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Derivation of the Laplace-Beltrami Operator for the Zonal Polynomials of Positive Definite Hermitian Matrix Argument

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Abstract

Some aspects of the complex linear structure theory, extending the real case due to Magnus (1988), are defined and studied. This theory provides complete proofs of conjectures given in literature around the derivation of the complex Laplace-Beltrami operator, which has the zonal polynomials of positive definite hermitian matrix argument as eigenfunctions. An explicit expression for the matrix $G(\operatorname{vec} X)$, which appears in the metric $(ds)^2 = d\operatorname{vec}^* X G(\operatorname{vec} X) d\operatorname{vec} X$, is obtained; also, the invariance of $(ds)^2$ under congruence transformations is proved. Explicit forms for $(ds)^2$ and $G(\operatorname{vec} X)$ are also derived under the spectral decomposition $X = UYU^*$.

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1 INTRODUCTION

In more than forty years the real and complex zonal polynomials have been a notable subject in statistical multivariate analysis and other areas. Their theoretical achievements and multiple possible applications have motivated different approaches for computing them in an efficient way, see Dumitriu, Edelman and Shuman (2004) and Demmel and Koev (2006). In particular, the derivation of the zonal polynomials as eigenfunctions of a Laplace-Beltrami-type operator become of interest, and in the next lines we give a summary about the literature of the complex case, which was inspired by the same method given for zonal polynomials of positive definite matrix argument. For the positive definite symmetric case, the source of the subsequent works is James (1968) (except for an error in its equation (3.9), see Díaz-García and Caro-Lopera (2006)), which was fully detailed by Muirhead (1982); and it motivated Definition 2.10 in Dumitriu, Edelman and Shuman (2004) for α-Jack polynomials and the algorithm for computing them. In such definition those polynomials are considered as the only homogeneous polynomial eigenfunctions of a Laplace-Beltrami operator indexed by the parameter α; we must recall that Jack polynomials reduce to real and complex zonal polynomials of positive definite symmetric and hermitian matrix argument when $\alpha = 2$ and $\alpha = 1$, respectively. However, no proofs or published references on the derivation of the α-Laplace-Beltrami operator are provided in Dumitriu, Edelman and Shuman (2004). Historically, a few years after the publication of James (1968), some papers conjectured the 1-Laplace-Beltrami operator and used it in further results, for example: Sugiura (1973), equation (4.16); Chikuse (1976), Lemma 2.1. But even for this case a complete study of the complex operator is not published and an extension of the detailed derivation given by Muirhead (1982) is not straightforward.

In that sense, the proposal of the present paper is to derive completely the 1-Laplace-Beltrami operator. The approach presented here is an extension of a new method, different to James (1968) and Muirhead (1982), which resulted successful not only in deriving again the 2-Laplace-Beltrami operator for the definite positive symmetric zonal polynomials, but, in deriving the semidefinite positive symmetric zonal polynomials (see Díaz-García and Caro-Lopera (2006)); this method for the general real symmetric polynomials is based in a recent theory due to Magnus (1988). However, for the extension of Magnus (1988) we required new definitions and properties of the complex linear structure theory, see for example Subsection 2.1 below, the remaining concepts are dispersed in the proofs of theorems in Section 2. Then, in Section 2 the fundamental complex linear structure elements are studied in order to express the 1-Laplace-Beltrami operator in terms of the latent roots of the Hermitian matrix; i.e, the following highlights are derived: the complex version of the operator Δ_X of Díaz-García and Caro-Lopera (2006); the invariance property of Δ_X^*; the matrix $G(\operatorname{vec} X)$, which appears in the metric $(ds)^2 = d\operatorname{vec}^* X G(\operatorname{vec} X) d\operatorname{vec} X$; the invariance of $(ds)^2$ under congruence transformations; the matrix $\tilde{D}_m$; and, explicit forms for $(ds)^2$ and $G(\operatorname{vec} X)$, under the spectral decomposition $X = UYU^*$. With this, the conjectures given in literature (Sugiura (1973), Chikuse (1976), Dumitriu, Edelman and Shuman (2004) for $\alpha = 1$) are proved; and even one of them are corrected, just compare Theorem 2.5 below with the conjectured equation (4.15) by Sugiura (1973), it seems an inherited error, derived from the error in equation (3.9) of James (1968) (see Díaz-García and Caro-Lopera (2006)).

