Property of Equation Systems in Proportionally Restricted BLUP Using Canonical Transformation

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Abstract In this paper, we describe how the procedure using canonical transformation for the restricted best linear unbiased prediction with the so-called zero restrictions considered (RBLUP CT) can be applied to the proportionally restricted best linear unbiased prediction of breeding values. Then we examine the property of simultaneous equation systems required in the presented procedure (PRBLUP CT) by investigating the ranks and the numbers of positive eigenvalues of the key matrices. Denoting the numbers of traits in the multi-trait animal model and the restricted traits by q and r , respectively, it is shown that while in the RBLUP CT with zero restrictions the number of the independent equation systems is $q-r$, that in the PRBLUP CT becomes $q-r+1$. That is, as r increases, the number of the independent equation systems to be solved decreases, and in the case of all traits restricted proportionally, for instance, the rank and the number of positive eigenvalues of the key matrix become unity and it is needed to solve only one system of the usual BLUP equations for the single transformed variable.

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Restricted selection is used to control genetic changes in some of traits to be improved. The theory of restricted selection index was formally presented by Kempthorne and Nordskog⁸⁾. The original index of Kempthorne and Nordskog allows maximum response to selection in certain traits, while keeping the change in other traits zero. The theory assumes known means and (co) variances of phenotypic records, unrelated candidates for selection, and no missing records. Indices with different types of restrictions were also considered by

several researchers (for a review, *e.g.*, see Brascamp¹⁾).

On the other hand, the best linear unbiased prediction (BLUP) of breeding values^{4,5)} is the viable alternative to the selection index approach and is applicable to more complicated data in animal breeding applications. Accordingly, the restricted best linear unbiased prediction (RBLUP) procedure, which is a BLUP counterpart of the restricted selection index, was derived by Quaas and Henderson¹⁰⁾. The RBLUP procedure generally requires the

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system of simultaneous equations of relatively high order to be solved, and then an application of canonical transformation to RBLUP has also been proposed⁷⁾. With the transformation technique, traits are transformed to be independent so that the equation system for each transformed variable is solved separately.

Restricted selection index and therefore RBLUP is known to be able to treat the more general case in addition to the case of the so-called zero restrictions. Mallard⁹⁾ showed that Kempthorne and Nordskog's restricted index can handle the case of proportional constraints, which was suggested by Kempthorne and Nordskog themselves⁸⁾. Moreover, Itoh and Yamada⁶⁾ presented the details of its property to handle proportional or desired gains.

Describing how the RBLUP method for zero restrictions using canonical transformation⁷⁾ (which will be referred to as RBLUP CT) can be applied to the case of proportional constraints imposed, the main purpose of this paper is to examine the nature of the current procedure, that is the proportionally restricted BLUP with canonical transformation used (denoted as PRBLUP CT), in the point of reducing the number of the transformed variables to be analyzed.

Theory

Multi-trait animal model

Assume that there are q traits to be analyzed. The number of individuals to be evaluated is denoted by p and the number of individuals with records by n .

For all q traits, when observations are ordered by animals within traits, the multi-trait animal model is written in matrix notation as

$$\mathbf{y} = (\mathbf{I}_q \otimes \mathbf{X})\boldsymbol{\beta} + (\mathbf{I}_q \otimes \mathbf{Z})\mathbf{a} + \mathbf{e} \quad (1)$$

with

$$\begin{aligned} \mathbf{y}' &= [\mathbf{y}_1' \quad \mathbf{y}_2' \quad \cdots \quad \mathbf{y}_i' \quad \cdots \quad \mathbf{y}_q'], \\ \boldsymbol{\beta}' &= [\boldsymbol{\beta}_1' \quad \boldsymbol{\beta}_2' \quad \cdots \quad \boldsymbol{\beta}_i' \quad \cdots \quad \boldsymbol{\beta}_q'], \\ \mathbf{a}' &= [\mathbf{a}_1' \quad \mathbf{a}_2' \quad \cdots \quad \mathbf{a}_i' \quad \cdots \quad \mathbf{a}_q'], \end{aligned}$$

and

$$\mathbf{e}' = [\mathbf{e}_1' \quad \mathbf{e}_2' \quad \cdots \quad \mathbf{e}_i' \quad \cdots \quad \mathbf{e}_q'],$$

where $\mathbf{y}_i$ is a vector of observations, $\boldsymbol{\beta}_i$ is a vector of unknown fixed effects, $\mathbf{a}_i$ is a vector of unknown random animal effects (breeding values), and $\mathbf{e}_i$ is a vector of random residuals for the i^{th} trait, $\mathbf{X}$ and $\mathbf{Z}$ are incidence matrices and are assumed to be the same for all traits, $\mathbf{I}_q$ is the identity matrix of order $q \times q$, and $\otimes$ denotes the direct product operator.

