On the Marginal Distribution of the Diagonal Blocks in a Blocked Wishart Random Matrix

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Abstract: Let A be a $(m_1+m_2)\times(m_1+m_2)$ blocked Wishart random matrix with diagonal blocks of size $m_1\times m_1$ and $m_2\times m_2$. The goal of the paper is to find the exact marginal distribution of the two diagonal blocks of A. We find an expression for this marginal density involving the matrix-variate generalized hypergeometric function. We became interested in this problem because of an application in spatial interpolation of random fields of positive-definite matrices, where this result will be used for parameter estimation, using composite likelihood methods.

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1. Introduction

The goal of this paper is to find an exact and useful form for the marginal distribution of the diagonal blocks of a 2×2 blocked Wishart random matrix. This problem arises in an applied problem, to estimate the parameters of a Wishart random field, which will be reported elsewhere.

Let A be a $(m_1+m_2)\times(m_1+m_2)$ Wishart random matrix, where the diagonal blocks are of size $m_1\times m_1$ and $m_2\times m_2$, respectively. In our intended application m_1, m_2 will be small integers, (and $m_1=m_2$, but we choose to treat the more general case). Write $A=\begin{pmatrix} A_1 & A_{12} \\ A_{12}^\top & A_2\end{pmatrix}$.

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Denote the number of freedom parameter by n and the scale parameter, which is a matrix blocked in the same way as A, by $\Sigma = \begin{pmatrix} \Sigma_1 & \Sigma_{12} \\ \Sigma_{12}^\top & \Sigma_2 \end{pmatrix}$. We are mostly interested in the special case $\Sigma = \begin{pmatrix} \Sigma_0 & \rho\Sigma_0 \\ \rho\Sigma_0 & \Sigma_0 \end{pmatrix}$ where the absolute value of ρ is less than one, but the general case is no more difficult.

All matrices are real. Notation: we use $\mathrm{Tr}(A)$ for the trace of the square matrix A, and $\mathrm{etr}(A) = \exp(\mathrm{Tr}(A))$. We write $\mathcal{P}^+(m)$ for the convex cone of real $m \times m$ positive definite matrices, and we write $\mathcal{O}(m)$ for the orthogonal group, that is, the set of $m \times m$ orthogonal matrices. The Stiefel manifold, that is the set of $m_1 \times m_2$ column orthogonal matrices, in which case necessarily $m_2 \leq m_1$, is written $\mathcal{V}_{m_2,m_1}$. We indicate the transpose of a matrix by an upperscript $^\top$.

In the convex cone of positive definite matrices, we use the cone order, defined by $A < B$ meaning that $B - A$ is positive definite, written $B - A > 0$. Integrals over cones are written as $\int_0^I g(A)\ (\mathrm{dA})$ meaning the integral is taken over the cone $0 < A < I$. The multivariate gamma function is denoted by $\Gamma_m(a)$ for $\Re(a) > \frac{m-1}{2}$, see (Muirhead, 1982) for proofs and properties.

In the second section we give some background information, especially about the Jacobians which we need to evaluate the integrals. In section three we state our results, and give proofs. In the final section we give some comments on the result.

2. Background

The single most important reference for background material for this paper is (Muirhead, 1982). Some results therefrom will not be cited directly.

When doing change of variables in a multiple integral we need to know the Jacobian. Here we will list the ones we need, most can be found in (Muirhead, 1982) or in (Mathai, 1997). We are following the notation of (Muirhead, 1982). First a very brief summary.

For any matrix X, let dX denote the matrix of differentials dx_{ij}. For an arbitrary $m_1 \times m_2$ matrix X, the symbol (dX) denotes the exterior product of the mn elements of dX:

$$(dX) \equiv \wedge_{j=1}^{m_2} \wedge_{i=1}^{m_1} dx_{ij}. \tag{1}$$

If X is a symmetric $m_2 \times m_2$ matrix, the symbol (dX) will denote the exterior product of the $\frac{m_2(m_2+1)}{2}$ distinct elements of dX:

$$(dX) \equiv \wedge_{1 \leq i \leq j \leq m_2} dx_{ij}. \tag{2}$$

With similar definitions for other kinds of structured matrices.

