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Integral representations and approximations for multivariate gamma distributions

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Abstract Let R be a $p \times p$-correlation matrix with an "m-factorial" inverse $R^{-1} = D - BB'$ with diagonal D minimizing the rank m of B. A new $\binom{m+1}{2}$-variate integral representation is given for p-variate gamma distributions belonging to R, which is based on the above decomposition of R^{-1} without the restriction $D > 0$ required in former formulas. This extends the applicability of formulas with small m. For example, every p-variate gamma cdf can be computed by an at most $\binom{p-1}{2}$-variate integral if $p = 3$ or $p = 4$. Since computation is only feasible for small m, a given R is approximated by an m-factorial R_0. The cdf belonging to R is approximated by the cdf associated with R_0 and some additional correction terms with the deviations between R and R_0.

Keywords Multivariate gamma distribution · Multivariate chi-square distribution · Multivariate Rayleigh-distribution · Approximation for positive definite matrices · m-factorial matrices

1 Introduction and notations

For any $p \times p$-matrix $A = (a_{ij})$ the determinant is denoted by $|A|$ and the trace by $\mathrm{tr}(A)$, $A > 0$ means positive definiteness, and $(a^{ij}) = A^{-1}$. I_p or I is a unit matrix and $\mathcal{E}$ denotes the expectation of a random variable (r.v.). A cumulative distribution function is abbreviated by cdf and a probability density by pdf. Formulas from the handbook of mathematical functions by Abramowitz and Stegun (1965) are cited by "A.S" and their number.

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The p-variate chi-square distributon $(\chi_p^2(\nu, \Sigma))$ is defined as the joint distribution of the diagonal elements of a $W_p(\nu, \Sigma)$-Wishart matrix with ν degrees of freedom and covariance matrix $\Sigma > 0$. It has the Laplace transform (L.t.) $|I_p + 2\Sigma T|^{-\nu/2}$ with $T = \text{diag}(t_1, \ldots, t_p)$. This distribution is of much interest in some multiple test procedures but it is also encountered in a slightly modified form as the multivariate Rayleigh-distribution in electrical engineering (Nomoto Kishi, and Nanba, 2004; Miller, 1975).

The p-variate gamma-distribution of order $\alpha(\Gamma_p(\alpha, \Sigma))$ in the sense of Krishnamoorthy and Parthasarathy (1951) differs from the $\chi_p^2(2\alpha, \Sigma)$-distribution only by a scale factor 2 and the extension of the parameter values $\nu = 2\alpha$ to non-integer values. In this paper w.l.o.g. Σ is restricted to irreducible regular correlation matrices R. The $\Gamma_p(\alpha, R)$-density $f_p(x_1, \ldots, x_p; \alpha, R)$ has the L.t.

$$\begin{aligned}
&\hat{f}_p(t_1, \ldots, t_p; \alpha, R) = |I_p + RT|^{-\alpha}, \\
&T = \text{diag}(t_1, \ldots, t_p), t_1, \ldots, t_p \geq 0, \\
&\text{positive integer } 2\alpha \text{ or } 2\alpha > p - 2 \geq 0.
\end{aligned} \tag{1}$$

Necessary and sufficient conditions for R associated with an infinitely divisible $\Gamma_p(\alpha, R)$-distribution are found in Griffiths (1984) and Bapat (1989). In this case all $\alpha > 0$ are admissible. For a given R not allowing infinite divisibility the exact set of admissible non-integer values 2α is unknown but some general sufficient conditions for α can be established. If a $\Gamma_p(\alpha, R)$-distribution is derived from a $W_p(2\alpha, R)$-distribution then $2\alpha > p-1$ is admissible. See also corollary 2.2.3.1 in Siotani, Hayakawa, and Fujikoshi (1985) with m instead of α. However for $p \geq 2$ this condition can be improved to $2\alpha > p - 2$ according to Royen (1997). This is also recognized by the remark following Eq. (4) leading to a probability mixture representation of the $\Gamma_p(\alpha, R)$-cdf in Eq. (6) with a $(p-1) \times (p-1)$-Wishart matrix S.

Unfortunately, the cdf and even the pdf of the $\Gamma_p(\alpha, R)$-distribution are difficult to compute at least for $p \geq 4$. It is the aim of this paper to provide new integral representations for the pdf and the cdf $F_p(x_1, \ldots, x_p; \alpha, R)$, which do not depend on some unnecessary restrictions as some former formulas in Royen (1991a,1995,1997). By the new general formula (20), e.g. almost every $\Gamma_p(\alpha, R)$-cdf can be computed by an at most $\binom{p-1}{2}$-variate integral if $p = 3$ or $p = 4$. For some special structures of R (e.g. tridiagonal matrices) different integral representations and series expansions are found in Royen (1994). See also Kotz, Balakrishnan, and Johnson (2000) and in particular for tridiagonal R^{-1} in Blumenson and Miller (1963). The computation is further simplified for half-integers α, which is seen from Eqs. (20), (22) and (23). In particular with $\alpha = 1/2$ formulas for normal probabilities of symmetrical rectangular regions are obtained in Eq. (26).

For general p the representations for the pdf and the cdf are given by $\binom{m+1}{2}$-variate integrals in Eqs. (15) and (20), where m is the rank of B in a decomposition $R^{-1} = D - BB'$ with a diagonal $p \times p$-matrix D. Minimizing the rank m of $R^{-1} - D$ by a variable D is important to reduce the computing effort. For this, the assumption $D > 0$, used in former formulas, is now removed by the new formulas in Sect. 4. Further details on "m-factorial decompositions" of R^{-1} or R with real or complex D are found in Sect. 3.

Since the computing effort increases rapidly with m, a given R can frequently be approximated by a correlation matrix $R_0 = D^{-1} + AA'$ with a very small rank m of A. Using R_0 instead of R, a first approximation for the $\Gamma_p(\alpha, R)$-cdf is obtained, which can be improved further by the first terms of a series expansion with the deviations between R and R_0. The general expansion with conditions for convergence is given in Sect. 5.

