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General analysis of unbalanced lattices and lattice squares including the recovery of interblock information*

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SUMMARY

In a more geometrical fashion than by the customary matrix approach the analysis of lattice and lattice square designs is revisited. Pointing out canonical subspaces in treatment effects subspace contained in observation space of which any canonical vector \mathbf{c} by orthogonal projection on block effects subspace followed by orthogonal projection on treatment space will be turned into $\lambda \mathbf{c}$, where $0 \le \lambda < 1$ is the associated canonical value, forms a central theme. Best estimator of the treatment effect vector in intra-block analysis follows immediately, as well as the residual variance factors for estimated treatment pair differences after an advantageous reparameterization. Block effects within superblocks supposed to be random lead to a reformulation of using interblock information, and the value of all λ will be reduced by a positive factor w smaller than 1 (or w_r and w_c for lattice squares), canonical spaces remaining unaltered. For exploring the required ratio of block variance(s) to residual variance under the normality assumption, application of REML, modified by Kitanidis to an iterative Gauss-Newton procedure extended with line search, is recommended in preference to relying on expected mean squares which may only provide initial values.

KEY WORDS: lattice design, canonical values and spaces, treatment reparameterization for pairwise comparison variances, recovery of interblock information, REML estimation of variance components, Gauss-Newton iteration, lattice square design.

1. Lattices: definition and notation

A lattice design is an incomplete block design consisting of at least two superblocks each of which contains all p^2 treatments exactly once: within each superblock the treatments are arranged in p blocks of size p according to at least two and at most p+1 orthogonal classifications.

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For p prime or the power of a prime there exist p+1 mutually orthogonal classifications; for p equal to 6 there are at most 3 possible, and for p equal to 10, 12, 14 or 15 there are at least 4. It is not feasible to look at lattices with a value of p larger than 17, to say the least. Let the number of superblocks or replicates be s and let the subscript of a particular block classification be denoted as k. Let the number of superblocks with block classification k be s_k ; obviously

$$\sum_{k=1}^{m} s_k = s \quad \text{with} \quad 2 \le m \le p+1.$$

For the specific values of p above, the upper bound of m will be smaller than p+1.

2. Estimation of treatment effects; canonical spaces

We consider first the problem of finding the best estimates of treatment and block effects under the assumption of additivity of those effects and on the basis of an observation vector \mathbf{y} in R^n with $n = sp^2$ whose disturbances with respect to expectation (the sum of the relevant treatment and block effects) have zero expectation and are mutually uncorrelated with unknown common variance σ^2 . The additivity assumption is equivalent to the statement that the expectation $\mathcal{E}\mathbf{y}$ is an element of the subspace $\langle A, B \rangle$ of R^n spanned by A and B, where A is generated by the p^2 orthogonal vectors $\mathbf{x}_i (i = 1, ..., p^2)$ consisting of merely ones within treatment class i and zeroes elsewhere, and B similarly by the ps orthogonal vectors \mathbf{z}_j (j = 1, ..., ps) with merely ones within block class j and zeroes elsewhere.

The solution of the above estimation problem by least squares is equivalent to finding a vector $\alpha \in A$ with coordinate p^2 -vector τ , and a vector $\beta \in B$ with coordinate ps-vector η such that $\alpha + \beta$ is the orthogonal projection of \mathbf{y} on $\langle A, B \rangle$, i.e. find $\alpha \in A$ and $\beta \in B$ such that

$$y - (\alpha + \beta) \perp \langle A, B \rangle$$
.

