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Asymptotic behavior of tails and quantiles of quadratic forms of Gaussian vectors

Stefan Jaschke,^a Claudia Klüppelberg,^b and Alexander Lindner^{b,*}

^a Federal Financial Supervisory Authority (BaFin), Graurheindorfer Str. 108, 53117 Bonn, Germany ^b Center of Mathematical Sciences, Munich University of Technology, D-85747 Garching, Germany

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Abstract

We derive results on the asymptotic behavior of tails and quantiles of quadratic forms of Gaussian vectors. They appear in particular in delta–gamma models in financial risk management approximating portfolio returns. Quantile estimation corresponds to the estimation of the Value-at-Risk, which is a serious problem in high dimension. © 2003 Elsevier Inc. All rights reserved.

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1. Introduction

Quadratic forms $X^T Q X$ of Gaussian vectors $X \sim N(\mu, \Sigma)$ play an important role in probability theory and statistics. These forms appear in (central and non-central) χ^2 -statistics, likelihood ratios, and power spectra, which are used in many different applications and models throughout statistics.

Traditional applications include "ballistic analysis of multiple weapon systems", the "detection of signals from noise in multichannel receivers", "the study of bone

(C. Klüppelberg), lindner@mathematik.tu-muenchen.de (A. Lindner).

^{*}Corresponding author.

E-mail addresses: stefan@jaschke-net.de (S. Jaschke), cklu@mathematik.tu-muenchen.de

URL: http://www.mathematik.tu-muenchen.de.

lengths determined in vivo using X-ray stereography" [13] as well as numerous applications in communication theory cited by Raphaeli [19] and Gao and Smith [7].

This paper was motivated by a problem from financial mathematics. The so-called delta–gamma method approximates the Value-at-Risk, which is nothing else but a small quantile, e.g. the 1%-quantile. The approximation is based on a second-order Taylor expansion of the price of a financial derivative, for instance, a European option. The expansion is for the price of the derivative at a particular time and at a certain price level of the underlying security, which may be an index or an asset price. See Duffie and Pan [6] for details.

In a Gaussian framework, the second-order approximation leads to

$$V(X) = \theta + \Delta^T X + \frac{1}{2} X^T \Gamma X, \qquad (1.1)$$

where X is an *m*-dimensional Gaussian vector with mean 0 and covariance matrix Σ , Δ is a vector in \mathbb{R}^m , and Γ is some symmetric $m \times m$ -matrix. The Gaussian model is usually based on the central limit theorem. Such quadratic approximations are extremely popular in risk management for financial institutions [17].

Eq. (1.1) can be brought into the diagonal form

$$V = \theta + \delta^T Y + \frac{1}{2} Y^T \Lambda Y = \theta + \sum_{j=1}^m \left(\delta_j Y_j + \frac{1}{2} \lambda_j Y_j^2 \right), \tag{1.2}$$

where $Y = (Y_1, ..., Y_m)^T$ is a standard normal vector, $\delta = (\delta_1, ..., \delta_m)^T \in \mathbb{R}^m$, and $\Lambda = \text{diag}(\lambda_1, ..., \lambda_m)$ is a diagonal matrix. This can be done by solving the *generalized* eigenvalue problem

$$CC^{T} = \Sigma,$$
$$C^{T} \Gamma C = \Lambda,$$

and putting X = CY, $\delta = C^T \Delta$.

Approximations to the probability distribution of V include series expansions [16, Section 4.2], numerical Fourier inversion [10,20], Monte Carlo simulation [8], and numerous approximations with limited accuracy based on moment matching (see [12] for references). The two approaches used in practice, which in principle can achieve any desired accuracy are numerical Fourier inversion and Monte Carlo simulation. For small quantiles, special Monte Carlo simulation methods, such as importance sampling (see e.g. [8]), have been developed to reduce the required amount of simulations.

The Fourier inversion method starts with the characteristic function $\phi(t) = Ee^{itV}$, $t \in \mathbb{R}$, which is known analytically in the case (1.1). Then the inversion formula

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-itx} \phi(t) dt$$
(1.3)

holds for the probability density f. The key to an error analysis of trapezoidal, equidistant approximations to the integral (1.3)

$$\tilde{f}(x,\Delta_t) \coloneqq \frac{\Delta_t}{2\pi} \sum_{k=-\infty}^{\infty} \phi(k\Delta_t) e^{-ik\Delta_t x}$$
(1.4)

is the Poisson summation formula

$$\tilde{f}(x,\Delta_t,t) = \sum_{j=-\infty}^{\infty} f\left(x + \frac{2\pi}{\Delta_t}j\right).$$
(1.5)

The infinite sum (1.4) has to be truncated, so the resulting errors consist in a discretization error and a truncation error. The discretization error is described by all terms in the infinite sum in (1.5) except that for j = 0. Thus, the question how the discretization error decreases asymptotically with Δ_t tending to 0 is identical to the question of the tail behavior of f. On the other hand, the truncation error can be read off (1.4) and is obviously related to the tail behavior of ϕ . The influence of these errors on accuracy is investigated theoretically as well as numerically in [1, p. 22]. For a modified approach using Fourier inversion, see Jaschke [11].

This paper proposes a different approach to the problem in providing an asymptotic approximation to the density f, to the tails of the distribution function F and to the α -quantile x_{α} for α close to 0 or 1. This approach is in the spirit of Beran [4], who derives the asymptotic right tail behavior of the distribution of V and its density function in the positive definite case, i.e. when $\lambda_1, \ldots, \lambda_m$ appearing in (1.2) are all strictly positive. The contribution of this paper is to develop the asymptotic tail behavior for the general case (1.2), without any restrictions on the λ_i 's. The extension of Beran's result was motivated by a real life example in risk management as mentioned before.

Our paper is organized as follows. In Section 2, we present V as being essentially a sum of independent non-central χ^2 -distributed random variables with different degrees of freedom and non-centrality parameters. In Section 3, the main asymptotic results are derived. The behavior of the lower and upper tails of V are obtained for the relevant regimes, which are determined by the lowest/highest eigenvalue being negative, zero or positive. Section 4 is devoted to quantile approximation based on the results in Section 3. Examples and some discussion on our results included in Section 5 conclude the paper. These examples show that our proposed approximations work well for extremely small/large quantiles, but even for quantiles such as 1% they may still not be precise enough. On the other hand, in contrast to numerical Fourier inversion, which in principle can achieve any desired accuracy, our approach yields explicit expressions for the extreme quantiles.

2. An alternative representation

Suppose that the (generalized) eigenvalues λ_i of V appearing in (1.2) are sorted in increasing order. Suppose there are $n \leq m$ distinct eigenvalues, and denote by i_i the

highest index of the *j*th distinct eigenvalue, and by μ_j its multiplicity $(\mu_j = i_j - i_{j-1}, i_0 = 0, i_n = m)$; thus $\lambda_{i_1} < \cdots < \lambda_{i_n}$. For $j = 1, \dots, n$, define

$$V_{j} \coloneqq \begin{cases} \frac{1}{2}\lambda_{i_{j}} \sum_{l=i_{j-1}+1}^{i_{j}} \left(\frac{\delta_{l}}{\lambda_{i_{j}}}+Y_{l}\right)^{2}, & \text{if } \lambda_{i_{j}}\neq 0, \\ \sum_{l=i_{j-1}+1}^{i_{j}} \delta_{l}Y_{l}, & \text{if } \lambda_{i_{j}}=0, \end{cases}$$

$$(2.1)$$

and $\bar{\delta}_j^2 \coloneqq \sum_{l=i_{j-1}+1}^{i_j} \delta_l^2$. Then the V_j are independent and

$$V = \theta - \sum_{\substack{j=1\\\lambda_{i_j} \neq 0}}^n \frac{\delta_j^2}{2\lambda_{i_j}} + \sum_{j=1}^n V_j.$$

If $\lambda_{i_j} = 0$, then V_j is Gaussian. If $\lambda_{i_j} \neq 0$, then V_j is a scaled version of a (non-central) χ^2 -variable with μ_j degrees of freedom and non-centrality parameter $a_j^2 = \bar{\delta}_j^2 / \lambda_{i_j}^2$. Specifically, if $g(\cdot; a_j^2, \mu_j)$ denotes the $\chi^2_{\mu_i}(a_j^2)$ -density, then

$$f_j(x) = \frac{2}{|\lambda_{i_j}|} g\left(\frac{2}{\lambda_{i_j}} x; a_j^2, \mu_j\right),\tag{2.2}$$

where f_j denotes the density of V_j .