Finally, Sect. 6 ends the paper with a short speculative view to approximations for the cdf by the real parts of certain complex measures associated with symmetrical complex matrices R_0.

2 Former integral representations of the $\boldsymbol{\Gamma_p(\alpha, R)}$-distribution

The new formulas in Sect. 4 are better understood by comparison with former ones. Throughout this paper the univariate standard gamma density of order α is denoted by

$$g_\alpha(x) = (\Gamma(\alpha))^{-1} x^{\alpha-1} e^{-x}, \quad x > 0, \alpha > 0, \tag{2}$$

with the cdf $G_\alpha(x)$,

and the non-central gamma density with non-centrality parameter $y \geq 0$ by

$$g_\alpha(x, y) = e^{-y} \sum_{n=0}^{\infty} g_{\alpha+n}(x) y^n/n! = e^{-y} g_\alpha(x) {}_0F_1(\alpha; xy) \tag{3}$$

with the cdf $G_\alpha(x, y)$.

Now let R be a given regular $p \times p$-correlation matrix representable by

$$R = D^{-1} + AA' \tag{4}$$

with $D = \operatorname{diag}(d_1, \ldots, d_p) > 0$ and a $p \times m$-matrix A of rank $m < p$ with rows a_j. With the lowest eigenvalue λ of R and $D^{-1} = \lambda I_p$ obviously $m \leq p - 1$ is always possible. The components Y_j of a $N_p(0, R)$ normal r.v. Y can be represented by

$$Y_j = d_j^{-1/2} U_j + \sum_{\mu=1}^{m} a_{j\mu} Z_\mu, \quad d_j^{-1} = 1 - |a_j|^2, \tag{5}$$

with i.i.d. $N(0, 1)$ r.v. U_j, Z_μ. Because of the "common factors" Z_μ, Eq. (4) is sometimes called an "m-factorial" representation of R. Now let $Y_\kappa, \kappa = 1, \ldots, \nu$, be i.i.d. $N_p(0, R)$ r.v. with components $Y_{j\kappa}$. With fixed values in the $m \times \nu$-matrix $Z = (Z_{\mu\kappa})$ the r.v.

$$X_j := \frac{1}{2} \sum_{\kappa=1}^{\nu} Y_{j\kappa}^2$$

are conditionally distributed as p independent non-central gamma variables with scale factors d_j and non-centrality parameters $\frac{1}{2}d_j a_j ZZ'a_j'$. Integrating over the $W_m(\nu, I_m)$-Wishart matrix $S = ZZ'$ the joint cdf of the X_j is

$$F_p(x_1, \ldots, x_p; \alpha, R) = \mathcal{E}\left(\prod_{j=1}^{p} G_\alpha\left(d_j x_j, \frac{1}{2} d_j a_j S a_j'\right)\right), \ \alpha = \nu/2. \quad (6)$$

With $m = 1$ this is simplified to

$$F_p(x_1, \ldots, x_p; \alpha, R) = \int_0^\infty \left(\prod_{j=1}^{p} G_\alpha(d_j x_j, d_j a_j^2 y)\right) g_\alpha(y)\mathrm{d}y. \quad (7)$$

Extending the functions $G_\alpha(x, y)$ to $y \in \mathbb{C}$ and using the L.t. (1) formula (6) was shown also to hold at least for all $\alpha > (p-2)/2$ and for indefinite AA' in Eq. (4), Royen (1991a, 1995). With an orthogonal matrix U and the diagonal matrix Λ of the eigenvalues of AA' the version $A = U\Lambda^{1/2}$ may contain some pure imaginary columns. The term "m-factorial representation of R" was retained for Eq. (4) also without the underlying model with m-factors.

As an example for this extension the $\Gamma_3(\alpha, (r_{jk}))$-distribution with $\prod_{j<k} r_{jk} \neq 0$ is considered. The three equations $r_{jk} = a_j a_k$ can always be solved by

$$\begin{aligned} a_j &= \sqrt{s}\, s_{k\ell}|r_{jk}r_{j\ell}/r_{k\ell}|^{1/2}, \quad j, k, \ell \text{ any permutation of } 1, 2, 3, \\ s_{k\ell} &= \mathrm{sgn}(r_{k\ell}), \quad s = \prod_{k<\ell} s_{k\ell}. \end{aligned} \quad (8)$$

This leads to the one-factorial decomposition $R = D^{-1} + aa'$ with a pure imaginary column a if $s = -1$ and Eq. (7) can be applied. However, with real a at most one $|a_j| \geq 1$ can occur, corresponding to $d_j^{-1} = 1 - a_j^2 \leq 0$, and Eq. (7) is not applicable. It was just this gap, which has motivated the search for a more general integral representation, now based on decompositions

$$R^{-1} = D - BB' \quad (9)$$

with any real or complex diagonal D.

The relation between Eq. (4) with any diagonal D, $|D| \neq 0$, and Eq. (9) is given by:

Lemma 1 *If a regular correlation matrix R has an m-factorial representation $D^{-1} + AA'$, then R^{-1} has also an m-factorial representation $D - BB'$ with the same D.*

Proof With the diagonal matrix Γ of the eigenvalues of $D^{1/2}AA'D^{1/2}$ it follows $|D^{1/2}RD^{1/2}| = |I + \Gamma| \neq 0$. There exists a not necessarily real matrix U with $U'U = I$ and a version $A = D^{-1/2}U\Gamma^{1/2}$. Then $R^{-1} = D - BB'$ is verified with $B = DA(I + \Gamma)^{-1/2}$.

3 General *m*-factorial representations of covariance matrices

Definition 1 *A regular $p \times p$-covariance matrix Σ is called "m-factorial" if m is the lowest integer allowing a representation*

$$\Sigma = D + AA' \tag{10}$$

with any real or complex diagonal matrix D and a $p \times m$-matrix A of rank m. Σ is called "real-m-factorial", if m is the lowest rank of A, which can be reached by a real diagonal D.

