Commun. Fac. Sci. Univ. Ank. Series A1
V. 49. pp. 117 - 122 (2000)

SPECTRAL DECOMPOSITION OF DISPERSION MATRIX FOR THE MIXED ANALYSIS OF VARIANCE MODEL

B. GÜVEN

Department of Statistics, Middle East Technical University 06531, Ankara Turkey.

(Received June 27, 2000; Accepted Oct. 11, 2000)

ABSTRACT

The spectral decomposition of the variance-covariance matrix for a balanced mixed analysis of variance model is presented. The model consists of crossed and/or nested factors with either replicated or nonreplicated.

1. INTRODUCTION

The spectral decomposition of a variance-covariance matrix (dispersion matrix) **V** is useful for finding its powers $\mathbf{V}^{\alpha}$ where α is any real number. In particular, $\alpha=-1$, $\mathbf{V}^{-1}$is useful for estimation or $\alpha=-\frac{1}{2}$, $\mathbf{V}^{-1/2}$ is useful for the transforming a linear model to a model with i.i.d. error terms.

The problem has been discussed before by Searle and Henderson [1] and Wansbeek and Kapteyn [2]. In both studies, it is supposed that the form of the spectral decomposition of **V** is of the same form of **V**. Then they obtained idempotent matrices in the spectral decomposition of **V** by equating **V** and its assumed spectral decomposition.

However our solution is based on deriving an idempotent matrix from eigenvectors for the corresponding eigenvalue in the spectral decomposition of **V** without assuming any form of the spectral decomposition of **V**.

2. THE DISPERSION MATRIX

The variance-covariance matrix **V** for a balanced k-factor mixed analysis of variance model is of the following structure

$$\mathbf{V}=\sum_{\mathbf{d}}\boldsymbol{\lambda}_{\mathbf{d}}\mathbf{N}_{\mathbf{d}} \tag{1}$$

where $\mathbf{d}$ is a k-vector of zeros and ones. The summation is taken over 2^k -elements. The $\lambda_\mathbf{d}$ are nonnegative parameters. Let $\mathbf{d}=(i_1,i_2,\ldots,i_k)$ with i_r or 1 for r=1,2...k. Then the matrix $\mathbf{N_d}$ in (1) are defined as

$$\mathbf{N_d}=\mathbf{J}_1^{i_1}\otimes\mathbf{J}_2^{i_2}\otimes\ldots\otimes\mathbf{J}_k^{i_k}$$

with $\mathbf{J}_r^0=\mathbf{I}_r$, where $\mathbf{J}_r$ and $\mathbf{I}_r$ are respectively a matrix of ones and an identity matrix of order n_r for r=1,2,...,k, the symbol $\otimes$ denotes the Kronecker product of matrices.

The full rank of (1), leading that all eigenvalues of (1) are nonzero, is provided by $\mathbf{N}_{00\ldots00}=\mathbf{I}_{12\ldots k}$ where $\mathbf{I}_{12\ldots k}$ is an identity matrix of order $\prod_{r=1}^k n_r$. A linear space generated by the columns of (1) is the sum of linear subspaces generated by the columns of 2^k matrices of order $\prod_{r=1}^k n_r$ given by $\mathbf{I}_{12\ldots k},\mathbf{N}_{00\ldots01},\ldots,\mathbf{N}_{11\ldots11}$ and then is spanned by the set of basis $\mathbf{I}_{12\ldots k},\mathbf{N}_{00\ldots01},\ldots,\mathbf{N}_{11\ldots11}$. However the basis for any $\mathbf{N}_{i_1i_2\ldots i_k}$ are the linear combination of the basis for $\mathbf{I}_{12\ldots k}$. As a result, a linear space generated by the columns of (1) is spanned by the set of basis for $\mathbf{I}_{12\ldots k}$.

3. THE SPECTRAL DECOMPOSIITION

Let $t_1,t_2,\ldots,t_k$ be denoted by $\mathbf{t}$ with $t_r=0$ or 1. The 2^k (possibly) distinct eigenvalues of (1) given by [1] are:

$$\phi_\mathbf{t}=\sum_\mathbf{d}\lambda_\mathbf{d}x_{t_1}^{i_1}x_{t_2}^{i_2}\ldots x_{t_k}^{i_k} \tag{2}$$

with multiplicity $\prod_{r=1}^k(n_r-1)^{1-t_r}$ and where $x_{t_r}^{i_r}$ is the eigenvalue of the matrix $\mathbf{J}_r^{i_r}$ given by

$$x_{t_r}^{i_r}=\begin{cases}0 & \text{if } t_r=0\\ n_r & \text{if } t_r=1\end{cases}$$

with multiplicity $(n_r-1)^{1-t_r}$ if $i_r=1$. $x_{t_r}^{i_r}=1$ for $t_r=0{,}1$ with multiplicity n_r if $i_r=0$.

