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An Orthogonal Representation of Estimable Functions†

Seongbaek Yi[1)]

Abstract

Students taking linear model courses have difficulty in determining which parametric functions are estimable when the design matrix of a linear model is rank deficient. In this note a special form of estimable functions is presented with a linear combination of some orthogonal estimable functions. Here, the orthogonality means the least squares estimators of the estimable functions are uncorrelated and have the same variance. The number of the orthogonal estimable functions composing the special form is equal to the rank of the design matrix. The orthogonal estimable functions can be easily obtained through the singular value decomposition of the design matrix.

Keywords: Estimable functions; linear model; singular value decomposition.

1. Introduction

Consider the linear model

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

where $\boldsymbol{X}$ is an $n \times k$ design matrix with rank $r(\leq k)$, $\boldsymbol{y}$ is an n-dimensional observation vector, $\boldsymbol{\beta}$ is a k-dimensional parameter vector and $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2, \ldots, \epsilon_n)^t$ is a random vector of errors. Assume that $\epsilon_1, \epsilon_2, \ldots, \epsilon_n$ are uncorrelated and have mean 0 and variance σ^2. One of the main problems in analysis of variance is to estimate a parametric function $\boldsymbol{c}^t\boldsymbol{\beta}$, where $\boldsymbol{c}$ is a given vector. A parametric function $\boldsymbol{c}^t\boldsymbol{\beta}$ is called an estimable function if it has an unbiased linear estimator. If $\boldsymbol{X}$ has full rank, then any parametric function $\boldsymbol{c}^t\boldsymbol{\beta}$ is estimable and its least squares(LS) estimator is $\boldsymbol{c}^t\left(\boldsymbol{X}^t\boldsymbol{X}\right)^{-1}\boldsymbol{X}^t\boldsymbol{y}$. However, if $\boldsymbol{X}$ has rank deficiency, then some parametric functions are not estimable.

The singular value decomposition(SVD) is concerned with the factorization of a matrix into a product of two orthogonal matrices and a diagonal matrix. The SVD of a design matrix has been widely applied to both teaching and research in linear models. Mandel (1982) discussed it in multiple linear regression with a special reference to the problems of collinearity. Eubank and Webster (1985) presented a simple method for solving the estimability problems in least squares estimation. Nelder (1985) took simpler least squares equations by joint orthogonal transformations of data and parameters using the SVD. Elswick *et al.* (1991) used the row reduced echelon form of a design matrix in order to find the sturcture of all estimable functions.

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1) Associate Professor, Division of Mathematical Sciences, Pukyong National University, Busan 608-737, Korea. E-mail: sbyi@pknu.ac.kr

In this note a special form of estimable functions is presented with a linear combination of some orthogonal estimable functions when the design matrix of a linear model is rank deficient. Here, the orthogonality means the least squares estimators of the estimable functions are uncorrelated and have the same variance. The orthogonal estimable functions are obtained through the SVD of the design matrix.

2. A Special Form of Estimable Functions

The following is a very useful lemma to decide whether a parametric function is estimable or not when the rank deficiency exists (see, *e.g.*, Scheffé, 1959).

Lemma 2.1 A parametric function $\boldsymbol{c}^t\boldsymbol{\beta}$ is estimable if and only if there exists an $n \times 1$ vector $\boldsymbol{a}$ such that

$$\boldsymbol{c}^t = \boldsymbol{a}^t\boldsymbol{X}.$$

When $\boldsymbol{X}$ has full rank, Lemma 2.1 guarantees that any parametric function is estimable with

$$\boldsymbol{a}^t = \boldsymbol{c}^t\left(\boldsymbol{X}^t\boldsymbol{X}\right)^{-1}\boldsymbol{X}^t.$$

There are infinitely many parametric functions satisfying the condition of Lemma 2.1. The purpose of this note is to present an orthogonal basis of such parametric functions through the singular value decomposition(SVD). For the existence of the SVD of any matrix, readers may refer to Hill (1996) or Mulcahy and Rossi (1998).

