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SINGULAR RANDOM MATRIX DECOMPOSITIONS: JACOBIANS.

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Abstract

For a singular random matrix Y, we find the Jacobians associated with the following decompositions; QR, Polar, Singular Value (SVD), L´U, L´DM and modified QR (QDR). Similarly, we find the Jacobinas of the following decompositions: Spectral, Cholesky´s, L´DL and symmetric non-negative definite square root, of the cross-product matrix S = Y´Y.

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1 Introduction

During the last decades, several problems on the distribution theory for random matrices have found solutions. For example, the noncentral distributions were found using zonal polynomials or the hypergeometric function with matrix argument, James (1961) and Herz (1955). However, the case of doble noncentral distributions and those associated with eigenvalues of some specific matrices, took more time and were solved through the application of a generalization of zonal polynomials called invariant polynomials with matrix argument, Davis (1980) and Chikuse (1980). A problem that has not been solved completely is the one related to the distribution of random singular matrices, which are not unusual to find in practical and theoretical problems. For example, when we have a sample matrix $Y \in I\!\!R^{N \times m}$, with N subjects and m variables, and there is linear dependence among variables or subjects, Y will be a singular matrix. Usually this case is solved eliminating individuals or variables, accordingly. This kind of solutions was forced due to the fact of not having enough theory to deal with singular matrices. As a matter of fact, the distributions of such Y, do not exist with respect to the Lebesgue measure in $I\!\!R^{Nm}$. Recently, some distributions for singular random matrices has been established, see Uhlig (1994), Díaz-García and Gutiérrez-Jáimez (1997), Díaz-García et al. (1997) and Díaz-García and Gutiérrez-Jáimez (2001). As we can notice from those references, the main problem to determine the distributions for random matrices has been the search for a new basis and the corresponding coordinates, for the rows and the columns of Y, since as a function of the new coordinates it is possible to define the measure for which the density function of Y, will exist. To do this, it is necessary to give a factorization of Y (which it is not unique) and calculate the corresponding jacobian. This has not been an easy task, due to the natural complications of working with this kind of distributions, see Billingsley (1979, Section 19) and Spivak (1965, Chapter 5).

Formally, if Y has a distribution with respect to the Lebesgue measure, and $\mathcal{K}$ and $\mathcal{N}$, are two given subspaces, then, when we factorize Y, what we are doing is rewrite Y as a product of at least two new matrices, e.g. $Y = KN$, such that $K \in \mathcal{K}$ and $N \in \mathcal{N}$, and the main problem is to find the image of the Lebesgue measure $\nu(dY)$ defined on $I\!\!R^{Nm}$ under the mapping $(K \in \mathcal{K}) \times (N \in \mathcal{N})$. In other words, we have to find the jacobian of the transformation or equivalently, the volumen element. To work out this problem, we can find different approaches: taking derivatives element by element, Deemer and Olkin (1951), Roy (1957) and Srivastava and Khatri (1979); calculating the Gram determinant on Riemannian manifolds, which is the square of the Jacobian, Cadet (1996); by the use of matrix differential calculus and taking into account the linear structures of the transformations, Magnus (1988); or using the external product of the differential forms, James (1954) and Muirhead (1982, Chapter 2). This last method has proved to be a very powerful technique when we are

dealing with the factorization of singular random matrices and therefore we will use it here, Uhlig (1994) and Díaz-García et al. (1997).

In the present work, we extend the above ideas and some new ones, to the case in which Y has a distribution with respect to the Hausdorff measure, that is, when Y is a singular random matrix. In particular, we extend for singular matrices, the Jacobians associated with the QR, SV and Polar decompositions; also, for singular and nonsingular matrices, we propose the Jacobians associated with the modified QR, called (QDR), the $L'U$ and $L'DM$ decompositions, as well as some other decompositions closely related to these, namely: the spectral, Cholesky's, $L'DL$ and symmetric positive square root decompositions, and some of their modifications, Díaz-García and González-Farias (1999).

2   New Jacobians

Notation. Let $\mathcal{L}_{m,N}(q)$ be the linear space of all $N \times m$ real matrices of rank $q \leq \min(N, m)$; $\mathcal{L}_{m,N}^+(q)$ be the linear space of all $N \times m$ real matrices of rank $q \leq \min(N, m)$ with q distinct singular values. The set of matrices $H_1 \in \mathcal{L}_{m,N}$ such that $H_1'H_1 = I_m$ is a manifold denoted $\mathcal{V}_{m,N}$, called Stiefel manifold. In particular, $\mathcal{V}_{m,m}$ is the group of orthogonal matrices $\mathcal{O}(m)$. Denote by $\mathcal{S}_m$, the homogeneous space of $m \times m$ positive definite symmetric matrices; $\mathcal{S}_m^+(q)$, the $(mq - q(q-1)/2)$-dimensional manifold of rank q positive semidefinite $m \times m$ symmetric matrices with q distinct positive eigenvalues; $\mathcal{T}_m$ denotes the group of $m \times m$ upper triangular matrices and $\mathcal{T}_m^+$ is the group of $m \times m$ upper triangular matrices with positive diagonal elements; $\mathcal{T}_{m,N}^+$ the set of $N \times m$ upper quasi-triangular matrices such that $T = (T_1|T_2) \in \mathcal{T}_{m,N}^+$, with $T_1 \in \mathcal{T}_N^+$ and $T_2 \in \mathcal{L}_{m-N,N}(N)$; $\mathcal{T}_m^{a_{ii}}$ denote the group of $m \times m$ upper triangular matrices with fixed ith diagonal elements a_{ii} and $\mathcal{T}_{m,N}^{a_{ii}}$ the set of $N \times m$ upper quasi-triangular matrices with fixed ith elements a_{ii}; in particular if $a_{ii} = 1$ for all i, those matrices are called unit upper triangular or unit quasi-triangular matrices and are denoted by $\mathcal{T}_m^1$ and $\mathcal{T}_{m,N}^1$ respectively; $\mathcal{D}(m) \subset \mathcal{T}_m$ the diagonal matrices.