An eigenvector $\mathbf{v}_{t_r}$ for $x_{t_r}^{i_r}$ will be:

$$\mathbf{v}_{t_r}=\begin{cases}\xi_{n_rk} \quad k=1,2,\ldots,n_r-1 & \text{if } t_r=0\\ \\ \frac{1}{\sqrt{n_r}}\mathbf{1}_r & \text{if } t_r=1\end{cases} \tag{3}$$

and $\xi_{n_r1},\xi_{n_r2},\ldots,\xi_{n_rn_r-1},\frac{1}{\sqrt{n_r}}\mathbf{1}_r$ is an orthonormal set, $\mathbf{1}_r$ is a $n_r\times1$ vector of ones.

Let

$$\nu_\mathbf{t}=\mathbf{v}_{t_1}\otimes\mathbf{v}_{t_2}\otimes\ldots\otimes\mathbf{v}_{t_k}. \tag{4}$$

Then ν_t is an eigenvector for ϕ_d in (2) since $J_r^{i_r} v_{t_r} = x_{t_r}^{i_r} v_{t_r}$ and

$$N_d \nu_t = (J_1^{i_1} \otimes J_2^{i_2} \otimes \ldots \otimes J_k^{i_k})(v_{t_1} \otimes v_{t_2} \otimes \ldots \otimes v_{t_k})$$
$$= J_1^{i_1} v_{t_1} \otimes J_2^{i_2} v_{t_2} \otimes \ldots \otimes J_k^{i_k} v_{t_k}$$
$$= x_{t_1}^{i_1} v_{t_1} \otimes x_{t_2}^{i_2} v_{t_2} \otimes \ldots \otimes x_{t_k}^{i_k} v_{t_k} = (x_{t_1}^{i_1} x_{t_2}^{i_2} \ldots x_{t_k}^{i_k})(v_{t_1} \otimes v_{t_2} \otimes \ldots \otimes v_{t_k}).$$

Consequently,

$$V\nu_t = \sum_d \lambda_d N_d \nu_t = \phi_t \nu_t .$$

Let $P_{t_r} = v_{t_r} v'_{t_r}$ for r=1,2,...,k where v_{t_r} in (3) is an eigenvector of $J_r^{i_r}$ and $M_t = \nu_t \nu'_t$ where ν_t in (4) is an eigenvector of (1). Then both P_{t_r} and M_t are idempotent matrices and the spectral decomposition of (1) is:

$$V = \sum_t \phi_t M_t$$

where

$$M_t = P_{t_1} \otimes P_{t_2} \otimes \ldots \otimes P_{t_r} \tag{5}$$

with

$$P_{t_r} = \begin{cases} \sum_{\ell=1}^{n_r-1} \xi_{n_r\ell} \xi'_{n_r\ell} & \text{if} \quad t_r = 0 \\ \frac{1}{n_r} J_r & \text{if} \quad t_r = 1 \end{cases} \tag{6}$$

Consider a matrix $I_r + J_r$ having eigenvalues 1 with multiplicity $n_r - 1$ and $1 + n_r$ and the respective orthonormal eigenvectors $\xi_{n_r\ell}, \ell = 1,2,\ldots,n_r - 1$ for 1 and $1/\sqrt{n_r}\, 1_r$. Then the spectral decomposition of $I_r + J_r$ is:

$$I_r + J_r = \sum_{\ell=1}^{n_r-1} \xi_{n_r\ell} \xi'_{n_r\ell} + (1+n_r)\frac{1}{n_r} J_r \tag{7}$$

Using (7),(6) can be rewritten as:

$$P_{t_r} = \begin{cases} I_r - \frac{1}{n_r} J_r & \text{if} \quad t_r = 0 \\ \frac{1}{n_r} J_r & \text{if} \quad t_r = 1 \end{cases} \tag{8}$$

where the rank of P_{t_r} is $(n_r - 1)^{1-t_r}$. From (5) with (8), it can be seen that M_t has rank $\sum_{r=1}^{k} (n_k - 1)^{1-t_r}$ and $M_t M_{t^*} = 0$ for $t \neq t^*$.