2 ZONAL PLYNOMIALS OF POSITIVE DEFINITE HERMITIAN MATRIZ ARGUMENT

To follow this section we recommend the reading of the Laplace-Beltrami operator given in Díaz-García and Caro-Lopera (2006).

Let $X \in S_m$ an $m \times m$ positive definite Hermitian matrix, the metric differential for S_m is defined to be

$$(ds)^2 = \operatorname{tr}(X^{-1}dXX^{-1}dX), \tag{1}$$

where $dX = (dx_{ij})$. Then we have

Theorem 2.1. *Let $L \in Gl(m, \mathbb{C})$, (with $Gl(m, \mathbb{C})$ the group of non-singular complex matrices) and L^* be the conjugate transpose of L, then the metric form (1) is invariant under the congruence transformation*

$$X \to LXL^*, \tag{2}$$

Proof. Given that $dX \to LdXL^*$ then

$$\begin{aligned}(ds)^2 &= \operatorname{tr}(X^{-1}dXX^{-1}dX)\\ &\to \operatorname{tr}((LXL^*)^{-1}LdXL^*(LXL^*)^{-}LdXL^*))\\ &= \operatorname{tr}(LX^{-1}L^*LdXL^*LX^{-1}L^*LdXL^*)\\ &= \operatorname{tr}(X^{-1}dXX^{-1}dX)\end{aligned}$$

which proves the invariance or $(ds)^2$. ■

Now, we present the complex version of the linear structure approach given in section 3 of Díaz-García and Caro-Lopera (2006).

We start with the complex operator Δ_X, see Díaz-García and Caro-Lopera (2006) and Muirhead (1982, eq. (24), p. 240):

Theorem 2.2. *Let X an $m \times m$ definite positive Hermitian matrix, then the complex version of the operator Δ_X of Díaz-García and Caro-Lopera (2006) is*

$$\Delta_X^* = (\det(X))^m \frac{\partial^*}{\partial \operatorname{vec} X}\left((\det(X))^{-m}(X \otimes X)\frac{\partial}{\partial \operatorname{vec} X}\right). \tag{3}$$

where $\det(X)$ is the determinant of X, $\operatorname{vec} X$ is the vectorization of X and $\otimes$ denotes the Kronecker product, see Muirhead (1982) and Magnus (1988).

Proof. The quadratic form $(ds)^2$ can be written in terms of a certain matrix $G(\cdot)$ as follows:

$$\begin{aligned}(ds)^2 &= \operatorname{tr}(X^{-1}dXX^{-1}dX)\\ &= d\operatorname{vec}^* X\left(X^{-1}\otimes X^{-1}\right)d\operatorname{vec}X\\ &= d\operatorname{vec}^* XG(\operatorname{vec}X)d\operatorname{vec}X\end{aligned}$$

Then

$$\begin{aligned}\det G(\operatorname{vec}X) &= \det\left(X^{-1}\otimes X^{-1}\right)\\ &= (\det X)^{-m}(\det X)^{-m}\\ &= (\det X)^{-2m}\end{aligned}$$

and

$$\begin{aligned}G^{-1}(\operatorname{vec}X) &= \left(X^{-1}\otimes X^{-1}\right)^{-1}\\ &= X\otimes X\end{aligned}$$

By substituting $\det G(\operatorname{vec}X)$ and $G^{-1}(\operatorname{vec}X)$ in the general definition of the operator Δ_X^* given in Muirhead (1982), (eq. (24), p.240), we obtain the required result.

■

As in the real case we have the invariance property of Δ_X^*:

Theorem 2.3. *The operator Δ_X^* in (3) is invariant under the congruence transformation (2), this is: for $L\in Gl(m,\mathbb{C})$ we have that $\Delta_X^*=\Delta_{LXL^*}^*$*

Proof. Take $Z=LXL^*$ and note that $\operatorname{vec}Z=(L\otimes L)\operatorname{vec}X$, then $d\operatorname{vec}Z=(L\otimes L)d\operatorname{vec}X$.

