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# CALCULATION OF ZONAL POLYNOMIALS OF 3×3 POSITIVE DEFINITE SYMMETRIC MATRICES

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## Abstract

A zonal polynomial identity is derived and is used to construct algorithms for the calculation of the zonal polynomials of $2\times 2$ and $3\times 3$ positive definite symmetric matrices.

## 1. Introduction

Many multivariate distributions involve functions which can be expanded in series of zonal polynomials. Examples of these are the noncentral distribution of the latent roots in multiple discriminant analysis, and the distribution of the canonical correlation coefficients, both of which were derived by Constantine [1]. The expository paper by James [3] and also the book by Johnson and Kotz [5] provide a large number of additional examples together with the definition and various properties of zonal polynomials. Thus, we see that explicit formulae or algorithms to calculate zonal polynomials are of extreme importance in multivariate analysis. So far there are three kinds of methods developed for calculating the zonal polynomial coefficients for general orders and degrees: (i) the method using the Young symmetrizer, James [2]; (ii) the method using the orthogonality relation satisfied by the zonal polynomial coefficients, James [3]; and (iii) the method using Laplace-Beltrami operator, James [4]. Parkhurst and James [6] have tabulated zonal polynomials of order 1 through 12. However, explicit formulae are available only for the special zonal polynomials corresponding to the highest and lowest partitions and for the case of order 2, see James [3], [4].

In this paper, we obtain a zonal polynomial identity which is used to construct algorithms for the calculation of zonal polynomials of $2\times 2$ and $3\times 3$ positive definite symmetric matrices.

## 2. A zonal polynomial identity

Throughout the paper, we shall use the following notation: $S$ is a $p\times p$ positive definite symmetric matrix with latent roots $\lambda_1, \lambda_2, \cdots, \lambda_p$; $s_j=\lambda_1^j+\cdots+\lambda_p^j$ $(j=1, 2, \cdots)$ are the power sums of the latent roots; $C_\kappa(S)$ is the zonal polynomials of $S$ corresponding to the partition $\kappa=(k_1, k_2, \cdots, k_p)$ of an integer $k$ such that $k_1\geqq\cdots\geqq k_p\geqq 0$ and $k_1+\cdots+k_p=k$. Also,

$$(\alpha)_k=\alpha(\alpha+1)\cdots(\alpha+k-1)\ ,$$

and for each partition $\kappa$ of $k$,

$$(\alpha)_\kappa=\prod_{i=1}^{p}\left(\alpha-\frac{1}{2}(i-1)\right)_{k_i}\ .$$

THEOREM. *For any real (or complex) number* $\alpha$,

$$\sum_\kappa (\alpha)_\kappa C_\kappa(S)=k!\sum_{\nu_1+2\nu_2+\cdots+k\nu_k=k}\frac{(\alpha s_1)^{\nu_1}}{\nu_1!}\frac{(\alpha s_2/2)^{\nu_2}}{\nu_2!}\cdots\frac{(\alpha s_k/k)^{\nu_k}}{\nu_k!} \tag{2.1}$$

*where the sum on the left-hand side of* (2.1) *is taken over all partitions* $\kappa$ *of* $k$, *while the sum on the right is over all non-negative integral* $\nu_1, \cdots, \nu_k$ *such that* $\nu_1+2\nu_2+\cdots+k\nu_k=k$.

PROOF. Consider the generating function

$$g(t)=\sum_{k=0}^{\infty}\frac{t^k}{k!}\sum_\kappa(\alpha)_\kappa C_\kappa(S)\ . \tag{2.2}$$

