tag{3.3}$$

which holds for any intermediate k, and where $P_{k,\bullet}$ is an asymptotically standard normal r.v. Given the results presented in Corollary 3.1, the Asymptotic Mean Square Error (AMSE) of $\widehat{\gamma}_{\bullet(q)}(k)$ is

$$AMSE\big(\widehat{\gamma}_{\bullet(q)}(k)\big) \;:=\; \begin{cases} \dfrac{\sigma_\bullet^2}{k} + c_\bullet^2 \dfrac{(\chi_q)^2}{U^2(n/k)}, & \text{in } \mathcal{R}_1 \\[2mm] \dfrac{\sigma_\bullet^2}{k} + b_\bullet^2 A^2(n/k), & \text{in } \mathcal{R}_2 \\[2mm] \dfrac{\sigma_\bullet^2}{k} + \left(b_\bullet + c_\bullet \dfrac{\chi_q}{C\gamma\beta}\right)^2 A^2(n/k), & \text{in } \mathcal{R}_3\ , \end{cases}$$

where $\text{Var}_\infty\big(\widehat{\gamma}_{\bullet(q)}(k)\big) := \sigma_\bullet^2/k$ and

$$\text{Bias}_\infty\big(\widehat{\gamma}_{\bullet(q)}(k)\big) \;:=\; \begin{cases} c_\bullet \dfrac{\chi_q}{U(n/k)} =: d_\bullet^{(1)}/U(n/k), & \text{in } \mathcal{R}_1 \\[2mm] b_\bullet A(n/k) =: d_\bullet^{(2)} A(n/k), & \text{in } \mathcal{R}_2 \\[2mm] \left(b_\bullet + c_\bullet \dfrac{\chi_q}{C\gamma\beta}\right) A(n/k) =: d_\bullet^{(3)} A(n/k), & \text{in } \mathcal{R}_3\ . \end{cases}$$

Let $k_{0,\bullet(q)} := \arg\min_k AMSE\big(\widehat{\gamma}_{\bullet(q)}(k)\big)$ be the so-called optimal level for the estimation of γ through $\widehat{\gamma}_{\bullet(q)}(k)$, i.e., the level associated with a minimum asymptotic mean squared error, and let us denote $\widehat{\gamma}_{n0,\bullet(q)} := \widehat{\gamma}_{\bullet(q)}\big(k_{0,\bullet(q)}\big)$, the estimator computed at its optimal level. The use of regular variation theory enabled Dekkers and de Haan (1989) to prove that, whenever $d_\bullet^{(i)} \neq 0$, $i = 1,2,3$ in this study, there exists a function $\varphi(n) = \varphi(n;\rho,\gamma)$, dependent only on the underlying model, and not on the estimator, but dependent here on $i = 1,2,3$, such that $\lim_{n\to\infty} \varphi(n)\, AMSE\big(\widehat{\gamma}_{n0,\bullet(q)}\big) =: LMSE\big(\widehat{\gamma}_{n0,\bullet(q)}\big)$ exists, with LMSE standing for *limiting mean-squared error*. Moreover,

$$LMSE\big(\widehat{\gamma}_{n0,\bullet(q)}\big) = \begin{cases} \dfrac{1+2\,\gamma}{2\,\gamma}\, \big(\sigma_\bullet^2\big)^{\frac{2\gamma}{1+2\gamma}} \Big(\big(d_\bullet^{(1)}\big)^2\Big)^{\frac{1}{1+2\gamma}}, & \text{in } \mathcal{R}_1 \\ \dfrac{2\rho-1}{2\rho}\, \big(\sigma_\bullet^2\big)^{-\frac{2\rho}{1-2\rho}} \Big(\big(d_\bullet^{(2)}\big)^2\Big)^{\frac{1}{1-2\rho}}, & \text{in } \mathcal{R}_2 \\ \dfrac{2\rho-1}{2\rho}\, \big(\sigma_\bullet^2\big)^{-\frac{2\rho}{1-2\rho}} \Big(\big(d_\bullet^{(3)}\big)^2\Big)^{\frac{1}{1-2\rho}}, & \text{in } \mathcal{R}_3\ . \end{cases} \tag{3.4}$$

It is then sensible to consider the following:

Definition 3.1. Given $\widehat{\gamma}_{n0,T_1(q)} = \widehat{\gamma}_{T_1(q)}\big(k_{0,T_1(q)}\big)$ and $\widehat{\gamma}_{n0,T_2(q)} = \widehat{\gamma}_{T_2(q)}\big(k_{0,T_2(q)}\big)$, two biased PORT-estimators $\widehat{\gamma}_{T_1(q)}$ and $\widehat{\gamma}_{T_2(q)}$ for which distributional representations of the type (3.3) hold with constants $\big(\sigma_{T_1}, d_{T_1}\big)$ and $\big(\sigma_{T_2}, d_{T_2}\big)$, $d_{T_1}, d_{T_2} \neq 0$, respectively, both computed at their optimal levels, the Asymptotic Root Efficiency (*AREFF*) of $\widehat{\gamma}_{T_1(q)}$ relatively to $\widehat{\gamma}_{T_2(q)}$ is

$$AREFF_{T_1(q)\,|\,T_2(q)} \equiv AREFF_{\widehat{\gamma}_{T_1(q)}\,|\,\widehat{\gamma}_{T_2(q)}} := \sqrt{\frac{LMSE\big(\widehat{\gamma}_{n0,T_2(q)}\big)}{LMSE\big(\widehat{\gamma}_{n0,T_1(q)}\big)}}\ ,$$

with LMSE given in (3.4).

Remark 3.1. Note that this measure was devised so that the higher the AREFF measure is, the better the first estimator is.

Remark 3.2. The optimal levels $k_{0,T(q)}$ for the estimation of γ through $\widehat{\gamma}_{T(q)}(k)$, with T denoting either H or M are denoted by $k_{0,H(q)}$ and $k_{0,M(q)}$ and are given in Table 1.

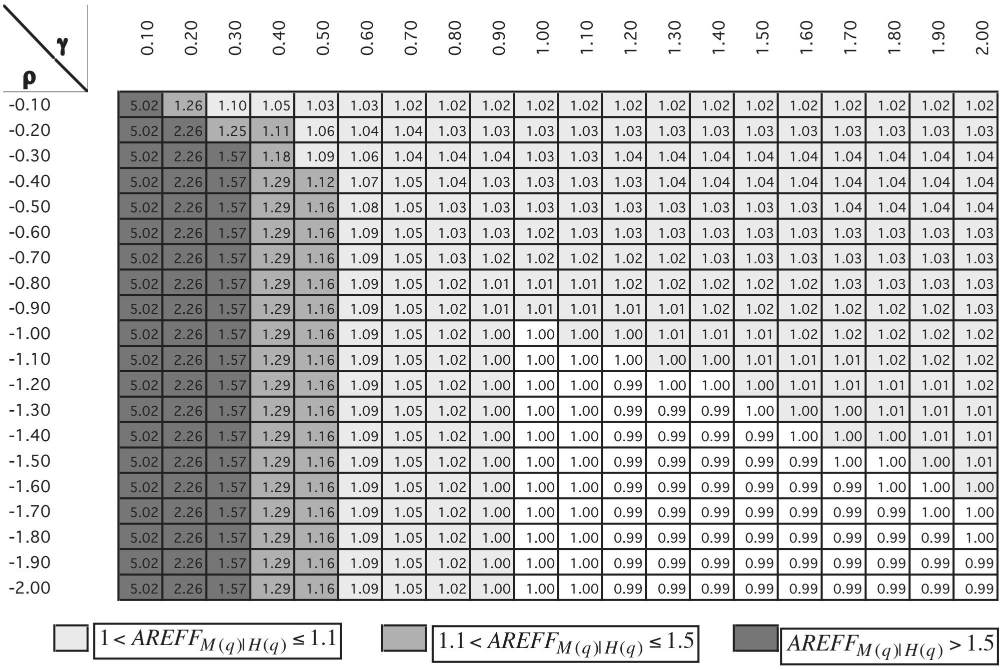
Table 1: Optimal levels for the estimation of γ through PORT-Hill and PORT-moment estimators.

Region	$k_{0,H(q)}$	$k_{0,M(q)}$
$\mathcal{R}_1$	$\left(\dfrac{C\,(1+\gamma)\,n^{\gamma}}{\lvert\chi_q\rvert\,\sqrt{2\,\gamma}}\right)^{2/(1+2\gamma)}$	$\left(\dfrac{C\,\sqrt{1+\gamma^2}\,(1+\gamma)^2\,n^{\gamma}}{\gamma^2\,\lvert\chi_q\rvert\,\sqrt{2\,\gamma}}\right)^{2/(1+2\gamma)}$
$\mathcal{R}_2$	$\left(\dfrac{(1-\rho)\,n^{-\rho}}{\lvert\beta\rvert\,\sqrt{-2\,\rho}}\right)^{2/(1-2\rho)}$	$\left(\dfrac{\sqrt{1+\gamma^2}\,(1-\rho)^2\,n^{-\rho}}{\lvert\gamma(1-\rho)+\rho\rvert\,\lvert\beta\rvert\,\sqrt{-2\,\rho}}\right)^{2/(1-2\rho)}$
$\mathcal{R}_3$	$\left(\dfrac{C\,(1-\rho)\,n^{-\rho}}{\lvert\beta C+\chi_q\rvert\,\sqrt{-2\,\rho}}\right)^{2/(1-2\rho)}$	$\left(\dfrac{C\,\sqrt{1+\rho^2}\,(1-\rho)^2\,n^{-\rho}}{\rho^2\,\lvert\beta C+\chi_q\rvert\,\sqrt{-2\,\rho}}\right)^{2/(1-2\rho)}$

Proposition 3.1. *The AREFF-indicator of* $\widehat{\gamma}_{M(q)}$ *relatively to* $\widehat{\gamma}_{H(q)}$ *is:*

$$AREFF_{M(q)\,|\,H(q)} = \begin{cases} \left(\dfrac{\gamma^2}{1+\gamma^2}\right)^{\frac{\gamma}{1+2\gamma}} \left(\dfrac{1+\gamma}{\gamma}\right)^{\frac{1}{1+2\gamma}}, & \textit{in } \mathcal{R}_1 \\ \left(\dfrac{\gamma^2}{1+\gamma^2}\right)^{\frac{-\rho}{1-2\rho}} \left(\dfrac{\gamma(1-\rho)}{\gamma(1-\rho)+\rho}\right)^{\frac{1}{1-2\rho}}, & \textit{in } \mathcal{R}_2 \\ \left(\dfrac{\rho^2}{1+\rho^2}\right)^{\frac{-\rho}{1-2\rho}} \left(\dfrac{1-\rho}{|\rho|}\right)^{\frac{1}{1-2\rho}}, & \textit{in } \mathcal{R}_3 \ . \end{cases}$$

This $AREFF$-measure is presented in Figure 1, where we can see that the gain in efficiency for the PORT-moment estimator happens for a large region of values of (γ, ρ).