Lemma 2.2 (SVD) If $\boldsymbol{X}$ is a real $n \times k$ matrix where $n \geq k$, then there exists an $n \times n$ orthogonal matrix $\boldsymbol{U}$ and a $k \times k$ orthogonal matrix $\boldsymbol{V}$ such that

$$\boldsymbol{X} = \boldsymbol{U\Sigma V}^t,$$

where $\boldsymbol{\Sigma}$ is an $n \times k$ matrix of the special form

$$\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Delta} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix}.$$

Here, $\boldsymbol{\Delta}$ is an $r \times r$ diagonal matrix with diagonal elements

$$\delta_1 \geq \delta_2 \geq \cdots \geq \delta_r > 0,$$

where r is the rank of $\boldsymbol{X}$.

We call δ_i the i^{th} singular value of $\boldsymbol{X}$. Also, the i^{th} column vector $\boldsymbol{u}_i$ of $\boldsymbol{U}$ and the j^{th} column vector $\boldsymbol{v}_j$ of $\boldsymbol{V}$ are called the i^{th} left singular vector and the j^{th} right singular vector, respectively. Applying Lemma 2.2 to Lemma 2.1, we obtain the following corollary.

Corollary 2.1 Let $\boldsymbol{U\Sigma V}^t$ be the SVD of $\boldsymbol{X}$. A parametric function $\boldsymbol{c}^t\boldsymbol{\beta}$ is estimable if and only if there exists a vector $\boldsymbol{d}$ such that

$$\boldsymbol{c}^t = \boldsymbol{d}^t\boldsymbol{\Sigma V}^t.$$

Since only the diagonal elements of the diagonal matrix $\boldsymbol{\Delta}$ are nonzero, Corollary 2.1 implies the following theorem.

Theorem 2.1 A parametric function is estimable if and only if it is a linear combination of $\delta_1\boldsymbol{v}_1^t\boldsymbol{\beta},\ \delta_2\boldsymbol{v}_2^t\boldsymbol{\beta},\dots,\delta_r\boldsymbol{v}_r^t\boldsymbol{\beta}$.

Theorem 2.1 shows that a special form of estimable functions can be represented by $\sum_{i=1}^r d_i\delta_i\boldsymbol{v}_i^t\boldsymbol{\beta}$, where $d_1, d_2, \dots, d_r$ are constants.

The following theorem shows the orthogonality of the estimable functions $\delta_1\boldsymbol{v}_1^t\boldsymbol{\beta}$, $\delta_2\boldsymbol{v}_2^t\boldsymbol{\beta},\dots,\delta_r\boldsymbol{v}_r^t\boldsymbol{\beta}$. Here, the orthogonality means the LS estimators of the estimable functions are uncorrelated. Its proof is in the Appendix.

Theorem 2.2 The LS estimators of the estimable functions $\delta_1\boldsymbol{v}_1^t\boldsymbol{\beta},\ \delta_2\boldsymbol{v}_2^t\boldsymbol{\beta},\dots,\delta_r\boldsymbol{v}_r^t\boldsymbol{\beta}$ are uncorrelated and they have the same variance σ^2.

Because of Theorems 2.1 and 2.2, we may call $\{\delta_1\boldsymbol{v}_1^t\boldsymbol{\beta},\ \delta_2\boldsymbol{v}_2^t\boldsymbol{\beta},\dots,\delta_r\boldsymbol{v}_r^t\boldsymbol{\beta}\}$ an orthogonal basis of estimable functions and call each $\delta_i\boldsymbol{v}_i^t\boldsymbol{\beta}$ a basic orthogonal estimable function.