The following invariant form on the orthogonal group represents the Haar measure, $\left(H^\top \mathrm{d}H\right) = \wedge_{i=1}^m \wedge_{j=i+1}^m h_j^\top dh_i$. Here H represents an orthogonal matrix. This form normalized to have total mass unity is represented by (dH). We also need to integrate over a Stiefel manifold, then $\left(H^\top dH\right)$ represents a similarly defined invariant form, see (Muirhead, 1982).

Some needed jacobians are not in (Muirhead, 1982), so we give them here, from (Díaz-García, González-Farias, 2005) and (Díaz-Garzía, Jaimez, Mardia, 1997).

Lemma 1. *(Jacobian of the symmetric square root of a positive definite matrix). Let S and R be in $\mathcal{P}^+(m)$ such that $S = R^2$ and let Δ be a diagonal matrix with the eigenvalues of R on the diagonal. Then,*

$$(dS) = 2^m \det(\Delta) \prod_{i<j}^{m} (\Delta_i + \Delta_j)\,(dR) = \prod_{i\le j}^{m} (\Delta_i + \Delta_j)\,(dR)$$

This result can also be found in (Mathai, 1997). We need the generalized polar decomposition of a rectangular matrix. Let C be an $m_1 \times m_2$ rectangular matrix with $m_2 \le m_1$. Then we always have $C = UH$ where H is positive semi-definite, positive definite if C has full rank, and U is a $m_1 \times m_2$ column-orthogonal matrix. In that last case, U is unique. See (Higham, 2008).

Lemma 2. *(Generalized Polar decomposition) Let X be an $m_1 \times m_2$ matrix with $m_1 \ge m_2$ and of rank m_2, with m_2 distinct singular values. Write $X = UH$, with $U \in \mathcal{V}_{m_2,m_1}$ and $H \in \mathcal{P}^+(m_2)$. Then H has m_2 distinct eigenvalues. Also let Δ be the diagonal matrix with the eigenvalues of H on the diagonal. Then*

$$(dX) = \det(\Delta)^{m_1 - m_2} \prod_{i<j}^{m_2} (\Delta_i + \Delta_j)\,(dH)\left(U^\top dU\right).$$

Note that since this results are used for integration, the assumption of distinct singular values is unimportant, since the subset where the singular values are equal has measure zero.

3. Results

Let us state our main result:

Theorem 1. *(The Marginal Distribution of the Diagonal Blocks of a Blocked Wishart Random Matrix with Blocks of unequal sizes) Let $A = \begin{pmatrix} A_1 & A_{12} \\ A_{12}^\top & A_2 \end{pmatrix}$ be a $(m_1 + m_2) \times (m_1 + m_2)$ blocked Wishart random matrix, where the diagonal blocks are of size $m_1 \times m_1$ and $m_2 \times m_2$, respectively. The Wishart distribution of A have $n \ge m_1 + m_2$ degrees of freedom and positive definite scale matrix $\Sigma = \begin{pmatrix} \Sigma_1 & \Sigma_{12} \\ \Sigma_{12}^\top & \Sigma_2 \end{pmatrix}$ blocked in the same way as A. The marginal distribution of the* *two diagonal blocks A_1 and A_2 have density function given by*

$$c \cdot \mathrm{etr}\left\{-\frac{1}{2}(\Sigma_1^{-1}A_1 + F^\top C_2 F A_1 + C_2^{-1}A_2)\right\} \cdot \det(A_1)^{(n-m_2-1)/2}$$
$$\det(A_2)^{(n-m_1-1)/2}\,{}_0\mathrm{F}_1\left(\left.\begin{matrix} \\ n/2\end{matrix}\right| \frac{1}{4}G\right) \quad (3)$$

where $C_2 = \Sigma_2 - \Sigma_{12}^\top\Sigma_1^{-1}\Sigma_{12}$, $F = C_2^{-1}\Sigma_{12}^\top\Sigma_1^{-1}$ *and* $G = A_2^{1/2}FA_1F^\top A_2^{1/2}$. $c^{-1} = 2^{(m_1+m_2)n/2}\Gamma_{m_1}(n/2)\Gamma_{m_2}(n/2)\,(\det\Sigma)^{n/2}$. ${}_0\mathrm{F}_1$ *is the generalized matrix-variate hypergeometric function, as defined in (Muirhead, 1982).*