Observe that, if $X \in \mathcal{L}_{m,N}^+(q)$, we can write X as

$$X_1 = \begin{pmatrix} \underset{q \times q}{X_{11}} & \underset{q \times m-q}{X_{12}} \\ \underset{N-q \times q}{X_{21}} & \underset{N-q \times m-q}{X_{11}} \end{pmatrix} \tag{1}$$

such that $r(X_{11}) = q$. This is equivalent to the right product of the matrix X with a permutation matrix Π, (see Golub and Van Loan, 1996, section 3.4.1),

that is $X_1 = X\Pi$. Note that the external product of the elements from the differential matrix dX are not affected by the fact that we multiply X (right or left) by a permutation matrix, that is, $(dX_1) = (d(X\Pi)) = (dX)$, since Π is an orthogonal matrix. We use this fact through the different factorizations proposed in this section, i.e. the X matrix for which the factorization it is sought, it is assumed that has being pre or post (or both) multiplied by the corresponding permutation matrix, Π. Then, without loss of generality, (dX) will be defined as the external product for the differentials dx_{ij}, such that x_{ij} are mathematically independent. It is important to note that we will have $Nq + mq - q^2$ mathematically independent elements in the matrix $X \in \mathcal{L}_{m,N}^{+}(q)$, corresponding to the elements of X_{11}, X_{12} and X_{21}. Explicitly,

$$(dX) \equiv (dX_{11}) \wedge (dX_{12}) \wedge (dX_{21}) = \bigwedge_{i=1}^{N} \bigwedge_{j=1}^{q} dx_{ij} \bigwedge_{i=1}^{q} \bigwedge_{j=q+1}^{m} dx_{ij}$$

Similarly, given $S \in \mathcal{S}_m^{+}(q)$, we define (dS) as

$$(dS) \equiv \bigwedge_{i=1}^{q} \bigwedge_{j=i}^{m} ds_{ij}$$

Again, we should note that, for this case, the matrix S can be written as

$$S \equiv \begin{pmatrix} S_{11} & S_{12} \\ {\scriptstyle q\times q} & {\scriptstyle q\times m-q} \\ S_{21} & S_{22} \\ {\scriptstyle m-q\times q} & {\scriptstyle m-q\times m-q} \end{pmatrix} \qquad \text{with} \qquad r(S_{11}) = q. \tag{2}$$

such that, the number of mathematically independent elements in S are, $mq - q(q-1)/2$ corresponding to the mathematically independent elements of S_{12} and S_{11}. Recall that $S_{11} \in \mathcal{S}_m$, in such a way that S_{11} has $q(q+1)/2$, therefore,

$$(dS) \equiv (dS_{11}) \wedge (dS_{12})$$

Since we will need some of the ideas later on, we include here the results corresponding to the jacobians for the singular value and spectral decompositions.

Theorem 1 (Singular value decomposition, SVD.) *Let $X \in \mathcal{L}_{m,N}^{+}(q)$, then there exist $V_1 \in \mathcal{V}_{q,N}$, $W_1 \in \mathcal{V}_{q,m}$ and $D \in \mathcal{D}(q)$, such that $X = V_1 D W_1'$, it is called non-singular part of the SVD, Rao (1973, p. 42) and Eaton (1983, p. 58). Let $V_2 \in \mathcal{V}_{N-q,N}$ (a function of V_1) and $W_2 \mathcal{V}_{m-q,m}$ (a function of W_1) such that $V = (V_1|V_2) \in \mathcal{O}(N)$ and $W = (W_1|W_2) \in \mathcal{O}(m)$. Writing by columns, $V_1 = (v_1 \cdots v_q)$, $V_2 = (v_{q+1} \cdots v_N)$, $W_1 = (w_1 \cdots w_q)$ and $W_2 = (w_{q+1} \cdots w_m)$, we have that*

$$(dX) = 2^{-q} |D|^{N+m-2q} \prod_{i<j}^{q} (D_{ii}^2 - D_{jj}^2)(dD)(V_1' dV_1)(W_1' dW_1)$$

where $D = \mathrm{diag}(D_{11}, \ldots, D_{qq})$, $(dD) \equiv \bigwedge\limits_{i=1}^{q} dD_{ii}$, and

$$(V_1'dV_1) \equiv \bigwedge_{i=1}^{q} \bigwedge_{j=i+1}^{N} v_j'dv_i \quad and \quad (W_1'dW_1) \equiv \bigwedge_{i=1}^{q} \bigwedge_{j=i+1}^{m} w_j'dw_i$$

define an invariant measure on $\mathcal{V}_{q,N}$ and on $\mathcal{V}_{q,m}$, respectively, James (1954) and Farrell (1985)).

For a proof see Díaz-García et al. (1997).

Remark 2 When $N \geq m = q$, the Jacobian given in Theorem 1 has been studied by James (1954, Section 8.1); Roy (1957, A.6.3, p. 183); Le and Kendall (1993, Section 4.) and by Uhlig (1994, Theorem 5). In Theorem 1, observe that when $X = X'$ then $W_1 = V_1$, thus obtaining the non- singular part of the spectral decomposition of X.