The series converges if the maximum of the absolute values of the characteristic roots of $tS$ is less than one. Then, Constantine [1] has shown that

$$g(t)=|I_p-tS|^{-\alpha}\ , \tag{2.3}$$

where $I_p$ denotes the identity matrix of order $p$. Therefore,

$$\ln g(t)=-\alpha\ln|I-tS|=\alpha\left\{t\ \mathrm{tr}\,(S)+\frac{t^2}{2}\mathrm{tr}\,(S^2)+\frac{t^3}{3}\mathrm{tr}\,(S^3)+\cdots\right\}$$

and hence,

$$g(t)=\exp(\alpha t s_1)\exp(\alpha t^2 s_2/2)\exp(\alpha t^3 s_3/3)\cdots\ . \tag{2.4}$$

Expanding each of the exponentials in (2.4) as a power series in $t$ and taking Cauchy products, we obtain

$$g(t)=\sum_{k=0}^{\infty}t^k\sum_{\nu_1+2\nu_2+\cdots+k\nu_k=k}\frac{(\alpha s_1)^{\nu_1}}{\nu_1!}\frac{(\alpha s_2/2)^{\nu_2}}{\nu_2!}\cdots\frac{(\alpha s_k/k)^{\nu_k}}{\nu_k!} \tag{2.5}$$

and the result is obtained by equating the coefficient of $t^k$ in (2.2) and (2.5).

Since $\alpha$ can be chosen arbitrarily, then to calculate $C_\kappa(S)$ for a particular partition $\kappa$, we simply choose $\alpha$ such that $(\alpha)_\zeta=0$ for all $\zeta\neq\kappa$, and $(\alpha)_\kappa\neq 0$. Substituting this value of $\alpha$ on both sides of (2.1) would then yield $C_\kappa(S)$ in terms of the power sums of the latent roots of $S$. Unfortunately, this method does not work in general, since there are only two such values, viz. $\alpha=1/2$ and $\alpha=-1$. Using these values, we obtain

(2.6) $$C_{(k)}(S)=f(1/2, k)/(1/2)_{(k)}$$

and

(2.7) $$C_{(1^k)}(S)=f(-1, k)/(-1)_{(1^k)}$$

where $f(\alpha, k)$ denotes the right-hand side of (2.1), while $(k)$ and $(1^k)$ are the partitions of $k$ having one and $k$ non-zero entries respectively. We note that (2.6), given in James ([3], p. 493), was obtained by Ruben [7], and that the $f(\alpha, k)$ can be easily calculated using the following recurrence relations

$$f(\alpha, 0)=1\ ;\quad f(\alpha, k)=(k-1)!\alpha\sum_{r=0}^{k-1} s_{k-r}f(\alpha, r)/r!\ ,\qquad k\geqq 1\ .$$

Let us now consider various values of $k$ ($<p$). When $k=1$, (2.1) reduces to

$$\alpha C_{(1)}(S)=f(\alpha, 1)=\alpha s_1$$

and hence, $C_{(1)}(S)=s_1$. For $k=2$, the partitions are (2) and $(1^2)$, and $C_{(2)}(S)$, $C_{(1^2)}(S)$ are as given in (2.6) and (2.7) respectively with $k=2$. When $k=3$, the partitions are (3), (21) and $(1^3)$. $C_{(3)}(S)$ and $C_{(1^3)}(S)$ are already given in (2.6) and (2.7), and using the fact that

(2.8) $$\sum_\kappa C_\kappa(S)=s_1^k\ ,$$

it follows that

(2.9) $$C_{(21)}(S)=s_1^3-C_{(3)}(S)-C_{(1^3)}(S)\ .$$

Note that (2.8) is a direct consequence of (2.1), since ${}_0F_0(S)=\lim_{n\to\infty} {}_1F_0(n; (1/n)S)$. One could also obtain $C_{(21)}(S)$ by substituting any value of $\alpha$ such that $(\alpha)_{(21)}=\alpha(\alpha+1)(\alpha-1/2)\neq 0$ into (2.1) and solving the resulting equation with the aid of (2.6) and (2.7).