Besides,

$$\frac{\partial}{\partial\operatorname{vec}X}=(L\otimes L)^*\frac{\partial}{\partial\operatorname{vec}Z}\quad\text{or}\quad\frac{\partial}{\partial\operatorname{vec}Z}=(L\otimes L)^{*-1}\frac{\partial}{\partial\operatorname{vec}X},$$

Thus

$$\begin{aligned}G(\operatorname{vec}Z) &= G((L\otimes L)\operatorname{vec}X)\\ &= (LXL^*)^{-1}\otimes(LXL^*)^{-1}\\ &= L^{*-1}X^{-1}L^{-1}\otimes L^{*-1}X^{-1}L^{-1}\\ &= (L\otimes L)^{*-1}(X^{-1}\otimes X^{-1})(L\otimes L)^{-1}\end{aligned}$$

Then,

$$\begin{aligned}\det(G(\operatorname{vec}Z)) &= (\det(L^*\otimes L^*))^{-1}\det(X^{-1}\otimes X^{-1})(\det(L\otimes L))^{-1}\\ &= (\det(L^*L\otimes L^*L))^{-1}\det(X^{-1}\otimes X^{-1})\\ &= (\det(L^*L))^{-m}(\det(L^+L))^{-m}(\det(X))^{-2m}\\ &= (\det(L^*L))^{-2m}(\det(X))^{-2m}\end{aligned}$$

And

$$\begin{aligned} G^{-1}(\operatorname{vec} Z) &= ((L\otimes L)^{*-1}(X^{-1}\otimes X^{-1})(L\otimes L)^{-1})^{-1} \\ &= (L\otimes L)(X\otimes X)(L\otimes L)^{*} \end{aligned}$$

Thus we get the required invariance, because

$$\begin{aligned} \Delta_Z^* &= \Delta_{LXL^*}^* \\ &= (\det(G(\operatorname{vec} Z)))^{-1/2}\frac{\partial^*}{\partial \operatorname{vec} Z}\left[(\det(G(\operatorname{vec} X)))^{1/2}\ G^{-1}(\operatorname{vec} Z)\frac{\partial}{\partial \operatorname{vec} Z}\right] \\ &= (\det(L^*L))^m(\det(X))^m\frac{\partial^*}{\partial \operatorname{vec} X}(L\otimes L)^{-1}\Big[((\det(L^*L))^{-m} \\ &\qquad (\det(X))^{-m}(L\otimes L)(X\otimes X)(L\otimes L)^*(L\otimes L)^{*-1}\frac{\partial}{\partial \operatorname{vec} X}\Big] \\ &= (\det X)^m\frac{\partial^*}{\partial \operatorname{vec} X}\left[(\det(X))^{-m}(L\otimes L)(X\otimes X)\frac{\partial}{\partial \operatorname{vec} X}\right] \\ &= \Delta_X^* \end{aligned}$$

■

Now if we proceed as Díaz-García and Caro-Lopera (2006) in the real case, we arrive at the following result

Theorem 2.4. *Let U be an unitary matrix, i.e. $U^*U = UU^* = I_m$ and consider the spectral decomposition of X given by $X = UYU^*$, with $Y = \operatorname{diag}(y_1,\dots,y_m)$, then*

$$(ds)^2 = d^*\operatorname{vec} Y(Y^{-1}\otimes Y^{-1})d\operatorname{vec} Y - 2d^*\operatorname{vec}\Theta((Y\otimes Y^{-1}) - I_{m^2})d\operatorname{vec}\Theta \qquad (4)$$