γ ρ	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
-0.10	5.02	1.26	1.10	1.05	1.03	1.03	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	5.02	2.26	1.25	1.11	1.06	1.04	1.04	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	5.02	2.26	1.57	1.18	1.09	1.06	1.04	1.04	1.04	1.03	1.03	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04
-0.40	5.02	2.26	1.57	1.29	1.12	1.07	1.05	1.04	1.03	1.03	1.03	1.03	1.04	1.04	1.04	1.04	1.04	1.04	1.04	1.04
-0.50	5.02	2.26	1.57	1.29	1.16	1.08	1.05	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.04	1.04	1.04	1.04
-0.60	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.03	1.03	1.02	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03	1.03
-0.70	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.03	1.02	1.02	1.02	1.02	1.02	1.03	1.03	1.03	1.03	1.03	1.03	1.03
-0.80	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.03	1.03	1.03	1.03
-0.90	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.01	1.01	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02	1.02	1.03
-1.00	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.00	1.00	1.00	1.00	1.01	1.01	1.01	1.02	1.02	1.02	1.02	1.02
-1.10	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.00	1.00	1.00	1.00	1.00	1.00	1.01	1.01	1.01	1.02	1.02	1.02
-1.20	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.00	1.00	1.00	0.99	1.00	1.00	1.00	1.01	1.01	1.01	1.01	1.02
-1.30	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.00	1.00	1.00	0.99	0.99	0.99	1.00	1.00	1.00	1.01	1.01	1.01
-1.40	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.00	1.00	1.00	0.99	0.99	0.99	0.99	1.00	1.00	1.00	1.01	1.01
-1.50	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.00	1.00	1.00	0.99	0.99	0.99	0.99	0.99	1.00	1.00	1.00	1.01
-1.60	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.00	1.00	1.00	0.99	0.99	0.99	0.99	0.99	0.99	1.00	1.00	1.00
-1.70	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.00	1.00	1.00	0.99	0.99	0.99	0.99	0.99	0.99	0.99	1.00	1.00
-1.80	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.00	1.00	1.00	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.99	1.00
-1.90	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.00	1.00	1.00	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.99
-2.00	5.02	2.26	1.57	1.29	1.16	1.09	1.05	1.02	1.00	1.00	1.00	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.99

☐ $1 < AREFF_{M(q)|H(q)} \le 1.1$

▨ $1.1 < AREFF_{M(q)|H(q)} \le 1.5$

■ $AREFF_{M(q)|H(q)} > 1.5$

Figure 1: Asymptotic efficiency of $\widehat{\gamma}_{M(q)}$ relatively to $\widehat{\gamma}_{H(q)}$ in the (γ, ρ)-plane whenever $\chi_q \neq 0$.

4. ASYMPTOTIC BEHAVIOUR OF THE PORT-QUANTILE ESTIMATORS

We first present the following result, proved in Ferreira *et al.* (2003), on the asymptotic behaviour of intermediate order statistics:

Proposition 4.1 (Ferreira *et al.*, 2003)**.** *Under the second order framework in* (1.4) *and for intermediate sequences of positive integers k, i.e. if* (1.3) *holds,*

$$X_{n-k:n} \stackrel{d}{=} U(n/k)\left(1+\frac{\gamma B_k}{\sqrt{k}}+o_p\big(A(n/k)\big)\right),$$

where B_k is asymptotically standard normal, and

$$\mathbb{C}\mathrm{ov}(B_i,B_j) = \sqrt{ij}\,\left(\frac{1-j/n}{j-1}\right), \qquad i<j\ .$$

We shall now consider and study the new PORT-quantile estimator, in (1.14). We can state the following result:

Theorem 4.1. *Let us assume that the second order condition in* (1.4) *holds, with $A(t)=\gamma\beta t^\rho$, that k is an intermediate sequence of integers, i.e.* (1.3) *holds, and that $\ln(np_n)/\sqrt{k}\to 0$, as $n\to\infty$, with p_n given in* (1.2)*. Then, for any real q, $0\le q<1$, and with T denoting either H or M,*

$$\text{(4.1)}\qquad \frac{\sqrt{k}}{\ln\!\left(\frac{k}{np_n}\right)}\left(\frac{\widetilde{Q}_{k,p_n,T(q)}}{\chi_{1-p_n}}-1\right) \stackrel{d}{=}$$

$$\stackrel{d}{=}\ \sigma_T\,P_{k,T}+\sqrt{k}\left(b_T\,A(n/k)+c_T\frac{\chi_q}{U(n/k)}\right)\big(1+o_p(1)\big)$$

$$-\left\{\frac{\sqrt{k}\,A(n/k)}{\ln\!\left(\frac{k}{np_n}\right)}\left(b_T\frac{2^\gamma\ln 2}{2^\gamma-1}-\frac{2^{\gamma+\rho}-1}{\rho(2^\gamma-1)}\right)+\frac{\sqrt{k}\;\chi_q}{U(n/k)\ln\!\left(\frac{k}{np_n}\right)}\,\frac{2^\gamma\ln 2}{2^\gamma-1}\right\}\big(1+o_p(1)\big),$$

with (b_T,σ_T) and c_T given in (1.10) *and* (3.2)*, respectively, and where $P_{k,T}$ is asymptotically standard normal.*

Proof: The PORT-quantile estimator in (1.14) can be written as

$$\widetilde{Q}_{k,p_n,T(q)} := X_{n-k:n}\left\{\left(\frac{X_{n-[k/2]:n}}{X_{n-k:n}}-1\right)\frac{1}{2^{T(q)}-1}\left(\frac{k}{np_n}\right)^{T(q)}+\frac{X_{n_q:n}}{X_{n-k:n}}\right\}.$$

Therefore,

$$\frac{\widetilde{Q}_{k,p_n,T(q)}-\chi_{1-p_n}}{X_{n-k:n}} = \left(\frac{X_{n-[k/2]:n}}{X_{n-k:n}}-1\right)\frac{1}{2^{T(q)}-1}\left(\frac{k}{np_n}\right)^{T(q)}+\frac{X_{n_q:n}}{X_{n-k:n}}-\frac{\chi_{1-p_n}}{X_{n-k:n}}\ .$$

As (2.2) holds, we can say that $X_{n_q:n}/X_{n-k:n}=o_p(1)$, and using the second order condition in (1.4), we can guarantee that

$$\frac{X_{n-[k/2]:n}}{X_{n-k:n}} = \frac{U\big(2\,\frac{n}{k}\big)}{U\big(\frac{n}{k}\big)} \stackrel{d}{=} 2^\gamma\left(1+\frac{2^\rho-1}{\rho}A(n/k)\big(1+o(1)\big)\right).$$

Since $\chi_{1-p_n} = U(1/p_n)$, the result in Proposition 4.1 enables us to write

$$\begin{aligned}
\frac{\chi_{1-p_n}}{X_{n-k:n}} &= \frac{U\left(\frac{n}{k}\,\frac{k}{np_n}\right)}{U\left(\frac{n}{k}\right)}\;\frac{U\left(\frac{n}{k}\right)}{X_{n-k:n}} \\
&\overset{d}{=} \left(\frac{k}{np_n}\right)^{\gamma}\left(1-\frac{A(n/k)}{\rho}\,\big(1+o(1)\big)\right)\left(1-\frac{\gamma B_k}{\sqrt{k}}+o_p\big(A(n/k)\big)\right) \\
&= \left(\frac{k}{np_n}\right)^{\gamma}\left(1-\frac{\gamma B_k}{\sqrt{k}}-\frac{A(n/k)}{\rho}\,\big(1+o_p(1)\big)\right),
\end{aligned}$$

and the use of the delta method leads us to

$$\frac{\left(\frac{k}{np_n}\right)^{T(q)}}{2^{T(q)}-1} \overset{d}{=} \frac{\left(\frac{k}{np_n}\right)^{\gamma}}{2^{\gamma}-1}\left(1+\big(T(q)-\gamma\big)\left(\ln\!\left(\frac{k}{np_n}\right)-\frac{2^{\gamma}\ln 2}{2^{\gamma}-1}\right)\big(1+o_p(1)\big)\right).$$