3. Examples

3.1. Balanced one-way model

Consider the following balanced one-way model

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij}, \quad i = 1, 2,\ j = 1, 2, 3.$$

Then the parameter vector $\boldsymbol{\beta}$ is $(\mu,\ \alpha_1,\ \alpha_2)^t$ and the design matrix $\mathbf{X}$ is

$$\mathbf{X}' = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix}.$$

The SVD of the design matrix $\boldsymbol{X}$ is computed using the built-in function SingularValues of Mathematica (Wolfram, 1999). We have two singular values 3.0000, 1.73205. The resulting two basic orthogonal estimable functions are

$$\eta_1 = 3.0000\,(0.816497\mu + 0.408248\alpha_1 + 0.408248\alpha_2)\,,$$
$$\eta_2 = 1.73205\,(0.0000\mu + 0.707107\alpha_1 - 0.707107\alpha_2)\,.$$

Any estimable functions for the above balanced one-way model can be represented by the linear combination of the two basic orthogonal estimable functions η_1 and η_2. For example the estimable function $\mu + \alpha_1$ can be represented by $0.4083\eta_1 + 0.4083\eta_2$ and $\alpha_1 - \alpha_2$ by $0.8166\eta_2$ using the relationship

$$\begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \end{bmatrix} = \begin{bmatrix} 0.272166 & 0.000000 \\ 0.136083 & 0.408248 \\ 0.136083 & -0.408248 \end{bmatrix} \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix}.$$

3.2. Unbalanced two-way model

Now, consider the unbalanced two-way classification model

$$y_{ijk} = \mu + \alpha_i + \beta_j + \epsilon_{ijk}, \quad (i = 1, 2, 3,\ j = 1, 2, 3, 4,\ k = 1, \ldots, K_{ij}),$$

where $K_{11} = 2$, $K_{12} = 3$, $K_{13} = 3$, $K_{14} = 2$, $K_{21} = 2$, $K_{22} = 3$, $K_{23} = 2$, $K_{24} = 3$, $K_{31} = 3$, $K_{32} = 2$, $K_{33} = 2$, $K_{34} = 3$. The parameter vector $\boldsymbol{\beta}$ is $(\mu, \alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3, \beta_4)^t$. Then, the design matrix $\mathbf{X}'$ is

$$\mathbf{X}' = \begin{bmatrix}
1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\
1&1&1&1&1&1&1&1&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&1&1&1&1&1&1&1&1&1&1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&1&1&1&1&1&1&1&1&1\\
1&1&0&0&0&0&0&0&0&0&1&1&0&0&0&0&0&0&0&0&1&1&1&0&0&0&0&0&0&0\\
0&0&1&1&1&0&0&0&0&0&0&0&1&1&1&0&0&0&0&0&0&0&0&1&1&0&0&0&0&0\\
0&0&0&0&0&1&1&1&0&0&0&0&0&0&0&1&1&0&0&0&0&0&0&0&0&0&1&1&0&0\\
0&0&0&0&0&0&0&0&1&1&0&0&0&0&0&0&0&1&1&1&0&0&0&0&0&0&0&1&1&1
\end{bmatrix}$$

We compute the SVD of the design matrix $\mathbf{X}'$ using the call function SVD of SAS (SAS Institute Inc, 1990). There are six singular values 6.895, 3.264, 3.200, 2.780, 2.687, 2.573. Also, the basic orthogonal estimable functions are

