The Annals of Mathematical Statistics
1968, Vol. 39, No. 5, 1711–1718

CALCULATION OF ZONAL POLYNOMIAL COEFFICIENTS BY USE OF THE LAPLACE-BELTRAMI OPERATOR

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1. Summary. The zonal polynomials of the positive definite real symmetric matrices, which appear in the expansions of the functions occurring in many multivariate non null distributions and moment formulae are eigenfunctions of the Laplace Beltrami operator. The resulting differential equation gives a recurrence relation between the coefficients from which they can be calculated.

2. Introduction. Many multivariate distributions involve functions which can be expanded in zonal polynomials. Examples are the distributions of the latent roots of the covariance matrix, (James (1960)), the non central distribution of the latent roots in multiple discriminant analysis (Constantine (1963) and for a special case, James (1961b)), the distributions of the canonical correlation coefficients (Constantine (1966)), the non central multiple correlation matrix (Srivastava (1968), the non central multivariate F or Studentized Wishart distribution (James (1964)), the non central Hotelling's T_0^2 (Constantine (1966)), and other test criteria (Khatri and Pillai (1968)), the distribution of the largest and smallest root of a Wishart distribution or a multivariate beta distribution (Constantine (1963), (1968) Sugiama (1966), (1967a), (1967b) and Pillai (1967)), and distributions of quadratic functions (Khatri (1966) and Hayakawa (1966)).

A number of moments of statistics in multivariate analysis are also expressible in zonal polynomials, such as the non central moments of the generalized variance (Herz (1955)), and likelihood ratio criterion (Constantine (1963)), non central moments of Hotelling's T_0^2 (Constantine (1966)), and other test criteria (Khatri and Pillai (1968)).

Zonal polynomials have been studied by Hua (1963) and James (1961). For a definition of them, see James (1964). They are a particular case of spherical functions, a general theory of which is given in Helgason (1962).

3. The Laplace Beltrami operator. From its group theoretic-nature, a zonal polynomial must be an eigenfunction of the Laplace Beltrami operator (see Helgason (1962) p. 387 equation (4)).

$$\Delta = (\det G)^{-\frac{1}{2}} \textstyle\sum_{k=1}^{n} (\partial/\partial x_k)\, (\det G)^{\frac{1}{2}} \sum_{i=1}^{n} g^{ik} (\partial/\partial x_i) \tag{3.1}$$

where $x_1, \cdots, x_n$ are coordinates of a point in a space with metric differential form

$$(ds)^2 = \textstyle\sum_{i=1}^{n} \sum_{j=1}^{n} g_{ij}\, dx_i\, dx_j\,; \tag{3.2}$$

$$G = (g_{ij}) \qquad \text{and} \qquad (g^{ij}) = G^{-1}. \tag{3.3}$$

Received 11 December 1967.

Maass (1955) has shown that the metric differential form on the space of $m \times m$ positive definite symmetric matrices X which is invariant under congruence transformation

$$X \to LXL' \tag{3.4}$$

where L is a $m \times m$ nonsingular matrix, is

$$(ds)^2 = \operatorname{tr}(X^{-1}\,dXX^{-1}\,dX). \tag{3.5}$$

If we write

$$X = HYH' \tag{3.6}$$

with H orthogonal and $Y = \operatorname{diag}(y_i)$, then the metric differential form becomes

$$\operatorname{tr}(Y^{-1}\,dYY^{-1}\,dY) + \text{terms in } dH \quad \text{and hence} \tag{3.7}$$

$$G = \left[\begin{array}{cccc|c} y_1^{-2} & & & 0 & \\ & \cdot & & & \\ & & \cdot & & 0 \\ & & & \cdot & \\ 0 & & & y_m^{-2} & \\ \hline & & 0 & & \begin{array}{c}\text{terms} \\ \text{in } dH\end{array} \end{array}\right] \tag{3.8}$$

Also we have

$$(\det G)^{\frac{1}{2}} = \text{invariant volume element} \tag{3.9}$$

$$= \textstyle\prod_{i=1}^m y_i^{-\frac{1}{2}(m+1)} \prod_{i<j}^m (y_i - y_j)\,(dH)$$

where (dH) is the invariant measure on the orthogonal group $O(m)$, as we know from derivations of latent roots distributions.