Therefore

$$\begin{aligned}
&\widetilde{Q}_{k,p_n,T(q)}-\chi_{1-p_n} \overset{d}{=} \\
&\overset{d}{=} \left(\frac{k}{np_n}\right)^{\gamma} X_{n-k:n}\left\{\big(T(q)-\gamma\big)\left(\ln\!\left(\frac{k}{np_n}\right)-\frac{2^{\gamma}\ln 2}{2^{\gamma}-1}\right)\big(1+o_p(1)\big)\right. \\
&\qquad \left.+\frac{\gamma B_k}{\sqrt{k}}+\frac{A(n/k)\,(2^{\gamma+\rho}-1)}{\rho(2^{\gamma}-1)}\,\big(1+o_p(1)\big)\right\} \\
&\overset{d}{=} \left(\frac{k}{np_n}\right)^{\gamma} U(n/k)\left(1+\frac{\gamma B_k}{\sqrt{k}}+\frac{A(n/k)}{\rho}\,\big(1+o_p(1)\big)\right) \\
&\qquad \times\left\{\big(T(q)-\gamma\big)\left(\ln\!\left(\frac{k}{np_n}\right)-\frac{2^{\gamma}\ln 2}{2^{\gamma}-1}\right)\big(1+o_p(1)\big)\right. \\
&\qquad \left.+\frac{\gamma B_k}{\sqrt{k}}+\frac{A(n/k)\,(2^{\gamma+\rho}-1)}{\rho(2^{\gamma}-1)}\,\big(1+o_p(1)\big)\right\},
\end{aligned}$$

using also the result presented in Proposition 4.1. Since

$$\Big(\gamma B_k/\sqrt{k}+\big(A(n/k)/\rho\big)\,\big(1+o_p(1)\big)\Big) = o_p\big(1/\sqrt{k}\big)\,,$$

then

$$\begin{aligned}
&\widetilde{Q}_{k,p_n,T(q)}-\chi_{1-p_n} \overset{d}{=} \\
&\overset{d}{=} \left(\frac{k}{np_n}\right)^{\gamma} U(n/k)\left\{\big(T(q)-\gamma\big)\left(\ln\!\left(\frac{k}{np_n}\right)-\frac{2^{\gamma}\ln 2}{2^{\gamma}-1}\right)\big(1+o_p(1)\big)\right. \\
&\qquad \left.+\frac{\gamma B_k}{\sqrt{k}}+\frac{A(n/k)\,(2^{\gamma+\rho}-1)}{\rho(2^{\gamma}-1)}\,\big(1+o_p(1)\big)\right\}.
\end{aligned}$$

Notice that $\chi_{1-p_n} = U(1/p_n) = \big(k/(np_n)\big)^{\gamma}\, U(n/k)$, and then

$$\frac{\sqrt{k}}{\ln\!\left(\frac{k}{np_n}\right)} \left(\frac{\widetilde{Q}_{k,p_n,T(q)}}{\chi_{1-p_n}} - 1\right) \overset{d}{=} \sqrt{k}\,\big(T(q)-\gamma\big) - \frac{\sqrt{k}}{\ln\!\left(\frac{k}{np_n}\right)}\,\big(T(q)-\gamma\big)\,\frac{2^{\gamma}\ln 2}{2^{\gamma}-1} + \frac{\gamma\, B_k}{\ln\!\left(\frac{k}{np_n}\right)} + \frac{\sqrt{k}}{\ln\!\left(\frac{k}{np_n}\right)}\,\frac{A(n/k)\,(2^{\gamma+\rho}-1)}{\rho(2^{\gamma}-1)}\ .$$

Using the distributional representation of $T(q)$ in (3.1) and since $\ln\big(k/(np_n)\big) \to \infty$, (4.1) follows. ☐

Corollary 4.1. *Under the conditions of* Theorem 4.1, *the following results hold:*

- *In $\mathcal{R}_1$, i.e. for values of $\gamma+\rho<0$ and $\chi_q \neq 0$,*

$$\frac{\sqrt{k}}{\ln\!\left(\frac{k}{np_n}\right)} \left(\frac{\widetilde{Q}_{k,p_n,T(q)}}{\chi_{1-p_n}} - 1\right) \overset{d}{=} \sigma_{T}\, P_{k,T} + \sqrt{k}\left(c_{T}\,\frac{\chi_q}{U(n/k)}\right)\big(1+o_p(1)\big) - \frac{\sqrt{k}\;\chi_q}{U(n/k)\,\ln\!\left(\frac{k}{np_n}\right)}\,\frac{2^{\gamma}\ln 2}{2^{\gamma}-1}\,\big(1+o_p(1)\big)\ .$$

  If $\sqrt{k}\big/U(n/k) \to \lambda_1$ finite, then

$$\frac{\sqrt{k}}{\ln\!\left(\frac{k}{np_n}\right)} \left(\frac{\widetilde{Q}_{k,p_n,T(q)}}{\chi_{1-p_n}} - 1\right) \underset{n\to\infty}{\xrightarrow{d}} \mathrm{Normal}\big(\lambda_1 c_{T}\chi_q, \sigma^2_{T}\big)\ .$$

- *In $\mathcal{R}_2$, i.e. for values of $\gamma+\rho>0$ or $\gamma+\rho\leq 0$ and $\chi_q = 0$,*

$$\frac{\sqrt{k}}{\ln\!\left(\frac{k}{np_n}\right)} \left(\frac{\widetilde{Q}_{k,p_n,T(q)}}{\chi_{1-p_n}} - 1\right) \overset{d}{=}$$
$$\overset{d}{=} \sigma_{T}\, P_{k,T} + \sqrt{k}\,\big(b_{T}\,A(n/k)\big)\,\big(1+o_p(1)\big) - \frac{\sqrt{k}\;A(n/k)}{\ln\!\left(\frac{k}{np_n}\right)}\left(b_{T}\,\frac{2^{\gamma}\ln 2}{2^{\gamma}-1} - \frac{2^{\gamma+\rho}-1}{\rho(2^{\gamma}-1)}\right)\big(1+o_p(1)\big)\ ,$$

  If $\sqrt{k}\,A(n/k) \to \lambda_2$ finite, then

$$\frac{\sqrt{k}}{\ln\!\left(\frac{k}{np_n}\right)} \left(\frac{\widetilde{Q}_{k,p_n,T(q)}}{\chi_{1-p_n}} - 1\right) \underset{n\to\infty}{\xrightarrow{d}} \mathrm{Normal}\big(\lambda_2 b_{T}, \sigma^2_{T}\big)\ .$$

- *In $\mathcal{R}_3$, i.e. for values of $\gamma+\rho=0$ and $\chi_q\neq 0$,*

$$\frac{\sqrt{k}}{\ln\!\left(\frac{k}{np_n}\right)}\left(\frac{\widetilde{Q}_{k,p_n,T(q)}}{\chi_{1-p_n}}-1\right)\overset{d}{=}$$

$$\overset{d}{=}\ \sigma_T\,P_{k,T}+\sqrt{k}\left(b_T\,A(n/k)+c_T\,\frac{\chi_q}{U(n/k)}\right)\big(1+o_p(1)\big)$$

$$-\left\{\frac{\sqrt{k}\,A(n/k)}{\ln\!\left(\frac{k}{np_n}\right)}\left(b_T\,\frac{2^\gamma\ln 2}{2^\gamma-1}-\frac{2^{\gamma+\rho}-1}{\rho(2^\gamma-1)}\right)+\frac{\sqrt{k}\;\chi_q}{U(n/k)\ln\!\left(\frac{k}{np_n}\right)}\,\frac{2^\gamma\ln 2}{2^\gamma-1}\right\}\big(1+o_p(1)\big)\,,$$

If $\sqrt{k}/U(n/k)\to\lambda_1$ and $\sqrt{k}\,A(n/k)\to\lambda_2$, with λ_1 and λ_2 both finite, then

$$\frac{\sqrt{k}}{\ln\!\left(\frac{k}{np_n}\right)}\left(\frac{\widetilde{Q}_{k,p_n,T(q)}}{\chi_{1-p_n}}-1\right)\ \xrightarrow[n\to\infty]{d}\ \text{Normal}\big(\lambda_1 c_T\chi_q+\lambda_2 b_T,\,\sigma_T^2\big)\,.$$

Remark 4.1. Notice that, under a second order framework, the mean value and the variance of the r.v. $\sqrt{k}\left(\widehat{\gamma}_{k,n,T(q)}-\gamma\right)$, provided in Corollary 3.1, are equal to the ones of $\sqrt{k}\left(\widetilde{Q}_{k,p_n,T(q)}/\chi_{1-p_n}-1\right)/\ln\!\big(k/(np_n)\big)$.

Since $\ln\!\big(k/(np_n)\big)$ goes to infinity very slowly, we can state a pre-asymptotic distributional representation, for moderate k and n:

Corollary 4.2. *Under the conditions of* Theorem 4.1 *and for moderate values of k and n, the following pre-asymptotic results hold:*

- *In $\mathcal{R}_1$, if $\sqrt{k}/U(n/k)\to\lambda_1$, finite, and with*

$$\mu_1\ :=\ \lambda_1\,c_T\,\chi_q\left(1-\frac{2^\gamma\ln 2}{2^\gamma-1}\,\frac{1}{c_T\ln\!\big(k/(np_n)\big)}\right)\,,$$

$$\frac{\sqrt{k}}{\ln\!\big(k/(np_n)\big)}\left(\frac{\widetilde{Q}_{k,p_n,T(q)}}{\chi_{1-p_n}}-1\right)\ \overset{d}{\approx}\ \text{Normal}\left(\mu_1,\,\sigma_T^2\left(1+\frac{\gamma^2}{\sigma_T^2\ln^2\!\big(k/(np_n)\big)}\right)\right)\,.$$

- *In $\mathcal{R}_2$, if $\sqrt{k}\;A(n/k)\to\lambda_2$, finite, and with*

$$\mu_2\ :=\ \lambda_2\,b_T\left(1+\frac{1}{\ln\!\big(k/(np_n)\big)}\left(\frac{2^\gamma\ln 2}{2^\gamma-1}-\frac{2^{\gamma+\rho}-1}{\rho\,(2^\gamma-1)\,b_T}\right)\right)\,,$$

$$\frac{\sqrt{k}}{\ln\!\big(k/(np_n)\big)}\left(\frac{\widetilde{Q}_{k,p_n,T(q)}}{\chi_{1-p_n}}-1\right)\ \overset{d}{\approx}\ \text{Normal}\left(\mu_2,\,\sigma_T^2\left(1+\frac{\gamma^2}{\sigma_T^2\ln^2\!\big(k/(np_n)\big)}\right)\right)\,.$$

- *In $\mathcal{R}_3$, if $\sqrt{k}/U(n/k) \to \lambda_1$ and $\sqrt{k}\,A(n/k) \to \lambda_2$, with λ_1 and λ_2 both finite, then, with*

$$\begin{aligned}\mu_1+\mu_2 \;&=\; \lambda_1\, c_{_T}\, \chi_q \left(1-\frac{2^\gamma \ln 2}{2^\gamma-1}\,\frac{1}{c_{_T}\ln\bigl(k/(np_n)\bigr)}\right)\\ &\qquad + \lambda_2\, b_{_T}\left(1+\frac{1}{\ln\bigl(k/(np_n)\bigr)}\left(\frac{2^\gamma \ln 2}{2^\gamma-1}-\frac{2^{\gamma+\rho}-1}{\rho(2^\gamma-1)\,b_{_T}}\right)\right),\end{aligned}$$

$$\frac{\sqrt{k}}{\ln\bigl(k/(np_n)\bigr)}\left(\frac{\widetilde{Q}_{k,p_n,T(q)}}{\chi_{1-p_n}}-1\right) \overset{d}{\approx} \text{Normal}\left(\mu_1+\mu_2,\, \sigma_{_T}^2\left(1+\frac{\gamma^2}{\sigma_{_T}^2 \ln^2\bigl(k/(np_n)\bigr)}\right)\right).$$

5. CONCLUSIONS

The new PORT-quantile estimator, defined in (1.14), is asymptotically equivalent to the PORT-quantile estimator in (1.13), studied in Araújo Santos *et al.* (2006). Consequently, and for finite sample sizes, we do not expect a much better behaviour of this new estimator comparatively to the one in (1.13). However, the use, in (1.14), of a PORT-version of a minimum-variance reduced-bias extreme value index estimator, like the ones in Caeiro *et al.* (2005), Gomes *et al.* (2007a) and Gomes *et al.* (2008b), leads to quantile estimators which overpass the estimator in Caeiro and Gomes (2008) and enjoy the adequate behaviour in the presence of linear transformations of the data. Also, the use of subsampling procedures, similar to the ones in Hall and Scotto (2008), can improve this estimation procedure. These are however topics out of the scope of this paper.