Theorem 3 (Spectral decomposition.) Let $S \in \mathcal{S}_m^+(q)$, then $S = W_1 L W_1'$, where $W_1 \in \mathcal{V}_{q,m}$ and $L \in \mathcal{D}(q)$, it is called the non-singular part of the spectral decomposition, Díaz-García et al. (1997). Also, let $X \in \mathcal{L}_{m,N}^+(q)$ and write $X = V_1 D W_1'$ (SVD) and $S = X'X$. Then

(1) $(dS) = 2^{-q}|L|^{m-q}\prod\limits_{i<j}^{q}(L_{ii} - L_{jj})(dL)(W_1'dW_1)$

(2) $(dX) = 2^{-q}|L|^{(N-m-1)/2}(dS)(V_1'dV_1)$

where $L = \mathrm{diag}(L_{11}, \ldots, L_{qq})$ and $(dL) = \bigwedge\limits_{i=1}^{q} dL_{ii}$.

Remark 4 Observe that the Jacobian in Theorem 3(1) is a particular case of Theorem 1, considering the symmetry of S. This Jacobian was demonstrated by Uhlig (1994). When $m = q$, the Jacobian has been studied by James (1954, Section 8.2), James (1964, eq. (93)) (when S is Hermitian), Srivastava and Khatri (1979, p. 31) and by Muirhead (1982, pp. 104-105). Proof for Theorem 4 part(2) is given in Díaz-García et al. (1997).

The following result, becomes very handy to establish some other important results in this section, it shows the Jacobian associated with a quasi-triangular matrix when it is written as the product of a diagonal matrix and a unit quasi-triangular matrix.

Theorem 5 Let $J \in \mathcal{T}_{m,q}^+$ with $r(J) = q$ such that $J = BG$ where $B \in \mathcal{D}(q)$ and $G \in \mathcal{T}_{m,q}^{g_{ii}}$, then we have

(1) $\qquad (dJ) = \prod_{i=1}^{q} b_{ii}^{m-i} \prod_{i=1}^{q} g_{ii}(dB)(dG).$ $\hfill (3)$

(2) if $G \in \mathcal{T}_{m,q}^{1}$

$$(dJ) = \prod_{i=1}^{q} b_{ii}^{m-i}(dB)(dG). \hfill (4)$$

where $(dJ) \equiv \bigwedge_{i=1}^{q} \bigwedge_{j=i}^{m} dj_{ij}$, $(dG) \equiv \bigwedge_{i=1}^{q} \bigwedge_{j=i+1}^{m} dg_{ij}$ and $(dB) \equiv \bigwedge_{i=1}^{q} db_{ii}$.

Proof.

(1) Writing J and G by rows, B through its diagonal elements and taking the product we get,

$$J = \begin{pmatrix} J_1' \\ \vdots \\ J_q' \end{pmatrix} = \begin{pmatrix} b_{11}G_1' \\ \vdots \\ b_{qq}G_q' \end{pmatrix},$$

therefore

$$J_1 = b_{11}G_1 \quad \text{so} \quad dT_1 = db_{11}G_1 + b_{11}dG_1 \quad \text{and similarly}$$

$$J_2 = b_{22}G_2 \qquad\qquad dT_2 = db_{22}G_2 + b_{22}dG_2$$

$$\vdots \qquad\qquad\qquad\qquad \vdots$$

$$J_q = b_{qq}G_q \qquad\qquad dT_q = db_{qq}G_q + b_q dG_q$$

taking the external product of the differentials; recalling that g_{ii} are fix for all i, $i = 1, 2, \ldots, q$; and that the product of repeated differentials is zero, we get

$$(dJ_i) \equiv \bigwedge_{j=i}^{m} dt_{ij} = g_{ii} db_{ii} \wedge b_{ii}^{m-i}(dG_i)$$

with $(dG_i) \equiv \bigwedge_{j=i+1}^{m} dg_{ij}$. Finally,

$$(dJ) \equiv \bigwedge_{i=1}^{q} \bigwedge_{j=i}^{m} dt_{ij} = \bigwedge_{i=1}^{q}(dJ_i) = \prod_{i=1}^{q} g_{ii} \prod_{i=1}^{q} b_{ii}^{m-i} \bigwedge_{i=1}^{q} db_{ii} \bigwedge_{i=1}^{q}(dG_i)$$

(2) The proof follows immediately. $\qquad\qquad\qquad\qquad\qquad\qquad\blacksquare$

Remark 6 *For square full rank matrices D and G, Magnus (1988, Theorem 810, p.141) the Jacobian is given in his Theorem 5(1) by using linear structures.*

Theorem 7 [$L'U$ decomposition, Doolittle's version.] Let $X \in \mathcal{L}^+_{m,N}(q)$, and write $X = \Delta'\Upsilon$, where $\Delta \in \mathcal{T}^1_{N,q}$ and $\Upsilon \in \mathcal{T}^+_{m,q}$, Golub and Van Loan (1996, Secction 3.4.9). Then

(1) $\quad (dX) = \displaystyle\prod_{i=1}^{q} v_{ii}^{N-i}(d\Upsilon)(d\Delta)$ $\hspace{4cm}$ (5)

(2) if $\Delta \in \mathcal{T}^{\delta_{ii}}_{q,N}$

$$(dX) = \prod_{i=1}^{q} v_{ii}^{N-i} \prod_{i=1}^{q} \delta_{ii}^{m-i+1}(d\Upsilon)(d\Delta). \hspace{2cm} (6)$$

where $(d\Delta) \equiv \displaystyle\bigwedge_{i=1}^{q}\bigwedge_{j=i+1}^{m} d\delta_{ij}$, $(d\Upsilon) \equiv \displaystyle\bigwedge_{i=1}^{q}\bigwedge_{j=i}^{m} d\Upsilon_{ij}$.