Consider a mixed model representing an experiment that is replicated n_k-times. (1) can be rewritten as

$$\mathbf{V} = \lambda_{00\ldots00}\mathbf{I}_n + \sum_{\mathbf{d}} \lambda_{\mathbf{d}}\mathbf{N}_{\mathbf{d}}\,. \tag{9}$$

since $\lambda_{00\ldots00}$ is positive and $\lambda_{t_1t_2\ldots t_{k-1}0}$ is zero for at least one of nonzero t_r where $r=1,2,\ldots,k-1$. Here $\mathbf{d}=(i_1i_2\ldots i_{k-1})$ with $i_r=0$ for $r=0,1,\ldots k-1$, the summation on the right hand side of (9) is taken over 2^{k-1}-elements and

$$\mathbf{N}_{\mathbf{d}} = \mathbf{J}_1^{i_1}\otimes\mathbf{J}_2^{i_2}\otimes\ldots\otimes\mathbf{J}_{k-1}^{i_{k-1}}\otimes\mathbf{J}_k\,.$$

It follows that (2) can be:

$$\phi_{\mathbf{t}} = \lambda_{00\ldots00}\sum_{\mathbf{d}}\lambda_{\mathbf{d}}x_1^{i_1}x_2^{i_2}\ldots x_{k-1}^{i_{k-1}}x_k \tag{10}$$

From (10), $\phi_{t_1t_2\ldots t_{k-1}0} = \lambda_{00\ldots00}$ with multiplicity

$$(n_k-1)\sum_{t_1t_2\ldots t_{k-1}=0}^{1}\prod_{r=1}^{k-1}(n_r-1)^{1-t_r} = (n_k-1)\prod_{r=1}^{k-1}n_r\,.$$

So 2^{k-1}-eigenvalues of (9) are the same and equal to the smallest eigenvalue $\lambda_{00\ldots00}$. The corresponding idempotent matrix for $\lambda_{00\ldots00}$ will be

$$\mathbf{M}_{k-1}\otimes(\mathbf{I}_r - \frac{1}{n_r}\mathbf{J}_r)$$

where a matrix $\mathbf{M}_{k-1}$ of order $\prod_{r=1}^{k-1}n_r$ is:

$$\mathbf{M}_{k-1} = \sum_{t_1t_2\ldots t_{k-1}=0}^{1}\mathbf{P}_{t_1}\otimes\mathbf{P}_{t_2}\otimes\ldots\otimes\mathbf{P}_{t_{k-1}}$$

with

$$\begin{aligned}\mathrm{rank}(\mathbf{M}_{k-1}) &= \sum_{t_1t_2\ldots t_{k-1}=0}^{1}\mathrm{rank}(\mathbf{P}_{t_1})\mathrm{rank}(\mathbf{P}_{t_2})\ldots\mathrm{rank}(\mathbf{P}_{t_{k-1}})\\ &= \sum_{t_1t_2\ldots t_{k-1}=0}^{1}\prod_{r=1}^{k-1}(n_r-1)^{1-t_r} = \prod_{r=1}^{k-1}\sum_{t_r=0}^{1}(n_k-1)^{1-t_r} = \prod_{r=1}^{k-1}n_r\,.\end{aligned}$$

Then $\mathbf{M}_{k-1}$ is an identity matrix since the full rank idempotent matrix is unique and equal to an identity matrix.

The eigenvalue of (9) is of the form

$$\phi^*_{t_1t_2\ldots t_{k-1}} = \phi_{t_1t_2\ldots t_{k-1}1} = \lambda_{00\ldots00} + n_k\sum_{\mathbf{d}}\lambda_{\mathbf{d}}x_{t_1}^{i_1}x_{t_2}^{i_2}\ldots x_{t_{k-1}}^{i_{k-1}}\,. \tag{11}$$

Then the spectral decomposition of (9) according to $2^{k-1}+1$ (possibly) distinct eigenvalues of (9}is:

$$\begin{aligned}\mathbf{V} &= \lambda_{00\ldots00}\,\mathbf{I}_{12\ldots k-1}\otimes(\mathbf{I}_k - \frac{1}{n_k}\mathbf{J}_k)\\ &+ \sum_{t_1t_2\ldots t_k-1}^{1}\phi^*_{t_1t_2\ldots t_{k-1}}\mathbf{P}_{t_1}\otimes\mathbf{P}_{t_2}\otimes\ldots\otimes\mathbf{P}_{t_{k-1}}\otimes\frac{1}{n_k}\mathbf{J}_k\end{aligned} \tag{12}$$

where $\mathbf{I}_{12\ldots k\text{-}1}$ is an identity matrix of order $\prod_{r=1}^{k-1} n_r$ and $\mathbf{P}_{t_r}$ is in (8).

4. CONCLUDING REMARKS

The spectral decomposition of **V** provides easily the computation of $\mathbf{V}^{\alpha}$ for any real α since

$$\mathbf{V}^{\alpha} = \sum_t \phi_t^{\alpha} \mathbf{M}_t$$

where ϕ_t and $\mathbf{M}_t$ are defined in (2) and (5) respectively.