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TOWARD THE DEFINITION OF A STRUCTURAL EQUATION MODEL OF PATENT VALUE: PLS PATH MODELLING WITH FORMATIVE CONSTRUCTS

Authors: Alba Martinez-Ruiz
– Department of Statistics and Operations Research,
Technical University of Catalonia, Barcelona, Spain
Universidad Católica de la Ssma. Concepción, Chile
alba.martinez-ruiz@upc.edu

Tomas Aluja-Banet
– Department of Statistics and Operations Research,
Technical University of Catalonia, Barcelona, Spain
tomas.aluja@upc.edu

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Abstract:

- This paper aims to propose a structural equation model which relates the variables that determine the patent value. Even though some patent indicators have been directly used to infer the private or social value of innovations, the results suggest that patent value is a more complex variable that may be modeled as an endogenous unobservable variable in a first- and in a second-order model, and which depends respectively on three and four constructs. Such variables include the knowledge used by companies to create their inventions, the technological scope of the inventions, the international scope of protection, and the technological usefulness of the inventions. The model allows the conceptualization of patent value into a potential and a recognized value of intangible assets, aiming toward an index construction approach. Partial least square (PLS) path modelling is performed as an exploratory model-building procedure. We use a sample of 2,901 patents granted in the United States in the field of renewable energy.

Key-Words:

- *patent value; patent indicators; PLS path modelling; structural equations models.*

AMS Subject Classification:

- 62H25, 62P20.

1. INTRODUCTION

Patents are one of the main sources of technological information. A patent is an exclusive right granted to inventors by a state only when the invention fulfils three basic requirements: the invention is new, it involves an inventive activity and it is useful for industry. Until now research involving patent data has been associated with the analysis of information contained in the patent document, such as backward and forward citations or number of claims, and the relationship between patents and research and development (R&D), innovation or economic growth. In recent years, patent indicators have been used to study the economical value of patents. In most cases, analytical approaches have been based on standard econometric analysis techniques such as probit or logit models, and survey analysis. However, patent value may be seen as a complex construct depending on a variety of elements. General and specific market conditions, countries' legal frameworks, geographic proximity or accumulated scientific and technological knowledge are different dimensions that have shown to affect patent value.

This paper proposes that a holistic and multidimensional model may offer a robust understanding of the different variables that determine patent value. For the moment, and considering patent document information, two path models are built considering five dimensions represented by five constructs. They are: patent value, technological usefulness of the invention, knowledge stock used by the company to create the technology, technological scope of the invention, and international scope of protection. The models are strongly based on the theory developed by the technological change scientific community and a thorough review of the literature on patent valuation. Each construct is associated with a set of observable variables. So, they can be estimated by these indicators. Manifest variables are mainly built from information contained in patent documents. A set of patents granted in the United States (U.S.) in the area of renewable energies was retrieved from Delphion database. The proposed path models are replicable because they could be repeated for different technological fields or countries. Moreover, the models may allow one to distinguish between: (a) those variables related to patent value at the time of application, i.e. those variables that could deliver a measure of potential value of patents, and (b) those that determine the value after the patent's application.

In the literature, research that addresses patent value using a structural equation model (SEM) approach is quite scarce. Moreover, rather traditional methods based on multivariate normal distribution assumption have been implemented. The advantage of SEM is flexibility in working with theory and data, approaching the whole phenomenon, and a more complete representation of the complex theory. Additionally, and contrary to a covariance-based approach such as the linear structural relation model (LISREL), PLS path modelling is theorybuilding-oriented and causal-predictive-oriented. Therefore, the exploratory nature of this procedure allows for the first formulation of a structural model of patent value. Finally, the PLS path modelling algorithm is a powerful technique for the analysis of skewed or long-tail data, such as patent data. Therefore, we also attempt to show the benefits of PLS path modelling as a tool for exploration and prediction of skewed data.

In this research, the models specification is made from a PLS perspective. So, we are posing PLS models. Section 2 provides background on patent indicators and constructs, and section 3 reviews the PLS path modelling procedure for hierarchical component models with repeated manifest variables and formative constructs. Section 4 addresses the first- and second-order model formulation, while also postulating on the indicators, latent variables (LVs) and causal relationships among variables. In particular, formative and reflective relationships among manifest and latent variables are justified. A description of patent data is given in Section 5. Section 6 reports the results, and shows the performance and effectiveness of PLS path modelling when working with patent data characterized by long tails. Finally, section 7 gives final remarks and some directions for future research.

2. PATENT INDICATORS AND CONSTRUCTS

Patent indicators have been used by scientific communities to study phenomena such as technological change or the growth of science and technology. Forward citations, i.e. the number of times that each patent has been cited by another patent, are the most widely used indicator to measure the value or importance of patents. Nevertheless, other indicators have also been introduced as a measure of value, such as family size, number of claims, number of international patent classification (IPC) codes where the patent is classified, and backward citations. Here, family size refers to the number of countries where a patent is sought for the same invention [27]. As a general patenting strategy, companies protect their inventions in their local countries first and then in other jurisdictions. Patents with a large family size tend to be more valuable or important [21], although Guellec *et al.* reported that this relationship might sometimes be inaccurate and “may reflect a lack of maturity of the applicant” [18, p. 114]. Even so, family size may be proposed as a proxy variable for the international scope of patent rights, and as a measure of patent value. The number of backward citations or references in a patent represents “all of the important prior art upon which the issued patent improves” [35, p. 318], and allows one to demonstrate that the invention is genuinely new. Claims are made in a special section in the patent document, where the thing that is being protected is specified. The claims section consists of a numbered list. Therefore, the number of claims is in fact the number of inventions protected [42, p. 134]. Patents with a large number of claims have a higher likelihood of being litigated, so they can be considered more valuable [22, 28, 38]. International patent classification classes were introduced as a proxy variable for the scope of protection by Lerner [31]. An invention with a larger technological scope should be more valuable due to its broader potential applications. The number of inventors and the number of applicants have also been used as indicators of the patent value [38].

Most patent indicators have been used to explain a conceptual variable or a construct. The relationship between patent citations and patent value has been deeply studied [1, 4, 18, 20, 21, 37, 38, 43]. Carpenter *et al.* [4], Albert *et al.* [1] and Harhoff *et al.* [20] have successfully shown that those patents that are related to important technological developments are most highly cited. Harhoff *et al.* [21] was the first to use backward and forward citations together as proxy variables for patent value, and Trajtenberg [43] established the role of citations as an indicator of the value of innovations. Patent citations and patent value have also been associated with market value and/or the R&D expenditures of companies [10, 15, 19, 31]. The relationship among patent value and patenting strategy, technological diversity (through the IPC), domestic and international R&D collaborations and/or co-applications (analyzing the country of residence of the authors) and the mix of designated states for protection (through the family size), have been studied by Guellec and van Pottelsberghe [18]. Reitzig [37, 38] studied the factors that determine an individual patent value. Analyzing the results of a questionnaire, he found that novelty and inventive activity are the most important factors in patents that are used as “bargaining chips”. Connolly *et al.* [10] showed that patent statistics are significantly related to companies’ market value. In addition, Griliches [15] found a significant relation among companies’ market value, the book value of R&D expenditures and the number of patents. He based his research on a time-series cross-section analysis of United States firm data. Lerner [31] reported that patent scope has a significant impact on the valuation of firms, while Hall *et al.* [19] investigated the trend in US patenting activities over the last 30 years, finding that the ratios of R&D to asset stock, patents to R&D, and citations to patents significantly affect companies’ market value.

On the other hand, some of these indicators have been related to other constructs. The number of inventors and applicants, backward citations and the number of claims have been related to patent novelty, i.e. the technological distance between a protected invention and prior art. A patent’s protection level or its technological scope or breadth can be measured by the number of claims or number of IPC classes into which the patent is classified [31]. Furthermore, patent stocks or knowledge stocks have been associated with the economic growth of a country as well as the economical activity [16], research and development results [29] and the value of innovation [40] and technological performance [42]. In this last case, the researchers found that the number of claims is a better indicator than the number of patents in the national technological capacity.

Finally, little research has reported on the structural relationship among latent variables which influence patent value using a multidimensional approach. The recent investigations of Harhoff [21, 22] and Reitzig [37, 38] used a large number of indicators of patent value aimed mainly at estimating the probability of opposition to a patent. In most cases, analytical approaches have been based on standard econometric analysis techniques (probit or logit models) or survey analysis. One reason that could explain why a multidimensional and structural approach has not been applied to technology/patent valuation is that more general structural models are based on maximum likelihood estimation and the multivariate normal distribution of data. Patent indicators are very heterogeneous and asymmetric, and, in general, they exhibit a large variance and skew. Consequently, assuming that this type of data has a multivariate normal distribution may lead to biased results. As seen below, PLS path modelling overcomes this drawback because it is an iterative algorithm that makes no assumptions about data distribution. Moreover, unlike other methods such as probit or logit models, it allows researchers to depict the relationship among a set of latent variables. Thus, we have the possibility of modelling the patent value as an unobservable variable.