$$\begin{aligned}
\eta_1 &= 6.895\,(0.794\mu + 0.265\alpha_1 + 0.265\alpha_2 + 0.265\alpha_3 \\
&\quad +0.183\beta_1 + 0.214\beta_2 + 0.183\beta_3 + 0.214\beta_4)\,, \\
\eta_2 &= 3.264\,(0.000\mu + 0.641\alpha_1 + 0.000\alpha_2 - 0.641\alpha_3 \\
&\quad -0.176\beta_1 + 0.242\beta_2 + 0.176\beta_3 - 0.242\beta_4)\,, \\
\eta_3 &= 3.200\,(0.008\mu + 0.394\alpha_1 - 0.781\alpha_2 + 0.394\alpha_3 \\
&\quad +0.143\beta_1 - 0.139\beta_2 + 0.143\beta_3 - 0.139\beta_4)\,, \\
\eta_4 &= 2.780\,(0.000\mu - 0.176\alpha_1 + 0.000\alpha_2 + 0.176\alpha_3 \\
&\quad +0.242\beta_1 + 0.641\beta_2 - 0.242\beta_3 - 0.641\beta_4)\,, \\
\eta_5 &= 2.687\,(0.024\mu - 0.107\alpha_1 + 0.238\alpha_2 - 0.107\alpha_3 \\
&\quad +0.485\beta_1 - 0.474\beta_2 + 0.485\beta_3 - 0.474\beta_4)\,, \\
\eta_6 &= 2.573\,(0.000\mu + 0.242\alpha_1 + 0.000\alpha_2 - 0.242\alpha_3 \\
&\quad +0.641\beta_1 - 0.176\beta_2 - 0.641\beta_3 + 0.176\beta_4)\,.
\end{aligned}$$

Any estimable functions for the above unbalanced two-way classification model can be represented by the linear combination $\sum_{i=1}^{6} d_i\eta_i$, where $d_1, d_2, \ldots, d_6$ are any constants.

4. Conclusions

In this note, the basic orthogonal estimable functions are defined. Any estimable function can be represented by a linear combination of the basic orthogonal estimable functions, which can be easily calculated through the SVD of the design matrix. The number of the basic orthogonal functions equals the rank of the design matrix.

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Appendix: Proof of Theorem 2.2

The SVD implies that

$$\boldsymbol{v}_i^t \boldsymbol{X}^t = \begin{cases} \delta_i \boldsymbol{u}_i^t, & i = 1, 2, \ldots, r, \\ 0, & i > r. \end{cases}$$

$$\boldsymbol{u}_i^t \boldsymbol{X} = \begin{cases} \delta_i \boldsymbol{v}_i^t, & i = 1, 2, \ldots, r, \\ 0, & i > r. \end{cases}$$

Let $\hat{\boldsymbol{\beta}}$ be an LS estimator of $\boldsymbol{\beta}$. For $i = 1, 2, \ldots, r$, the normal equations and the above relations imply the following.

$$\begin{aligned} \boldsymbol{X}^t \boldsymbol{X} \hat{\boldsymbol{\beta}} &= \boldsymbol{X}^t \boldsymbol{y} \\ \Rightarrow \quad \boldsymbol{v}_i^t \boldsymbol{X}^t \boldsymbol{X} \hat{\boldsymbol{\beta}} &= \boldsymbol{v}_i^t \boldsymbol{X}^t \boldsymbol{y} \\ \Rightarrow \quad \delta_i \boldsymbol{u}_i^t \boldsymbol{X} \hat{\boldsymbol{\beta}} &= \delta_i \boldsymbol{u}_i^t \boldsymbol{y} \\ \Rightarrow \quad \delta_i \boldsymbol{v}_i^t \hat{\boldsymbol{\beta}} &= \boldsymbol{u}_i^t \boldsymbol{y}. \end{aligned}$$

Therefore, the orthogonality of the left singular vectors $\{\boldsymbol{u}_i\}$ implies that, for $i, j = 1, 2, \ldots, r$,

$$\begin{aligned} \mathrm{Cov}\left(\delta_i \boldsymbol{v}_i^t \hat{\boldsymbol{\beta}},\, \delta_j \boldsymbol{v}_j^t \hat{\boldsymbol{\beta}}\right) &= \mathrm{Cov}\left(\boldsymbol{u}_i^t \boldsymbol{y},\, \boldsymbol{u}_j^t \boldsymbol{y}\right) \\ &= \boldsymbol{u}_i^t \mathrm{Var}(\boldsymbol{y}) \boldsymbol{u}_j \\ &= \sigma^2 \boldsymbol{u}_i^t \boldsymbol{u}_j \\ &= \begin{cases} \sigma^2, & i = j, \\ 0, & i \neq j. \end{cases} \end{aligned}$$

This completes the proof of Theorem 2.2.

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