Proof. Using the invariance of the metric and the spectral decomposition of X we obtain

$$\begin{aligned} (ds)^2 &= \operatorname{tr}(X^{-1}dXX^{-1}dX) \\ &= \operatorname{tr}((UYU^*)^{-1}d(UYU^*)(UYU^*)^{-1}d(UYU^*)); \end{aligned}$$

following the same procedure presented in Díaz-García and Caro-Lopera (2006) for the real case ($U = H \in \mathcal{O}(m)$ group of orthogonal matrices) and noting that $\operatorname{tr} A = \operatorname{tr} A^*$, $\operatorname{tr} AB = \operatorname{tr} BA$, the metric takes the form

$$(ds)^2 = 2\operatorname{tr}(U^*dUU^*dU) + \operatorname{tr}(Y^{-1}dYY^{-1}dY) - 2\operatorname{tr}(Y^{-1}U^*dUYU^*dU),$$

where we used the fact that $U^*dU = -dU^*U$, because $U^*U = I_m$ and by differentiation $dU^*U + U^*dU = 0$; so $U^*dU = -dU^*U = -(U^*dU)^*$ and it means that U^*dU is an skew-Hermitian matrix. See Khatri (1965, (iv), p.99), (observe that $B^* = dB$ in Khatri's notation).

So, if we denote $U^*dU = d\Theta$ we get the desired result

$$\begin{aligned}
(ds)^2 &= \operatorname{tr}(Y^{-1}dYY^{-1}dY) - 2\operatorname{tr}(Y^{-1}U^*dUYU^*dU) + 2\operatorname{tr}(U^*dUU^*dU)\\
&= \operatorname{tr}(Y^{-1}dYY^{-1}dY) - 2\operatorname{tr}(Y^{-1}d\Theta Y d\Theta) + 2\operatorname{tr}(d\Theta d\Theta)\\
&= d^*\operatorname{vec}Y(Y^{-1}\otimes Y^{-1})d\operatorname{vec}Y - 2d^*\operatorname{vec}\Theta(Y\otimes Y^{-1})d\operatorname{vec}\Theta\\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad +2d^*\operatorname{vec}\Theta d\operatorname{vec}\Theta\\
&= d^*\operatorname{vec}Y(Y^{-1}\otimes Y^{-1})d\operatorname{vec}Y - 2d^*\operatorname{vec}\Theta((Y\otimes Y^{-1}) - I_{m^2})d\operatorname{vec}\Theta
\end{aligned}$$

■

2.1 THE MATRIX $\tilde{D}_m$

To reach the main result: the matrix $G(w(Y))$, we need to define new topics on complex linear structure (see Magnus (1988) for the real case) . We start with the matrix $\tilde{D}_m$.

Definition 2.1. Let A be an $m \times m$ skew-Hermitian matrix, then the matrix $\tilde{D}_m$ is defined from the decomposition of $\operatorname{vec} A$, and $\tilde{\mathbf{v}}(A)$,i.e

$$\operatorname{vec} A = \tilde{D}_m\tilde{\mathbf{v}}(A) \tag{5}$$

and

$$\tilde{\mathbf{v}}(A) = \tilde{D}_m^+\operatorname{vec} A \tag{6}$$

Here, the action of $\tilde{D}_m^+$ over $\operatorname{vec} A$ just removes from $\operatorname{vec} A$ the elements a_{ii}, $i = 1, \ldots, m$.

Note that for our propose we do not need something else for $\tilde{D}_m$, because all the calculations can be expressed as function of $\tilde{D}_m$ and this is the foundation for the linear structure of the skew-symmetric matrices (see Magnus (1988),p.94), i.e. we just need to apply twice the computation of $\tilde{D}_m\tilde{\mathbf{v}}(A)$, knowing that the diagonal and the under-diagonal elements of a skew-Hermitian matrix are mathematically independent.

2.2 THE MATRIX $G(\cdot)$

Now, we have all the tools for finding the main matrix $G(\cdot)$. Extending the result of real linear structure, we see that if Y is a diagonal matrix, then $\operatorname{vec} Y = \psi_m^*\,\mathbf{w}(Y)$ (see Magnus (1988), p.109 and Díaz-García and Caro-Lopera (2006)) and knowing that Θ is skew-Hermitian, then $\operatorname{vec}\Theta = \tilde{D}_m\tilde{\mathbf{v}}(\Theta)$ for a matrix $\tilde{D}_m : m^2 \times m(m-1)$, because an unitary matrix U has $m^2 - m = m(m-1)$ independently mathematical elements, the same ones of Θ. So the metric form $(ds)^2$ in (4) can be written as follows