2.1. Patent value

Patents are intellectual assets that do not necessarily have an immediate return. A patent may protect a product that can be manufactured and sold. But a patent may also protect technologies which, together with other technologies, enable the manufacture of a final product. In both cases, to obtain an economic value from patents may be extremely difficult. In studying patent value, different approaches have been taken throughout the literature. Some of the approaches focus on the private value of a patent while others concentrate on a patent's social value. Lanjouw *et al.* [27, p. 407] defined the private value of a patent in terms of "the difference in the returns that would accrue to the innovation with and without patent protection". The magnitude of this difference would be crucial in applying or renewing the protection. Reitzig [38] also focused on the private value of patents, and specifies the need to consider the patent value as a construct. Technical experts were surveyed and, according to them, the research showed that the factors that determine patent value are: state of the art (existing technologies), novelty, inventiveness, breadth, difficulty of inventing, disclosure and dependence on complementary assets[1]. Additionally, Trajtenberg [43] showed that patent data was highly correlated with some indicators of the social benefits of innovations. Guellec *et al.* [18] presented a value scale proposing

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[1] We attempt to consider these variables as constructs in the proposed structural model. However, recall that in this research, the manifest variables are mainly obtained from the patent document. So, latent and manifest variables are subject to this constraint.

that technology increases its own value as it passes through different stages: from invention to application, examination, publication and decision to grant, and finally to the high value stage if the patent is granted. The distinction is made between the intrinsic value of the patent simply for being granted (and thereby having proven novelty, inventive activity and applicability) and the potential value of technology (dependent on its potential for generating future returns).

Some patent indicators have been used to directly infer the patent's value, such as forward citations or family size (see Table 1). Even though this may be useful and may give an approximation of the patent value, many elements may affect the invention and protection process. We consider some of these factors based on the presented background, and represent their interactions proposing a multidimensional analysis of the problem. It is worth noting that this research does not seek to determine the value of an individual patent or to obtain a monetary value of the assets. Rather, the patent value is proposed in terms of the technological usefulness of the inventions. This model, however, allows us to compare and rank the value of a company's patent portfolios. We address the question of what variables determine the patent value and how they relate to each other. These variables are modeled as unobserved variables. So, they and their relationships set up a structural equation model.

Table 1: Brief summary of different approaches used to study the patent value.

Author	**Construct**	**Indicators**	**Dependent variable**	**Method**
Trajtenberg (1990)	Social value of innovations	Patent count weighted by citations	Consumer surplus	Multinomial logit model
Guellec *et al.* (2000)	Patent value, patenting strategy, technological diversity, R&D collaboration	Number of IPC, family size, dummy variables, etc.	Probability that a EPO patent application is granted	Probit model
Reitzig (2003)	Patent value, novelty, inventive activity, invent around, disclosure	—	'present patent value'	Survey, probit model
Harhoff *et al.* (2003)	Private value of patents, value of renewed patent protection and asset value of patent right	Survey of patent-holders, backward and forward citations, family size, IPC, outcome of opposition proceedings	Patent right as a price to sell the patent right	Survey, probit model
Hall *et al.* (2005)	Market value	Patent citations, R&D expenditures, total assets	Tobin's q	Tobin's Q equation

3. THE PLS PATH MODELLING APPROACH FOR MODEL FORMULATION

PLS path modelling is a component-based procedure for estimating a sequence of latent variables developed by the statistician and econometrician Herman Wold [45, 46, 47]. During the last few years, it has proved to be useful for estimating structural models, in marketing and information system research in particular, and in the social sciences in general [6, 12, 23, 24, 33, 41]. Some of its features have encouraged its use, such as: (1) it is an iterative algorithm that offers an explicit estimation of the latent variables, and their relationships, (2) it works with few cases and makes no assumptions about data distribution — in contrast with LISREL that makes strong assumptions about data distribution and where hundreds of cases are necessary for its application, and (3) it overcomes the identification problems when formative measurement models are included. Wold [47] emphasizes that "using prior knowledge and intuition the investigator is free to specify the LVs, to design the inner relations, and to compile a selection of indicators for each LV" [p. 582]. The path model "is usually tentative since the model construction is an evolutionary process. The empirical content of the model is extracted from the data, and the model is improved by interactions through the estimation between the model and the data and the reactions of the researcher" [45, p. 70].

In a PLS path modelling approach, the structural model or inner model — also called the inner relations and substantive theory — depicts the relationship among latent variables as multiple regressions:

$$\xi_j = \beta_{j0} + \sum_i \beta_{ji}\,\xi_i + \nu_j \tag{3.1}$$

where ξ_j and ξ_i are the endogenous and exogenous latent variables, respectively, and β_{ji} are called path coefficients and measure the relationship among constructs. The arrangement of the structural model is strongly supported by theory at the model specification stage. So, PLS path modelling is used to explore if these relationships hold up or whether other theory-based specifications, that may be proposed, help in providing a better explanation for a particular phenomenon. The condition imposed is $E(\xi_j/\xi_i) = \sum_i \beta_{ji}\,\xi_i$. There is no linear relationship between predictor and residual, $E(\nu_j/\forall\xi_i) = 0$ and $\text{cov}(\nu_j, \xi_i) = 0$.

The measurement model or outer model — also called the outer relations — describes the relationship between latent (ξ_i) and manifest (x_{ih}) variables in two different ways: mode A and mode B. "Mode A is often used for an endogenous LV and mode B for an exogenous one. Mode A is appropriate for a block with a reflective measurement model and mode B for a formative one" [41, p. 268]. Reflective relationships seek to represent variance and covariances between the manifest variables that are generated or caused by a latent variable. So, observed variables are treated as an effect of unobserved variables [2, 9]. In a reflective measurement model, the manifest variables are measured with error. Alternatively, formative relationships are used to minimize residuals in the structural relationships [14], and here, manifest variables are treated as forming the unobserved variables. MacCallum and Browne [32] said that observed variables in a formative model are exogenous measured variables. In a formative outer model the manifest variables are presumed to be error-free and the unobserved variable is estimated as a linear combination of the manifest variables plus a disturbance term, so they are not true latent variables (as in the traditional factorial approach). As in this case all variables forming the construct should be considered, the disturbance term represents all those non-modeled causes.

In mode A or in reflective relationships, manifest and latent variables relationships are described by ordinary least square regressions:

$$x_{ih} = \pi_{ih0} + \pi_{ih}\,\xi_i + \epsilon_{ih} \;. \tag{3.2}$$

The parameters π_h are called loadings. The condition imposed is $E(x_h/\xi) = \pi_{h0} + \pi_h\,\xi$, ϵ_h with zero mean and uncorrelated with ξ. Loadings indicate the extent to which each indicator reflects the construct, and represent the correlation between indicators and component scores.

In mode B or in formative relationships, unobserved variables are generated by their own manifest variables as a linear function of them and a residual:

$$\xi_i = \sum_h w_{ih}\,x_{ih} + \delta_i \;. \tag{3.3}$$

The parameters w_h are called weights, and allow us to determine the extent to which each indicator contributes to the formation of the constructs. Each block of manifest variables may be multidimensional. The condition imposed is $E(\xi/x_h) = \sum_h w_h\,x_h$. This implies that the residuals δ_i have zero mean and they are uncorrelated with the manifest variables x_i.

Wold's basic-design of PLS path modelling [45, 46, 47] does not consider higher-order latent variables. Therefore, in Wold's algorithm each construct must be related to a set of observed variables in order to be estimated. However, Lohmöller [30] proposed a procedure for the case of hierarchical constructs; that is to say, for cases where there is a construct that does not have a block of measurement variables, or more simply: it is only related to other constructs. In hierarchical component modelling, manifest variables of first-order latent variables are repeated for the second-order latent variable. So, a set of "auxiliary" variables is introduced for estimation purposes. After that, the model is estimated using PLS path modelling in the usual way. Hence, the specification of PLS has an additional equation that Lohmöller [30] called the cross-level relation:

$$y_{jl} = \pi_{jl0} + \pi_{jl}\,\xi_j + \epsilon_{jl} \;. \tag{3.4}$$

The condition imposed is $E(\xi_j \epsilon_{jl}) = 0$. We are interested in this type of model because, as seen below, the patent value construct may be modeled as a second-order latent variable, i.e. the value can only be estimated through linear relations with other latent variables.

Reliability of reflective measurement models is evaluated by examining loadings. A rule of thumb generally accepted is 0.7 or more. This implies that "there is more shared variance between construct and variable than error variance" [24, p. 198]. A low value in a loading factor suggests that the indicator has little relation to the associated construct. All indicators of a block of variables must reflect the same construct. Therefore, there should be high collinearity within each block of variables. Thus, the internal consistency of a reflective measurement model is related to the coherence between constructs and their measurement variables. The unidimensionality of the block of variables may be assessed by using Cronbach's alpha coefficient (should be > 0.7), and composite reliability (should be > 0.7). According to Chin [6, p. 320] "alpha tends to be a lower bound estimate of reliability whereas composite reliability is a closer approximation under the assumption that the parameter estimates are accurate".

To represent the extent to which measures of a given construct differ from measures of other constructs (discriminant validity), the average variance extracted (AVE) may be calculated. Therefore, as suggested by Fornell and Larcker [13], the percentage of variance captured by the construct in relation to the variance due to random measurement error is computed (should be > 0.5). Likewise when models have more than two reflective constructs, cross loadings may be obtained by calculating the correlations between component scores and indicators associated with other reflective constructs. If an indicator has higher correlation with another latent variable instead of the associated latent variable, its position should be reconsidered in the model. Therefore, each indicator has to be more related to its construct than another one in the same model. To assess the significance of loadings, weights and path coefficients, standard errors and t-values may be computed by bootstrapping (200 samples; t-value > 1.65 significant at the 0.05 level; t-value > 2 significant at the 0.01 level).