Due to Lemma 1 with minimal m an m-factorial Σ with $|D| \neq 0$ has an m-factorial inverse $\Sigma^{-1} = D^{-1} - BB'$.

For some examples with randomly generated 6×6-correlation matrices 3-factorial representations were computed with a complex diagonal D. With only real D no 3-factorial representation did exist.

Thus, by the extension of the term "m-factorial" in Definition 1 more matrices R are representable as m-factorial with a small value of m, which is useful for the $\binom{m+1}{2}$-variate integral representation in Sect. 4

What can be said generally on the minimal value m for a given irreducible regular $\Sigma_{p\times p} = (\sigma_{jk})$ apart from $m \leq p-1$? A tridiagonal Σ with $\prod_{j=1}^{p-1} \sigma_{j,j+1} \neq 0$ shows the existence of cases with $m = p-1$. On the other hand set, eventually after a permutation of rows and columns,

$$\Sigma - D = \begin{pmatrix} \widetilde{\Sigma}_{11} & \Sigma_{12} \\ \Sigma_{21} & \widetilde{\Sigma}_{22} \end{pmatrix}$$

with an $m \times m$-matrix $\widetilde{\Sigma}_{11}$ and a variable $D = \mathrm{diag}(d_1, \ldots, d_p)$. If $\widetilde{\sigma}_{11}, \ldots, \widetilde{\sigma}_{mm}$-and therefore $d_1, \ldots, d_m$-can be chosen in such a way that $\widetilde{\Sigma}_{11}$ and $\Sigma - D$ have the same rank m, then there exists a matrix X with $\widetilde{\Sigma}_{11}X = \Sigma_{12}$, $\Sigma_{21}X = \widetilde{\Sigma}_{22}$ and consequently $\Sigma_{21}\widetilde{\Sigma}_{11}^{-1}\Sigma_{12} = \widetilde{\Sigma}_{22}$. Thus, $d_{m+1}, \ldots, d_p$ are functions of $d_1, \ldots, d_m$. After multiplication by $|\widetilde{\Sigma}_{11}|$ the $\binom{p-m}{2}$ remaining equations with the off-diagonal elements of the symmetrical $\widetilde{\Sigma}_{22}$ must be satisfied by $d_1, \ldots, d_m$. For this, $m \geq \binom{p-m}{2}$ should be necessary apart from exceptions. The lowest integer m satisfying this condition is

$$m_p := p - \left[\frac{1}{2}\left(\sqrt{8p+1} - 1\right)\right]. \tag{11}$$

In particular $m_p = \binom{k}{2}$ is obtained from $p = \binom{k+1}{2}$.

The conjecture "Almost all (w.r.t. Lebesgue measure) irreducible regular covariance matrices $\Sigma_{p\times p}$ are m-factorial with $m \leq m_p$" follows from Lemma 2 for $p = 4$ and is proved here only for $p = 6$, $m_p = 3$.

Proof W.l.o.g. let $\Sigma_{6\times 6}$ be a random correlation matrix R without zeros. Let be D a variable diagonal matrix, $R - D = \binom{\widetilde{R}_{11}, R_{12}}{R_{21}, \widetilde{R}_{22}}$ with a 3×3-matrix $\widetilde{R}_{11}$ and $(c_{jk}) := R_{21}(|\widetilde{R}_{11}|\widetilde{R}_{11}^{-1})R_{12}$.

Following the procedure before Eq. (11) the equations

$$c_{jk} = |\widetilde{R}_{11}| r_{j+3,k+3}, \quad 1 \leq j < k \leq 3, \tag{12}$$

have to be solved with $|\widetilde{R}_{11}| \neq 0$ to find a 3-factorial representation of R. Additionally the equations

$$c_{jk} = 0 \tag{13}$$

are considered. It can be shown—supported by a computer algebra system—that Eq. (12) has six general solutions $(\widetilde{r}_{11}, \widetilde{r}_{22}, \widetilde{r}_{33})$ and Eq. (13) has five ones, four of them coinciding with solutions of Eq. (12). Within the space of random R the solutions of Eq. (12) are almost sure different. Therefore, at least one solution of Eq. (12) is left with $|\widetilde{R}_{11}| \neq 0$. (Normally, one solution of Eq. (13) provides a value $|\widetilde{R}_{11}| \neq 0$ and consequently it is no solution of Eq. (12). Then two solutions of Eq. (12) are left).

If $3 \leq p \leq 5$ only one equation has to be solved with real values $d_1, \ldots, d_{p-2}$ to obtain an at most $(p-2)$-factorial representation of $\Sigma_{p\times p}$ with real D. For $p = 4$ or 5 there are $p - 3$ free parameters among the d_j. Besides, a given $R_{5\times 5}$ has frequently a good approximation by a 2-factorial correlation matrix R_0, which leads to the general approximation method in Sect. 5.

An m-factorial representation for a given Σ can also be found by equations for the unknown elements of A instead of looking for D. This method, given below, is applied in the proof of the following lemma providing exact conditions for $\Sigma_{4\times 4}$ to be at most 2-factorial.

Lemma 2 *If $\Sigma = (\sigma_{jk})$ is a regular irreducible 4×4-covariance matrix, not equivalent to a tridiagonal matrix (i.e. not tridiagonal after any permutation of rows and columns), then there exists a representation $\Sigma = D + AA'$ with a real diagonal D and a $4 \times m$-matrix A with rank $m \leq 2$ and real or imaginary columns.*