We further suppose

$$\mathbf{E} \begin{bmatrix} \mathbf{y} \\ \mathbf{a} \\ \mathbf{e} \end{bmatrix} = \begin{bmatrix} (\mathbf{I}_q \otimes \mathbf{X})\boldsymbol{\beta} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} \quad \text{and} \quad \text{Var} \begin{bmatrix} \mathbf{a} \\ \mathbf{e} \end{bmatrix} = \begin{bmatrix} \mathbf{G} & \mathbf{0} \\ \mathbf{0} & \mathbf{R} \end{bmatrix}$$

with $\mathbf{G} = \mathbf{G}_0 \otimes \mathbf{A}$ and $\mathbf{R} = \mathbf{R}_0 \otimes \mathbf{I}_n$, where $\mathbf{A}$ is the additive relationship matrix among animals to be evaluated, $\mathbf{G}_0$ and $\mathbf{R}_0$ are the additive genetic and residual variance-covariance matrices among traits, respectively, and $\mathbf{I}_n$ is the identity matrix of order $n \times n$.

Proportionally restricted BLUP (PRBLUP)

For the case of the RBLUP procedure with zero changes in some traits considered, when denoting the set of restrictions on $\mathbf{a}$ by $\mathbf{C}'\mathbf{a}$ with $\mathbf{C} = \mathbf{C}_0 \otimes \mathbf{I}_p$, $\mathbf{C}_0$ is as defined by Kempthorne and Nordskog⁸⁾ and whose elements are unity or zero.

Mallard⁹⁾ demonstrated that the equations for proportional constraints can be converted into those for zero restrictions on linear combinations of traits. For the case of proportional constraints, let the set of the constraints on $\mathbf{a}$ be $\mathbf{T}'\mathbf{a}$ with $\mathbf{T} = \mathbf{T}_0 \otimes \mathbf{I}_p$, assuming that the vector of relatively desired changes for traits 1, 2, ..., $r \leq q$ is $\mathbf{k}' = [k_1 \ k_2 \ \cdots \ k_r]$. Then $\mathbf{T}_0'$ is given as $[\mathbf{T}_r' \ \mathbf{0}']$. The matrix $\mathbf{T}_r'$ is expressed, for instance, as

$$\mathbf{T}_r' = \begin{bmatrix} k_2 & -k_1 & 0 & \cdots & 0 \\ k_3 & 0 & -k_1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ k_r & 0 & 0 & \cdots & -k_1 \end{bmatrix} \quad (2)$$

such that

$$\mathbf{T}_r' \mathbf{k} = \mathbf{0}. \quad (3)$$

Note that T_r is not unique and can be written in various forms⁶⁾.

Based on these facts, denoting the proportionally restricted best linear unbiased predictor by $\hat{\mathbf{a}}$, it is already known that a general form of the mixed model equations to be solved is straightforwardly written as

$$\begin{bmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{X}'\mathbf{R}^{-1}\mathbf{Z} & \mathbf{X}'\mathbf{R}^{-1}\mathbf{Z}\mathbf{G}\mathbf{T} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z} + \mathbf{G}^{-1} & \mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z}\mathbf{G}\mathbf{T} \\ \mathbf{T}'\mathbf{G}\mathbf{Z}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{T}'\mathbf{G}\mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z} & \mathbf{T}'\mathbf{G}\mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z}\mathbf{G}\mathbf{T} \end{bmatrix} \begin{bmatrix} \hat{\beta} \\ \hat{\mathbf{a}} \\ \hat{\mathbf{v}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{y} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{y} \\ \mathbf{T}'\mathbf{G}\mathbf{Z}'\mathbf{R}^{-1}\mathbf{y} \end{bmatrix}, \quad (4)$$

where $\hat{\beta}$ is a vector of some solution to β and $\mathbf{v}$ is analogous to a vector of LaGrange multipliers.