Thus

$$g^{ii} = y_i^2, \tag{3.10}$$

and

$$g^{ij} = 0, \qquad i \neq j. \tag{3.11}$$

On substituting in the part of the Laplace Beltrami operator concerned with the roots, we have

$$\Delta = \sum [y_i^2(\partial^2/\partial y_i^2) - \tfrac{1}{2}(m-3)y_i(\partial/\partial y_i) + \textstyle\sum_{j=1,\,j\neq i}^m y_i^2\,(y_i - y_j)^{-1}\,(\partial/\partial y_i)]. \tag{3.12}$$

4. Eigenvalues and differential equation. Now any homogeneous polynomial of degree k is an eigenfunction of Euler's operator

$$\sum y_i(\partial/\partial y_i) \tag{4.1}$$

with eigenvalue k, hence if we leave this term out of (3.12), we merely change the eigenvalue. Thus the zonal polynomials must be eigenfunctions of the operator

$$\sum_{i=1}^{n} y_i^2(\partial^2/\partial y_i^2) + \sum_{i=1}^{m} \sum_{j=1, j\neq i}^{m} y_i^2(y_i - y_j)^{-1} (\partial/\partial y_i). \tag{4.2}$$

The zonal polynomial $C_\kappa(Y)$ is of the form

$$C_\kappa(Y) = c_\kappa y_1^{k_1} y_2^{k_2} \cdots y_m^{k_m} + \text{terms of lower weight.} \tag{4.3}$$

For a discussion of weights of monomials see e.g. James (1964) p. 491.

On applying the operator (4.2) to the monomial $y_1^{k_1} \cdots y_m^{k_m}$ of highest weight, and comparing coefficients, we see that the eigenvalue is

$$\sum k_i(k_i + m - i - 1). \tag{4.4}$$

Hence the zonal polynomial satisfies the differential equation

$$\sum y_i^2(\partial^2/\partial y_i^2)C_\kappa(Y) + \sum_{i,j=1, i\neq j}^{m} y_i^2(y_i - y_j)^{-1}(\partial/\partial y_i)C_\kappa(Y) - \sum k_i(k_i + m - i - 1)C_\kappa(Y) = 0. \tag{4.5}$$

5. Recurrence relations. The term

$$\sum y_i^2(\partial^2/\partial y_i^2) \tag{5.1}$$

is weight preserving and its effect on a monomial

$$y_1^{l_1} \cdots y_m^{l_m} \tag{5.2}$$

is simply to multiply it by

$$\sum_{i=1}^{m} l_i(l_i - 1). \tag{5.3}$$

The effect of the operator

$$\sum_{i,j=1, i\neq j}^{m} y_i^2(y_i - y_j)^{-1}(\partial/\partial y_i) \tag{5.4}$$

can be seen by considering the expression

$$\begin{aligned}(y_i - y_j)^{-1}(y_i^2(\partial/\partial y_i) - y_j^2(\partial/\partial y_j))(y_i^{l_i}y_j^{l_j} + y_i^{l_j}y_j^{l_i}) &= l_i\{y_i^{l_i}y_j^{l_j} + \text{symmetric terms}\} \\ &\quad + (l_i - l_j)\{y_i^{l_i-1}y_j^{l_j+1} + \text{symmetric terms}\} \\ &\quad + (l_i - l_j)\{y_i^{l_i-2}y_j^{l_j+2} + \text{symmetric terms}\} \\ &\quad + \cdots .\end{aligned} \tag{5.5}$$

It can be seen that the operator multiplies the monomial (5.2) by

$$\sum l_i(m - i), \tag{5.6}$$

and adds on $(l_i - l_j)$ times the monomial

$$y_1^{l_1} \cdots y_i^{l_i - r} \cdots y_j^{l_j + r} \cdots y_m^{l_m} \tag{5.7}$$

for any such admissible monomials.

The recurrence relation determines the zonal polynomial uniquely once a normalizing constant, such as the coefficient of the term of highest weight is given.

The recurrence relation betweens the coefficients C_λ, C_μ of the monomial symmetric functions M_λ, M_μ which corresponds to the differential equation is thus

$$c_\lambda = \sum_\mu ((l_i + r) - (l_j - r))c_\mu(\rho_\kappa - \rho_\lambda)^{-1} \tag{5.8}$$

where

$$\rho_\lambda = \sum_{i=1}^m l_i(l_i - i), \qquad \lambda = (l_1 \cdots l_m), \tag{5.9}$$

and

$$\mu = (l_1 \cdots l_i + r \cdots l_j - r \cdots l_m) \tag{5.10}$$

for all r such that, when the partition μ is arranged in descending order, μ is above λ and below or equal to κ. The summation is over all such μ, including possibly, non descending ones.