The inner model is assessed by examining the path coefficients among latent variables. The value of path coefficients provides evidence regarding the strength of the association among latent variables. Moreover, the coefficient of determination (R-square) of each endogenous variable gives the overall fit of the model or the percentage of variance explained by the model. In this research, PLS path modelling and bootstrapping were carried out in SmartPLS [39] with a centroid weighting scheme.

3.1. A brief overview of formative and reflective outer models

The distinction between reflective and formative measurement models for structural equation models is an issue that has been addressed by several scientific communities. Major contributions have been made by researchers from statistics [9], psychology and sociology [2, 3], information science [36], and business and marketing research [11, 14]. There are some decision rules criteria to determine if a relationship should be modeled as formative or reflective (mode B or mode A in the Wold's PLS approach). The guidelines can be summarized in five points as follows [9, 14, 34]. (1) The strong theory and the previous knowledge of a phenomenon under study should help to clarify the generative nature of the construct. When a formative relationship is considered, manifest variables must cover the entire scope of construct. (2) Correlations among manifest variables. In a reflective outer model, manifest variables have to be highly correlated; in contrast this condition must not be applied in a formative outer model. (3) Within-construct correlations versus between-construct correlations. This is a common practice in the model specification stage by means of cross-validation; the applied rule is that the former should be greater than the latter. However, Bollen and Lennox [2] show that this may lead to an incorrect indicator selection for reflective and formative outer models, because this rule may have exceptions. So, the condition must be applied with caution. (4) Sample size and multicollinearity affect the stability of indicator coefficients, and they are a frequent problem in multiple regressions. So, multicollinearity will influence the quality of the estimates in formative relationships. (5) Interchangeability. This concept refers to whether or not the manifest variables share the same concept [11, 25]. All manifest variables in a reflective model explain the same construct. So, removing an indicator from the block of variables should not have a significant effect on the construct. The situation is completely different when considering formative outer models. The indicators do not have to be interchangeable or share the same concept. That is what [2] called "sampling facets of a construct"; in other words manifest variables of a formative block of variables should represent all the aspects that form the concept. Finally, Gudergan *et al.* [17] recently proposed a procedure based on tetrad analysis to distinguish between a reflective and formative measurement model in a component-based approach. However, when an outer model has less than four observed variables, this procedure requires adding manifest variables from other outer models. Therefore, the discussion on the reflective and formative nature of the constructs studied here is based mainly on the five rules presented previously.

4. PATENT VALUE MODELS

Two models were tested. First of all, we are interested in knowing the relationships among patent indicators, patent value, and different constructs which up to now have been studied and identified as patent value determinants[2]. In previous research, these constructs have not been modeled as unobservable variables, such as in a structural equation model approach. So, the model formulation began by defining the patent value as an endogenous latent variable, since it is the primary variable to be estimated in the model. Summarizing the results of previous researchers, three unobserved variables related to the dependent variable were identified as exogenous: the knowledge stock of the patent, the technological scope of the invention, and the international scope of the protection (see Figure 1). We took into account all of the measurement variables found in the state of the art, and which can be computed from information contained in the patent document. Nevertheless, indicators constructed from the patent text, such as from the abstract or technical description, are excluded from this study.

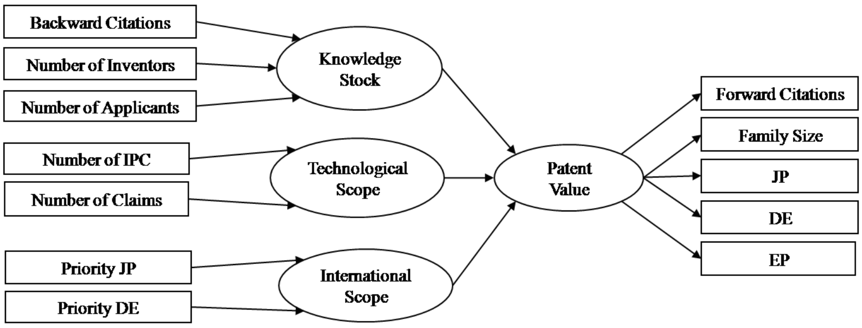

Figure 1: First-order model of patent value; patent value is an endogenous latent variable; knowledge stock, technological scope, and international scope are formative exogenous constructs.

The knowledge stock represents the base of knowledge that was used by the applicant to create an invention. This would be the content domain. This existing knowledge encourages the inventive activity and may come from within or outside the company. We would like to find those indicators that are value determinants, and that companies may use to make decisions. Since we are considering the patent document as the main data source, the applicants and inventors — that have contributed their knowledge to the creation of the invention — may be considered as forming this construct. The same applies to the backward citations.

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[2] It is worth noting that we are not interested in explaining the variance and covariance among manifest variables as in a covariance-based approach, at least not at this stage.

The previous works, cited in the patent document, are the scientific and technical knowledge units that must exist before the creation of an invention, and they may be used as knowledge inputs within the invention process. Moreover, backward citations represent the prior art, and demonstrate that the invention had not been protected before. These three indicators have been related to the patent value for other authors (see for instance [38]). However, they still have not been used to estimate an unobserved variable as they are in a structural equation model.

From a theoretical standpoint, the knowledge stock is an exogenous latent variable, and affects the value of a patent. Keeping in mind the backward citations, it seems reasonable to think that an invention that is protected in an area where a lot of inventions are applied — hence with a large knowledge stock — will have less value than a potential radical innovation or a breakthrough invention, and therefore having a smaller knowledge stock. The number of inventors and applicants are revealed first in time, and cause a change on the knowledge stock, and not vice-versa. Additionally, it is not difficult to see that there is no covariance among backward citations, and the number of inventors and applicants. For instance, a patent may contain a large number of references, but the invention may be created only by one inventor or by one applicant. So, a reflective approach would fail to meet the unidimensionality condition. For this construct, however, multicollinearity would not be a problem. Hence, a formative mode is suitable for modelling the relationship between the indicators and the knowledge stock.

The technological scope of the invention is related to the potential utility of an invention in some technological fields. So, the manifest variables for this construct are the number of four-digit IPC classes where the patent is classified, and the number of claims of the patent. The IPC classes allow us to know the technical fields related to the invention, and therefore the number of potential application fields. This does not mean that an invention ultimate use is restricted to a determined area. A company may protect an invention for strategic purposes, for example to prevent its being used by a competitor. Here, the underlying issue is that the larger the number of classification codes, the larger the number of potential application fields, and hence, the greater the technological scope of the patent. On the other hand, and according to Tong and Frame [42, p. 134], "each claim represents a distinct inventive contribution, so patents are, in effect, bundles of inventions". Claims are a description of what the inventors actually claim to have invented and describe the potential application of the invention. As seen in the literature review, the number of claims should reflect the inventive activity of the invention. So, under the assumption that a highly sophisticated invention will require much inventiveness, the patent will also have a considerable amount of claims. Thus, this variable will also give information about the technological scope of the patents. It is arguable that this is not always so. Probably there are sophisticated inventions that have not required a large number of claims to be protected. But this may be unusual in the renewable energy field. As seen in Table 1 below, the number of claims is a skewed variable (skewness = 4.29, kurtosis = 43.65), with median 14. Following the rules presented before to distinguish between formative and reflective outer models, in this case, the manifest variables are revealed first, and cause a change in the technological scope of the inventions. When defining the manifest variables determining the technological scope. Probably, inventors have an idea of the applicability of the invention long before the time of protecting it. But, it is the patent value, therefore the protected invention, that is being analyzed here. So, a formative relationship is modeled between the indicators and the constructs. Additionally, as with the knowledge stock, there is no collinearity among manifest variables, and the block of variables is not one-dimensional.

The international scope refers to the geographic zones where the invention is protected. Inventions are usually protected in the local country first and then in others, as part of the companies' patenting strategy. All the patents considered in the sample are granted in the U.S. So, we defined two dummy variables that consider whether the invention had been protected in Japan (priority JP) or in Germany (priority DE) during the priority period. Japan and Germany are large producers of renewable energy technologies. Hence, it is interesting to examine whether these variables affect the patent value. Variables indicating whether inventions have been protected through the European Patent Office (EPO) or by the World Intellectual Property Organization (WIPO) have been excluded from the analysis because they provide little information. This means that for the international scope, not all the variables that could form the construct are being considered. So, higher disturbance terms are expected in this case. The international scope is clearly caused by the manifest variables. Here, again there is no collinearity among manifest variables, the block of variables is not one-dimensional. Therefore, formative relationships are considered in this block of variables.

On the other hand, the importance of a patent for future technological developments will be reflected in the number of times that the patent is cited, since the patent is useful for the development of other technologies [18], and in the patenting strategy pursued by the company over time. The latter is measured by taking into account the size of the patent family or the number of countries where the protection is sought. For the block of variables of patent value, a reflective relationship is considered between manifest and latent variables. As in this case all the indicators should explain the same construct (aside from the variables that have traditionally been used to infer the patent value), dummy variables are defined by considering whether the patent has been protected in Japan (JP), Germany (DE) or through the European Patent Office (EP). So, in this research, the first analyzed case is a first-order model composed by four constructs: knowledge stock, technological scope, international scope, and patent value (Figure 1).

It is worth noting that the first three constructs — knowledge stock, technological scope, and international scope — give an *a priori* value of patents. Thus, the intrinsic characteristics of the patent at the time of its application, along with the patenting strategy of the company in the priority period, may give a preliminary idea of patent value. In contrast, patent value estimated through forward citations and family size gives an *a posteriori* value for patents. This value (recognized value) is obtained over time and is given by others through the number of times that the patent is cited and the number of countries where the protection is sought. Estimating the patent value only through these manifest variables seems too ambitious. Rather, it is reasonable to think that the patent value is jointly given by those variables that determine the *a priori* and the *a posteriori* patent value. Using this approach, the influence of the *a posteriori* relative to the *a priori* patent value may also be assessed. Hence, the indicators that were initially related to the patent value are also associated with a fifth underlying latent variable related to the potential usefulness of the patent. The more useful a patent is, the more it is cited by others and the more important it is to the company's patenting strategy. We call this latent variable "technological usefulness". From a methodological standpoint, this means that the patent value is not directly related to a block of observed variables. So, this construct is regarded as a second-order latent variable that is influenced by all of the other constructs in a second-order model. The proposed model is shown in Figure 2. We explore the veracity of the assumptions with PLS path modelling.