3. Approximation of the tails

In this section, we shall determine the tail behavior of the density f(x) of V as x approaches the left and right endpoints of its support. It will turn out that the left, resp. right, tail behavior of f differs according whether λ_{i_1} , resp. λ_{i_n} , is negative, zero, or positive. For $\lambda_{i_1} < 0$, f(x) behaves like a constant times $f_1(x)$ as $x \to -\infty$, and for $\lambda_{i_1} \ge 0$ it behaves like a constant times a power of x times $f_1(x)$, as x approaches the left endpoint.

3.1. Case 1: the lowest eigenvalue is negative

For our results, we shall need the tail behavior of (non-)central χ^2 -distributions, whose density is known analytically, see for example [14, p. 416]; [15, p. 436]:

$$g(x;a^{2},\mu) = \mathbf{1}_{(0,\infty)}(x) \begin{cases} \frac{1}{2} (\sqrt{x}/a)^{\mu/2-1} I_{\mu/2-1}(a\sqrt{x}) e^{-(x+a^{2})/2} & (a \neq 0), \\ \frac{1}{2^{\mu/2} \Gamma(\mu/2)} x^{\mu/2-1} e^{-x/2} & (a = 0), \end{cases}$$
(3.1)

where $a \coloneqq \sqrt{a^2}$ and

$$I_{\nu}(x) = \sum_{n=0}^{\infty} \frac{1}{n! \Gamma(n+\nu+1)} \left(\frac{x}{2}\right)^{2n+\nu}$$
(3.2)

is the modified Bessel function of the first kind.

The tail behavior of $I_v(x)$ for $x \to \infty$ is independent of v, see e.g. [2, (9.7.1)]:

$$I_{\nu}(x) = e^{x} (2\pi x)^{-1/2} (1 + O(1/x)), \quad x \to \infty,$$
(3.3)

which leads to

$$g(x; a^{2}, \mu) = (2\sqrt{2\pi})^{-1} a^{(1-\mu)/2} e^{-a^{2}/2} x^{(\mu-3)/4} e^{-x/2 + a\sqrt{x}} (1 + O(1/\sqrt{x})),$$

$$x \to \infty,$$
(3.4)

in the case $a \neq 0$. Together with (2.2) this leads to the tail behavior of f_i (if $\lambda_{i_i} \neq 0$):

$$f_j(x) = f_j^{\mathsf{t}}(x)(1 + O(1/\sqrt{|x|})), \quad x \to (\operatorname{sgn} \lambda_{i_j}) \infty,$$
(3.5)

where f_i^t is defined by

$$f_{j}^{t}(x) \coloneqq c_{j} \mathbf{1}_{(0,\infty)}(\lambda_{i_{j}} x) \begin{cases} |x|^{(\mu_{j}-3)/4} e^{-x/\lambda_{i_{j}}+a_{j}}\sqrt{|2/\lambda_{i_{j}}|}\sqrt{|x|} & (a_{j} \neq 0), \\ |x|^{\mu_{j}/2-1} e^{-x/\lambda_{i_{j}}} & (a_{j} = 0), \end{cases}$$
(3.6)

with

$$c_j \coloneqq \begin{cases} (2\sqrt{2\pi})^{-1} e^{-a_j^2/2} a_j^{(1-\mu_j)/2} (\frac{2}{|\lambda_{i_j}|})^{(\mu_j+1)/4} & (a_j \neq 0), \\ \\ |\lambda_{i_j}|^{-\mu_j/2} / \Gamma(\mu_j/2) & (a_j = 0) \end{cases}$$

and $a_j = \sqrt{a_j^2} = |\bar{\delta}_j/\lambda_{i_j}|$. Note also that the support of f_j is $[0, \infty)$ if $\lambda_{i_j} > 0$, and $(-\infty, 0]$ if $\lambda_{i_j} < 0$. If $\lambda_{i_j} = 0$, then f_j is Gaussian. The following theorem shows that the left tail behavior of f is determined by the tail behavior of f_1 .

Theorem 3.1. For $\lambda_1 = \lambda_{i_1} < 0$, the density f of V has the asymptotic left tail behavior

$$f(x) = b_1 f_1(x) (1 + O(1/\sqrt{|x|})) = b_1 f_1^{\mathsf{t}}(x) (1 + O(1/\sqrt{|x|})), \quad x \to -\infty, \quad (3.7)$$

and for $\lambda_m = \lambda_{i_n} > 0$, it has the asymptotic right tail behavior

$$f(x) = b_n f_n(x)(1 + O(1/\sqrt{x})) = b_n f_n^{t}(x)(1 + O(1/\sqrt{x})), \quad x \to \infty,$$
(3.8)

where the constant b_k , $k \in \{1, n\}$, is given by

$$b_k \coloneqq e^{\theta/\lambda_{i_k} - a_k^2/2} \prod_{j \in \{1, \dots, n\} \setminus \{k\}} \left(\left(1 - \frac{\lambda_{i_j}}{\lambda_{i_k}}\right)^{-\mu_j/2} e^{\tilde{\delta}_j^2 (2(\lambda_{i_k} - \lambda_{i_j})\lambda_{i_k})^{-1}} \right).$$
(3.9)

Proof. Let $\lambda_1 < 0$. Our proof is inspired by an example given in [3, p. 573]. We claim that, whenever a probability density *h* has asymptotic behavior $h(x) = c_h f_1^t(x)(1 + O(1/\sqrt{|x|}))$ (for some constant $c_h \neq 0$ and $x \to -\infty$), then, for j > 1, the convolution $h * f_j$ has asymptotic behavior

$$(h * f_j)(x) = \left(\int_{-\infty}^{\infty} e^{y/\lambda_1} f_j(y) \, dy\right) h(x)(1 + O(1/\sqrt{|x|})), \quad x \to -\infty.$$
(3.10)

In other words, we show that

$$\int_{-\infty}^{\infty} \sqrt{|x|} \left(\frac{h(x-y)}{h(x)} - e^{y/\lambda_1} \right) f_j(y) \, dy = O(1), \quad x \to -\infty.$$
(3.11)

To show (3.11), split the integral into the two integrals ranging over $(-\infty, x + c)$ and $[x + c, \infty)$, for some sufficiently large positive constant c. The first integral can be bounded as

$$\int_{-\infty}^{x+c} \sqrt{|x|} \left| \frac{h(x-y)}{h(x)} - e^{y/\lambda_1} \right| f_j(y) \, dy$$

$$\leq \frac{\sqrt{|x|}}{h(x)} \left(\sup_{-\infty < y \le x+c} f_j(y) \right) \int_{-\infty}^{x+c} h(x-y) \, dy + \sqrt{|x|} \int_{-\infty}^{x+c} e^{y/\lambda_1} f_j(y) \, dy.$$

The first term in this sum converges to 0 for $x \to -\infty$, since $\int_{-\infty}^{x+c} h(x-y) dy \leq 1$, and since $h(x)/\sqrt{|x|}$ decreases slower than f_j , see (3.5), (3.6). If we choose $\tilde{\lambda}_j \in (\lambda_1, \lambda_j), \tilde{\lambda}_j < 0$, then (3.5) and (3.6) show that $e^{y/\lambda_1} f_j(y) = O(e^{v(\lambda_1^{-1} - \tilde{\lambda}_j^{-1})}), y \to -\infty$, and thus $\int_{-\infty}^{x+c} e^{y/\lambda_1} f_j(y) dy = O(e^{(x+c)(\lambda_1^{-1} - \tilde{\lambda}_j^{-1})}), x \to -\infty$, showing that the second term above converges to 0 for $x \to -\infty$, too.