Proportionally restricted BLUP using canonical transformation (PRBLUP CT)

Eliminating $\hat{\mathbf{v}}$ from eq.(4) by absorption gives

$$\begin{bmatrix} \mathbf{X}'\mathbf{H}\mathbf{X} & \mathbf{X}'\mathbf{H}\mathbf{Z} \\ \mathbf{Z}'\mathbf{H}\mathbf{X} & \mathbf{Z}'\mathbf{H}\mathbf{Z} + \mathbf{G}^{-1} \end{bmatrix} \begin{bmatrix} \hat{\beta} \\ \hat{\mathbf{a}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{H}\mathbf{y} \\ \mathbf{Z}'\mathbf{H}\mathbf{y} \end{bmatrix}, \quad (5)$$

where $\mathbf{H} = \mathbf{H}_0 \otimes \mathbf{I}_n$, and

$$\mathbf{H}_0 = \mathbf{R}_0^{-1} - \mathbf{R}_0^{-1}\mathbf{G}_0\mathbf{T}_0(\mathbf{T}_0'\mathbf{G}_0\mathbf{R}_0^{-1}\mathbf{G}_0\mathbf{T}_0)^{-1}\mathbf{T}_0'\mathbf{G}_0\mathbf{R}_0^{-1}. \quad (6)$$

Now, $\mathbf{G}_0$ is a positive definite matrix, and $\mathbf{H}_0$ is positive semi-definite. So, there exists a matrix $\mathbf{Q}$ which satisfies

$$\mathbf{Q}'\mathbf{G}_0^{-1}\mathbf{Q} = \mathbf{I}_r \text{ and } \mathbf{Q}'\mathbf{H}_0\mathbf{Q} = \mathbf{D}, \quad (7)$$

where $\mathbf{D}$ is a diagonal matrix whose diagonal elements, λ_i , are the characteristic roots or the eigenvalues of the following equations

$$|\mathbf{H}_0 - \lambda\mathbf{G}_0^{-1}| = 0. \quad (8)$$

With the positive λ_i , the mixed model equations to be solved are given as

$$\begin{bmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Z} \\ \mathbf{Z}'\mathbf{X} & \mathbf{Z}'\mathbf{Z} + \mathbf{A}^{-1}\lambda_i^{-1} \end{bmatrix} \begin{bmatrix} \hat{\beta}_i^* \\ \hat{\mathbf{a}}_i^* \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{y}_i^* \\ \mathbf{Z}'\mathbf{y}_i^* \end{bmatrix}, \quad (9)$$

where $\mathbf{y}_i^*$ is obtained by $(\mathbf{Q}^{-1} \otimes \mathbf{I}_n)\mathbf{y}$. When λ_i is zero, the equations become

$$\begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}^{-1} \end{bmatrix} \begin{bmatrix} \hat{\beta}_i^* \\ \hat{\mathbf{a}}_i^* \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \quad (10)$$

which leads to $\hat{\mathbf{a}}_i^* = \mathbf{0}$ and indefinite $\hat{\beta}_i^*$. The solutions on the original scale are given by the backtransformation, as follows

$$\hat{\mathbf{a}} = (\mathbf{Q} \otimes \mathbf{I}_p) \hat{\mathbf{a}}^*. \quad (11)$$

Ranks of the key matrices and the numbers of positive eigenvalues

Since $\mathbf{H}_0$ is a symmetric and positive semi-definite matrix, its eigenvalues are all non-negative, and the number of the positive eigenvalues is equal to its rank. From the notion of rank, rank of the product of a matrix and a non-singular matrix equals rank of the former matrix. So, the rank of $\mathbf{H}_0\mathbf{R}_0$ is the same as that of $\mathbf{H}_0$. Because of

$$(\mathbf{H}_0\mathbf{R}_0)^2 = \mathbf{H}_0\mathbf{R}_0, \quad (12)$$

or $\mathbf{H}_0\mathbf{R}_0$ is idempotent, the rank of $\mathbf{H}_0\mathbf{R}_0$ becomes

$$\begin{aligned} \text{rank}(\mathbf{H}_0\mathbf{R}_0) &= \text{rank}[\mathbf{I} - \mathbf{R}_0^{-1}\mathbf{G}_0\mathbf{T}_0(\mathbf{T}_0'\mathbf{G}_0\mathbf{R}_0^{-1}\mathbf{G}_0\mathbf{T}_0)^{-1}\mathbf{T}_0'\mathbf{G}_0] \\ &= q - \text{rank}(\mathbf{T}_0) \\ &= q - r + 1. \end{aligned} \quad (13)$$

Therefore, the number of positive eigenvalues of $\mathbf{H}_0$ is expressed as $q - r + 1$. Using Sylvester's law of inertia, the number of positive eigenvalues of a matrix is not altered by multiplying a non-singular matrix. Consequently, the number of positive eigenvalues of $\mathbf{G}_0\mathbf{H}_0$ is given as $q - r + 1$, which is the rank of $\mathbf{H}_0$. From this consideration, the number of positive eigenvalues concerning eq.(8) depends on the rank of $\mathbf{H}_0$, and the number of sets of eq.(9) to be solved becomes $q - r + 1$.