Proof. We will only work the proof for part (2), since part (1) follows from (2) taking $\delta_{ii} = 1$ for all i. Let X and Δ be denoted by columns, $X = (X_1 X_2 \cdots X_q \cdots X_m)$, $\Delta = (\Delta_1 \Delta_2 \cdots \Delta_q)$, and $\Upsilon = (v_{ij})$, then,

$$
\begin{aligned}
X_1 &= v_{11}\Delta_1 \\
X_2 &= v_{12}\Delta_1 + v_{22}\Delta_2 \\
X_3 &= v_{13}\Delta_1 + v_{23}\Delta_2 + v_{33}\Delta_3 \\
&\vdots \qquad\qquad \vdots \\
X_{q-1} &= v_{1q-1}\Delta_1 + v_{2q-1}\Delta_2 + v_{3q-1}\Delta_3 + \cdots + v_{q-1q-1}\Delta_{q-1} \\
X_q &= v_{1q}\Delta_1 + v_{2q}\Delta_2 + v_{3q}\Delta_3 + \cdots + v_{qq}\Delta_q \\
X_{q+1} &= v_{1q+1}\Delta_1 + v_{2q+1}\Delta_2 + v_{3q+1}\Delta_3 + \cdots + v_{qq+1}\Delta_q \\
&\vdots \qquad\qquad \vdots \\
X_m &= v_{1m}\Delta_1 + v_{2m}\Delta_2 + v_{3m}\Delta_3 + \cdots + v_{qm}\Delta_q
\end{aligned}
$$

taking differentials and then omitting those differentials that appear previ-

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ously, we get the following expressions

$$
\begin{aligned}
dX_1 &= dv_{11}\Delta_1 + v_{11}d\Delta_1 \\
dX_2 &= dv_{12}\Delta_1 + dv_{22}\Delta_2 + v_{22}d\Delta_2 \\
dX_3 &= dv_{13}\Delta_1 + dv_{23}\Delta_2 + dv_{33}\Delta_3 + v_{33}d\Delta_3 \\
&\vdots \qquad\qquad\qquad \vdots \\
dX_{q-1} &= dv_{1q-1}\Delta_1 + dv_{2q-1}\Delta_2 + dv_{3q-1}\Delta_3 + \cdots + dv_{q-1q-1}\Delta_{q-1} \\
&\quad + v_{q-1q-1}d\Delta_{q-1} \\
dX_q &= dv_{1q}\Delta_1 + dv_{2q}\Delta_2 + dv_{3q}\Delta_3 + \cdots + dv_{qq}\Delta_q + v_{qq}d\Delta_q \\
dX_{q+1} &= dv_{1q+1}\Delta_1 + dv_{2q+1}\Delta_2 + dv_{3q+1}\Delta_3 + \cdots + dv_{qq+1}\Delta_q \\
&\vdots \qquad\qquad\qquad \vdots \\
dX_m &= dv_{1m}\Delta_1 + dv_{2m}\Delta_2 + dv_{3m}\Delta_3 + \cdots + dv_{qm}\Delta_q
\end{aligned}
$$

Taking external products of the differentials, recalling that the product of repeated differentials is zero and noticing that the differentials that appear before do not have to be taken into account again, we get,

$$
\begin{aligned}
(dX_1) &= \delta_{11}dv_{11} \wedge v_{11}^{N-1}d\Delta_1 \\
(dX_2) &= \delta_{11}dv_{12} \wedge \delta_{22}dv_{22} \wedge v_{22}^{N-2}d\Delta_2 \\
(dX_3) &= \delta_{11}dv_{13} \wedge \delta_{22}dv_{23} \wedge \delta_{33}dv_{33} \wedge v_{33}^{N-3}d\Delta_3 \\
&\vdots \qquad\qquad\qquad\qquad \vdots \\
(dX_{q-1}) &= \delta_{11}dv_{1q-1} \wedge \delta_{22}dv_{2q-1} \wedge \delta_{33}dv_{3q-1} \wedge \cdots \wedge \delta_{q-1q-1}dv_{q-1q-1} \\
&\quad \wedge v_{q-1q-1}^{N-(q-1)}d\Delta_{q-1} \\
(dX_q) &= \delta_{11}dv_{1q} \wedge \delta_{22}dv_{2q} \wedge \delta_{33}dv_{3q} \wedge \cdots \wedge \delta_{qq}dv_{qq} \wedge v_{qq}^{N-q}d\Delta_q \\
(dX_{q+1}) &= \delta_{11}dv_{1q+1} \wedge \delta_{22}dv_{2q+1} \wedge \delta_{33}dv_{3q+1} \wedge \cdots \wedge \delta_{qq}dv_{qq+1} \\
&\vdots \qquad\qquad\qquad\qquad \vdots \\
(dX_m) &= \delta_{11}dv_{1m} \wedge \delta_{22}dv_{2m} \wedge \delta_{33}dv_{3m} \wedge \cdots \wedge \delta_{qq}dv_{qm}
\end{aligned}
$$

with $d\Delta_j = \bigwedge\limits_{i=j+1}^{N} d\delta_{ij}$. Therefore,

$$
(dX) \equiv \bigwedge_{i=1}^{N}\bigwedge_{j=1}^{q} dx_{ij} \bigwedge_{i=1}^{q}\bigwedge_{j=q+1}^{m} dx_{ij} = \prod_{i=1}^{q}\delta_{ii}^{m-i+1}\prod_{i=1}^{q}v_{ii}^{N-i}\bigwedge_{i=1}^{N}\bigwedge_{j=i+1}^{q} d\delta_{ij}\bigwedge_{i=1}^{q}\bigwedge_{j=i}^{q} dv_{ij} \blacksquare
$$

Remark 8 *Note that if $\Delta \in \mathcal{T}_{N,q}^+$ and $\Upsilon \in \mathcal{T}_{m,q}^1$ in Theorem 7, we get a variant*

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of the decomposition $L'U$, known as Crout's decomposition, see Harville (1997, p.228).