Now (3.11) will follow if we show that there is an integrable function bounding

$$G: y \mapsto f_j(y) e^{y/\lambda_1} \sup_{x \leqslant x_0} \left\{ \sqrt{|x|} \left| \frac{h(x-y)}{h(x)} e^{-y/\lambda_1} - 1 \right| \mathbf{1}_{[x+c,\infty)}(y) \right\}$$
(3.12)

for some suitably chosen $x_0 < 0$. We will choose $x_0 = -2c$. Thus, we can assume $x \le -2c$ and $x - y \le -c$ in the following calculations. Write $h(x) = c_h f_1^t(x)(1 + \rho(x))$, where

$$|\sqrt{|x|\rho(x)|} \leqslant C \quad \forall x \leqslant -c \tag{3.13}$$

(c sufficiently large, C some constant). Then we have from (3.6)

$$\frac{h(x-y)}{h(x)} e^{-y/\lambda_{1}} - 1$$

$$= \left|\frac{x-y}{x}\right|^{(\mu_{1}-3)/4} e^{a_{1}\sqrt{2/|\lambda_{1}|}(\sqrt{y-x}-\sqrt{|x|})} \frac{1+\rho(x-y)}{1+\rho(x)} - 1$$

$$= \left\{ \left|\frac{x-y}{x}\right|^{(\mu_{1}-3)/4} e^{a_{1}\sqrt{2/|\lambda_{1}|}(\sqrt{y-x}-\sqrt{|x|})} - 1$$

$$+ \left|\frac{x-y}{x}\right|^{(\mu_{1}-3)/4} e^{a_{1}\sqrt{2/|\lambda_{1}|}(\sqrt{y-x}-\sqrt{|x|})}\rho(x-y)$$

$$- \rho(x) \right\} \frac{1}{1+\rho(x)}$$

$$=: \left\{ H_{1}(x,y) + H_{2}(x,y) + H_{3}(x,y) \right\} \frac{1}{1+\rho(x)},$$
(3.14)

where $H_i(x, y)$ is defined to be the summand appearing in the *i*th row of the preceding sum. We claim that for any $\lambda' > 0$, there is a constant $C_{\lambda'} > 0$

such that

$$\sqrt{|x|}|H_i(x,y)| \le C_{\lambda'} e^{\lambda'|y|}, \quad \forall x \le -2c, \ x-y \le -c, \ i=1,2,3.$$
(3.15)

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For H_3 this is clear, since $\sqrt{|x|}|H_3(x,y)| \leq C$ by (3.13). To show this for H_2 , note that

$$\sqrt{|x|}\rho(x-y) = \frac{\sqrt{x}}{\sqrt{|x-y|}}\sqrt{|x-y|}\rho(x-y) \leqslant C \left|\frac{x-y}{x}\right|^{-1}$$

by (3.13), and hence

$$\sqrt{|x|}|H_2(x,y)| \leq \left|\frac{x-y}{x}\right|^r e^{p(\sqrt{y-x}-\sqrt{|x|})},$$

for some $r \in \mathbb{R}$ and $p := a_1 \sqrt{2/|\lambda_1|}$. Now if $y \ge 0$, then $1 \le |(x - y)/x| \le 1 + y/(2c)$. If y < 0, and $x \le 2y$, then $1/2 \le |(x - y)/x| \le 2$. If y < 0 and $x \ge 2y$, then $c/(2|y| + c) \le |(x - y)/x| \le 2$. Thus, for all $x \le -2c$ and $x - y \le -c$, the following inequalities hold:

$$\frac{c}{2|y|+2c} \leqslant \left|\frac{x-y}{x}\right| \leqslant 2 + \frac{|y|}{2c}.$$
(3.16)

Together with

$$\sup_{x \leqslant -2c} e^{p(\sqrt{y-x} - \sqrt{|x|})} \leqslant \sup_{x \leqslant -2c} e^{p(\sqrt{|y|+|x|} - \sqrt{|x|})} \leqslant e^{p\sqrt{|y|}}$$

this implies that (3.15) holds for H_2 . Next we shall show that it also holds for H_1 : An application of the mean value theorem to the function $y \mapsto (1 - y/x)^{(\mu_1 - 3)/4}$ shows that

$$\left(1 - \frac{y}{x}\right)^{(\mu_1 - 3)/4} = 1 - \frac{\mu_1 - 3}{4} \left(1 - \frac{\xi_1}{x}\right)^{(\mu_1 - 3)/4 - 1} \frac{y}{x} =: 1 + \psi_1(x, y), \tag{3.17}$$

where ξ_1 is some number between 0 and y. Since $1 - \xi_1/x$ lies between 1 and 1 - y/x, it follows from (3.16) and $x \leq -2c$, that

$$\sqrt{|x|}|\psi_1(x,y)| \le C_1 \left(2 + \frac{2|y|}{c}\right)^{C_1'}$$
(3.18)

for some constants C_1, C_1' . Applying the mean value theorem to the function $y \mapsto e^{p(\sqrt{y-x}-\sqrt{-x})}$, where $p = a_1\sqrt{2/|\lambda_1|}$, shows that

$$e^{p(\sqrt{y-x}-\sqrt{-x})} = 1 + e^{p(\sqrt{\xi_2 - x} - \sqrt{-x})} \frac{py}{2\sqrt{\xi_2 - x}} =: 1 + \psi_2(x, y),$$
(3.19)

where ξ_2 is some number between 0 and y. Now since

$$e^{p(\sqrt{\xi_2-x}-\sqrt{-x})} \leqslant e^{(p\sqrt{|y|+|x|}-\sqrt{|x|})} \leqslant e^{p\sqrt{|y|}},$$

and since $\sqrt{|x|/(\xi_2 - x)} = (1 - \xi_2/x)^{-1/2}$, where $1 - \xi_2/x$ lies between 1 and 1 - y/x, it follows as for ψ_1 that

$$\sqrt{|x|}|\psi_2(x,y)| \le C_2 \left(2 + \frac{2|y|}{c}\right)^{C_2'} e^{p\sqrt{|y|}},\tag{3.20}$$

for some constants C_2 and C_2' . Now (3.14), (3.17) and (3.19) show that

$$\sqrt{|x|}H_1(x,y) = \sqrt{|x|}(\psi_1(x,y) + \psi_2(x,y) + \psi_1(x,y)\psi_2(x,y)),$$

and (3.18), (3.20) then immediately imply (3.15) for H_1 .

Since $\lim_{x\to-\infty} \rho(x) = 0$ it follows from (3.12), (3.14) and (3.15), that for any $\lambda' > 0$ there exists a constant $C_{\lambda'} > 0$ such that $G(y) \leq C_{\lambda'} f_j(y) e^{y/\lambda_1} e^{\lambda'|y|}$. But it is clear that this is an integrable majorant for sufficiently small λ' . Hence, we obtain (3.11) and (3.10). It then follows by induction and from (3.5) that the density of $\sum_{j=1}^{n} V_j$ has asymptotic behavior

$$\left(\prod_{j=2}^{n} \int_{-\infty}^{\infty} e^{y/\lambda_{1}} f_{j}(y) \, dy\right) f_{1}^{t}(x) (1 + O(1/\sqrt{|x|})), \tag{3.21}$$

as $x \to -\infty$. There remains to calculate $\int_{-\infty}^{\infty} e^{y/\lambda_1} f_j(y) dy$: For $\lambda_{i_j} \neq 0$, (2.2) gives

$$\int_{-\infty}^{\infty} e^{y/\lambda_1} f_j(y) \, dy$$

= $\int_{-\infty}^{\infty} e^{x\lambda_{i_j}/(2\lambda_1)} g(x; a_j^2, \mu_j) \, dx$
= $E\left(\exp\left\{\frac{\lambda_{i_j}}{2\lambda_1}\chi_{\mu_j}^2(a_j^2)\right\}\right)$
= $e^{\tilde{\delta}_j^2/(2\lambda_{i_j}\lambda_1)} \left(1 - \frac{\lambda_{i_j}}{\lambda_1}\right)^{-\mu_j/2} e^{\tilde{\delta}_j^2/(2(\lambda_1 - \lambda_{i_j})\lambda_1)},$ (3.22)

where we used the fact that the moment generating function of $\chi^2_{\mu_j}(a_j^2)$ at $t \leq \frac{1}{2}$ is given by