Proof The existence of $A = (a_{j\mu})$ is shown with a zero $a_{\ell 2}$ in its second column and a free real or imaginary parameter $a_{\ell 1}$. The matrix Σ can be mapped to a connected graph $\mathcal{G}(\Sigma)$ with vertices $1, \ldots, 4$ containing the edge $[i, j]$ iff $\sigma_{ij} \neq 0, i \neq j$. Let $G_{i_1 i_2 i_3 i_4}$ denote the class of matrices Σ with the vertex degrees $i_1 \geq \cdots \geq i_4$ in the corresponding graph. By assumption $\Sigma \in G_{2211}$ was excluded. Let i, j, k, ℓ be any permutation of 1,2,3,4. If there is at least one vertex ℓ of degree 3 then $\prod_{i\neq\ell} \sigma_{i\ell} \neq 0$. With $a_{\ell 2} := 0$ and a real variable $a_{\ell 1}^2 \neq 0$ set $a_{i1} = \sigma_{i\ell}/a_{\ell 1}$, $i \neq \ell$. Then the three equations

$$\sigma_{ij} - \sigma_{i\ell}\sigma_{j\ell}/a_{\ell 1}^2 = \sigma_{ij} - a_{i1}a_{j1} = a_{i2}a_{j2}, \quad i, j \neq \ell, \tag{14}$$

can be solved for the a_{i2}, a_{j2} because the left-hand sides (lhs) are different from zero if certain values of $a_{\ell 1}^2$ are excluded. If the three lhs vanish simultaneously with a suitable $a_{\ell 1}$ then Σ is one-factorial. Now only $\Sigma \in G_{2222}$ is left. In this case let be $\sigma_{k\ell} = \sigma_{ij} = 0$ and $\sigma_{ik}, \sigma_{jk}, \sigma_{i\ell}, \sigma_{j\ell} \neq 0$. With the above defined $a_{\ell 2}, a_{\ell 1}, a_{i1}, i \neq \ell$, it follows $a_{k1} = 0$ and $a_{i1}, a_{j1} \neq 0$. Then the lhs of Eq. (14) are $\neq 0$ and Eq. (14) can be solved again, which concludes the proof.

A general way to compute $A_{p\times m} = (a_{j\mu})$ in Eq. (10) is as follows: Set $a_{j\mu} = 0$, $j < \mu \leq m$ and consider $x_\mu = a_{\mu\mu}^{-2}$ as complex variables, $\mu = 1, \dots, m$. Then

$$\begin{aligned} \sigma_{1j} &= a_{11}a_{j1} \quad \text{implies} \\ a_{j1} &= \sigma_{1j}\sqrt{x_1} \quad \text{and} \\ a_{j1}a_{k1} &= \sigma_{1j}\sigma_{1k}x_1, \quad 2 \leq j < k \leq p, \end{aligned}$$

$$\begin{aligned} \sigma_{2j} &= a_{21}a_{j1} + a_{22}a_{j2} \quad \text{implies} \\ a_{j2} &= (\sigma_{2j} - \sigma_{12}\sigma_{1j}x_1)\sqrt{x_2} = \sigma_{2j}^{(1)}\sqrt{x_2} \quad \text{and} \\ a_{j2}a_{k2} &= \sigma_{2j}^{(1)}\sigma_{2k}^{(1)}x_2, \quad 3 \leq j < k \leq p, \end{aligned}$$

$$\begin{aligned} \sigma_{3j} &= a_{31}a_{j1} + a_{32}a_{j2} + a_{33}a_{j3} \quad \text{implies} \\ a_{j3} &= (\sigma_{3j}^{(1)} - \sigma_{23}^{(1)}\sigma_{2j}^{(1)}x_2)\sqrt{x_3} = \sigma_{3j}^{(2)}\sqrt{x_3} \quad \text{and} \\ a_{j3}a_{k3} &= \sigma_{3j}^{(2)}\sigma_{3k}^{(2)}x_3, \quad 4 \leq j < k \leq p. \end{aligned}$$

The last $\binom{p-m}{2}$ equations with the "residuals of order m" are

$$\sigma_{jk}^{(m)} = \sigma_{jk}^{(m-1)} - \sigma_{mj}^{(m-1)}\sigma_{mk}^{(m-1)}x_m = 0, \quad m+1 \leq j < k \leq p.$$

To solve them for $x_1, \dots, x_m$, $\binom{p-m}{2} \leq m$ is supposed, satisfied by $m = m_p$ from Eq. (11).

With $6 \leq p \leq 9$ only $\binom{p-m}{2} = 3$ occurs. The solution of these three equations is very simple by elimination of x_m and x_{m-1}. With the three indices i, j, k involved and $\sigma'_{ij}, \sigma''_{ij}$ instead of $\sigma_{ij}^{(m-1)}, \sigma_{ij}^{(m-2)}$, we obtain after having eliminated x_m:

$$\begin{aligned} \sigma'_{ij}\sigma'_{mk} &= \sigma'_{ik}\sigma'_{mj} \\ \sigma'_{jk}\sigma'_{mi} &= \sigma'_{ik}\sigma'_{mj}. \end{aligned}$$

Inserting $\sigma'_{ij} = \sigma''_{ij} - \sigma''_{m-1,i}\sigma''_{m-1,j}x_{m-1}$ and likewise for the remaining terms, both the equations become linear in x_{m-1}. Thus, after elimination of x_{m-1}, only one algebraic equation $p(x_1, \dots, x_{m-2}) = 0$ remains to be solved for x_{m-2} with any free parameter values $x_1, \dots, x_{m-3}$ if $m > 3$.

In addition to an m-factorial representation of an m-factorial Σ some further solutions of the final equations of the above computing procedures might be found because of non-equivalent manipulations, as multiplication by terms, nullified later by some solutions. Therefore, a careful check of the solutions is indispensable.

For larger values of p and m the finding of m-factorial decompositions of an m-factorial Σ seems to be more difficult, but at present the resulting $\binom{m+1}{2}$-variate integrals for the $\Gamma_p(\alpha, R)$-cdf in Eq. (20) would hardly be computable if $m > 3$.