$$(ds)^2 = d^*\,\mathbf{w}(Y)\psi_m(Y^{-1}\otimes Y^{-1}\psi_m^* d\,\mathbf{w}(Y) - 2d^*\tilde{\mathbf{v}}(\Theta)\tilde{D}_m^*((Y\otimes Y^{-1} - I_{m^2}))\tilde{D}_m d\tilde{\mathbf{v}}(\Theta)$$

$$= \quad (d^{*}\,\mathbf{w}(Y)\ d^{*}\tilde{\mathbf{v}}(\Theta)) \begin{pmatrix} \psi_m(Y^{-1}\otimes Y^{-1})\psi_m^{*} & 0 \\ 0 & -2\tilde{D}_m^{*}((Y\otimes Y^{-1})-I_{m^2})\tilde{D}_m) \end{pmatrix} \begin{pmatrix} d\,\mathbf{w}(Y) \\ d\tilde{\mathbf{v}}(\Theta) \end{pmatrix}$$

$$= \quad (d\,\mathbf{w}^{*}(Y)\ d^{*}\tilde{\mathbf{v}}(\Theta))G(\mathbf{w}(Y)) \begin{pmatrix} d\,\mathbf{w}(Y) \\ d\tilde{\mathbf{v}}(\Theta) \end{pmatrix}.$$

Thus,

$$G(\mathbf{w}(Y)) = \begin{pmatrix} \psi_m(Y^{-1}\otimes Y^{-1})\psi_m^{*} & 0 \\ 0 & -2\tilde{D}_m^{*}((Y\otimes Y^{-1})-I_{m^2})\tilde{D}_m) \end{pmatrix}; \tag{7}$$

by Magnus (1988), p.113, Th. 7.7 (i):

$$\psi_m(Y^{-1}\otimes Y^{-1})\psi_m^{*} = Y^{-1}\odot Y^{-1} = \operatorname{diag}(y_1^{-2},\dots,y_m^{-2}),$$

then

$$\det(\psi_m(Y^{-1}\otimes Y^{-1})\psi_m^{*}) = \prod_{i=1}^{m} y_i^{-2}. \tag{8}$$

For finding an explicit expression of the matrix $-2\tilde{D}_m^{*}((Y\otimes Y^{-1})-I_{m^2})\tilde{D}_m$ let us take a look at the (skew-Symmetric) real case proved in Díaz-García and Caro-Lopera (2006):

$$-2\tilde{D}_m'((Y\otimes Y^{-1})-I_{m^2})\tilde{D}_m =$$

$$\operatorname{diag}\left[\left(\frac{2(y_i-y_j)^2}{y_iy_j}\right), 1\le j<i\le m\right] \in \Re^{\frac{1}{2}m(m-1)\times\frac{1}{2}m(m-1)}. \tag{9}$$

That matrix considers only the mathematically independent elements lying under the main diagonal.

Similarly, if we take in count the mathematically independent elements above the diagonal, we obtain the required complex version to be

$$M = -2\tilde{D}_m^{*}((Y\otimes Y^{-1})-I_{m^2})\tilde{D}_m =$$

$$\operatorname{diag}\left\{\begin{array}{ll} \dfrac{2(y_i-y_j)^2}{y_iy_j}, & 1\le j<i\le m \\ \dfrac{2(y_j-y_i)^2}{y_iy_j}, & 1\le i<j\le m \end{array}\right\} \in \Re^{m(m-1)\times m(m-1)}, \tag{10}$$

(except for a permutation of the diagonal elements).

By permuting the elements of the diagonal we have

$$\begin{aligned} M &= \operatorname{diag}\left[\frac{2(y_1-y_2)^2}{y_1y_2}, \frac{2(y_1-y_3)^2}{y_1y_3}, \dots, \frac{2(y_1-y_m)^2}{y_1y_m},\right. \\ &\qquad \frac{2(y_2-y_1)^2}{y_2y_1}, \frac{2(y_2-y_3)^2}{y_2y_3}, \dots, \frac{2(y_2-y_m)^2}{y_2y_m}, \dots, \\ &\qquad \left.\frac{2(y_m-y_1)^2}{y_my_1}, \frac{2(y_m-y_2)^2}{y_my_2}, \dots, \frac{2(y_m-y_{m-1})^2}{y_my_{m-1}}\right] \end{aligned}$$