$$E(\exp\{t\chi^2_{\mu_j}(a_j^2)\}) = (1-2t)^{-\mu_j/2} \exp(a_j^2 t(1-2t)^{-1}),$$

see e.g. [15, p. 437]. Similar calculations, using the moment generating function of the normal distribution, show that

$$\int_{-\infty}^{\infty} e^{y/\lambda_1} f_j(y) \, dy = e^{\overline{\delta}_j^2/(2\lambda_1^2)}$$

for $\lambda_{ij} = 0 \neq \bar{\delta}_j^2$. Then it follows with b_1 as defined in (3.9), that the density of $\sum_{j=1}^n V_j$ has the asymptotic behavior $\exp\{-\theta/\lambda_1 + a_1^2/2 + \sum_{\lambda_{ij}\neq 0}^n \frac{\bar{\delta}_j^2}{2\lambda_{ij}\lambda_1}\}b_1 f_1^{t}(x)$

$$(1 + O(1/\sqrt{|x|}))$$
, as $x \to -\infty$. Thus, since $V = \theta - \sum_{\substack{j=1\\\lambda_{ij}\neq 0}}^{n} \frac{\tilde{\delta}_j^2}{2\lambda_{ij}} + \sum_{j=1}^{n} V_j$,

$$f(x) = \exp\left\{-\theta/\lambda_1 + \sum_{j=1 \atop \lambda_{i_j} \neq 0}^n \frac{\bar{\delta}_j^2}{2\lambda_{i_j}\lambda_1}\right\} b_1 f_1^{\mathsf{t}}\left(x - \theta + \sum_{j=1 \atop \lambda_{i_j} \neq 0}^n \frac{\bar{\delta}_j^2}{2\lambda_{i_j}}\right) \times (1 + O(1/\sqrt{|x|})),$$

as $x \to -\infty$. Then it follows immediately that $\lim_{x\to -\infty} f(x)(b_1 f_1^t(x))^{-1} = 1$. More precise arguments, similar to the ones we used to show (3.15) for H_1 , together with (3.5) then imply (3.7). The proof of (3.8) is similar. \Box

Remark 3.2. (a) By (3.22) and (3.9), for $k \in \{1, n\}$,

$$b_k = E\left(\exp\left\{\frac{1}{\lambda_{i_k}}(V-V_k)\right\}\right);$$

thus, b_k is nothing else than the moment generating function of $V - V_k$ evaluated at the point $1/\lambda_{i_k}$.

(b) Eq. (3.7) is trivially true if $\lambda_1 > 0$, since then the support of f as well as that of f_1 are both bounded from the left.

(c) Eq. (3.7) shows that there is a function ρ and constants c, C>0 such that $f(x) = b_1 f_1^t(x)(1 + \rho(x))$ and $|\sqrt{|x|}\rho(x)| \leq C$ for all $x \leq -c$. The constant *C* gives error bounds for the approximation. The proof presented here is actually constructive, i.e. explicit values for *c* and *C* could be derived by exact bookkeeping in the proof. Bounds for the starting constants needed in (3.3) can be found in [18], for example.

(d) Similar results have been derived in the context of tail distributions; see Goldie and Klüppelberg [9] and references therein.

3.2. Case 2: the lowest eigenvalue is positive

Suppose that $\lambda_1 > 0$. In this subsection, we shall derive the tail behavior of f(x) as x approaches the left endpoint of its support: It follows from (3.2) that the modified Bessel function of the first kind $I_v(x)$ behaves like $2^{-\nu}(\Gamma(\nu+1))^{-1}x^{\nu}(1+O(x^2))$ as $x \searrow 0$. Then (3.1) shows that

$$g(x;a^2,\mu) = \frac{2^{-\mu/2}}{\Gamma(\mu/2)} e^{-a^2/2} x^{\mu/2-1} (1+O(x)), \quad x \searrow 0,$$

and with (2.2) we obtain for j = 1, ..., n,

$$f_j(x) = \frac{\lambda_{i_j}^{-\mu_j/2}}{\Gamma(\mu_j/2)} e^{-a_j^2/2} x^{\mu_j/2-1} (1+\psi_j(x)),$$

where ψ_j is a function for which there exist constants $d_j, D_j > 0$ such that $|\psi_j(x)| \leq D_j |x|$ for all $x \in [0, d_j]$. Then we obtain for $j, k \in \{1, ..., n\}$,

$$f_j * f_k(x) = \frac{\lambda_{i_j}^{-\mu_j/2} \lambda_{i_k}^{-\mu_k/2} e^{-(a_j^2 + a_k^2)/2}}{\Gamma(\mu_j/2) \Gamma(\mu_k/2)} \int_0^x y^{\mu_j/2 - 1} (x - y)^{\mu_k/2 - 1} (1 + \psi_j(y)) \times (1 + \psi_k(x - y)) \, dy.$$

Now one has

$$\begin{split} &\int_0^x y^{\mu_j/2-1} (x-y)^{\mu_k/2-1} \, dy \\ &= x^{(\mu_j+\mu_k)/2-1} \int_0^1 z^{\mu_j/2-1} (1-z)^{\mu_k/2-1} \, dz \\ &= x^{(\mu_j+\mu_k)/2-1} \, \mathcal{B}(\mu_j/2,\mu_k/2) \\ &= x^{(\mu_j+\mu_k)/2-1} \, \frac{\Gamma(\mu_j/2)\Gamma(\mu_k/2)}{\Gamma(\frac{\mu_j+\mu_k}{2})}, \end{split}$$

where $B(\cdot, \cdot)$ denotes the Beta-function. For the remaining terms, similar calculations show that e.g.

$$\left| \int_0^x y^{\mu_j/2-1} (x-y)^{\mu_k/2-1} \psi_j(y) \, dy \right| \leq D_j \frac{\Gamma(\mu_j/2+1)\Gamma(\mu_k/2)}{\Gamma(\frac{\mu_j+\mu_k}{2}+1)} x^{(\mu_j+\mu_k)/2}$$

for $x \in [0, d_i]$, implying that

$$f_j * f_k(x) = \frac{\lambda_{i_j}^{-\mu_j/2} \lambda_{i_k}^{-\mu_k/2}}{\Gamma(\frac{\mu_j + \mu_k}{2})} e^{-(a_j^2 + a_k^2)/2} x^{(\mu_j + \mu_k)/2 - 1} (1 + O(x)), \quad x \searrow 0.$$

Now we immediately obtain the tail behavior of f:

Proposition 3.3. For $\lambda_1 = \lambda_{i_1} > 0$, the density f of V has the asymptotic left tail behavior

$$f\left(x+\theta-\sum_{j=1}^{n}\frac{\bar{\delta}_{j}^{2}}{2\lambda_{i_{j}}}\right)=d|x|^{m/2-1}\left(1+O(x)\right), \quad x\searrow 0$$
(3.23)

with the constant

$$d = \frac{\prod_{j=1}^{n} |\lambda_{i_j}|^{-\mu_j/2}}{\Gamma(m/2)} e^{-\sum_{j=1}^{n} a_j^2/2}.$$
(3.24)

If $\lambda_m = \lambda_{i_n} < 0$, then (3.23) holds for the right tail as $x \nearrow 0$.

3.3. Case 3: the lowest eigenvalue is 0

Now suppose that $\lambda_1 = 0$ and $\bar{\delta}_1^2 \neq 0$. Since $V_1 = \sum_{l=1}^{i_1} \delta_l Y_l$ is normally distributed with mean zero and variance $\bar{\delta}_1^2$, it follows that $f_1(x) = (\sqrt{2\pi}|\bar{\delta}_1|)^{-1}e^{-x^2/(2\bar{\delta}_1^2)}$. We shall see that the left tail behavior of f(x) is essentially determined by the tail behavior of f_1 .