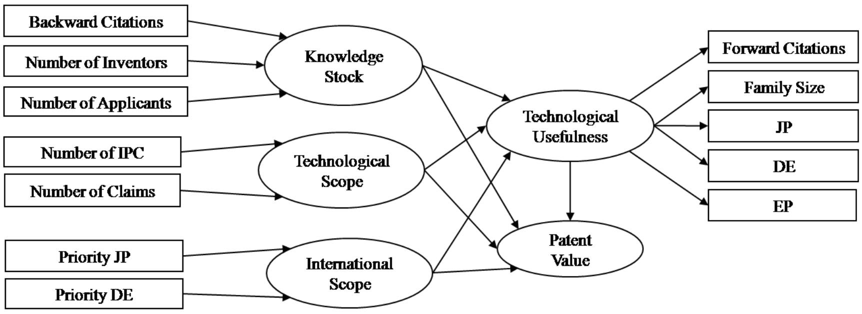

Figure 2: Hierarchical component model of patent value; patent value is an endogenous second-order latent variable; technological usefulness is a reflective endogenous latent variable; knowledge stock, technological scope, and international scope are formative exogenous constructs.

5. PATENT DATA

Renewable energy patents include wind, solar, geothermal, wave / tide, biomass, and waste energy. To select suitable patent data, we use the IPC classes for renewable energies listed by Johnstone *et al.* [26]. The sample comprises a total of 2,901 patents (sample 1), published in 1990–1991, 1995–1996, 1999–2000 and 2005–2006, and granted in the U.S. (source: Delphion database). We retrieved these data, and the indicators described above were computed. The number of claims was collected manually for each patent.

Table 2 provides descriptive statistics for patent indicators. The results indicate that some variables are very heterogeneous and asymmetric, and they also exhibit large variance. So, normality is not a good assumption. Positive values of skewness indicate positive/right skew (notice how the medians are always smaller than the means). Likewise, positive kurtosis indexes show distributions that are sharper than the normal peak.

Table 2: Descriptive statistics of patent data.

Manifest Variable	Mean	Standard Deviation	Minimum	Mediam	Maximum	Skewness	Kurtosis
Number of applicants	1.04	0.29	1	1	9	12.85	260.81
Number of inventors	2.21	1.58	1	2	14	1.76	4.23
Backward citations	15.36	18.97	0	11	327	5.54	50.79
Number of IPC	6.28	4.52	1	5	48	2.09	7.71
Number of claims	17.02	15.08	1	14	279	4.29	43.65
Priority JP	0.19	0.39	0	0	1	1.54	0.37
Priority DE	0.08	0.27	0	0	1	3.09	7.55
Forward citations	5.63	10.16	0	2	158	5.3	46.83
Family size	8.53	11.62	1	6	202	5.58	51.27
Dummy JP	0.44	0.49	0	0	1	0.23	−1.95
Dummy DE	0.32	0.46	0	0	1	0.75	−1.44
Dummy EP	0.43	0.49	0	0	1	0.25	−1.94

Additionally, the priority countries of these patents are U.S. (59%), Japan (19%), Germany (9%), Great Britain (2%), France (1%) and so on. Patents belong to 1,581 applicants. Patents have been granted to companies (69%), individuals (25%) and universities, research centers or governmental institutions (6%). Due to the manner in which the sample was selected, the sample is homogenous in terms of technological area and the country where the patents were granted. However, the sample is heterogeneous in terms of the type of applicant or the industry in which the companies are classified, and this heterogeneity could affect the results. This also means that there are companies belonging to different industries that are interested in developing renewable energy innovations. At any rate, it is worth noting that at this stage, the patent value model is being tested in general at the level of renewable energy technologies. We estimate the model using the total sample (2,901 patents, sample 1). However, providing that time is an important factor that may affect the findings, three additional samples were taken. Patent indicator matrices were selected in the following application years: 1990–1991 ($N = 129$, sample 2), 1995–1996 ($N = 128$, sample 3) and 1999–2000 ($N = 536$, sample 4). So, in order to analyze whether it is possible to find a pattern in the parameter estimates, the proposed models were estimated with all data, and with time-period data (notice that cases are different in each time-period).

6. RESULTS

The internal consistency of reflective outer models, technological usefulness and patent value was assessed by using Cronbach's alpha and composite reliability. For the first-order, the Cronbach's alpha coefficients for patent value are 0.68, 0.79, 0.76 and 0.68 for samples 1, 2, 3 and 4, respectively. Moreover, composite reliability coefficients are 0.77, 0.85, 0.84 and 0.79 for each sample, respectively. So, the patent value is unidimensional. AVE scores are 0.48, 0.56, 0.54 and 0.48 for patent value and for samples 1, 2, 3 and 4, respectively. So, the constructs capture on average more than 50% of the variance in relation to the amount of variance due to measurement error. In the second-order model, technological usefulness has the same Cronbach's alpha and composite reliability coefficients that patent value has in the first-order model. Cronbach's alpha coefficients for the patent value are 0.59, 0.68, 0.7 and 0.58 for samples 1, 2, 3 and 4, respectively. Composite reliability coefficients are 0.72, 0.76, 0.79 and 0.71 for each sample, respectively. Therefore, both technological usefulness and patent value are unidimensional. The technological usefulness captures on average a 54% of the variance in relation to the amount of variance due to measurement error (see the AVE scores for patent value in the first-order model). However, AVE scores for patent value (second-order latent variable) are quite different, 0.24, 0.29, 0.3 and 0.22 for samples 1, 2, 3 and 4, respectively. So, this block of variables is unidimensional, and the latent variable captures on average a 26% of the variance in relation to the amount of variance due to measurement error. This low percentage may be because reflective and formative indicators have been repeated for the second-order latent variable.

Table 3 reports the cross loadings for the reflective block of variables in the second-order model of patent value in the three analyzed time-periods. Forward citations, family size and dummy variables JP, DE and EP are slightly more correlated in the three time-periods, with the technological usefulness of the patents rather than the patent value itself. In regards to other indicators, quite the opposite happens: the correlation between indicators and patent value are always higher than the correlation between indicators and technological usefulness. This is adequate even though patent value indicators are used as auxiliary variables in order to estimate the model. It is worth noting that cross loadings of some variables are very similar over time, suggesting a pattern. This phenomenon is interesting because it indicates that the number of inventors; the number of IPC classes; dummy variables JP, DE and EP; forward citations and family size are strongly and constantly correlated with the patent value and its technological usefulness throughout time. This empirical evidence supports the relationships between latent and manifest variables as proposed in the models.

Table 3: Cross loadings between indicators for reflective block of variables.

Manifest Variable	**1990–1991**		**1995–1996**		**1999–2000**	
	Patent Value	**Technological Usefulness**	**Patent Value**	**Technological Usefulness**	**Patent Value**	**Technological Usefulness**
Number of inventors	0.572	0.279	0.611	0.424	0.492	0.135
Backward citations	0.064	0.129	0.092	0.067	0.141	0.091
Number of IPC	0.587	0.387	0.465	0.357	0.495	0.228
Number of claims	−0.074	−0.027	0.403	0.257	0.131	0.048
Dummy priority JP	0.527	0.258	0.391	0.253	0.414	0.162
Dummy priority DE	0.205	0.127	0.103	0.127	0.154	0.136
Forward citations	0.229	0.292	0.295	0.29	0.085	0.085
Family size	0.775	0.894	0.741	0.825	0.714	0.859
Dummy JP	0.816	0.836	0.818	0.833	0.727	0.774
Dummy DE	0.692	0.775	0.754	0.808	0.559	0.681
Dummy EP	0.666	0.818	0.739	0.799	0.658	0.809

Tables 4 and 5 present the standardized loadings and weights by PLS estimation and t-values by bootstrapping for the first- and second-order models, respectively. Loadings and weights reveal the strength of the relationship between manifest and latent variables. The number of inventors, the number of IPC classes and the dummy priority variables JP and DE are strongly and significantly related to their constructs in all cases in the first- and in the second-order models. Some authors [5, 7, 44] have studied the performance of the PLS path modelling algorithm using Monte Carlo simulations. Among others, the factors analyzed have been the sample size and the number of manifest variables per latent variable. In general, researchers agree and recommend having at least three indicators per construct. However, only Chin *et al.* [8] considered in their study the case of two observed variables per latent variables in their study of interaction effects with reflective outer models. However, as a result of their simulation study, Vilares *et al.* [44, p. 13] reported that "PLS always produces good estimates for perceived value loadings [a latent variable with two indicators, the author]. This is an interesting result, since PLS is presented as being 'consistent at large' ...". In the formative outer models analyzed here, there are few indicators available per construct. However, the magnitudes of the weights are large enough to infer that there may be a formative relationship between indicators and constructs. Additionally, these results suggest that the patent value and the technological usefulness are evident since the patent is applied. Therefore, the value can be assessed at an early stage. The number of claims shows a weaker association with the technological scope than the number of IPC classes. Perhaps this indicator is more related to the "quality" of the invention, not in the sense of how inventions have an impact on different technological fields (scope) but rather on how important this impact is in a given technological field. Regarding the international scope, this variable seems to be formed by its indicators. The manifest variables are statistically significant in all cases in the two analyzed models. So, this could mean that in the renewable energy field, besides protecting the invention in the U.S., it is important as a value determinant for early protection of the inventions which originate in the other two largest producers of these technologies: Japan and Germany.

Table 4: Standardized loadings and weights for outer models for the first-order model of the patent value, t-values in parenthesis, * at the 0.01 significance level, ** at the 0.05 significance level.