When $k=4$, the partitions are (4), (31), $(2^2)$, $(21^2)$, $(1^4)$. As usual, $C_{(4)}(S)$ and $C_{(1^4)}(S)$ are known from (2.6), (2.7). Let $\alpha_1$, $\alpha_2$, $\alpha_3$ be any three different values of $\alpha$. Then from (2.1), we have the system of equations

$$
\begin{pmatrix} (\alpha_1)_{(31)} & (\alpha_1)_{(2^2)} & (\alpha_1)_{(21^2)} \\ (\alpha_2)_{(31)} & (\alpha_2)_{(2^2)} & (\alpha_2)_{(21^2)} \\ (\alpha_3)_{(31)} & (\alpha_3)_{(2^2)} & (\alpha_3)_{(21^2)} \end{pmatrix} \begin{pmatrix} C_{(31)}(S) \\ C_{(2^2)}(S) \\ C_{(21^2)}(S) \end{pmatrix} = \begin{pmatrix} f(\alpha_1, 4) - (\alpha_1)_{(4)} C_{(4)}(S) - (\alpha_1)_{(1^4)} C_{(1^4)}(S) \\ f(\alpha_2, 4) - (\alpha_2)_{(4)} C_{(4)}(S) - (\alpha_2)_{(1^4)} C_{(1^4)}(S) \\ f(\alpha_3, 4) - (\alpha_3)_{(4)} C_{(4)}(S) - (\alpha_3)_{(1^4)} C_{(1^4)}(S) \end{pmatrix} . \tag{2.10}
$$

One can easily check that there is no unique solution to (2.10), since the matrix on the left-hand side is of rank 2. Thus, (2.1) fails to generate the zonal polynomials corresponding to the partitions (31), $(2^2)$ and $(21^2)$. When $k$ exceeds 4, the same problem arises and (2.1) alone cannot generate the zonal polynomials corresponding to any partitions of $k$ except for $(k)$ and $(1^k)$, which are as given in (2.6) and (2.7). Even use of (2.1) along with the results on some weighted sum of zonal polynomials given by Sugiura [8] failed to generate the zonal polynomials.

## 3. Calculation of zonal polynomials of 2×2 matrices

We take $k=2m$ or $2m+1$ according as $k$ is even or odd. In this case, the possible partition of $k$ are

$$
\begin{aligned}
&(k), (k-1, 1), (k-2, 2), \cdots, (m, m) , && \text{if } k=2m . \\
&(k), (k-1, 1), (k-2, 2), \cdots, (m+1, m) , && \text{if } k=2m+1 .
\end{aligned}
$$

In either case, i.e., $k$ even or odd, the zonal polynomials can be successively obtained by substituting the values $\alpha=1/2, -1/2, -3/2, \cdots, -(2m-1)/2$ into (2.1). Then, we obtain the system of equations

$$
\begin{pmatrix} (1/2)_{(k)} & 0 & 0 & \cdots & \cdots 0 \\ (-1/2)_{(k)} & (-1/2)_{(k-1,1)} & 0 & \cdots & \cdots 0 \\ (-3/2)_{(k)} & (-3/2)_{(k-1,1)} & (-3/2)_{(k-2,2)} & 0 & \cdots 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ ((1-2m)/2)_{(k)} & ((1-2m)/2)_{(k-1,1)} & ((1-2m)/2)_{(k-2,2)} & \cdots & ((1-2m)/2)_{(k-m,m)} \end{pmatrix} \begin{pmatrix} C_{(k)}(S) \\ C_{(k-1,1)}(S) \\ C_{(k-2,2)}(S) \\ \cdots \\ \cdots \\ C_{(k-m,m)}(S) \end{pmatrix} = \begin{pmatrix} f(1/2, k) \\ f(-1/2, k) \\ f(-3/2, k) \\ \cdots \\ \cdots \\ f((1-2m)/2, k) \end{pmatrix} \tag{3.1}
$$

and the zonal polynomials can now be easily obtained since the matrix on the left-hand side of (3.1) is lower triangular. For various special cases, we have used the recurrence relation

$$s_k = s_1 s_{k-1} - (s_1^2 - s_2)s_{k-2}/2\ , \qquad k=3, 4, \cdots \tag{3.2}$$

to verify that the polynomials obtained from (3.1) coincide with those given by James [3].