Proposition 3.4. Let h be a probability density with support in $[0, \infty)$ such that

$$h(x) = c_h x^{\mu} (1 + O(x)), \quad x \searrow 0 \tag{3.25}$$

for some $\mu > -1$ and some constant $c_h \neq 0$. Further, suppose that h is bounded on every interval $[\Delta, \infty)$ for every $\Delta > 0$. Then

$$(f_1 * h)(x) = c_h \frac{\Gamma(\mu + 1)(\bar{\delta}_1^2)^{\mu + 1}}{\sqrt{2\pi}|\bar{\delta}_1|} |x|^{-(\mu + 1)} e^{-x^2/(2\bar{\delta}_1^2)} (1 + O(1/|x|)),$$

$$x \to -\infty.$$
(3.26)

Proof. For simplicity, we assume that $\delta_1^2 = 1$. The proof for general δ_1^2 is similar or alternatively can be deduced by a simple dilation argument.

Note that (3.25) is equivalent to

$$h(x) = c_h x^{\mu} e^{x^2/2} (1 + O(x)), \quad x \searrow 0.$$

Write

$$h(x) = c_h x^{\mu} e^{x^2/2} (1 + \psi(x)),$$

where

$$|\psi(x)| \leqslant Dx \quad \forall x \in [0, \Delta] \tag{3.27}$$

and $D, \Delta > 0$ are suitable constants. Also, let

 $h(x) \leq E \quad \forall x \in [\Delta, \infty) \tag{3.28}$

for some E > 0. Then we have for negative x,

$$(f_{1} * h)(x) = \int_{0}^{\infty} h(y)f_{1}(x - y) dy$$

$$= \frac{1}{\sqrt{2\pi}} \int_{0}^{4} c_{h} y^{\mu} e^{y^{2}/2} e^{-(x - y)^{2}/2} dy$$

$$+ \frac{1}{\sqrt{2\pi}} \int_{0}^{4} c_{h} y^{\mu} e^{y^{2}/2} \psi(y) e^{-(x - y)^{2}/2} dy$$

$$+ \frac{1}{\sqrt{2\pi}} \int_{4}^{\infty} h(y) e^{-(x - y)^{2}/2} dy$$

$$= \frac{c_{h}}{\sqrt{2\pi}} e^{-x^{2}/2} |x|^{-(\mu + 1)} \int_{0}^{4|x|} z^{\mu} e^{-z} dz$$

$$+ \frac{c_{h}}{\sqrt{2\pi}} e^{-x^{2}/2} |x|^{-(\mu + 1)} \int_{0}^{4|x|} z^{\mu} \psi(z/|x|) e^{-z} dz$$

$$+ \frac{1}{\sqrt{2\pi}} e^{-x^{2}/2} \int_{4}^{\infty} h(y) e^{xy} e^{-y^{2}/2} dy.$$

Noting that $\Gamma(\mu+1) = \int_0^\infty z^\mu e^{-z} dz$, we obtain

$$\frac{(f_1 * h)(x) - c_h \Gamma(\mu + 1) e^{-x^2/2} |x|^{-(\mu+1)} / \sqrt{2\pi}}{c_h \Gamma(\mu + 1) e^{-x^2/2} |x|^{-(\mu+1)} / \sqrt{2\pi}}$$

= $\frac{-\int_{A|x|}^{\infty} z^{\mu} e^{-z} dz}{\Gamma(\mu + 1)} + \frac{\int_0^{A|x|} z^{\mu} \psi(z/|x|) e^{-z} dz}{\Gamma(\mu + 1)} + \frac{\int_A^{\infty} h(y) e^{xy} e^{-y^2/2} dy}{c_h \Gamma(\mu + 1) |x|^{-(\mu+1)}}$
=: $A_1(x) + A_2(x) + A_3(x)$.

There remains to show that $|x|(A_1(x) + A_2(x) + A_3(x))$ is bounded as $x \to -\infty$: Since

$$|x| \int_{\Delta|x|}^{\infty} z^{\mu} e^{-z} dz \leq \frac{1}{\Delta} \int_{\Delta|x|}^{\infty} z^{\mu+1} e^{-z} dz \to 0, \quad x \to -\infty,$$

we have $A_1(x) = O(1/x)$ as $x \to -\infty$. From (3.27) we obtain

$$|x| \int_0^{\Delta|x|} z^{\mu} \psi(z/|x|) e^{-z} \, dz \leq D \int_0^{\Delta|x|} z^{\mu+1} e^{-z} \, dz \leq D\Gamma(\mu+2),$$

showing that $A_2(x) = O(1/x)$ as $x \to -\infty$. Finally, (3.28) gives

$$|x|^{\mu+2} \int_{\Delta}^{\infty} h(y) e^{xy} e^{-y^2/2} \, dy \leq E|x|^{\mu+2} \int_{\Delta}^{\infty} e^{xy} \, dy = E|x|^{\mu+1} e^{\Delta x} \to 0, \quad x \to -\infty,$$

showing that $A_3(x) = O(1/x)$ as $x \to -\infty$. This gives (3.26). \Box

Combining Propositions 3.3 and 3.4, we obtain the left tail behavior of f:

Theorem 3.5. For $\lambda_1 = \lambda_{i_1} = 0$, the density f of V has the asymptotic left tail behavior

$$f\left(x+\theta-\sum_{j=2}^{n}\frac{\bar{\delta}_{j}^{2}}{2\lambda_{i_{j}}}\right)$$

= $\frac{e^{-\sum_{j=2}^{n}a_{j}^{2}/2}}{\sqrt{2\pi}|\bar{\delta}_{1}|}\left(\prod_{j=2}^{n}|\bar{\delta}_{1}^{2}/\lambda_{i_{j}}|^{\mu_{j}/2}\right)|x|^{-\sum_{j=2}^{n}\mu_{j}/2}e^{-x^{2}/(2\bar{\delta}_{1}^{2})}(1+O(1/x))$

as $x \to -\infty$. For $\lambda_m = \lambda_{i_n} = 0$, the density of V has the asymptotic right tail behavior

$$\begin{split} f\left(x+\theta-\sum_{j=1}^{n-1}\frac{\bar{\delta}_{j}^{2}}{2\lambda_{i_{j}}}\right) \\ &=\frac{e^{-\sum_{j=1}^{n-1}a_{j}^{2}/2}}{\sqrt{2\pi}|\bar{\delta}_{n}|}\left(\prod_{j=1}^{n-1}|\bar{\delta}_{n}^{2}/\lambda_{i_{j}}|^{\mu_{j}/2}\right)x^{-\sum_{j=1}^{n-1}\mu_{j}/2}e^{-x^{2}/(2\bar{\delta}_{n}^{2})}(1+O(1/x)) \end{split}$$

as $x \to \infty$.

4. Approximation of the quantiles

In this section, we give an approximation of the α - and $(1 - \alpha)$ -quantile of V as $\alpha \rightarrow 0$. As before, denote the density of V by f and its distribution function by F. The α -quantile of V will be denoted by x_{α} , thus

$$x_{\alpha} = F^{\leftarrow}(\alpha) \coloneqq \inf\{x \in \mathbb{R}: F(x) \ge \alpha\}, \quad \alpha \in (0, 1).$$

Since for $\lambda_{i_1} < 0$, Theorem 3.1 expressed the left tail behavior of f in terms of the tail behavior of f_1^t , it is natural to approximate x_{α} using the quantile of some suitable function \tilde{F}_1^t , where $\frac{d}{dx}\tilde{F}_1^t(x) = f_1^t(x)(1 + O(1/\sqrt{|x|}))$ as $x \to -\infty$. This is done in the following theorem. Note that the function $\tilde{F}_1^t(x)$ is given explicitly and that its quantiles can easily be calculated numerically:

Theorem 4.1. Suppose $\lambda_1 = \lambda_{i_1} < 0$, or $\lambda_m = \lambda_{i_n} > 0$, respectively. Define on the relevant range (i.e. for large negative x, or for large positive x, respectively)

$$\begin{split} \tilde{F}_{1}^{t}(x) &:= |\lambda_{1}| f_{1}^{t}(x) = |\lambda_{1}| c_{1} |x|^{(\mu_{1}-3)/4} e^{-x/\lambda_{1}+a_{1}\sqrt{2/|\lambda_{1}|}\sqrt{|x|}}, \\ 1 - \tilde{F}_{n}^{t}(x) &:= |\lambda_{i_{n}}| f_{n}^{t}(x) = \lambda_{i_{n}} c_{n} x^{(\mu_{n}-3)/4} e^{-x/\lambda_{i_{n}}+a_{n}\sqrt{2/\lambda_{i_{n}}}\sqrt{x}}, \end{split}$$

where f_1^t and f_n^t are given by (3.6). Let b_1 and b_n be defined as in (3.9), and denote the α quantiles of \tilde{F}_1^t and $1 - \tilde{F}_n^t$ by $(\tilde{F}_1^t)^{\leftarrow}(\alpha)$ and $(1 - \tilde{F}_n^t)^{\leftarrow}(\alpha)$, respectively. Then, as $\alpha \to 0$,
the lower and upper quantiles of V satisfy the following asymptotic equations,

respectively:

$$x_{\alpha} = \lambda_{i_1} \log b_1 + (\tilde{F}_1^{t})^{\leftarrow}(\alpha) + O(1/\sqrt{|(\tilde{F}_1^{t})^{\leftarrow}(\alpha)|}),$$
(4.1)

$$x_{1-\alpha} = \lambda_{i_n} \log b_n + (1 - \tilde{F}_n^{\mathsf{t}}) \stackrel{\leftarrow}{} (\alpha) + O(1/\sqrt{(1 - \tilde{F}_n^{\mathsf{t}}) \stackrel{\leftarrow}{} (\alpha)}).$$
(4.2)

Proof. Define the shifted random variable $V_{(sh)} \coloneqq V - \lambda_{i_1} \log b_1$. Denote its density by $f_{(sh)}$, its distribution function by $F_{(sh)}$ and its α -quantile by $x_{\alpha,(sh)} = F_{(sh)}^{\leftarrow}(\alpha)$. Put $x_{\alpha,1} \coloneqq (\tilde{F}_1^{\dagger})^{\leftarrow}(\alpha)$. Since

$$x_{\alpha} = x_{\alpha,(\mathrm{sh})} + \lambda_{i_1} \log b_1,$$

(4.1) is equivalent to

$$x_{\alpha,(\mathrm{sh})} - x_{\alpha,1} = O(1/\sqrt{|x_{\alpha,1}|}), \quad x_{\alpha,1} \to -\infty.$$

$$(4.3)$$

There remains to show (4.3): an application of Theorem 3.1 to $V_{(\text{sh})}$ shows that $f_{(\text{sh})}(x) = b_{1,(\text{sh})}f_1^{t}(x)(1 + O(1/\sqrt{|x|}))$, where $b_{1,(\text{sh})} = b_1 \exp\{(-\lambda_{i_1} \log b_1)/\lambda_{i_1}\} = 1$, i.e.

$$f_{(sh)}(x) = f_1^t(x)(1 + O(1/\sqrt{|x|})), \quad x \to -\infty.$$
(4.4)

On the other hand, with $\tilde{f}_1^t(x) \coloneqq \frac{d}{dx} \tilde{F}_1^t(x) = |\lambda_1| \frac{d}{dx} f_1^t(x)$ we also obtain

$$\tilde{f}_1^{t}(x) = f_1^{t}(x)(1 + O(1/\sqrt{|x|})), \quad x \to -\infty.$$

Thus,

$$\tilde{f}_1^{t}(x) = f_{(sh)}(x)(1 + O(1/\sqrt{|x|})), \quad x \to -\infty,$$

holds, that is, there exist positive constants c, C > 0 such that

$$|f_{(\mathrm{sh})}(x) - \tilde{f}_1^{\mathrm{t}}(x)| \leq \frac{C}{\sqrt{|x|}} f_{(\mathrm{sh})}(x) \quad \forall x \leq -c.$$

Choose c such that in addition $f_{(sh)}(x) > 0$ for all $x \le -c$. Then $F_{(sh)}$ is strictly increasing on $(-\infty, -c)$ and hence $F_{(sh)}^{\leftarrow}(F_{(sh)}(x)) = x$ for all $x \le -c$. Defining

$$r(x) \coloneqq F_{(\mathrm{sh})}(x) - \tilde{F}_{1}^{\mathsf{t}}(x), \tag{4.5}$$

it follows that

$$|r(x)| \leq \int_{-\infty}^{x} |f_{(sh)}(y) - \tilde{f}_{1}^{t}(y)| \, dy \leq \frac{C}{\sqrt{|x|}} F_{(sh)}(x) \quad \forall x \leq -c.$$
(4.6)

Now let $0 < \alpha < 1$ such that $x_{\alpha,1} \leq -c$. Noting that

$$x_{\alpha,(\mathrm{sh})} - x_{\alpha,1} = F_{(\mathrm{sh})}^{\leftarrow}(F_{(\mathrm{sh})}(x_{\alpha,(\mathrm{sh})})) - F_{(\mathrm{sh})}^{\leftarrow}(F_{(\mathrm{sh})}(x_{\alpha,1})),$$

the mean value theorem implies the existence of some constant ξ between $F_{(sh)}(x_{\alpha,(sh)})$ and $F_{(sh)}(x_{\alpha,1})$ such that by (4.5) and (4.6),

$$\begin{aligned} |x_{\alpha,(sh)} - x_{\alpha,1}| &= |F_{(sh)}(x_{\alpha,(sh)}) - F_{(sh)}(x_{\alpha,1})| \cdot |(F_{(sh)}^{\leftarrow})'(\xi)| \\ &= |r(x_{\alpha,1})| \cdot |(F_{(sh)}^{\leftarrow})'(\xi)| \\ &\leqslant \frac{C}{\sqrt{|x_{\alpha,1}|}} \frac{F_{(sh)}(x_{\alpha,1})}{f_{(sh)}(F_{(sh)}^{\leftarrow}(\xi))} \\ &= \frac{C}{\sqrt{|x_{\alpha,1}|}} \frac{F_{(sh)}(x_{\alpha,1})}{\xi} \frac{F_{(sh)}(F_{(sh)}^{\leftarrow}(\xi))}{f_1^{t}(F_{(sh)}^{\leftarrow}(\xi))} \frac{f_1^{t}(F_{(sh)}^{\leftarrow}(\xi))}{f_{(sh)}(F_{(sh)}^{\leftarrow}(\xi))}. \end{aligned}$$
(4.7)

Since $|\xi - F_{(sh)}(x_{\alpha,1})| \leq |r(x_{\alpha,1})| \leq CF_{(sh)}(x_{\alpha,1})/\sqrt{|x_{\alpha,1}|}$, it follows that $\xi \in [F_{(sh)}(x_{\alpha,1})$ $(1 - C/\sqrt{|x_{\alpha,1}|}), F_{(sh)}(x_{\alpha,1})(1 + C/\sqrt{|x_{\alpha,1}|})]$, and hence $\lim_{x_{\alpha,1}\to-\infty} F_{(sh)}(x_{\alpha,1})/\xi = 1$. In particular, $\xi \to 0$ as $x_{\alpha,1}\to -\infty$, and thus $y \coloneqq F_{(sh)}^{\leftarrow}(\xi) \to -\infty$ as $x_{\alpha,1}\to -\infty$. Since

$$\lim_{y \to -\infty} \frac{F_{(\mathrm{sh})}'(y)}{(f_1^{\mathrm{t}})'(y)} = -\lambda_1 \neq 0$$

by (4.4), l'Hospital's rule implies that

$$\lim_{x_{x,1}\to-\infty}\frac{F_{(\mathrm{sh})}(F_{(\mathrm{sh})}(\xi))}{f_1^{\mathsf{t}}(F_{(\mathrm{sh})}(\xi))} = \lim_{y\to\infty}\frac{F_{(\mathrm{sh})}(y)}{f_1^{\mathsf{t}}(y)} = -\lambda_1.$$

Also, by (4.4),

$$\lim_{x_{z,1}\to-\infty}\frac{f_1^{\mathsf{t}}(F_{(\mathrm{sh})}(\xi))}{f_{(\mathrm{sh})}(F_{(\mathrm{sh})}(\xi))} = \lim_{y\to-\infty}\frac{f_1^{\mathsf{t}}(y)}{f_{(\mathrm{sh})}(y)} = 1.$$