Corollary 9 *[$L'U$ decomposition, Crout's version.] Let $X \in \mathcal{L}_{m,N}^{+}(q)$, such that $X = \Delta'\Upsilon$, where $\Delta \in \mathcal{T}_{N,q}^{+}$ and $\Upsilon \in \mathcal{T}_{m,q}^{1}$, see Golub and Van Loan (1996, Secction 3.4.9). Then*

(1) $$dX) = \prod_{i=1}^{q} \delta_{ii}^{m-i}(d\Upsilon)(d\Delta). \tag{7}$$

(2) If $\Upsilon \in \mathcal{T}_{q,N}^{\delta_{ii}}$

$$(dX) = \prod_{i=1}^{q} v_{ii}^{N-i+1} \prod_{i=1}^{q} \delta_{ii}^{m-i}(d\Upsilon)(d\Delta), \tag{8}$$

where $(d\Delta) \equiv \bigwedge_{i=1}^{q} \bigwedge_{j=i}^{m} d\delta_{ij}$, $(d\Upsilon) \equiv \bigwedge_{i=1}^{q} \bigwedge_{j=i+1}^{m} d\Upsilon_{ij}$.

Proof. The proof follows the steps of the one given in Theorem 7.

Theorem 10 ($L'DM$ decomposition.) *Let $X \in \mathcal{L}_{m,N}^{+}(q)$, such that $X = \Psi'\Pi\Xi$, where $\Psi \in \mathcal{T}_{N,q}^{1}$, $\Pi \in \mathcal{D}(q)$ and $\Xi \in \mathcal{T}_{m,q}^{1}$, Golub and Van Loan (1996, Secction 4.1.1). Then*

$$(dX) = \prod_{i=1}^{q} \pi_{ii}^{N+m-2i}(d\Psi)(d\Pi)(d\Xi).$$

Proof. Write $X = \Psi'\Pi\Xi = \Psi'U$ with $U = \Pi\Xi$ and observe that $U \in \mathcal{T}_{N,q}^{+}$, then, by Theorem 7

$$(dX) = \prod_{i=1}^{q} u_{ii}^{N-i}(dU)(d\Psi) \tag{9}$$

Now, $U = \Pi\Xi$, with $\Pi \in \mathcal{D}(q)$ and $\Xi \in \mathcal{T}_{m,q}^{1}$, therefore by Theorem 5,

$$(dU) = \prod_{i=1}^{q} \pi_{ii}^{m-i}(d\Pi)(d\Xi) \tag{10}$$

Note that $u_{ii} = \pi_{ii}$, since $\chi_{ii} = 1$ for all i. Therefore, substituting (10) in (9), we establish the result. ∎

Theorem 11 (QR decomposition.) *Let $X \in \mathcal{L}_{m,N}^{+}(q)$, then there exist $H_1 \in \mathcal{V}_{q,N}$ and $T \in \mathcal{T}_{m,q}$ with $t_{ii} \geq 0$, $i = 1, 2, \ldots, \min(q, N-1)$ such that*

$X = H_1T$, Golub and Van Loan (1996, Secction 5.4), Roy (1957, A.3.11, p.149) and Goodall and Mardia (1993). Then

$$(dX) = \prod_{i=1}^{q} t_{ii}^{N-i}(H_1'dH_1)(dT). \tag{11}$$

where $(dT) \equiv \bigwedge_{i=1}^{q}\bigwedge_{j=i}^{m} dt_{ij}$

Proof. Given that $X = H_1T$ we have $dX = dH_1T + H_1dT$. Let $H = (H_1 \vdots H_2)$ (H_2 a function of H_1), such that $H \in \mathcal{O}(N)$, then

$$H'dX = \begin{pmatrix} H_1'dH_1T + dT \\ H_2'dH_1T \end{pmatrix}$$

Now, observe that T can be written as $T = (T_1 \vdots T_2)$, where $T_1 \in \mathcal{T}_q$ and $T_2 \in \mathcal{L}_{m-q,q}$. Thus the demonstration reduces to the one given in Muirhead (1982, pp. 64-66), observing that

$$H_1'dH_1T = [H_1'dH_1T_1 \vdots H_1'dH_1T_2]$$

$$H_2'dH_1T = [H_2'dH_1T_1 \vdots H_2'dH_1T_2]$$

and computing the exterior product, column by column, $[H_1'dH_1T_2]$ and noticing that $[H_2'dH_1T_2]$ does not contribute at all to the exterior product, since its elements appear in previous columns. ∎

Remark 12 *When $N \geq m = q$, this result is given in Roy (1957, A.6.1, p. 170), Srivastava and Khatri (1979, Problem 1.33, p. 38), where in addition, an explicit form for the measure $(H_1'dH_1)$ is given. On the same context, Muirhead (1982, pp. 63-66) gives the demonstration under the same guidelines as the one given in James (1954, Section 8), for the SVD case. Finally, Goodall and Mardia (1993) establish, without proof, that the result is true when $q = \min(N, m)$.*

Theorem 13 (Cholesky's decomposition.) *Let $S \in \mathcal{S}_m^+(q)$, then $S = T'T$, where $T \in \mathcal{T}_{m,q}$, Golub and Van Loan (1996, p. 148). Also, let $X \in \mathcal{L}_{m,N}^+(q)$ with $X = H_1T$ (QR Decomposition) and $S = X'X = T'T$ such that*

$$S = \begin{pmatrix} \underset{q\times q}{S_{11}} & \underset{q\times m-q}{S_{12}} \\ \underset{m-q\times q}{S_{21}} & \underset{m-q\times m-q}{S_{22}} \end{pmatrix} \qquad with \qquad r(S_{11}) = q.$$

Then

(1) $(dS) = 2^q \prod_{i=1}^{q} t_{ii}^{m-i+1}(dT)$

(2) $(dX) = 2^{-q}|S_{11}|^{(N-m-1)/2}(dS)(H_1'dH_1)$

Proof.