By orthogonal projection on A and B, respectively, two equations emerge: $\mathbf{P}_A \mathbf{y} - \boldsymbol{\alpha} - \mathbf{P}_A \boldsymbol{\beta} = \mathbf{0}$, and $\mathbf{P}_B \mathbf{y} - \mathbf{P}_B \boldsymbol{\alpha} - \boldsymbol{\beta} = \mathbf{0}$. Orthogonal projection of the second equation on A and subtraction of the result from the first equation yields an equation involving $\boldsymbol{\alpha}$ only

$$(\mathbf{I} - \mathbf{P}_A \mathbf{P}_B) \alpha = \mathbf{P}_A (\mathbf{y} - \mathbf{P}_B \mathbf{y}), \tag{1}$$

while the second equation gives

$$\beta = \mathbf{P}_B(\mathbf{y} - \boldsymbol{\alpha}). \tag{2}$$

In the present situation the spaces A and B have only the space G spanned by $\mathbf{1}_n$

(consisting of merely ones) in common (in other words: block and treatment spaces are connected). By considering the orthogonal complements A^* and B^* of G in A and B, respectively, it is easily seen that the right hand side \mathbf{d} of (1) is orthogonal to G. The solution of (1) for $\mathbf{I} - \mathbf{P}_A \mathbf{P}_B$ restricted to A^* can be obtained by knowledge of an orthogonal canonical basis for A^* consisting of vectors \mathbf{u}_i for which $\mathbf{P}_A \mathbf{P}_B \mathbf{u}_i = \lambda_i \mathbf{u}_i$ with $0 \le \lambda_i < 1$. Then α will be

$$\sum_{i=1}^{p^2-1} (1 - \lambda_i)^{-1} \mathbf{u}_i.$$

In the present special case of the given general solution procedure for incomplete block designs we make the following observation. Let A_k be the p-dimensional subspace of A consisting of vectors constant within each class of the classification A_k . The (p-1)-dimensional subspace of A_k orthogonal to G satisfies $\sum_{j=1}^p a_j = 0$ where j runs through the p classes of A_k . Application of \mathbf{P}_B , i.e. replacing the elements within every block by their average, leaves the elements in the blocks generated by A_k unchanged while those in all other blocks will vanish. Subsequent application of \mathbf{P}_A (replacing the elements corresponding to any treatment by their average) assigns $s_k a_j/s$ to all elements corresponding to treatments occurring in class j of A_k . Consequently s_k/s is canonical value of $\mathbf{P}_A\mathbf{P}_B$ for the orthogonal complement of G in A_k . These m canonical spaces span a subspace of dimension m(p-1) in A. The orthogonal complement A_{m+1} of A_1, \ldots, A_m in A has dimension $p^2-1-m(p-1)=(p-1)(p+1-m)$ which vanishes for m=p+1. Since each block sum for any vector in A_{m+1} which is not void will vanish due to the orthogonality of A_{m+1} to every generator \mathbf{z}_j of B, the canonical value of $\mathbf{P}_A\mathbf{P}_B$ for A_{m+1} is zero.

Hence for m = p + 1

$$\alpha = \sum_{k=1}^{m} (1 - s_k/s)^{-1} \mathbf{P}_{A_k} \mathbf{d} = \sum_{k=1}^{m} s(s - s_k)^{-1} \mathbf{P}_{A_k} \mathbf{d}.$$
 (3)

Since, for $m , <math>\mathbf{d} = \sum_{k=1}^{m+1} \mathbf{P}_{A_k} \mathbf{d}$, we have

$$\alpha = \sum_{k=1}^{m} (1 - s_k/s) \mathbf{P}_{A_k} \mathbf{d} + (\mathbf{d} - \sum_{k=1}^{m} \mathbf{P}_{A_k} \mathbf{d}) = \mathbf{d} + \sum_{k=1}^{m} s_k (s - s_k)^{-1} \mathbf{P}_{A_k} \mathbf{d}.$$
 (4)

Recall that \mathbf{P}_{A_k} involves only replacing the elements corresponding to all treatments which occur together in one block according to the classification A_k by their average.

3. Variance of estimated treatment differences; reparameterization

For the establishment of the variance of treatment difference estimators it is convenient to apply a reparameterization of the treatment effect τ_i suggested by the form of the solutions (3) and (4) for the estimation problem. For m = p + 1 set τ_i equal to the sum of effects $\tau_{k(i)}$ (k = 1, ..., m) each due to the class of A_k to which treatment i belongs, and for $m add to such a sum a residual effect <math>\tau_{(i)}$. This implies the introduction of a seemingly excessive number mp or $mp + p^2$ of new parameters instead of the original number p^2 .