4 A new integral representation of the $\Gamma_p(\alpha, R)$-distribution

The announced integral representation is provided by the following theorem:

Theorem 1 *Let R be any regular $p \times p$-correlation matrix with an m-factorial representation $D - BB'$ of R^{-1} with a not necessarily real $D = diag(d_1, \ldots, d_p)$ and a $p \times m$-matrix B with rank $m < p$ and rows b_j. Then at least for positive integers 2α and for all $\alpha > (p-2)/2$ the $\Gamma_p(\alpha, R)$- pdf is given by*

$$f_p(x_1, \ldots, x_p; \alpha, R)$$
$$= |R|^{-\alpha} \prod_{j=1}^{p} \left(\exp(-d_j x_j) x_j^{\alpha-1} / \Gamma(\alpha)\right) \cdot \mathcal{E}\left(\prod_{j=1}^{p} {}_0F_1\left(\alpha; \tfrac{1}{2} x_j b_j S b_j'\right)\right), \quad (15)$$

where the expectation refers to a $W_m(2\alpha, I_m)$-Wishart matrix S.

Some remarks are inserted before the proof:

If $D > 0$ then $R - D^{-1} \geq 0$ and $D - R^{-1} \geq 0$ are equivalent conditions for B to be real. In this case at least all $\alpha > (m-1)/2$ are admissible.

The rank m of $R^{-1} - D$ should be minimized by D to reduce the computing effort. With a complex D frequently a lower m-value can be reached than by a real one if $p \geq 5$.

To integrate over S, the representation $\frac{1}{2}S = Y^{1/2} C Y^{1/2}$ can be used with $Y = \mathrm{diag}(Y_1, \ldots, Y_m)$, i.i.d.r.v. Y_j with pdf g_α and a random correlation matrix C, independent of Y, with density

$$\frac{(\Gamma(\alpha))^m}{\Gamma_m(\alpha)} |C|^{\alpha - \frac{m+1}{2}}, \quad \Gamma_m(\alpha) = \pi^{m(m-1)/4} \prod_{j=1}^{m} \Gamma\left(\alpha - \tfrac{j-1}{2}\right),$$

if $\alpha > (m-1)/2$. For example, with $m = 3$ integration over C is easily transformed to integration over a rectangular region of angles.

Formula (6) can be derived from Eq. (15) with $D > 0$. A series expansion of the $\Gamma_p(\alpha, R)$-pdf with univariate gamma densities is contained in Royen (1991b). With $R^{-1} = (r^{ij})$ and $Q = (q_{ij})$, $q_{ij} = r^{ij}/(r^{ii} r^{jj})^{1/2}$ this expansion is given—with the notations of the underlying paper—by the leading term $|Q|^\alpha \prod_{j=1}^{p} r^{jj} g_\alpha(r^{jj} x_j)$, multiplied by a power series $P(x_1, \ldots, x_p)$ with rather intricate coefficients. The rhs in Eq. (15) can also be written as

$$|Q|^\alpha \prod_{j=1}^{p} r^{jj} g_\alpha(r^{jj} x_j) \cdot \mathcal{E}\left(\prod_{j=1}^{p} \exp(-x_j b_j b_j') \, {}_0F_1\left(\alpha; \tfrac{1}{2} x_j b_j S b_j'\right)\right). \quad (16)$$

Thus, by comparison, the power series coincides with the above expectation. Besides $\mathcal{E}(\exp(-bb') \, {}_0F_1\left(\alpha; \frac{1}{2} bSb'\right)) = 1$ can be shown for any row $b \in \mathbb{C}^m$.

Proof of Theorem 1 With a suitable $c > 0$ all values $\mathrm{Re}(d_j + c) = \mathrm{Re}(r^{jj} + b_j b_j' + c)$ are positive. The L.t. with the variables $t_1, \ldots, t_p \geq 0$ of

$\exp\left(-c\sum_{j=1}^{p} x_j\right) f_p(x_1,\ldots,x_p;\alpha,R)$ is obtained by changing the order of integration and using the L.t. $t^{-\alpha}\exp(y/t)$ of $x^{\alpha-1}{}_0F_1(\alpha;xy)/\Gamma(\alpha)$.

With $D_{ct} := \mathrm{Diag}(\ldots,d_j+c+t_j,\ldots) = D + cI_p + T$ this L.t. is

$$|R|^{-\alpha}|D_{ct}|^{-\alpha}\,\mathcal{E}\left(\prod_{j=1}^{p}\exp\left(\tfrac{1}{2}(d_j+c+t_j)^{-1}b_jSb_j'\right)\right)$$
$$= |R|^{-\alpha}|D_{ct}|^{-\alpha}\,\mathcal{E}\left(\mathrm{etr}\left(\tfrac{1}{2}SB'D_{ct}^{-1}B\right)\right).$$

With $C := D_{ct}^{-1/2}B$, the substitution $\widetilde{S} := S(I_m - C'C)$ and $|I_m - C'C| = |I_p - CC'|$ the above expectation is $|I_p - CC'|^{-\alpha}$, which yields the L.t.

$$|R|^{-\alpha}|D+cI_p+T-BB'|^{-\alpha} = |R|^{-\alpha}|R^{-1}+cI_p+T|^{-\alpha} = |I_p+R(cI_p+T)|^{-\alpha}.$$

The substitution is justified by $\mathrm{Re}(I_m - C'C) > 0$ with a sufficiently large c. Now it follows $\widehat{f_p}(t_1,\ldots,t_p;\alpha,R) = |I_p+RT|^{-\alpha}$, concluding the proof.