The nonnegative parameters λ_d in (1) correspond to variance components. From (2), the eigenvalues of the variance-covariance matrix is the linear combination of variance components. It is not necessary to recompute the spectral decomposition of **V*** where a new variance-covariance matrix **V*** is obtained by removing some λ_d's from **V**. It can be obtained by removing the corresponding λ_d's from the spectral decomposition of **V**.

A half number of eigenvalues of **V** are same and equal to the smallest eigenvalue when there is a replication. In this case, the summations in both (11) and (12) are taken over 2^{k-1}, instead of 2^k. This facilitates the computation of the spectral decomposition of **V**.

5. AN EXAMPLE

Consider the two-way random effect model $y_{ijk} = \mu + a_i + b_j + c_{ij} + e_{ijk}$, $i = 1,2,\ldots,n_1$, $j = 1,2,\ldots,n_2$, $k = 1,2,\ldots,n_3$ where

$$a_i \sim N(0,\sigma_a^2),\ b_j \sim N(0,\sigma_b^2),\ c_{ij} \sim N(0,\sigma_c^2),\ e_{ijk} \sim N(0,\sigma_e^2)$$

and they are independent. The variance-covariance matrix for this model is:

$$V = \sigma_a^2 \mathbf{I}_1 \otimes \mathbf{J}_2 \otimes \mathbf{J}_3 \otimes \sigma_b^2 \mathbf{J}_1 \otimes \mathbf{I}_2 \otimes \mathbf{J}_3 \otimes \sigma_c^2 \mathbf{I}_1 \otimes \mathbf{I}_2 \otimes \mathbf{I}_3 \otimes \sigma_e^2 \mathbf{I}_1 \otimes \mathbf{I}_2 \otimes \mathbf{I}_3$$

where $\mathbf{I}_r$ and $\mathbf{J}_r$ for r=1,2,3 are a $n_r \times n_r$ identity matrix and a $n_r \times n_r$ matrix of ones respectively.

Define $\lambda_{000} = \sigma_e^2, \lambda_{001} = \sigma_c^2, \lambda_{011} = \sigma_a^2, \lambda_{101} = \sigma_b^2$ and the other λ_d's are zero. The 2^3 eigenvalues of **V** are:

$$\begin{aligned}\phi_{t_1t_2t_3} &= \sum_{i_1i_2i_3=0}^{1} \lambda_{i_1i_2i_3} x_{t_1}^{i_1} x_{t_2}^{i_2} x_{t_3}^{i_3} \\ &= \lambda_{000} + \lambda_{001}x_{t_3} + \lambda_{011}x_{t_2}x_{t_3} + \lambda_{101}x_{t_1}x_{t_3}\end{aligned}$$

where $x_{t_r} = 0$ if $t_r = 0, x_{t_r} = n_r$ if $t_r = 1$ for r=1,2,3. Then

$\phi_{000} = \phi_{010} = \phi_{100} = \phi_{110} = \lambda_{000}$, $\phi_{001} = \lambda_{000} + n_3\lambda_{001}$, $\phi_{011} = \lambda_{000} + n_3\lambda_{001} + n_2n_3\lambda_{011}$, $\phi_{101} = \lambda_{000} + n_3\lambda_{001} + n_1n_3\lambda_{101}$, $\phi_{111} = \lambda_{000} + n_3\lambda_{001} + n_1n_3\lambda_{101} + n_2n_3\lambda_{011}$.

The spectral decomposition of **V** is:

$$\mathbf{V} = \phi_{000}\,\mathbf{I}_{12} \otimes (\mathbf{I}_3 - \frac{1}{n_3}\mathbf{J}_3) + \phi_{001}\,\mathbf{I}_1 \otimes \mathbf{I}_2 \otimes \frac{1}{n_3}\mathbf{J}_3$$
$$+\phi_{011}(\mathbf{I}_1 - \frac{1}{n_1}\mathbf{J}_1) \otimes \frac{1}{n_2}\mathbf{J}_2 \otimes \frac{1}{n_3}\mathbf{J}_3$$
$$+\phi_{101}\frac{1}{n_1}\mathbf{J}_1 \otimes (\mathbf{I}_2 - \frac{1}{n_2}\mathbf{J}_2) \otimes \frac{1}{n_3}\mathbf{J}_3$$
$$+\phi_{111}\frac{1}{n_1}\mathbf{J}_1 \otimes \frac{1}{n_2}\mathbf{J}_2 \otimes \frac{1}{n_3}\mathbf{J}_3.$$

Acknowledgment
The author thanks the referee for making comments which clearify the paper.

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