If m = p + 1 a solution for $\tau_{k(i)}$ can be equal to any element corresponding to treatment i in the term with subscript k in (3), but for m one will use the term with subscript <math>k in the utmost right member of (4); for $\tau_{(i)}$ the term d in the same expression may be used.

It follows that the expression for the estimator of each new parameter in terms of treatment class sums or treatment sums occurring in the right hand member of the unreduced normal equations $\mathbf{X}'\mathbf{X}\mathbf{q} = \mathbf{X}'\mathbf{y}$ (in addition there are block sums involved which we do not bother about) is simply a multiplication of the relevant sum with some constant. In other words, the proposed estimators of the new treatment parameters correspond to the use of a weak inverse of $\mathbf{X}'\mathbf{X}$ with a diagonal submatrix \mathbf{C} concerning the new treatment effects. Note that the way the weak inverse acts upon block totals is irrelevant for our purposes. This submatrix \mathbf{C} can be used for the establishment of the variance factor for any identifiable treatment contrast, all new treatment effect estimators being seemingly uncorrelated.

If m = p + 1 the p estimators of $\tau_{k(i)}$ at fixed k follow from (3) as the p different elements occurring in $s(s - s_k)^{-1}\mathbf{P}_{A_k}\mathbf{d}$, and since ps is the divisor of treatment class sums required in $\mathbf{P}_{A_k}\mathbf{d}$ the estimation variance of the difference between two treatments occurring together in blocks according to classification $A_{k'}$ involving 2(m-1) parameters $\tau_{k(i)}$ will be as if these treatment effects are uncorrelated with a variance factor of σ^2 for each individual treatment equal to

$$p^{-1} \sum_{\substack{k=1\\k \neq k'}}^{m} (s - s_k)^{-1}. \tag{5}$$

It is noted that if in this case s_k is constant and thus equal to s/m then (5) reduces to (p+1)/(ps), and if in particular s=p+1 then (5) reduces to 1/p.

If m there are <math>2(m - 1) parameters $\tau_{k(i)}$ involved in the difference between two treatments occurring together in blocks arising from classification k' and in addition two parameters of type $\tau_{(i)}$. The associated variance factor for such a

treatment will be

$$s^{-1} \left\{ 1 + p^{-1} \sum_{\substack{k=1\\k \neq k'}}^{m} s_k (s - s_k)^{-1} \right\}.$$
 (6)

If m < p+1 and the two treatments do not occur together in any block the restriction $k \neq k'$ must be removed from (6) due to the presence of 2(m+1) parameters in such a difference.

Ideas similar to those in Sections 2 and 3 appeared incompletely in Corsten (1976). See also a related approach in Corsten (1985) as a reaction to Williams et al. (1980).

4. Testing orthogonal treatment components

For the estimation of σ^2 one needs the difference between (\mathbf{y}, \mathbf{y}) and $(\alpha + \beta, \alpha + \beta)$. The latter term is found as the square of the projection of $\alpha + \beta$ on B equal to $|\mathbf{P}_B\mathbf{y}|^2$ plus the square of the perpendicular from $\alpha + \beta$ on B. This perpendicular $\alpha + \beta - \mathbf{P}_B\mathbf{y}$ is due to (2) equal to $\alpha - \mathbf{P}_B\alpha$. Due to the orthogonality of $\alpha - \mathbf{P}_B\alpha$ and $\mathbf{P}_B\alpha$ the square $(\alpha - \mathbf{P}_B\alpha, \alpha - \mathbf{P}_B\alpha) = (\alpha, \alpha - \mathbf{P}_B\alpha)$ which by treatmentwise summation of products is seen to be equal to $(\alpha, \mathbf{P}_A(\alpha - \mathbf{P}_B\alpha))$ and due to (1) equal to (α, \mathbf{d}) . Hence $|\alpha + \beta|^2 = |\mathbf{P}_B\mathbf{y}|^2 + (\alpha, \mathbf{d})$. For lattices with m = p + 1 one finds from (3) that the squared perpendicular also needed for testing the nullity of treatment effects under the assumption of normality of the disturbances will be equal to $\sum_{k=1}^m s(s-s_k)^{-1} |\mathbf{P}_{A_k}\mathbf{d}|^2$. Obviously, each of these m terms can be used for testing in a quasi-independent manner the treatment effects corresponding to any of the classifications A_k , and similarly any contrast belonging to the effects of such a classification. A similar decomposition of the adjusted treatment sum of squares is possible for lattices with m and the <math>m + 1 terms which appeared in the middle part of (4), that is