Note that the definition of the matrix-variate hypergeometric function is by a series expansion, which is convergent in all cases we need, see (Muirhead, 1982). The rest of this section consists in a proof of this theorem.

Introduce the following notation: The Schur complements of $\Sigma = \left(\begin{smallmatrix}\Sigma_1 & \Sigma_{12}\\ \Sigma_{12}^\top & \Sigma_2\end{smallmatrix}\right)$ is $C_1 = \Sigma_1 - \Sigma_{12}\Sigma_2^{-1}\Sigma_{12}^\top$ and $C_2 = \Sigma_2 - \Sigma_{12}^\top\Sigma_1^{-1}\Sigma_{12}$. Then define $F = C_2^{-1}\Sigma_{12}^\top\Sigma_1^{-1}$. In the following we will be using some standard results on blocked matrices without quoting them.

The Wishart density function of A written as a function of the blocks:

$$\begin{aligned} c \cdot \mathrm{etr}\left(-\frac{1}{2}\left(\Sigma_1^{-1}A_1 + F^\top C_2 F A_1 - 2F^\top A_{12}^\top\right) + \left(C_2^{-1}A_2\right)\right) \\ \cdot \det(A_1)^\gamma \det(A_2 - A_{12}^\top A_1^{-1}A_{12})^\gamma \end{aligned} \quad (4)$$

where $c^{-1} = 2^{(m_1+m_2)n/2}\Gamma_{m_1+m_2}(\frac{1}{2}n)\,(\det\Sigma)^{n/2}$ and $\gamma = \frac{n-m_1-m_2-1}{2}$. In the following we will work with the density concentrating on the factors depending on A_{12}. To prove the theorem we need to integrate out the variable A_{12}. The other variables, which are constant under the integration, will be concentrated in one constant factor. So we repeat the formula (4) written as a differential form with the constants left out.

$$K_1 \cdot \mathrm{etr}(FA_{12})\det(A_2 - A_{12}^\top A_1^{-1}A_{12})^\gamma \;\; (dA_{12}) \quad (5)$$

where $K_1 = c \cdot \mathrm{etr}\left(-\frac{1}{2}(\Sigma_1^{-1}A_1 + F^\top C_2 F A_1\right)\mathrm{etr}\left(-\frac{1}{2}C_2^{-1}A_2)\right)\det(A_1)^\gamma$. Now, to find the marginal distribution of the diagonal blocks, we need to integrate over the off-diagonal block A_{12}. Under this integration the value of the diagonal blocks A_1 and A_2 will remain fixed, and the region of integration will be a subset of $\mathbb{R}^{m_1\times m_2}$ consisting of the matrices A_{12} such that the block matrix $A = \left(\begin{smallmatrix}A_1 & A_{12}\\ A_{12}^\top & A_2\end{smallmatrix}\right)$ is positive definite. This seems like a complicated set, but we can give a simple description of it using the polar decomposition of a matrix. Note that this is one of the key observations for the proof, and this authors has not seen any use of this observation earlier.