(1) The proof is analogous to the proof of Theorem 7. Alternatively, the Jacobian may be computed via patterned matrices, (see Henderson and Searle, 1979) .

(2) Observe that we can write $T = \left(\underset{q\times q}{T_1} \vdots \underset{q\times m-q}{T_2}\right)$ then

$$S = \begin{pmatrix} \underset{q\times q}{S_{11}} & \underset{q\times m-q}{S_{12}} \\ \underset{m-q\times q}{S_{21}} & \underset{m-q\times m-q}{S_{22}} \end{pmatrix} = \begin{pmatrix} T_1' \\ T_2' \end{pmatrix} \left(T_1 \vdots T_2\right) = \begin{pmatrix} T_1'T_1 & T_1'T_2 \\ T_2'T_1 & T_2'T_2 \end{pmatrix},$$

thus, $|S_{11}| = |T_1'T_1| = |T_1|^2 = \prod_{i=1}^{q} t_{ii}^2$ and from Theorem 3.2(1), $(dT) =$ $2^{-q}\prod_{i=1}^{q} t_{ii}^{-(m-i+1)}(dS)$. Then substituting into (11), we obtain the desired result. ∎

Theorem 14 (Modified QR decomposition (QDR).) *Let* $X \in \mathcal{L}_{m,N}^{+}(q)$, *then there exist* $H_1 \in \mathcal{V}_{q,N}$, $N \in \mathcal{D}(q)$ *and* $\Omega \in \mathcal{T}_{m,q}^{1}$ *with* $\omega_{ii} \geq 0$, $i = 1, 2, \ldots, \min(q, N-1)$ *such that* $X = H_1 N\Omega$. *For this decomposition we have*

$$(dX) = 2^{-q}\prod_{i=1}^{q} n_{ii}^{N+m-2i}(H_1'dH_1)(dN)(d\Omega)$$

Proof. Write $X = H_1 Z$ with $Z = N\Omega$ and observe that $Z \in \mathcal{T}_{m,q}^{+}$, then by Theorem 11,

$$(dX) = 2^{-q}\prod_{i=1}^{q} z_{ii}^{N-i}(H_1'dH_1)(dZ). \tag{12}$$

Now, $Z = N\Omega$, and $z_{ii} = N_{ii}$, since $\omega_{ii} = 1$ for all i. By means of the Theorem 5 we get,

$$(dZ) = \prod_{i=1}^{q} n_{ii}^{m-i}(d\Omega)(dN), \tag{13}$$

so, substituting (13) in (12), the result is established. ∎

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Theorem 15 ($L'DL$ decomposition.) *Let $S \in \mathcal{S}_m^+(q)$, with $S = \Omega'O\Omega$, where $\Omega \in \mathcal{T}_{m,q}^1$ and $O \in \mathcal{D}(q)$, see Golub and Van Loan (1996, Theorem 4.2.5, p. 143 and Section 4.2.9, pp. 148-149). Write $S = X'X = \Omega'O\Omega$, such that $X = H_1 N\Omega \in\in \mathcal{L}_{m,N}^+(q)$. Then*

(1) $(dS) = \prod_{i=1}^{q} o_{ii}^{m-i}(d\Omega)(dO)$

(2) $(dX) = 2^{-q}|O|^{(N-m-1)/2}(H_1'dH_1)(dS).$

Proof.

(1) Write $S = \Omega'O\Omega = G'G$, where $G = C\Omega$, $C = O^{1/2}$ and $C \in \mathcal{T}_{m,q}^+$. Then, by Theorem 13

$$(dS) = 2^q \prod_{i=1}^{q} g_{ii}^{m-i+1}(dG). \tag{14}$$

Now, $G = C\Omega$, with $g_{ii} = c_{ii}$, since $\omega_{ii} = 1$ for all i. Then, by Theorem 5

$$(dG) = \prod_{i=1}^{q} c_{ii}^{m-i}(dC)(d\Omega) \tag{15}$$

so, substituting (15) in (14), we get,

$$(dS) = 2^q \prod_{i=1}^{q} c_{ii}^{2m-2i+1}(dC)(d\Omega). \tag{16}$$

But $C = O^{1/2}$ with $(dC) = 2^{-q}|O|^{-1/2}(dO)$ and $c_{ii} = o_{ii}^{1/2}$, from here we get the result.

(2) The proof follows from Theorem 14 and Theorem 15(1). ■

Theorem 16 (Symmetric non-negative definite square root.) *If $S \in \mathcal{S}_m^+(q)$ then there exists $R \in \mathcal{S}_m^+(q)$, such that $S = R^2$, Srivastava and Khatri (1979, p. 38), Muirhead (1982, p. 588) and Golub and Van Loan (1996, p. 148)). Thus, we have that*

$$(dS) = 2^q|D|^{m-q+1} \prod_{i<j}^{q}(D_{ii} + D_{jj})(dR) = |D|^{m-q} \prod_{i\leq j}^{q}(D_{ii} + D_{jj})(dR) \tag{17}$$

where $R = Q_1 D Q_1'$ is the spectral decomposition of R, $Q_1 \in \mathcal{V}_{q,m}$ and $D = \text{diag}(D_{11}, \ldots, D_{qq})$.