In calculating the polynomials, it is convenient to use a polynomial $Z_\kappa(Y)$ with a different normalization constant, which is given in terms of $C_\kappa(Y)$ by the equation

$$C_\kappa(Y) = [\chi_{[2\kappa]}(1)2^k k!/(2k)!]Z_\kappa(Y) \tag{5.11}$$

from James (1964) equation (18) p. 478, where the symbol $\chi_{[2\kappa]}(1)$ is defined. From equations (18) and (132) (ibid.), the coefficient of the monomial of highest weight

$$y_1^{k_1}y_2^{k_2} \cdots y_m^{k_m}, \tag{5.12}$$

and thus of the monomial symmetry function

$$M_\kappa(Y) = y_1^{k_1}y_2^{k_2} \cdots y_m^{k_m} + \text{symmetric terms}, \tag{5.13}$$

in $Z_\kappa(Y)$ is

$$2^k \prod_{l=1}^{p} \prod_{i=1}^{l} (\tfrac{1}{2}l - \tfrac{1}{2}(i-1) + k_i - k_l)_{k_l - k_{l+1}} \tag{5.14}$$

where p is the number of non zero parts in the partition

$$\kappa = (k_1 k_2 \cdots k_m). \tag{5.15}$$

6. Example of the calculation of a zonal polynomial. Suppose we wish to calculate $Z_{(41)}$.

From equation (5.14), we have

$$Z_{(41)} = 120 y_1^4 y_2 + \text{terms of lower weight}. \tag{6.1}$$

From formula (5.9), we have the values of ρ

(6.2)							
	partition	41	32	31^2	$2^2 1$	21^3	1^5
	ρ	11	6	3	0	-4	-10.

Hence the coefficient of

$$M_{(32)} = y_1^3 y_2^2 + \text{symmetric terms} \tag{6.3}$$

is given by

$$(4 - 1)/(11 - 6) \times 120 = 72. \tag{6.4}$$

Now the coefficient of $M_{(31^2)}$ comes from the partitions (410), (401) and (320) and is thus

$$\tfrac{1}{8}(2 \times 4 \times 120 + 2 \times 72) = 138.$$

Continuing in this way, we have

$$Z_{(41)} = 120M_{(41)} + 72M_{(32)} + 138M_{(31^2)} + 108M_{(2^21)} + 126M_{(21^3)} + 120M_{(1^5)}\,.$$

The coefficient of the last term $M_{(1^k)}$ in Z_κ seems to be $k!$ and serves as a check.

7. The case of order two. This case is essentially treated by Helgason (1962) pp. 405–406. He deals with the spherical functions of the real 2×2 unimodular group, which are the same as our zonal polynomials with a power of the determinant, y_1y_2, factored out. To show the connection, we shall transform our differential equation to agree with his.

In the case of order 2, the differential equation (4.5) for the zonal polynomial $C_{(k_1k_2)}\begin{bmatrix} y_1 & \\ & y_2 \end{bmatrix}$ becomes

$$\begin{aligned} y_1^2(\partial^2C/\partial y_1^2) + y_2^2(\partial^2C/\partial y_2^2) + (y_1 - y_2)^{-1}(y_1^2(\partial C/\partial y_1) \\ - y_2^2(\partial C/\partial y_2)) - [k_1^2 + k_2(k_2 - 1)]C = 0. \end{aligned} \tag{7.1}$$

Put

$$\begin{aligned} a_1 &= y_1 + y_2 \\ a_2 &= y_1y_2\,, \end{aligned} \tag{7.2}$$

and the differential equation becomes

$$\begin{aligned} (a_1^2 - 2a_2)(\partial^2C/\partial a_1^2) + 2a_1a_2(\partial^2C/\partial a_1\partial a_2) + 2a_2^2(\partial^2C/\partial a_2^2) \\ + a_1(\partial C/\partial a_1) + a_2(\partial C/\partial a_2) - [k_1^2 + k_2(k_2 - 1)]C = 0. \end{aligned} \tag{7.3}$$