Thus (4.7) implies (4.3) and hence (4.1). The proof of (4.2) is similar. \Box

Theorem 4.1 gives an approximation of x_{α} in terms of the α -quantile of some function $\tilde{F}_1^t(x)$. There, $\tilde{F}_1^t(x) = |\lambda_1| f_1^t(x)$ was chosen. However, the proof of Theorem 4.1 showed that any function \tilde{F}_1^t could have been chosen, as long as

$$\frac{d}{dx}\tilde{F}_{1}^{t}(x) = f_{1}^{t}(x)(1 + O(1/\sqrt{|x|})), \quad x \to -\infty.$$

For example, one might choose

$$\tilde{F}_1^{\mathsf{t}}(x) \coloneqq \int_{-\infty}^x f_1(y) \, dy.$$

Then (2.2) implies

$$(\tilde{F}_1^{\mathrm{t}})^{\leftarrow}(\alpha) = \frac{\lambda_{i_1}}{2} \chi_{1-\alpha,\mu_1}^2(a_1^2),$$

where $\chi^2_{1-\alpha,\mu}(a^2)$ denotes the $(1-\alpha)$ -quantile of the χ^2 -distribution with μ degrees of freedom and non-centrality parameter a^2 . Thus, we obtain:

Corollary 4.2. Suppose $\lambda_1 = \lambda_{i_1} < 0$, or $\lambda_m = \lambda_{i_n} > 0$, respectively. Then $\alpha \to 0$ is equivalent to $\chi^2_{1-\alpha,\mu_k}(a_k^2) \to \infty$ for $k \in \{1,n\}$, and as $\alpha \to 0$, the lower and upper quantiles of V satisfy the following asymptotic equations for $\lambda_{i_1} < 0$ and $\lambda_{i_n} > 0$, respectively:

$$x_{\alpha} = \lambda_{i_1} \log b_1 + \frac{\lambda_{i_1}}{2} \chi^2_{1-\alpha,\mu_1}(a_1^2) + O(1/\sqrt{\chi^2_{1-\alpha,\mu_1}(a_1^2)}),$$
(4.8)

$$x_{1-\alpha} = \lambda_{i_n} \log b_n + \frac{\lambda_{i_n}}{2} \chi_{1-\alpha,\mu_n}^2(a_n^2) + O(1/\sqrt{\chi_{1-\alpha,\mu_n}^2(a_n^2)}).$$
(4.9)

Corollary 4.2 links the quantiles of V with the quantiles of non-central χ^2 distributions. The latter can be calculated with many software packages, such as **R**, *Electronic Tables* or *StaTable*, the latter two both reviewed in Boomsma and Molenaar [5]. The package *S-Plus* has a routine implemented to calculate the distribution function of a non-central χ^2 -distribution. However, it does not compute the inverse of this function, i.e. the quantiles. Nevertheless, using a bisection method, the quantiles can be approximated numerically.

The following theorem gives an approximation of the quantiles of V for the case that the lowest (or the largest) eigenvalue is 0:

Theorem 4.3. Suppose $\lambda_1 = \lambda_{i_1} = 0$, or $\lambda_m = \lambda_{i_n} = 0$, respectively. Define on the relevant range

$$\tilde{F}_{1}^{t}(x) \coloneqq \left(\frac{|\bar{\delta}_{1}|}{\sqrt{2\pi}}e^{-\sum_{j=2}^{n} a_{j}^{2}/2} \prod_{j=2}^{n} |\bar{\delta}_{1}^{2}/\lambda_{i_{j}}|^{\mu_{j}/2}\right) (-x)^{-1-\sum_{j=2}^{n} \mu_{j}/2}e^{-x^{2}/(2\bar{\delta}_{1}^{2})},$$

$$1 - \tilde{F}_{n}^{t}(x) \coloneqq \left(\frac{|\bar{\delta}_{n}|}{\sqrt{2\pi}}e^{-\sum_{j=1}^{n-1} a_{j}^{2}/2} \prod_{j=1}^{n-1} |\bar{\delta}_{n}^{2}/\lambda_{i_{j}}|^{\mu_{j}/2}\right) x^{-1-\sum_{j=1}^{n-1} \mu_{j}/2}e^{-x^{2}/(2\bar{\delta}_{n}^{2})}.$$

Denote by $(\tilde{F}_1^t)^{\leftarrow}(\alpha)$ and $(1 - \tilde{F}_n^t)^{\leftarrow}(\alpha)$ the α -quantiles of \tilde{F}_1^t and $1 - \tilde{F}_n^t$, respectively. Then, as $\alpha \to 0$, the lower and upper quantiles of V satisfy the following asymptotic equations, respectively:

$$x_{\alpha} = \theta - \sum_{j=2}^{n} \frac{\bar{\delta}_{j}^{2}}{2\lambda_{i_{j}}} + (\tilde{F}_{1}^{t})^{\leftarrow}(\alpha) + O(1/(\tilde{F}_{1}^{t})^{\leftarrow}(\alpha)^{2}),$$
(4.10)

$$x_{1-\alpha} = \theta - \sum_{j=1}^{n-1} \frac{\bar{\delta}_j^2}{2\lambda_{i_j}} + (\tilde{F}_n^{t})^{\leftarrow}(\alpha) + O(1/(1 - \tilde{F}_n^{t})^{\leftarrow}(\alpha)^2).$$
(4.11)

Proof. We only treat the case $\lambda_1 = 0$. The treatment of the upper tail for $\lambda_m = 0$ is similar. Since the proof is similar to the proof of Theorem 4.1, using Theorem 3.5

instead of Theorem 3.1, we only show how to modify that proof. Put $V_{(\text{sh})} := V + \sum_{j=2}^{n} \frac{\tilde{\delta}_{j}^{2}}{2\lambda_{i_{j}}} - \theta = \sum_{j=1}^{n} V_{j}$. Let $f_{(\text{sh})}$ and $F_{(\text{sh})}$ be the density and distribution function of $V_{(\text{sh})}$, and $x_{\alpha,(\text{sh})}$ the corresponding α -quantile. Define $\tilde{f}_{1}^{\text{t}}(x) := \frac{d}{dx} \tilde{F}_{1}^{\text{t}}(x)$ for x < 0. Then

$$\begin{split} \tilde{f}_{1}^{\text{rt}}(x) &= \frac{e^{-\sum_{j=2}^{n} a_{j}^{2}/2}}{\sqrt{2\pi} |\tilde{\delta}_{1}|} \bigg(\prod_{j=2}^{n} |\tilde{\delta}_{1}^{2}/\lambda_{i_{j}}|^{\mu_{j}/2} \bigg) |x|^{-\sum_{j=2}^{n} \mu_{j}/2} e^{-x^{2}/(2\tilde{\delta}_{1}^{2})} \\ &\times \bigg(1 + \bigg(1 + \sum_{j=2}^{n} \mu_{j}/2 \bigg) \tilde{\delta}_{1}^{2} x^{-2} \bigg), \end{split}$$

and Theorem 3.5 gives $\tilde{f}_1^t(x) = f_{(sh)}(x)(1 + O(1/x))$. Then with $x_{\alpha,1} = (\tilde{F}_1^t)^{\leftarrow}(\alpha)$ denoting the α -quantile of \tilde{F}_1^t and the same notations as in the proof of Theorem 4.1, (4.6) becomes $|r(x)| \leq \frac{C}{|x|} F_{(sh)}(x)$, and (4.7) changes to

$$\begin{aligned} |x_{\alpha,(\mathrm{sh})} - x_{\alpha,1}| &\leqslant \frac{C}{|x_{\alpha,1}|} \frac{F_{(\mathrm{sh})}(x_{\alpha,1})}{\xi} \frac{F_{(\mathrm{sh})}(F_{(\mathrm{sh})}^{\leftarrow}(\xi))}{-\tilde{f}_{1}^{\mathrm{t}}(F_{(\mathrm{sh})}^{\leftarrow}(\xi))(F_{(\mathrm{sh})}^{\leftarrow}(\xi))^{-1}} \frac{\tilde{f}_{1}^{\mathrm{t}}(F_{(\mathrm{sh})}^{\leftarrow}(\xi))}{f_{(\mathrm{sh})}(F_{(\mathrm{sh})}^{\leftarrow}(\xi))} \frac{1}{-F_{(\mathrm{sh})}^{\leftarrow}(\xi)} \\ &= \frac{C'}{|x_{\alpha,1}|} \frac{1}{-F_{(\mathrm{sh})}^{\leftarrow}(\xi)} (1+o(1)), \end{aligned}$$

where l'Hospital's rule was applied to $F_{(sh)}(F_{(sh)}^{\leftarrow}(\xi))/(-\tilde{f}_1^t(F_{(sh)}^{\leftarrow}(\xi))(F_{(sh)}^{\leftarrow}(\xi))^{-1})$. This implies (4.10). \Box

Finally, for $\lambda_{i_1} > 0$ or $\lambda_{i_n} < 0$, an approximation can be written down quite explicitly, which is done in the next Theorem.