Proof. From Corollary 3, $R = Q_1 D Q_1'$ with $D = \text{diag}(D_{11}, \ldots, D_{qq})$ and

$P_1 \in \mathcal{V}_{q,m}$. Applying Theorem 3

$$(dR) = 2^{-q}|D|^{m-q} \prod_{i<j}^{q} (D_{ii} - D_{jj})(dD)(Q_1'dQ_1). \tag{18}$$

Now let $S = R^2 = RR = Q_1 D Q_1' Q_1 D q_1' = Q_1 D^2 Q_1'$, applying Corollary 3 once again, we have

$$(dS) = 2^{-q}|D^2|^{m-q} \prod_{i<j}^{q} (D_{ii}^2 - D_{jj}^2)(dD^2)(Q_1'dQ_1).$$

Observing that $(dD^2) = \prod_{i=1}^{q} 2D_{ii}(dD) = 2^q|D|(dD)$, $(D_{ii}^2 - D_{jj}^2) = (D_{ii} + D_{jj})(D_{ii} - D_{jj})$, and from (18),

$$(dS) = 2^q|D|^{m-q+1} \prod_{i<j}^{q} (D_{ii} + D_{jj}) \left[2^{-q}|D|^{m-q} \prod_{i<j}^{q} (D_{ii} - D_{jj})(Q_1'dQ_1)(dD) \right]$$

$$= 2^q|D|^{m-q+1} \prod_{i<j}^{q} (D_{ii} + D_{jj})(dR).$$

The second expression for (dS) is found observing that

$$\prod_{i \le j}^{q} (D_{ii} + D_{jj}) = \prod_{i=1}^{q} 2D_{ii} \prod_{i<j}^{q} (D_{ii} + D_{jj}). \blacksquare$$

Remark 17 *The Jacobian for the case where $S \in \mathcal{S}_m$, i.e., $q = m$, was studied by Olkin and Rubin (1964), Henderson and Searle (1979) and Cadet (1996).*

Theorem 18 (Polar decomposition.) *Let $X \in \mathcal{L}_{m,N}^+(q)$, $N \ge m$, and write $X = P_1 R$, such that, $P_1 \in \mathcal{V}_{m,N}$, and $R \in \mathcal{S}_m^+(q)$, Herz (1955), Cadet (1996) and Golub and Van Loan (1996, p. 149). Also, let $S = X'X = R^2 \in \mathcal{S}_m^+(q)$ (Non-negative definite square root). Then*

(1) $(dX) = \dfrac{|D|^{N-q}}{\text{Vol}(\mathcal{V}_{m-q,N-q})} \prod_{i<j}^{q} (D_{ii} - D_{jj})(dR)(P_1'dP_1)$

(2) $(dX) = \dfrac{2^{-q}}{\text{Vol}(\mathcal{V}_{m-q,N-q})} |L|^{(N-m-1)/2}(dS)(P_1'dP_1)$

where $L = D^2$ and $\text{Vol}(\mathcal{V}_{m-q,N-q}) = \displaystyle\int\limits_{K_1 \in \mathcal{V}_{m-q,N-q}} (K_1'dK_1) = \dfrac{2^{(m-q)}\pi^{(m-q)(N-q)/2}}{\Gamma_{m-q}[\frac{1}{2}(N-q)]}.$

Proof.

(1) From Díaz-García et al. (1997) we have that the nondegenerate density of $S = X'X$ (central case) is

$$\frac{\pi^{qN/2}|L|^{(N-m-1)/2}}{\Gamma_q[\frac{1}{2}N]\left(\prod_{i=1}^{r}\lambda_i^{K/2}\right)}h(\operatorname{tr}\Sigma^- S)(dS).$$

Let $S = R^2$, with $(dS) = 2^q|D|^{m-q+1}\prod_{i<j}^{q}(D_{ii} + D_{jj})(dR)$ and $L = D^2$ (see Theorem 16). Then

$$\frac{\pi^{qN/2}|L|^{(N-m-1)/2}}{\Gamma_q[\frac{1}{2}N]\left(\prod_{i=1}^{r}\lambda_i^{N/2}\right)}h(\operatorname{tr}\Sigma^- S)(dS)$$

$$= \frac{2^q\pi^{qN/2}|D|^{(N-q)}\prod_{i<j}^{q}(D_{ii} + D_{jj})}{\Gamma_q[\frac{1}{2}N]\left(\prod_{i=1}^{r}\lambda_i^{N/2}\right)}h(\operatorname{tr}\Sigma^- R^2)(dR)$$

denote this function as $f_R(R)$.

Now, the nondegenerate density of X $(\mu_x = 0)$ is

$$\frac{1}{\prod_{i=1}^{r}\lambda_i^{N/2}}h(\operatorname{tr}\Sigma^- X'X)(dX).$$

Let $X = P_1 R$ with Jacobian, $(dX) = \alpha(dR)(P_1 dP_1)$, where α is independent of P_1. Then the nodegenerate joint density of R, P_1 is

$$\frac{\alpha}{\prod_{i=1}^{r}\lambda_i^{N/2}}h(\operatorname{tr}\Sigma^- R^2)(dR)(P_1 dP_1).$$

Integrating with respect to $P_1 \in \mathcal{V}_{m,k}$ we have that

$$\frac{\alpha 2^m \pi^{Nm/2}}{\Gamma_m[\frac{1}{2}N]\prod_{i=1}^{r}\lambda_i^{N/2}}h(\operatorname{tr}\Sigma^- R^2)(dR).$$

denote this function as $g_R(R)$. Thus considering the quotient

$$f_R(R)/g_R(R) = 1$$

and from the fact that $\mathcal{V}_{m,N}/\mathcal{V}_{m-q,N-q} = \mathcal{V}_{m,N}$, the result follows.