$$\sum_{k=1}^{m} s(s-s_k)^{-1} |\mathbf{P}_{A_k} \mathbf{d}|^2 + \left\{ |\mathbf{d}|^2 - \sum_{k=1}^{m} |\mathbf{P}_{A_k} \mathbf{d}|^2 \right\}.$$

Each of the first m components is a sum of squares based on class contrasts of treatment sums adjusted for blocks to be multiplied with the relevant factor $s(s-s_k)^{-1}$; for the last term the multiplication factor is 1.

The variance σ^2 will be estimated as the ratio of $|\mathbf{y}|^2 - |\mathbf{P}_B \mathbf{y}|^2 - (\alpha, \mathbf{d})$ and (p-1)(ps-p-1).

5. Lattice with random blocks within replicates

If the randomization procedure of blocks within superblocks permits the model with additive treatment and block effects both being fixed may be replaced with one with fixed treatment and superblock effects, but with block effects superblocks as random uncorrelated variables with common variance σ_1^2 and expectation zero; one hopes for estimation of treatment effects with smaller variance. In vector notation we have

$$\mathbf{y} = \boldsymbol{\mu} + \sigma_1 \sqrt{p} \mathbf{P}_B \mathbf{v}_1 + \sigma \mathbf{v}_0, \tag{7}$$

where $\mu \in E = \langle A, S \rangle$, S is the space of superblock effects, \mathbf{v}_1 and \mathbf{v}_0 are standardized random vectors consisting of $n(=p^2s)$ uncorrelated random variables with zero expectation and unit variance. Note that in the second term the individual terms within any block are identical, those of $\mathbf{P}_B\mathbf{v}_1$ having variance 1/p and hence those of the second term having variance σ_1^2 , as the model requires. Eq. (7) is equivalent to

$$\mathbf{y} = \boldsymbol{\mu} + \sigma_1 \sqrt{p} \mathbf{P}_B \mathbf{v}_1 + \sigma \mathbf{P}_B \mathbf{v}_0 + \sigma \mathbf{P}_{B^{\perp}} \mathbf{v}_0, \tag{7a}$$

where B^{\perp} is the orthogonal complement of B in \mathbb{R}^n . Since the second and the third term are component-wise uncorrelated, (7a) can be replaced with

$$\mathbf{y} = \boldsymbol{\mu} + \sqrt{p\sigma_1^2 + \sigma^2} \mathbf{P}_B \mathbf{v}_2 + \sigma \mathbf{P}_{B^{\perp}} \mathbf{v}_0, \tag{7b}$$

where \mathbf{v}_0 and \mathbf{v}_2 have the same properties as \mathbf{v}_0 and \mathbf{v}_1 had before. Since the coordinates of orthogonal projections of a vector \mathbf{v}_0 or \mathbf{v}_2 on orthogonal subspaces are uncorrelated one may instead of two vectors \mathbf{v}_0 and \mathbf{v}_2 as well use only one standardized vector \mathbf{v} . So we arrive at the final formulation of the model

$$\mathbf{y} = \boldsymbol{\mu} + \sqrt{p\sigma_1^2 + \sigma^2 \mathbf{P}_B \mathbf{v} + \sigma \mathbf{P}_{B^{\perp}} \mathbf{v}}.$$
 (8)