The $\Gamma_p(\alpha,R)$-cdf follows from Eq. (15) by changing the order of integration over S and $x_1,\ldots,x_p$. For this, the following functions are defined with the notations (2) and (3):

$$h_\alpha(z,y) := e^y g_\alpha(z,y) = e^{-z}(z/y)^{(\alpha-1)/2} I_{\alpha-1}(2\sqrt{yz}), \quad (y,z\in\mathbb{C}) \tag{17}$$

with the modified Bessel function $I_{\alpha-1}$.

$$H_\alpha(z,y) := \int_0^z h_\alpha(\zeta,y)\mathrm{d}\zeta = e^y G_\alpha(z,y)$$
$$= e^{-z}\sum_{k=0}^{\infty}(z/y)^{(\alpha+k)/2} I_{\alpha+k}(2\sqrt{yz}), \quad (y,z\in\mathbb{C}), \tag{18}$$

(Royen, 1991a)

$$K_\alpha(d,x,y) := \frac{1}{\Gamma(\alpha)}\int_0^x \exp(-\mathrm{d}\xi)\xi^{\alpha-1}\,{}_0F_1(\alpha;\xi y)\mathrm{d}\xi$$
$$= \left\{\begin{matrix} d^{-\alpha}H_\alpha(dx,y/d), & d\neq 0 \\ (x/y)^{\alpha/2}I_\alpha(2\sqrt{xy}), & d=0\end{matrix}\right\}, \quad (x\geq 0, d, y\in\mathbb{C}). \tag{19}$$

Now the $\Gamma_p(\alpha,R)$-cdf is given by

$$F_p(x_1,\ldots,x_p;\alpha,R) = |R|^{-\alpha}\mathcal{E}\left(\prod_{j=1}^{p} K_\alpha(d_j,x_j,\tfrac{1}{2}b_jSb_j')\right) \tag{20}$$

with the expectation referring to a $W_m(2\alpha, I_m)$-matrix S. With $m = 1$ and $|D| \neq 0$ the rhs is reduced to

$$|DR|^{-\alpha} \int_0^\infty \prod_{j=1}^p H_\alpha(d_j x_j, b_j^2 y/d_j) g_\alpha(y)\mathrm{d}y. \tag{21}$$

For actual computation the function $H_\alpha(z, y)$ should be available also for $y, z \in \mathbb{C}$. Some remarks on representations of the H_α may be helpful. It is easy to verify that

$$H_{\alpha+n}(z, y) = H_\alpha(z, y) - \sum_{k=1}^n h_{\alpha+k}(z, y), \quad \alpha > 0, \quad n \in \mathbb{N}_0 \tag{22}$$

and in particular with the error function

$$H_{1/2}(z, y) = \frac{1}{2} e^y \left(\operatorname{erf}(\sqrt{z} + \sqrt{y}) + \operatorname{erf}(\sqrt{z} - \sqrt{y})\right). \tag{23}$$

Since the $I_{k-1/2}$ are elementary functions (A.S.10.2.9) this holds also for the $h_{1/2+k}$, which simplifies the computation for half-integers α.

For integer α the function H_1 is needed. From $h_1(z, y) = e^{-z} I_0(2\sqrt{yz})$ and

$$I_0(2\sqrt{yz}) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp(x\mathrm{e}^{\mathrm{i}\varphi} + y\mathrm{e}^{-\mathrm{i}\varphi})\mathrm{d}\varphi$$

it follows

$$\begin{aligned} H_1(z, y) &= e^y - e^{-z} \sum_{n=0}^\infty \left(\sum_{j=0}^n z^j/j! \right) y^n/n! \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} w^{-1}(\exp(wz) - 1) \exp(y\mathrm{e}^{-\mathrm{i}\varphi})\mathrm{d}\varphi, \quad w := \mathrm{e}^{i\varphi} - 1. \end{aligned} \tag{24}$$

Besides

$$\begin{aligned} e^{-y} H_\alpha(z, y) = G_\alpha(z, y) &= \sqrt{\frac{z}{\pi}} \int_{-1}^{1} G_{\alpha-1/2}\left((1 - c^2)z)\right) \\ &\times \exp\left(-(c\sqrt{z} - \sqrt{y})^2\right) \mathrm{d}c, \quad \alpha \geq 1/2, \quad G_0 := 1, \end{aligned} \tag{25}$$

can be derived from A.S.6.5.29 and A.S.9.6.18.

Every $\Gamma_3(\alpha, R)$-cdf with $\prod_{j<k} r^{jk} \neq 0$ is computable by a univariate integral, since the equations $r^{jk} = -b_j b_k$ can always be solved. For example, with correlations $r_{12} = 1/\sqrt{2}, r_{13} = 1/\sqrt{2}, r_{23} = 1/4$ a negative $d_1 = -1$ is obtained in $D = R^{-1} + bb'$. With (21), (22), (23), e.g. $F_3(2.8, 6.4, 4.7; 3/2, R) = 0.857013\ldots$ can be computed.

As a by-product formulas for normal probabilities of p-variate symmetrical rectangular regions arise with $\alpha = 1/2$. With m-factorial R, a $\mathcal{N}_p(0, R)$-r.v. $(Y_1, \ldots, Y_p)$ with $R^{-1} = D - BB'$, $|D| \neq 0$, and a $\mathcal{N}_m(0, I_m)$-distributed column Z, it follows with $S = ZZ'$ from Eqs. (20) and (23):

$$P\left(\bigcap_{j=1}^{p}\{|Y_j| \leq \sqrt{2x_j}\}\right) = F_p(x_1, \ldots, x_p; \frac{1}{2}, R) = 2^{-p}|DR|^{-1/2}$$
$$\times\, \mathcal{E}\left(\exp(\tfrac{1}{2}Z'B'D^{-1}BZ)\prod_{j=1}^{p}\left(\operatorname{erf}(\sqrt{d_jx_j} + b_jZ/\sqrt{2d_j}) + \operatorname{erf}(\sqrt{d_jx_j} - b_jZ/\sqrt{2d_j})\right)\right) \tag{26}$$

with expectation referring to Z.

5 Approximation to R by m-factorial R_0 and Taylor approximations for the $\Gamma_p(\alpha, R)$-distribution

At present, actual computation of the $\Gamma_p(\alpha, R)$-cdf by Eq. (20) is only accomplished with very small values of m. By a good approximation to a given correlation matrix R by an m-factorial correlation matrix R_0 with small m, a first approximation to the $\Gamma_p(\alpha, R)$-cdf is obtained with R_0 instead of R. For example, a given $R_{5\times5}$ has frequently a good 2-factorial approximation R_0. The following considerations aim at this case, but general formulas will be derived. The $\Gamma_p(\alpha, R)$-probability measure P of any fixed area—and in particular the corresponding cdf-can be considered as a function of $R = R_0 + H$, and subsequent approximations to $P(R)$ can be computed by Taylor polynomials $P(R_0) + P_1(H; R_0) + P_2(H; R_0) + \cdots$, where the P_j are homogeneous polynomials of degree j with the deviations h_{ij} in H. Such a Taylor expansion was derived for multivariate normal probabilities of rectangular regions in Royen (1987). With a small value of $\mathrm{tr}(H^2)$ a reasonable approximation to the $\Gamma_p(\alpha, R)$-cdf should be obtained by sums of $\binom{m+1}{2}$-variate integrals with a much lower number of terms than needed by the known series expansions, e.g. in Royen (1991b).