Now substitute

$$\begin{aligned} u &= \tfrac{1}{2}a_1a_2^{-\frac{1}{2}}, \\ v &= a_2^{\frac{1}{2}}, \end{aligned} \tag{7.4}$$

and upon multiplying by (-2), we have

$$\begin{aligned} (1 - u^2)(\partial^2C/\partial u^2) - v^2(\partial^2C/\partial v^2) - 2u(\partial C/\partial u) \\ + 2[k_1^2 + k_2(k_2 - 1)]C = 0. \end{aligned} \tag{7.5}$$

Since the differential equation is homogeneous in v, we substitute

$$C = v^k P(u). \tag{7.6}$$

Then $P(u)$ satisfies the equation

$$(1 - u^2)\,(d^2P/du^2) - 2u\,(dP/du) + \rho(\rho + 1)P = 0 \tag{7.7}$$

where $\rho = k_1 - k_2$. This agrees with Helgason's equation (16) p. 405 except for the sign of $\rho(\rho + 1)$.

The solution which is regular at $u = 1$, is the Legendre function of the first kind

$$P_\rho(u) = (2\pi)^{-1} \int_0^{2\pi} (u + (u^2 - 1)^{\frac{1}{2}} \cos t)^\rho \, dt. \tag{7.8}$$

Hence

$$C_{(k_1k_2)}\left(\begin{bmatrix} y_1 & \\ & y_2 \end{bmatrix}\right) / C_{(k_1k_2)}(I_2) = (y_1 y_2)^{\frac{1}{2}k} P_{k_1-k_2}\left(\tfrac{1}{2}(y_1 + y_2)(y_1 y_2)^{-\frac{1}{2}}\right) \tag{7.9}$$

From Erdelyi et al. (1953) p. 150 equation (15), we have the formulae for the Legendre polynomials $P_{k_1-k_2}(u)$ as

$$P_{2n} = (-1)^n (2n)!(2^{2n}(n!)^2)^{-1} {}_2F_1(-n, n + \tfrac{1}{2}; \tfrac{1}{2}; u^2) \quad \text{for} \quad k_1 - k_2 = 2n \tag{7.10}$$

and

$$P_{2n+1} = (-1)^n (2n + 1)!(2^{2n}(n!)^2)^{-1} u \, {}_2F_1(-n, n + \tfrac{3}{2}; \tfrac{3}{2}; u^2) \quad \text{for} \quad k_1 - k_2 = 2n + 1. \tag{7.11}$$

For integral k_1 and k_2, this agrees with the formula (130) of James (1964). For non integral values of k_1 and k_2, whether real or complex, the function on the right hand side of (7.9) is the zonal function of an infinite dimensional representation of the group.

8. Conclusions. Formulae (5.14) and (5.8) show that the coefficients of zonal polynomials are all positive when expressed in terms of monomial symmetric functions and hence that the zonal polynomials are positive on the domain of positive definite symmetric matrices. The formulae would appear to give the best method so far known, of programing the calculation of the zonal polynomials on the computer.

The coefficients of the polynomials are listed up to order 5 in the appendix. They check against the coefficients given in James (1964) for the polynomials expressed as sums of powers and elementary symmetric functions.

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APPENDIX

Zonal polynomials Z_κ in terms of monomial symmetric functions. M_κ defined by equation (5.13).

	1st degree	
$Z_{(1)}$	$M_{(1)}$	

	2nd degree	
$Z_{(2)}$	$3M_{(2)} + 2M_{(1^2)}$	
$Z_{(1^2)}$	$2M_{(1^2)}$	

3rd degree	$M_{(3)}$	$M_{(21)}$	$M_{(1^3)}$
$Z_{(3)}$	15	9	6
$Z_{(21)}$		4	6
$Z_{(1^3)}$			6

4th degree

M	(4)	(31)	(2^2)	(21^2)	(1^4)
$Z_{(4)}$	105	60	54	36	24
$Z_{(31)}$		18	12	22	24
$Z_{(2^2)}$			24	16	24
$Z_{(21^2)}$				10	24
$Z_{(1^4)}$					24

5th degree

M	(5)	(41)	(32)	(31^2)	(2^21)	(21^3)	(1^5)
$Z_{(5)}$	945	525	450	300	270	180	120
$Z_{(41)}$		120	72	138	108	126	120
$Z_{(32)}$			72	48	88	96	120
$Z_{(31^2)}$				42	28	78	120
$Z_{(2^21)}$					40	60	120
$Z_{(21^3)}$						36	120
$Z_{(1^5)}$							120