Thus

$$G(\mathbf{w}(Y)) = \begin{pmatrix} \operatorname{diag}(y_1^{-2}, \dots, y_m^{-2}) & 0 \\ 0 & M \end{pmatrix} = \operatorname{diag}(y_1^{-2}, \dots, y_m^{-2}) \oplus M, \qquad (11)$$

where $\bigoplus$ denotes the direct sum of two matrices, see Srivastava and Khatri (1979), p.3, i.e $A \oplus B = \operatorname{diag}(A, B) = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}$ Then,

$$G(\mathbf{w}(Y))^{-1} = \operatorname{diag}(y_1^2, \dots, y_m^2) \oplus M^{-1},$$

where

$$\begin{aligned} M &= \operatorname{diag}\left[\frac{y_1y_2}{2(y_1-y_2)^2}, \frac{y_1y_3}{2(y_1-y_3)^2}, \dots, \frac{y_1y_m}{2(y_1-y_m)^2},\right. \\ &\qquad \frac{y_2y_1}{2(y_2-y_1)^2}, \frac{y_2y_3}{2(y_2-y_3)^2}, \dots, \frac{y_2y_m}{2(y_2-y_m)^2}, \dots, \\ &\qquad \left.\frac{y_my_1}{2(y_m-y_1)^2}, \frac{y_my_2}{2(y_m-y_2)^2}, \dots, \frac{y_my_{m-1}}{2(y_m-y_{m-1})^2}\right] \end{aligned}$$

Finally, we collect the highlights of the operator $\Delta^*_{X=UYU^*}$ in the following result:

Theorem 2.5. *1.*

$$\begin{aligned} G(\mathbf{w}(Y)) &= \operatorname{diag}(y_1^{-2}, \dots, y_m^{-2}) \oplus \\ &\qquad \operatorname{diag}\left(\frac{2(y_1-y_2)^2}{y_1y_2}, \frac{2(y_1-y_3)^2}{y_1y_3}, \dots, \frac{2(y_1-y_m)^2}{y_1y_m},\right. \\ &\qquad \frac{2(y_2-y_1)^2}{y_2y_1}, \frac{2(y_2-y_3)^2}{y_2y_3}, \dots, \frac{2(y_2-y_m)^2}{y_2y_m}, \dots, \\ &\qquad \left.\frac{2(y_m-y_1)^2}{y_my_1}, \frac{2(y_m-y_2)^2}{y_my_2}, \dots, \frac{2(y_m-y_{m-1})^2}{y_my_{m-1}}\right), \end{aligned}$$

2.

$$G(\mathbf{w}(Y))^{-1} = \operatorname{diag}(y_1^2, \dots, y_m^2) \oplus \operatorname{diag}\left(\frac{y_1y_2}{2(y_1-y_2)}, \dots, \frac{y_my_{m-1}}{2(y_m-y_{m-1})}\right)$$

and

3.

$$\det(G(\mathbf{w}(Y)))^{1/2} = \prod_{i=1}^{m} y_i^{-m} \prod_{i<j} 2(y_i - y_j)^2$$

We emphasize that expression (3) is not the same one proposed by Sugiura (1973) in equation (4.15). In fact it is an inherited error, derived from the error in equation (3.9) of James (1968), see Díaz-García and Caro-Lopera (2006).

Then, collecting the above results, we have proved exhaustively that the 1-Laplace-Beltrami operator, which has the complex zonal polynomials as eigenfunction, is given by

$$\Delta = \sum_{i=1}^{m} y_i^2 \frac{\partial^2}{\partial y_i^2} + 2\sum_{i=1}^{m} \sum_{j=1(j\neq i)}^{m} y_i^2 (y_i - y_j)^{-1} \frac{\partial}{\partial y_i} + (2-m)\sum_{i=1}^{m} y_i \frac{\partial}{\partial y_i}, \qquad (12)$$

see: Sugiura (1973), equation (4.16); Chikuse (1976), Lemma 2.1; Dumitriu, Edelman and Shuman (2004), Definition 2.10 with $\alpha = 1$.

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