To compute an m-factorial least square approximation $R_0 = D^{-1} + AA'$ with real D for a given $R_{p\times p} = (r_{ij})$ by minimization of

$$Q(A) := \sum_{1\leq i<j\leq p}(r_{ij} - a_ia_j')^2 = \frac{1}{2}\mathrm{tr}(H^2)$$

with the rows a_j of $A_{p\times m}$ is difficult by a lot of stationary points. Besides, the number of possibly pure imaginary columns of an optimal A is not known before. Here an algorithm is proposed which has provided frequently at least good approximations R_0 to $R_{5\times5}$. In a first step $\binom{p}{2} - \binom{p-m}{2}$ deviations h_{ij} are forced to vanish by the procedure described after Lemma 2 using m variables $x_\mu = a_{\mu\mu}^{-2}$. The remaining sum of squares $Q(A) = q(x_1, \ldots, x_m) = \sum_{m<i<j\leq p} h_{ij}^2$-now containing more than m squares—is minimized with respect to real variables x_μ. With $m = 2$ the equation $\partial q/\partial x_2 = 0$ is linear in x_2. Thus, only $\partial q/\partial x_1(x_1, x_2(x_1)) = 0$ has to be

solved for x_1. This step is repeated for all possible choices of $J = \{i_1, \ldots, i_m\} \subseteq \{1, \ldots, p\}$ with $q = \sum_{i<j} h_{ij}^2$, $i, j \notin J$. If $Q = q = 0$ is not reached—i.e. R is not real-m-factorial—then the matrices $A(J)$, obtained in this way, provide the starting points for further numerical minimization, e.g. by the steepest descent. Finally, a matrix A with the lowest reached value $Q(A)$ is selected. However, $R_0 = D^{-1} + AA' > 0$ has to be checked separately, but this is frequently satisfied for good approximations R_0. Sometimes it is more economical to abandon the last numerical minimization step and only to compute an A with as much zeros as possible in H. Then with $p = 5$ only one $h_{ij} \neq 0$ would be left. Then the first terms P_n in Eq. (29) are essentially simplified and lead to useful approximations to the $\Gamma_5(\alpha, R)$-cdf by 3-variate integrals if h_{ij} is small.

With all $r_{ij} > 0$ and $m = 1$ $\sum_{1\le i<j\le p}\left(\ln(a_i a_j / r_{ij})\right)^2$ is minimized by

$$a_k = \left(\prod_{\substack{i=1\\ i\neq k}}^{p} r_{ik} \Big/ \left(\prod_{1\le i<j\le p} r_{ij}\right)^{1/(p-1)}\right)^{1/(p-2)}, \quad k = 1, \ldots p, \tag{27}$$

but again, $R_0 = \mathrm{Diag}(\ldots, 1 - a_k^2, \ldots) + aa' > 0$ should be satisfied.

Now let R_0 be an m-factorial approximation to $R = R_0 + H$. Then, with $\delta_0 := |I_p + R_0 T|$ and

$$\tau_n(T; R_0, H) := \delta_0^n \operatorname{trace}\left(\left(-HT(I_p + R_0 T)^{-1}\right)^n\right) \tag{28}$$

the L.t. $|I_p + RT|^{-\alpha} = \delta_0^{-\alpha} \left|I_p + HT(I_p + R_0 T)^{-1}\right|^{-\alpha}$ has the formal series expansion

$$\begin{aligned}
\delta_0^{-\alpha} \exp\left(\alpha \sum_{n=1}^{\infty} \delta_0^{-n} \tau_n / n\right) &= \sum_{n=0}^{\infty} P_n(t_1, \ldots, t_p; \alpha, R_0, H)\delta_0^{-(\alpha+n)} \\
= \delta_0^{-\alpha}\Big(1 + \alpha\tau_1\delta_0^{-1} &+ \frac{\alpha}{2}\left(\tau_2 + \alpha\tau_1^2\right)\delta_0^{-2} \\
+ \frac{\alpha}{6}\left(2\tau_3 + 3\alpha\tau_2\tau_1 + \alpha^2\tau_1^3\right)\delta_0^{-3} + \cdots\Big)
\end{aligned} \tag{29}$$

which is uniformly convergent for all $T \ge 0$ if the spectral norm $\left\|HR_0^{-1}\right\| < 1$, being equivalent to $R_0 \pm H > 0$. Using a computer algebra system the reader can e.g. look at the polynomials P_1, P_2 with $p = 5$ and in particular with only one $h_{ij} \neq 0$.

The integration of the inverted n-th term of Eq. (29) yields

$$P_n\left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_p}; \alpha, R_0, H\right) F(x_1, \ldots, x_p; \alpha + n, R_0) \tag{30}$$

with the $\Gamma_p(\alpha + n, R_0)$-cdf F. With $R_0^{-1} = \mathrm{diag}(\ldots, d_j, \ldots) - BB'$ obtained from $R_0 = D^{-1} + AA'$ and the rows b_j of B Eq. (30) is a linear combination of terms

$$|R_0|^{-(\alpha+n)}\ \mathcal{E}\left(\prod_{j=1}^{p}\left(\frac{\partial}{\partial x_j}\right)^{k_j}\int_0^{x_j} e^{-d_j\xi}\xi^{\alpha-1+n}(\Gamma(\alpha+n))^{-1}\right.$$
$$\left.\times\ {}_0F_1\left(\alpha+n;\frac{1}{2}\xi b_j S_{2(\alpha+n)}b_j'\right)\mathrm{d}\xi\right) \tag{31}$$

with $0 \le k_1,\ldots,k_p \le n$ and the expectation referring to a $W_m(2(\alpha+n), I_m)$-Wishart matrix $S_{2(\alpha+n)}$.