## 4. Calculation of zonal polynomials of 3×3 matrices

The possible partitions of $k$ are

$$(k), (k-1, 1), (k-2, 2), (k-2, 1^2), (k-3, 3), \cdots, (m, m, m)\ , \qquad \text{if } k=3m\ .$$

$$(k), (k-1, 1), (k-2, 2), \cdots, (m+1, m, m)\ , \qquad \text{if } k=3m+1\ .$$

$$(k), (k-1, 1), (k-2, 2), \cdots, (m+1, m+1, m)\ , \qquad \text{if } k=3m+2\ .$$

As before, we observe that (2.1) alone cannot generate the zonal polynomials for any partition of $k$ except for $(k)$. Fortunately, if we now use the identity given by James ([3], eg. (129)), then it turns out that all the polynomials can be generated recursively by again substituting different values of $\alpha$ into (2.1). The procedure is as follows:
(a) First find the zonal polynomials corresponding to the partitions of $k$ into three parts by using James' identity

$$C_{(k_1, k_2, k_3)}(S) = \frac{\chi_{\{2k_1, 2k_2, 2k_3\}}(1)2^{6k_3}(k!)(2k_1+2k_2-4k_3)!}{\chi_{\{2k_1-2k_3, 2k_2-2k_3\}}(1)6^{k_3}(2k)!(k_1+k_2-2k_3)!} \cdot \prod_{i=1}^{3}\left(2-\frac{1}{2}i+k_i-k_3)_{k_3}(s_1^3-3s_1s_2+2s_3)^{k_3}\right) \cdot C_{(k_1-k_3, k_2-k_3)}(S) \tag{4.1}$$

where

$$\chi_{\{k_1, k_2, k_3\}}(1) = k! \prod_{i<j}^{3}(k_i-k_j-i+j)\Big/\prod_{i=1}^{3}(k_i+3-i)!\ , \tag{4.2}$$

and we note that the zonal polynomial $C_{(k_1-k_3, k_2-k_3)}(S)$ will certainly be known before. In particular, when $k_2=k_3$, then (4.1) reduces to

$$C_{(k_1, k_2, k_2)}(S) = \chi_{\{2k_1, 2k_2, 2k_2\}}(1)\frac{2^{6k_2}(k!)(2k_1-2k_2)!(k_1-k_2+3/2)_{k_2}}{6^{k_2}(2k)!(k_1-k_2)!(1/2)_{k_1-k_2}} \cdot (1)_{k_2}(1/2)_{k_2}(s_1^3-3s_1s_2+2s_3)^{k_2}f(1/2, k_1-k_2)\ . \tag{4.3}$$

(b) The remaining zonal polynomials are successively obtained by substituting the values $\alpha=1/2, -1/2, -3/2, \cdots, -(k-1)/2$ if $k$ is even, or $\alpha=1/2, -1/2, \cdots, -(k-2)/2$ if $k$ is odd into (2.1). This technique will yield the zonal polynomials in terms of $s_1, s_2, \cdots, s_k$ but the recurrence relation

$$s_k = s_1 s_{k-1} - \frac{1}{2}(s_1^2 - s_2)s_{k-2} + \frac{1}{6}(s_1^3 - 3s_1s_2 + 2s_3)s_{k-3} . \tag{4.4}$$

$k=4, 5, \cdots$, can be used to express the results in terms of $s_1, s_2, s_3$.