Theorem 4.4. Suppose $\lambda_1 = \lambda_{i_1} > 0$, or $\lambda_m = \lambda_{i_n} < 0$, respectively. Then, as $\alpha \to 0$, the lower and upper quantiles of V satisfy the following asymptotic equations, respectively:

$$\begin{aligned} x_{\alpha} &= \theta - \sum_{j=1}^{n} \frac{\bar{\delta}_{j}^{2}}{2\lambda_{i_{j}}} + \left(\frac{m}{2d}\alpha\right)^{2/m} + O(\alpha^{4/m}), \\ x_{1-\alpha} &= \theta - \sum_{j=1}^{n} \frac{\bar{\delta}_{j}^{2}}{2\lambda_{i_{j}}} - \left(\frac{m}{2d}\alpha\right)^{2/m} + O(\alpha^{4/m}), \end{aligned}$$

where d is the constant defined in (3.24).

The proof is similar to the proof of Theorem 4.3 and therefore omitted.



Fig. 1. The left part of the distribution function (CDF) in Example 5.1 (case 1: $\lambda_1 < 0$) as well as the normal approximation and the approximations of Theorem 4.1 and Corollary 4.2. The right graph shows probabilities in a log scale, the left in a linear scale.

Table 1 Quantiles in Example 5.2 (Case 3: $\lambda_1 = 0.$)

Probability	"true" quantile	Approximation	
		Normal	Tail
0.0500	-1.3602	-1.514526	-1.636064
0.0250	-1.6916	-1.900456	-1.900803
0.0100	-2.0745	-2.349183	-2.228890
0.0050	-2.3339	-2.654734	-2.461087
0.0010	-2.8662	-3.284746	-2.954294
0.0001	-3.5131	-4.054846	-3.572531



Fig. 2. The left part of the distribution function (CDF) in Example 5.2 (Case 3: $\lambda_1 = 0$) as well as the normal approximation and the approximation of Theorem 4.3. The right graph shows probabilities on a logarithmic scale, the left one on a linear scale.

5. Examples and discussion

In this section, we shall illustrate the results of the last section by means of specific examples. Our approximations will be compared to standard approximations, like a normal approximation for $\lambda_1 \leq 0$, and a gamma approximation for $\lambda_1 > 0$.

Example 5.1 (Illustration of Case 1). Suppose that in model (1.2) we have m = 15, n = 3, $\lambda_{i_1} = -2$, $\lambda_{i_2} = 1$, $\lambda_{i_3} = 2$, $\mu_1 = 5$, $\mu_2 = 4$, $\mu_3 = 6$, $a_1^2 = 4$, $\bar{\delta}_2^2 = 4$, $\bar{\delta}_3^2 = 16$, and $\theta = 0$. In Fig. 1, the left part of the distribution function of *V*, the normal approximation as well as the approximations according to Theorem 4.1 and Corollary 4.2 are plotted. The "true" distribution has been computed by numerical Fourier inversion with high accuracy. The left graph shows the probability on a

linear scale, while the right graph shows it on a logarithmic scale. From the left graph, it can be seen that the normal distribution approximates the true distribution well for small |x|, whereas the approximations of Theorem 4.1 and Corollary 4.2 approximate better for large negative x, which is shown by the right graph. The normal approximation is computed by moment matching: the cumulants of V can easily be read off the power series expansion of the cumulant generating function and are given by

$$\kappa_1 = \theta + \frac{1}{2} \sum_{j=1}^m \lambda_j \text{ and } \kappa_r = \frac{1}{2} \sum_{j=1}^m ((r-1)!\lambda_j^r + r!\delta_j^2\lambda_j^{r-2}).$$

Example 5.2 (Illustration of Case 3). Suppose that in model (1.2) we have m = n = 2, $\lambda_1 = 0$, $\lambda_2 = 1$, $\delta_1 = 1$, $\delta_2 = 0$, and $\theta = 0$. Again, a normal approximation is quite good at the center of the distribution, whereas the approximation of Theorem 4.3 works well for large negative x. Table 1 shows that the tail approximation becomes better than the normal approximation for probabilities approximately below 0.025. In Fig. 2, the distribution function of V, the normal approximation as well as the approximation of Theorem 4.3 are plotted on a linear and logarithmic scale.

Example 5.3 (Illustration of Case 2). Suppose that in model (1.2) we have m = 4, n = 2, $\lambda_1 = \lambda_2 = 1$, $\lambda_3 = \lambda_4 = 2$, $\delta_1 = \delta_2 = 1$, $\delta_3 = \delta_4 = 0$. $\theta = 1$ is chosen such that the left tail of the distribution ends at 0. A straightforward approximation of such a distribution is a gamma distribution (with shape parameter p and scale parameter β) with matching mean (βp) and variance ($\beta^2 p$). The gamma approximation fits very well at the center of the distribution, as seen from the left graph of Fig. 3, while the tail approximation of Theorem 4.4 is superior for $\alpha < 0.05$, approximately.

Remark 5.4. Since the tail approximations derived in the previous section are qualitatively different for $\lambda_1 < 0$, $\lambda_1 = 0$, and $\lambda_1 > 0$, it is clear that (for fixed α) the approximation of Theorem 4.1 must give bad results for $\lambda_1 < 0$, but close to zero. To be able to give explicit ranges for the quantiles for which our approximations work well, one would need precise error bounds. As pointed out in Remark 3.2(c), in principle it is possible to obtain such bounds, but very elaborate.

Example 5.5. This example shows that it can happen that (4.8) and (4.9) approximate well only for very small α : Let n = m = 2, $\mu_1 = \mu_2 = 1$, $-\lambda_1 = \lambda_2 = 2$, $\delta_1 = \delta_2 = 2a$, where $a \ge 3$ is positive, and $\theta = 0$. Then $V_1 = -(-a + Y_1)^2$, $V_2 = (a + Y_2)^2$, where Y_1 and Y_2 are independent standard normal variables. Then $P(Y_i \in [-3,3]) \ge \sqrt{0.99}$ and it follows that $P(V_2 \in [(a - 3)^2, (a + 3)^2]) = P(V_1 \in [-(a + 3)^2, -(a - 3)^2] \ge \sqrt{0.99}$. Since V_1 and V_2 are independent, it follows that $P(V_1 + V_2 \in [-12a, 12a]) \ge 0.99$, implying that the true 1%-quantile of $V_1 + V_2$ lies in [-12a, 12a]. However, if we use approximation (4.8), we have $b_1 = 2^{-1/2}e^{-a^2/4}$;



Fig. 3. The left part of the distribution function (CDF) in Example 5.3 (Case 2: $\lambda_1 > 0$), as well as the gamma approximation and the approximation of Theorem 4.4. The right graph shows x and the probabilities in a log scale, the left one in a linear scale.

hence, $\hat{x}_{1\%} = a^2/2 + \log 2 - \chi^2_{1-\alpha,1}(a^2)$, where $\hat{x}_{1\%}$ denotes the approximating quantity. Since the 1%-quantile of $\chi^2_1(a^2)$ lies in $[(a - 2.6)^2, (a + 2.6)^2]$, it follows that $\hat{x}_{1\%} \in [\log 2 - 6.76 - a^2/2 - 5.2a, \log 2 - 6.76 - a^2/2 + 5.2a]$. For large *a*, this differs clearly from the true quantile, which lies in [-12a, 12a]. So we see that the approximation (4.8) can lead to large errors in the approximation, if the level 1% is fixed, and if the non-centrality parameters are large, even if the eigenvalues λ_1 and λ_2 have the same modulus.

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