Now we need to assume that $m_1 \geq m_2$. For the opposite inequality a parallell development can be given, using the other factorization $\det A = \det(A_2)\det(A_1 - A_{12}A_2^{-1}A_{12}^\top)$. From for instance Theorem 1.12 in (Fuzhen Zhang et. al., 2005) it follows that the region of integration is the set

$$\{A_{12} \in \mathbb{R}^{m_1 \times m_2} \colon 0 < A_{12}^\top A_1^{-1} A_{12} < A_2\} \tag{6}$$

Introduce $E = A_2^{-1/2} A_{12}^\top A_1^{-1/2}$ where we use the usual symmetric square root. Then in terms of the new variable E the region of integration becomes

$$\{E^\top \in \mathbb{R}^{m_1 \times m_2} \colon 0 < EE^\top < I\} \tag{7}$$

and with the generalized polar decomposition in the form $E^\top = UP$ with $P \in \mathcal{P}^+(m_2), U \in \mathcal{V}_{m_2,m_1}$, $EE^\top = P^2$ so the region of integration can be written as

$$\{P \in \mathcal{P}^+(m_2), U \in \mathcal{V}_{m_2,m_1} \colon 0 < P^2 < I\} \tag{8}$$

which is a Cartesian product of a cone interval with a Stiefel manifold.

The Jacobian of the transformation from A_{12} to E is $(dE) = \left(dE^\top\right) = \det(A_2)^{-m_1/2}\det(A_1)^{-m_2/2}(dA_{12})$. The Jacobian of the polar decomposition $E^\top = UP$ is $(dE) = \left(dE^\top\right) = (\det\Delta)^{m_1-m_2}\prod_{i<j}^{m_2}(\Delta_i - \Delta_j)\,(dP)\left(U^\top dU\right)$ where Δ is a diagonal matrix with the eigenvalues of P on the diagonal. See lemma (2). A last transformation will be useful. Define $P^2 = X$. The Jacobian of this transformation is $(dX) = 2^{m_2}\det\Delta\prod_{i<j}^{m_2}(\Delta_i + \Delta_j)\,(dP)$, Δ is as above. See lemma (1)

Applying this transformations the integral of (5) can be written as

$$K_2 \cdot \int_0^I \int_{\mathcal{V}_{m_2,m_1}} \operatorname{etr}(X^{1/2} A_2^{1/2} F A_1^{1/2} U) \det(I - X)^\gamma \det(X)^{(m_1-m_2-1)/2}\,(\mathrm{d}X)\,\left(U^\top \mathrm{d}U\right) \tag{9}$$

where the constant
$K_2 = 2^{-m_2} c \operatorname{etr}\left(-\frac{1}{2}((\Sigma_1^{-1} + F^\top C_2 F)A_1 + C_2^{-1}A_2)\right) \cdot (\det A_1)^{\gamma + m_2/2}(\det A_2)^{\gamma + m_1/2}$

We are ready to perform the integration over the Stiefel manifold. For this purpose we need a generalization of the following result from (, Muirhead, 1982, Theorem 7.4.1, page 262), which we cite here.

Let X be an $m \times n$ real matrix with $m \leq n$ and $H = [H_1 \colon H_2]$ an $n \times n$ orthogonal matrix, where H_1 is $n \times m$. Then

$$\int_{\mathcal{O}(n)} \operatorname{etr}(XH_1)\,(\mathrm{d}H) = {}_0\mathrm{F}_1\left(\,{}_{n/2}\middle|\,\frac{1}{4}XX^\top\right). \tag{10}$$

But we have an integral over the Stiefel manifold, not the orthogonal group, so we need now to generalize the result (10) to an integral over the Stiefel manifold. What we need is the following. Let $\mathcal{V}_{m_2,m_1}$ be the manifold of $m_1 \times m_2$ column orthogonal matrices with $m_2 \leq m_1$, and let f be a function defined on the Stiefel manifold. We can extend this function to a function defined on $\mathcal{O}(m_1)$ in the following way. Let U be an $m_1 \times m_2$ orthogonal matrix, and write it in block form as $[U_1 : U_2]$ such that $U_1 \in \mathcal{V}_{m_2,m_1}$. How can we characterize the set of U_2 which is complementing U_1 to form an orthogonal matrix? First, let U_2 be an fixed, but arbitrary such matrix. Then clearly any other $m_1 \times (m_1 - m_2)$ column orthogonal matrix with the same column space also works. The common column space is the orthogonal complement of the column space of U_1. The set of such matrices can be described as $\{V \in \mathcal{V}_{m_1-m_2,m_1} : V = U_2 Q \text{ for } Q \in \mathcal{O}(m_1 - m_2)\ \}$. For this set we write $\mathcal{V}^{H_1}_{m_1-m_2,m_1}$. As a set we can identify this with $\mathcal{O}(m_1 - m_2)$. Specifically, we can identify U_2 with the very special column orthogonal matrix $\begin{pmatrix} 0_{m_2 \times m_1 - m_2} \\ Q \end{pmatrix}$ where $Q \in \mathcal{O}(m_1 - m_2)$ which clearly forms a proper submanifold of the Stiefel manifold $\mathcal{V}_{m_1-m_2,m_1}$. The function f can now be extended to the orthogonal group by defining $f(U) = f([U_1 : U_2]) = f(U_1)$ and for the integral we find that