For the intended numerical application with Taylor polynomials of a very low degree the convergence of Eq. (29) is not needed. Nevertheless, the convergence to the cdf is established by the following theorem. Let s_n denote the inverted partial sums of the expansion (29) and $S_n(x_1,\ldots,x_n)$ their integrals over $\times_{j=1}^{p}(0,x_j]$.

Theorem 2 *If* $\|HR_0^{-1}\| < 1$ *then the sequence* (S_n) *converges to the* $\Gamma_p(\alpha, R)$*-cdf* $F(x_1,\ldots,x_p)$ *for all values* $0 < x_j < \infty$.

Proof Let $\widehat{f}$ denote here the Fourier transform (F.t.) of f. For the eigenvalues $\lambda(T)$ of $-iHT(I_p - iR_0T)^{-1}$ it is shown $|\lambda(T)| \le 1-\epsilon$ with an $\epsilon > 0$ independent of T. Since the λ depend continuously on $t_1,\ldots,t_p$, $|T| \ne 0$ is assumed. Then

$$\left|\lambda I_p + iHT(I - iR_0T)^{-1}\right| = 0$$
$$\Longleftrightarrow |\lambda(I - iR_0T) + iHT| = 0 \Longleftrightarrow \left|R_0 - \lambda^{-1}H + iT^{-1}\right| = 0,$$

if $\lambda \ne 0$. With $\lambda^{-1} = \rho e^{i\varphi}$ the equation

$$\left|R_0 - \rho\cos\varphi H + i(T^{-1} - \rho\sin\varphi H)\right| = 0 \tag{32}$$

can only be solved with $\rho \ge (1-\epsilon)^{-1}$, because $R_0 - H > 0$, i.e. $|\lambda| \le 1-\epsilon$.

With $z_j := (1-it_j)^{-1}$, $\omega_j := z_j(1+it_j) = \exp(2i\arctan t_j)$, $j = 1,\ldots,p$, the corresponding diagonal matrices Z, Ω, $A := 2(I+R_0)^{-1}$ and $C := I - A$ the F.t. $\widehat{f_0} = |I - iR_0T|^{-\alpha}$ can be written as $\widehat{f_0} = |A|^{\alpha}|Z|^{\alpha}|I_p - C\Omega|^{-\alpha}$, (Royen, 1991b). Thus, $|I_p - C\Omega|^{-\alpha}$ is uniformly bounded on $\mathbb{R}^p$, since $\|C\Omega\| = \|C\| < 1$.

By the Fourier inversion formula we obtain

$$\prod_{j=1}^{p}\left(\frac{\partial}{\partial x_j}\right)^{k_j} F(x_1,\ldots,x_p;\alpha+n,R_0)$$
$$= (2\pi)^{-p}\int_{\mathbb{R}^p}|I - iR_0T|^{-(\alpha+n)}\prod_{j=1}^{p}(-it_j)^{k_j-1}\big(\exp(-it_jx_j)-1\big)\mathrm{d}t_j,$$

where the rhs is absolutely bounded by

$$K\int_{\mathbb{R}^p}\prod_{j=1}^{p}\left(1+t_j^2\right)^{-\alpha/2}\min\left(x_j, 2|t_j|^{-1}\right)\mathrm{d}t_j < \infty$$

with a constant K only depending on α, p and R_0, since all $k_j \leq n$. Now

$$\begin{aligned} &|F(x_1,\ldots,x_n;\alpha,R) - S_n(x_1,\ldots,x_n)| \\ &< \int\limits_{\mathbb{R}^p} |\widehat{f} - \widehat{s}_n| \prod_{j=1}^{p} \left|\left(\exp(-it_jx_j) - 1\right) / (-it_j)\right| \mathrm{d}t_j \\ &\leq \int\limits_{\mathbb{R}^p} \epsilon_n(t_1,\ldots,t_n) |I - iR_0T|^{-\alpha} \prod_{j=1}^{p} \min\left(x_j, 2|t_j|^{-1}\right) \mathrm{d}t_j, \end{aligned}$$

which tends to zero, since $\epsilon_n(t_1,\ldots,t_n) \to 0$ uniformly on $\mathbb{R}^p$ due to Eq. (32).

The proof is more simple if $\alpha > 1/2$, because then $\widehat{f} - \widehat{s}_n \in \mathcal{L}^2(\mathbb{R}^p)$. Thus, $\int_{\mathcal{A}} |f - s_n| dx_1, \ldots, dx_p \longrightarrow 0$ for any bounded region $\mathcal{A} \subseteq \mathbb{R}_+^p$ is obtained by Cauchy's inequality and Plancherels identity.

6 Approximation to $\Gamma_p(\alpha, R)$-distributions by complex measures

In Sect. 5 an m-factorial correlation matrix R_0 with small m was used as an approximation to a given R to obain approximations for the $\Gamma_p(\alpha, R)$-cdf by $\binom{m+1}{2}$-variate integrals.

If in the F.t. $\widehat{f}(t_1,\ldots,t_p;\alpha,R_0)$ the off-diagonal elements r_{0ij} of R_0 are replaced symmetrically by complex variables, then $\widehat{f}$ becomes the F.t. of a variable complex measure μ_0. If, with very small imaginary parts in R_0, smaller values $\sum_{i<j} |r_{ij} - r_{oij}|^2$ can be reached than only by correlation matrices R_0, then $\mathrm{Re}(\mu_0)$ might provide also a first approximation to the $\Gamma_p(\alpha, R)$-probability measure P. Even with $p = 5$ and $m = 2$ optimal approximations to R by symmetrical (not hermitian) complex 2-factorial R_0 are difficult to compute. Nevertheless, this method should be investigated further because it should be useful for other applications too.

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