Discussion

After Mallard's work⁹⁾, it is well known that Kempthorne and Nordskog's restricted selection index method⁸⁾ (and thus Quaas and Henderson's restricted BLUP procedure¹⁰⁾) can handle the cases of proportional constraints or relatively desired gains on traits. Accordingly, as described in this paper, RBLUP CT⁷⁾ is also a general procedure and is straight-

forwardly applicable to the situations of proportional constraints considered. Hence, the originality of this paper on the aspect of describing the outline of the PRBLUP CT procedure might be scarce, but it could be of certain value to have examined here the nature of ranks and the numbers of positive eigenvalues of the key matrices, and the number of independent systems of equations to be solved in the procedure with proportional constraints considered. In this context, this paper is a supplement to Itoh and Iwaisaki⁷⁾. We have not provided a numerical illustration on the current procedure. Except for the construction of an appropriate $\mathbf{T}_0$, however, one may make reference to the worked example given by Itoh and Iwaisaki⁷⁾.

For the case of zero restrictions with canonical transformation applied, the eigenvalues which are the diagonal elements of the diagonal matrix $\mathbf{D}$ in the transformation can become zero as a result of putting the restrictions. The number of equation systems to be solved is dependent upon the number of the restricted traits and is $q-r$ ⁷⁾. Similarly for the corresponding cases of proportional constraints, or PRBLUP CT, the number of the equation systems to be solved is affected by the number of non-zero eigenvalues of the product of $\mathbf{G}_0$ and the constraint-imposing matrix $\mathbf{H}_0$ which corresponds to the rank of $\mathbf{H}_0$. Although as the number of proportionally restricted traits becomes high, that of the equation systems to be solved becomes low, the actual number of the equation systems in the PRBLUP CT is not completely the same as that in the RBLUP CT. Converting relatively desired gains into zero gain constraints of linear combinations of the traits, the number of positive eigenvalues and consequently that of the equation systems to be solved in PRBLUP CT results in $q-r+1$. Note that each system of equations for the transformed variables is solved separately as a single-variable analysis. When one wishes to achieve relatively desired gains in all the traits,

or in the case of $q=r$, the rank of $\mathbf{H}_0$ is unity and only one system of equations for the single variable is needed to solve, in which the computational burden would be largely reduced. In this case, the final solutions back-transformed are proportional to each other for all the traits within each animal, because of $\mathbf{T}'\mathbf{a}=\mathbf{0}$, similarly as demonstrated by Quaas and Henderson¹⁰⁾.

The computation of the $\mathbf{A}$ matrix which is involved in eq.(4) as $\mathbf{G}=\mathbf{G}_0\otimes\mathbf{A}$, relatively compared to that of its inverse, is very time consuming with a large number of animals to be evaluated. Then Quaas and Henderson¹⁰⁾ showed that it is possible to eliminate $\mathbf{A}$ from eq.(4). The (P) RBLUP CT procedures also do not require $\mathbf{A}$. In addition, an advantage of the procedures is that the transformation matrix $\mathbf{Q}$ can easily be obtained using a general program package and then, without requiring any special computing program for (P) RBLUP, eq.(9) corresponding to the positive eigenvalues can be solved utilizing a conventional program written for a single-trait BLUP.

However, the use of the (P) RBLUP CT procedures requires the following conditions: 1) animal models, 2) no other random factors except for animals and residuals, 3) no partially missing records, and 4) for all traits the same design matrices concerning fixed effects. For these conditions, finally, we would like to comment that an animal model is becoming the predominant model in current systems for genetic evaluation, and that following some recent findings^{2,3)}, it might be possible to extend the procedures to the situations where the above conditions 2) to 4) are relaxed.

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正準変換を利用した比例制限付き BLUP における 連立方程式系の特徴

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本論文では、正準変換を利用したいわゆるゼロ制限に関する制限付き BLUP 法 (RBLUP CT) が、育種価の比例制限付き BLUP に対してどのように応用され得るかを示すとともに、記述された手法 (PRBLUP CT) においてキーとなる行列のランクおよび正の固有値数に関する性質を調べることにより、解くべき連立方程式系の特徴を明らかにした。多形質個体モデルにおける評価対象形質数を q 、制限付与形質数を r とすれば、RBLUP CT における独立な連立方程式系の個数は $q-r$ であるのに対して、PRBLUP CT におけるそれは $q-r+1$ として与えられた。すなわち、 r が増加すれば、応じて解くべき連立方程式系の個数は逆に減少し、例えばすべての形質に対して比例制限を付与する場合にはキー行列のランクおよび正の固有値数は 1 となり、通常の単一形質 BLUP に関する一組の連立方程式系のみを解けばよいことが示された。

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