$$\begin{aligned}
&\int_{\mathcal{O}(m_1)} f(U_1)\ \left(U^\top \mathrm{d}U\right) = \\
&\qquad \int_{\mathcal{V}_{m_2,m_1}} \int_{\mathcal{V}^{H_1}_{m_1-m_2,m_1}} f([U_1 : U_2])\ \left(U^\top \mathrm{d}U\right) = \\
&\qquad \int_{\mathcal{V}_{m_2,m_1}} f(U_1)\ \left(U_1^\top \mathrm{d}U_1\right) \int_{\mathcal{V}^{H_1}_{m_1-m_2,m_1}} \left(Q^\top \mathrm{d}Q\right) = \\
&\qquad \operatorname{Vol}\mathcal{O}(m_1 - m_2) \int_{\mathcal{V}_{m_2,m_1}} f(H_1)\ \left(H_1^\top \mathrm{d}H_1\right). \qquad (11)
\end{aligned}$$

Returning to our integral, the integral over the Stiefel manifold occurring in (9) can now be written as

$$\begin{aligned}
&\int_{\mathcal{V}_{m_2,m_1}} \operatorname{etr}(X^{1/2} A_2^{1/2} F A_1^{1/2} U)\ \left(U^\top \mathrm{d}U\right) \\
&\quad = \frac{1}{\operatorname{Vol}(\mathcal{O}(m_1 - m_2))} \int_{\mathcal{O}(m_1)} \operatorname{etr}(X^{1/2} A_2^{1/2} F A_1^{1/2} U_1)\left(U^\top \mathrm{d}U\right)
\end{aligned}$$

where U_1 consistes of the m_2 first columns of U

$$\begin{aligned}
&= \frac{\operatorname{Vol}(\mathcal{O}(m_1))}{\operatorname{Vol}(\mathcal{O}(m_1 - m_2))} \int_{\mathcal{O}(m_1)} \operatorname{etr}(X^{1/2} A_2^{1/2} F A_1^{1/2} U_1)\,(\mathrm{d}U) \\
&= \frac{\operatorname{Vol}(\mathcal{O}(m_1))}{\operatorname{Vol}(\mathcal{O}(m_1 - m_2))}\ {}_0\mathrm{F}_1\left(\tfrac{m_1}{2} \,\middle|\, \frac{1}{4} A_2^{1/2} F A_1^{1/2} X A_1^{1/2} F^\top A_2^{1/2} \right) \qquad (12)
\end{aligned}$$

where we did use (10). Here $\operatorname{Vol}(\mathcal{O}(m)) = \frac{2^m \pi^{m^2/2}}{\Gamma_m(m/2)}$ is the volume of the orthogonal group, see (Muirhead, 1982). The differential form (dU) denotes Haar measure normalized to total mass unity.

Now write $G = A_2^{1/2} F A_1 F^\top A_2^{1/2}$ then we can write (9) as

$$K_2 \frac{\mathrm{Vol}(\mathcal{O}(m_1))}{\mathrm{Vol}(\mathcal{O}(m_1 - m_2))} \int_0^I (\det X)^{(m_1-m_2-1)/2} \det(I-X)^\gamma \, {}_0\mathrm{F}_1 \left(\left. \frac{m_1}{2} \right| \frac{1}{4} GX \right) (\mathrm{d}X) \tag{13}$$

and to evaluate this integral we need another result from (, Muirhead, 1982, theorem 7.2.10, page 254), we do not state it here.