Construct	**Indicator**	**Sample 1**	**1990–1991**	**1995–1996**	**1999–2000**
Knowledge stock	Backward citations	0.541* (1.860)	0.420* (1.688)	0.128 (0.791)	0.499* (1.670)
	Number of inventors	0.807** (3.054)	0.920** (4.937)	0.988** (9.086)	0.872** (2.794)
Technological scope	Number of IPC	0.966** (5.935)	0.997** (13.746)	0.803** (5.455)	0.985** (4.502)
	Number of claims	0.176 (0.756)	−0.058 (0.364)	0.529 (1.432)	0.103** (0.354)
International scope	Priority JP	0.802** (3.662)	0.909** (5.492)	0.904** (7.844)	0.847** (3.630)
	Priority DE	0.725** (2.814)	0.512** (2.043)	0.502** (2.479)	0.660** (2.422)
Patent value	Forward citations	−0.108 (0.940)	0.274** (2.041)	0.299* (1.693)	0.096 (0.524)
	Family size	0.840** (9.464)	0.893** (36.017)	0.813** (15.126)	0.845** (5.297)
	Dummy JP	0.777** (6.593)	0.843** (19.572)	0.841** (21.277)	0.802** (4.549)
	Dummy DE	0.690** (5.530)	0.777** (11.126)	0.811** (18.389)	0.671** (4.087)
	Dummy EP	0.780** (7.921)	0.808** (11.975)	0.794** (12.513)	0.786** (5.272)

On the other hand, patent value and technological usefulness are always strongly and significantly reflected in their explanatory variables. Forward citations, patent family and dummy variables constantly reflect patent value in the first-order model and technological usefulness in the second-order model. The forward citations are not significant in the models evaluated in 1999–2000. But, this may be due to the fact that in recent years patents have been cited less, and the variable is less informative than in previous years. Moreover, loadings for the relationship between forward citations and technological usefulness are smaller

Table 5: Standardized loadings and weights for outer models for the second-order model of the patent value, t-values in parenthesis, * at the 0.01 significance level, ** at the 0.05 significance level.

Construct	**Indicator**	**Sample 1**	**1990–1991**	**1995–1996**	**1999–2000**
Knowledge stock	Backward citations	0.439 (1.619)	0.248 (1.103)	0.122 (0.991)	0.357 (1.114)
	Number of inventors	0.871** (3.828)	0.976** (8.060)	0.989** (24.728)	0.938** (3.214)
Technological scope	Number of IPC	0.952** (6.544)	0.995** (18.078)	0.761** (4.633)	0.974** (4.140)
	Number of claims	0.220 (1.028)	−0.078 (0.546)	0.584** (3.139)	0.150 (0.516)
International scope	Priority JP	0.867** (4.090)	0.931** (10.601)	0.947** (7.863)	0.915** (4.096)
	Priority DE	0.639** (2.422)	0.465** (2.709)	0.401* (1.701)	0.548* (1.943)
Technological usefulness	Forward citations	0.762** (6.833)	0.836** (22.739)	0.834** (24.167)	0.774** (5.177)
	Family size	0.795** (10.667)	0.818** (11.800)	0.799** (18.126)	0.809** (11.499)
	Dummy JP	0.705** (7.983)	0.775** (11.891)	0.809** (18.318)	0.681** (6.256)
	Dummy DE	−0.052 (0.488)	0.292** (2.280)	0.290** (2.190)	0.085 (0.616)
	Dummy EP	0.853** (13.577)	0.894** (36.226)	0.825** (21.104)	0.859** (11.526)
Patent value	Backward citations	0.232 (1.511)	0.064 (0.564)	0.092 (1.005)	0.141 (0.735)
	Number of inventors	0.476** (3.477)	0.572** (5.964)	0.611** (8.825)	0.492** (3.016)
	Number of IPC	0.549** (5.909)	0.587** (7.837)	0.465** (4.820)	0.495** (3.420)
	Number of claims	0.185 (1.296)	−0.074 (0.748)	0.403** (3.193)	0.131 (0.810)
	Priority JP	0.387** (2.723)	0.527** (5.466)	0.391** (3.604)	0.414** (2.461)
	Priority DE	0.202** (5.318)	0.205** (2.262)	0.103 (1.269)	0.154 (1.191)
	Forward citations	−0.085 (0.861)	0.229* (1.944)	0.295** (2.453)	0.085 (0.659)
	Family size	0.730** (8.250)	0.775** (15.351)	0.741** (11.612)	0.714** (5.952)
	Dummy JP	0.711** (6.083)	0.816** (20.264)	0.818** (18.295)	0.727** (4.349)
	Dummy DE	0.586** (5.318)	0.692** (8.318)	0.754** (11.977)	0.559** (4.349)
	Dummy EP	0.672** (7.196)	0.666** (6.650)	0.739** (13.752)	0.658** (6.341)

than, for instance, loadings for the relationship between family size and technological usefulness. These results may mean that the longitudinal nature of this variable — citations that are received throughout the time — is an important factor that should be taken into account when considering this indicator in the models. The quality of each outer model is measured through the communality index, i.e. the proportion of variance in the measurement variables accounted for by the latent variable. For the second-order model, communality indexes for patent value are 0.29, 0.30 and 0.22 for the 1990–1991, 1995–1996 and 1999–2000 models, respectively. Therefore, indicators have approximately 30% of the variance in common with its latent variable. As seen above, this low percentage may be because reflective and formative indicators have been repeated for the second-order latent variable. The communality indexes for technological usefulness are 0.57, 0.55 and 0.49 for each time-period, also giving evidence of an important percentage of shared variance.

Tables 6 and 7 show the findings for the inner relationships (standardized beta coefficients, significance levels and coefficients of determination) for the first- and second-order models respectively. Path coefficient of knowledge stock, technological scope and international scope as related to patent value are significant at 0.01 levels in almost all cases. Therefore, the patent value may be formed by constructs estimated from reliable patent indicators. The first-order model allows us to obtain an estimate of the patent value "in time equal to zero". As showed in the second-order model, the knowledge stock, the technological scope and the international scope are also related to technological usefulness. Moreover, technological usefulness and patent value are significantly related, indicating how the former is an important variable in the prediction of the latter. The second-order model allows us to obtain the patent value as the sum of the value in time equal to zero, and the value given by others, that is the technological usefulness.

Table 6: Standardized path coefficients for the first-order model of patent value, t-values in parenthesis, * at the 0.01 significance level, ** at the 0.05 significance level.

Latent Variable	**Sample 1**	**1990–1991**	**1995–1996**	**1999–2000**
Knowledge stock to Patent value	0.115 (1.248)	0.202* (1.987)	0.306** (2.263)	0.091 (1.040)
Technological scope to Patent value	0.238** (2.892)	0.314** (4.221)	0.335** (3.084)	0.200** (2.278)
International scope to Patent value	0.243** (3.199)	0.154* (1.998)	0.251** (3.044)	0.220** (2.420)
R^2 of patent value	0.161	0.234	0.35	0.114

Table 7: Standardized path coefficients for the second-order model of patent value, t-values in parenthesis, * at the 0.01 significance level, ** at the 0.05 significance level.

Latent Variable	**Sample 1**	**1990–1991**	**1995–1996**	**1999–2000**
Knowledge stock to Patent value	0.280** (9.979)	0.226** (9.510)	0.229** (12.349)	0.293** (8.281)
Technological scope to Patent value	0.278** (8.811)	0.227** (10.737)	0.226** (8.870)	0.271** (7.620)
International scope to Patent value	0.212** (5.505)	0.232** (11.314)	0.166** (7.659)	0.236** (5.160)
Knowledge stock to Technological usefulness	0.104 (1.162)	0.180* (1.752)	0.299** (3.771)	0.072 (0.783)
Technological scope to Technological usefulness	0.237** (2.686)	0.315** (3.290)	0.334** (3.387)	0.207** (2.133)
International scope to Technological usefulness	0.225** (2.486)	0.142 (1.376)	0.236** (3.042)	0.200** (2.252)
Technological usefulness to Patent value	0.683** (14.511)	0.668** (16.951)	0.697** (20.558)	0.698** (11.207)
R^2 of patent value	0.998	0.998	0.999	0.997
R^2 of usefulness	0.148	0.219	0.338	0.103

The determination coefficient for patent value is 0.9 in the second-order models, i.e. the model fit the data in an acceptable way. This result is not surprising; it confirms the aforementioned findings and indicates how the data is better explained by second-order models as compared with first-order models. However, we must consider this result carefully, because the patent value is estimated considering all the measurement variables of the models. Another explanation for this is that in the second-order models, the contribution of the recognized value of patents (technological usefulness) is considered, and this would help fit the data better. Unlike patent value, technological usefulness has a moderate coefficient of determination. Perhaps other indicators should help to better explain the model, or again the longitudinal nature of the forward citations is an important factor to be considered. However, we think that the results are acceptable, taking into account the literature review and the goodness of fit obtained using other models in the analysis of patent data. It is worth noting that the structural relationships are significant.

7. FINAL REMARKS

This research relates manifest variables that come from information contained in the patent document with latent variables into a single replicable model. The magnitude of this relationship and the importance of each construct are known, including the influence of knowledge stock, the technological and international scope in the value of the technology. In the first-order model, the variables that most affect the patent value are the technological and the international scope. In the second-order model, the technological usefulness is also important.

A distinction between two patent values can be made: an *a priori* and intrinsic value, which the patent has at the moment of its application (the potential value of the patent); and an *a posteriori* value that the patent acquires over time through the actions of a company or others (the value that is recognized). The potential value depends on the characteristics of the patent at the time of application -such as the patenting strategy of a company, the technological applicability of the patents in different technological fields and the base of knowledge that is necessary for the creation of a new invention. As time passes, the patent potentiality is recognized and reflected in the number of times that it is cited and in the number of countries where it is protected. This recognition is a reflection of its technological usefulness. Even though companies can assess the importance or impact of their inventions, these results and the procedure for obtaining them are becoming a tool for improving the strategy of developing new products and inventions, improving intellectual property policy and for comparing technologies with other competitors. The stability of results over time augur that this may be possible.

In order to assess companies' patent portfolios using a model that can be replicated, a follow-up to this research will study patent value evolution as well as the market-patent relationship and its implications. Furthermore, there are other indicators related to patent value that have been previously studied, but they cannot be computed from the information contained in the patent documents, such as the number of renewals and the number of opposition cases. Nevertheless, these variables could be related to another latent variable in the model, or be a reflection of the technological usefulness of an invention. Finally, PLS path modelling has proven to be a suitable approach for analyzing patent data.

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