To illustrate the above procedure we now consider the cases $k=4, 5$, since for $k=1$, 2 and 3, the zonal polynomials are given in Section 2. When $k=4$, the partitions are (4), (31), $(2^2)$, and $(21^2)$. Using (4.3), we have

$$C_{(21^2)}(S) = \frac{8}{9}\{s_1^4 - 3s_1^2 s_2 + 2s_1s_3\} .$$

Now, by substituting the values $\alpha=1/2, -1/2, -3/2$ into (2.1) and using (4.4), we get

$$\begin{aligned} C_{(4)}(S) &= f(1/2, 4)/(1/2)_4 \\ &= \frac{1}{105}\{s_1^4 + 12s_1^2s_2 + 12s_2^2 + 32s_1s_3 + 48s_4\} \\ &= \frac{1}{35}\{3s_1^4 - 12s_1^2s_2 + 12s_2^2 + 32s_1s_3\} , \end{aligned}$$

$$\begin{aligned} C_{(31)}(S) &= \frac{1}{(-1/2)_3(-1)}\{f(-1/2, 4) - (-1/2)_4 C_{(4)}(S) \\ &\qquad - (-1/2)_2(-1)(-3/2)C_{(21^2)}(S)\} \\ &= \frac{1}{63}\{-4s_1^4 + 156s_1^2s_2 - 72s_2^2 - 80s_1s_3\} , \end{aligned}$$

$$\begin{aligned} C_{(2^2)}(S) &= \frac{1}{(-3/2)_2(-2)_2}\{f(-3/2, 4) - (-3/2)_4 C_{(4)}(S) \\ &\qquad - (-3/2)_3(-2)C_{(31)}(S) - (-3/2)_2(-2)(-5/2)C_{(21^2)}(S)\} \\ &= \frac{1}{315}\{28s_1^4 + 168s_1^2s_2 + 252s_2^2 - 448s_1s_3\} . \end{aligned}$$

Note that $C_{(2^2)}(S)$ could have been obtained by using (2.8). For $k=5$, the partitions are (5), (41), (32), $(31^2)$ and $(2^21)$. From (4.1), we have

$$\begin{aligned} C_{(2^21)}(S) &= \frac{4}{3}(s_1^3 - 3s_1s_2 + 2s_3)C_{(1^2)}(S) \\ &= \frac{8}{9}\{s_1^5 - 4s_1^3s_2 + 2s_1^2s_3 + 3s_1s_2^2 - 2s_2s_3\} . \end{aligned}$$

Using (4.3), we get

$$C_{(31^2)}(S)=\frac{20}{9}(s_1^3-3s_1s_2+2s_3)f(1/2,\,2)$$
$$=\frac{5}{9}\{s_1^5-s_1^3s_2+2s_1^2s_3-6s_1s_2^2+4s_2s_3\}\;.$$

Substituting the values $\alpha=1/2,\,-1/2,\,-3/2$ into (2.1) and using (4.4), we have

$$C_{(5)}(S)=\frac{1}{3\cdot5\cdot7\cdot9}\{s_1^5+20s_1^3s_2+80s_1^2s_3+60s_1s_2^2+240s_1s_4+160s_2s_3+384s_5\}$$
$$=\frac{1}{63}\{7s_1^5-36s_1^3s_2+48s_1^2s_3+12s_1s_2^2+32s_2s_3\}\;,$$

$$C_{(41)}(S)=\frac{1}{(-1/2)_4(-1)}\{f(-1/2,\,5)-(-1/2)_5C_{(5)}(S)$$
$$-(-1/2)_3(-1)(-3/2)C_{(31^2)}(S)\}$$
$$=\frac{1}{9}\{-s_1^5+9s_1^3s_2+6s_1^2s_3+6s_1s_2^2-20s_2s_3\}\;,$$

$$C_{(32)}(S)=\frac{1}{(-3/2)_3(-2)_2}\{f(-3/2,\,5)-(-3/2)_5C_{(5)}(S)-(-3/2)_4(-2)C_{(41)}(S)$$
$$-(-3/2)_3(-2)(-5/2)C_{(31^2)}(S)-(-3/2)_2(-2)_2(-5/2)C_{(2^21)}(S)\}$$
$$=\frac{1}{63}\{-28s_1^5+232s_1^3s_2-272s_1^2s_3-12s_1s_2^2+80s_2s_3\}\;.$$

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