Using this we find a result we need for the integral of an hypergeometric function, by using the series expansion definition of the hypergeometric function and integrating term by term:

Theorem 2. *If Y is a symmetric $m \times m$ matrix we have that*

$$\int_0^I \det(X)^{a-(m+1)/2} \det(I-X)^{b-(m+1)/2} \, {}_p\mathrm{F}_q \left(\left. \begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix} \right| XY \right) (\mathrm{d}X) = \frac{\Gamma_m(a)\Gamma_m(b)}{\Gamma_m(a+b)} \, {}_{p+1}\mathrm{F}_{q+1} \left(\left. \begin{matrix} a_1, \dots, a_p, a \\ b_1, \dots, b_q, a+b \end{matrix} \right| Y \right) \tag{14}$$

so both degrees of the hypergeometric function are raised by one.

The proof is a simple calculation that we leave out.

Now using (14) to calculate (13) we get, finally, the result

$$K_2 \cdot \frac{\mathrm{Vol}(\mathcal{O}(m_1))}{\mathrm{Vol}(\mathcal{O}(m_1 - m_2))} \frac{\Gamma_{m_2}(m/2)\Gamma_{m_2}((n-m_1)/2)}{\Gamma_{m_2}(n/2)} \, {}_1\mathrm{F}_2 \left(\left. \begin{matrix} m_1/2 \\ m_1/2, n/2 \end{matrix} \right| \frac{1}{4} G \right) \tag{15}$$

but note that one pair of upper and lower arguments to the hypergeometric function are equal, those clearly cancels. With a little algebra we complete the proof of our main theorem.

4. Some Final Comments

To help interpret our main result, we calculated the conditional distribution of the matrix A_1 given the matrix A_2. We will not give the full details of the calculation here, but only give the result. The density of A_1 given that $A_2 = a_2$ has the density given by

$$\frac{1}{2^{mn/2}\Gamma_m(n/2)\det(C_1)^{n/2}} \mathrm{etr}(-\frac{1}{2} C_1^{-1} A_1) \det(A_1)^{(n-m-1)/2} \cdot \mathrm{etr}(-\frac{1}{2}\Omega) \, {}_0\mathrm{F}_1 \left(\left. n/2 \right| \frac{1}{4} \Omega C_1^{-1} A_1 \right), \tag{16}$$

where we have given the conditional density only for the special case $\Sigma = \begin{pmatrix} \Sigma_0 & \rho\Sigma_0 \\ \rho\Sigma_0 & \Sigma_0 \end{pmatrix}$. For this case we have, with the notation from the main theorem, $C_1 = C_2 = (1-\rho^2)\Sigma_0$, $F = \frac{\rho}{1-\rho^2}\Sigma_0^{-1}$, and $\mathrm{F}^\top C_2 F = \frac{\rho^2}{1-\rho^2}\Sigma_0^{-1}$. We have defined $\Omega = \rho^2 C_1^{-1} a_2$, which can be seen as a non-centrality parameter. The density above is equal to the non-central Wishart distribution given in (, Muirhead, 1982, Theorem 10.3.2). We see that the conditional distribution is a kind of non-central Wishart distribution, where the non-centrality parameter Ω depends on the conditioning matrix A_2. In this way, the effect of the conditioning is to change the distribution of A_1, which in the marginal case is central Wishart, to a noncentral Wishart distribution, with non-centrality parameter depending on the conditioning tensor.

As said in the introduction, this result will be used for modelling of a spatial random field of tensors, where we will estimate the parameters using composite likelihood. This application will be reported elsewhere. For that application we will need to calculate values of matrix-variate hypergeometric functions numerically. A paper giving an efficient method for summing the defining series is (Koev, Edelman, 2006), with associated matlab implementation. The paper [Butler and Wood (2003)) give a Laplace approximation for the case we need, the ${}_0\mathrm{F}_1$ function.

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