(2) The result is obtained substituting (dR), from (17), in Theorem 18(1). ∎

Remark 19 *(1) The Jacobian in Theorem 13(1) was studied by Cadet (1996) when $q = m$, computing Grams determinant on riemannian manifold. In*

Cadet's notation, ds denotes the riemannian measure on $\mathcal{V}_{q,m}$ (the invariant measure on $\mathcal{V}_{q,m}$), which has the normalizing constant

$$\int\limits_{\mathcal{V}_{q,m}} ds = \frac{2^{p(p+3)/4}\pi^{qm/2}}{\Gamma_q[\frac{1}{2}m]}.$$

Which differs from the normalizing constant proposed by James (1954), for $(P_1'dP_1)$, see also Srivastava and Khatri (1979, p. 75) and Muirhead (1982, p. 70). But it is known that the invariant measure on $\mathcal{V}_{q,m}$ is unique, in the sense that if there are two invariant measures on $\mathcal{V}_{q,m}$, one is a finite multiple of the other, see James (1954) and Farrell (1985, p. 43). In particular

$$ds = 2^{p(p-1)/4}(P_1'dP_1). \tag{19}$$

From expression (19) the Jacobian in Theorem 18(2) is found, when $q = m$, with respect to the measure $(P_1'dP_1)$, any of the Jacobians studied here may be expressed as a function of the ds measure proposed by Cadet, considering the different normalizing constants (see Cadet, 1996, Remark (4)). The result given in Theorem 18(2), and also the assumption of $q = m$, was proposed (without proof) by Herz (1955).

(2) On the other hand, observe that for any of the factorizations $X = KN \in \mathcal{L}_{m,N}^+(q)$, the number of mathematically independent elements in X ($Nq + mq - q^2$), must be equal to the number of mathematically independent elements in K, plus the number of mathematically independent elements in N. For example, in the QR decomposition, $X = H_1 T$, is such that the number of mathematically independent elements in $H_1 \in \mathcal{V}_{q,N}$ is $Nq - q(q+1)/2$ (see Muirhead, 1982, p. 67) and the number of mathematically independent elements $T \in \mathcal{T}_{m,q}^+$ is $mq - q(q-1)/2$ with the sum being $Nq + mq - q^2$ the number of mathematically independent elements. On a first look, it would seem like this rule does not hold for the Polar decomposition of a singular matrix, since, if $X = P_1 R$, with $P_1 \in \mathcal{V}_{q,N}$ with $Nm - m(m+1)/2$ elements mathematically independent and $R \in \mathcal{S}_m^+(q)$ with $mq - q(q-1)/2$ elements mathematically independent, we would have that the total sum equals $Nm - m(m+1)/2 + mq - q(q-1)/2 \neq Nq + mq - q^2$ elements mathematically independent. This is due to the conditions on the dimensionality of the matrix P_1 and R, in the definition of the Polar decomposition, $P_1 \in \mathcal{V}_{m,N}$ y $R \in \mathcal{S}_m^+(q)$. Note, however that the Polar decomposition of $X \in \mathcal{L}_{m,N}^+(q)$ can be written as

$$X = P_1 R$$

$$= \left(\underset{N \times q}{P_q} \mid \underset{N \times m-q}{P_*} \right) \begin{pmatrix} \underset{q \times m}{R_1} \\ \underset{m-q \times m}{R_2} \end{pmatrix}$$

$$= P_1 R_1 + P_2 R_2 \tag{20}$$

where $P_1 = (P_q|P_*)$, $R' = (R_1'|R_2')$ are such that R_1 contains the $mq -$ $q(q-1)/2$ mathematically independent elements in R, the $m - q$ columns of P_* are arbitrary and they also are functions of the columns of P_q, that is, the mathematically independent elements in the decomposition of $X = P_1 R$, are contained on the first summand of (20). If we proceed as in the case of the QR decomposition, dropping the second summand on the equation (20) (since $T_2 = 0$), it is easy to see that the Jacobian for the Polar decomposition will be proportional to $(P_q' dP_q') \wedge)(dR_1)$. However, since the Jacobian has to be a function of P_1 and R, it will be only necessary to put $(P_q' dP_q')$, as a function of P_1, since by definition $(dR) = (dR_1)$, see equation (2). In this way, we get the proportionality constants for Theorems 18(1) and 18(2). To see this, let P_2 and P_{N-q} such that $P = (P_1|P_2) \in \mathcal{O}(N)$ and let $P = (P_q|P_{N-q}) \in \mathcal{O}(N)$, then by Lemma 9.5.3 in Muirhead (1982, p. 397),

$$(P'dP) = (P_1'dP_1) \wedge (M'dM), \text{ with } M \in \mathcal{O}(N - m) \qquad (21)$$

similarly,

$$(P'dP) = (P_q'dP_q) \wedge (A'dA), \text{ with } A \in \mathcal{O}(N - q) \qquad (22)$$

and applying again Lemma 9.5.3 in Muirhead (1982, p. 397) to $(A'dA)$ in the equation (22) we have:

$$(P'dP) = (P_q'dP_q) \wedge (B_1'dB_1) \wedge (C'dC), \qquad (23)$$

with $B_1 \in \mathcal{V}_{m-q,N-q}$ and $C \in \mathcal{O}(N - q - (m - q)) \equiv \mathcal{O}(N - m)$. Now, equating (21) and (23), we get

$$(P_1'dP_1) \wedge (M'dM) = (P_q'dP_q) \wedge (B_1'dB_1) \wedge (C'dC), \qquad (24)$$

By the uniqueness of the Haar measure on $\mathcal{O}(N - m)$, we have that $(M'dM) = (C'dC)$ therefore $(P_1'dP_1) = (P_q'dP_q) \wedge (B_1'dB_1)$, and the result is established.

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