Now the best estimate \mathbf{m} of $\boldsymbol{\mu} = \boldsymbol{\alpha} + \boldsymbol{\gamma}$, where $\boldsymbol{\gamma} \in S$, will be presented while σ_1^2/σ^2 is supposed to be known for the time being. Set $g = \sigma^2/(\sigma^2 + p\sigma_1^2)$ with 0 < g < 1 and consider $\sqrt{g}\mathbf{P}_B\mathbf{y} + \mathbf{P}_{B^\perp}\mathbf{y}$ which equals $\sqrt{g}\mathbf{P}_B\boldsymbol{\mu} + \mathbf{P}_{B^\perp}\boldsymbol{\mu} + \sigma\mathbf{v}$. Least squares estimation based on covariance matrix $\sigma^2\mathbf{I}_n$ requires finding $\mathbf{m} \in E$ such that $\sqrt{g}\mathbf{P}_B(\mathbf{y} - \mathbf{m}) + \mathbf{P}_{B^\perp}(\mathbf{y} - \mathbf{m})$ is orthogonal to any similarly transformed element \mathbf{e} of a basis of E, i.e. to $\sqrt{g}\mathbf{P}_B\mathbf{e} + \mathbf{P}_{B^\perp}\mathbf{e}$. Equivalently, $g\mathbf{P}_B(\mathbf{y} - \mathbf{m}) + \mathbf{P}_{B^\perp}(\mathbf{y} - \mathbf{m})$ should be orthogonal to any \mathbf{e} in E which in turn is equivalent to $\mathbf{P}_E[g\mathbf{P}_B(\mathbf{y} - \mathbf{m}) + \mathbf{P}_{B^\perp}(\mathbf{y} - \mathbf{m})] = \mathbf{0}$. Orthogonal projection of the expression in square brackets on E and E0, respectively, using E1 in E2, and introducing E3 gives the equations:

$$\mathbf{P}_{S}(\alpha + \gamma) - w\mathbf{P}_{S}\mathbf{P}_{B}(\alpha + \gamma) = \mathbf{P}_{S}\mathbf{y} - w\mathbf{P}_{S}\mathbf{P}_{B}\mathbf{y}, \tag{9a}$$

$$\mathbf{P}_{A}(\alpha+\gamma) - w\mathbf{P}_{A}\mathbf{P}_{B}(\alpha+\gamma) = \mathbf{P}_{A}\mathbf{y} - w\mathbf{P}_{A}\mathbf{P}_{B}\mathbf{y}. \tag{9b}$$

By the unessential restriction of α to orthogonality to G, α will be orthogonal to S. Due to $\mathbf{P}_S \mathbf{P}_B = \mathbf{P}_S$ (9a) reduces to $\gamma = \mathbf{P}_S \mathbf{y}$. Inserting this outcome into (9b) and using $\mathbf{P}_A \mathbf{P}_S = \mathbf{P}_G$ one can reduce (9b) to

$$(\mathbf{I} - w\mathbf{P}_A\mathbf{P}_B)\alpha = \mathbf{P}_A[(\mathbf{y} - \mathbf{P}_G\mathbf{y}) - w\mathbf{P}_B(\mathbf{y} - \mathbf{P}_G\mathbf{y})]. \tag{10}$$

Equation (10) is similar to (1) but now \mathbf{P}_B has been replaced everywhere with $w\mathbf{P}_B$ and \mathbf{y} with $\mathbf{y} - \mathbf{P}_G \mathbf{y}$, i.e. subtraction of the general mean from the observations. The latter operation causes the right hand side of (10) \mathbf{d}_{10} to be orthogonal to G.

Now $w\mathbf{P}_A\mathbf{P}_B$ obviously has the orthogonal complements of G in $A_1, ..., A_{m+1}$ again as canonical spaces, the canonical values being ws_k/s for k=1,...,m, and 0 for k=m+1 if A_{m+1} is not void. The solutions of (10) will be modifications of those in (3) and (4) in the sense that \mathbf{d} will be replaced with \mathbf{d}_{10} and that all canonical values will be multiplied with w. Similarly, the variance factors of σ^2 for treatment pair comparisons will be straightforward modifications of (5) and (6) in replacing each s_k with ws_k . Obviously, these factors are monotone increasing in w.

Hence the largest values will be reached as w approaches unity, i.e. if $p\sigma_1^2$ grows large compared to σ^2 . This situation where little or nothing can be gained over intrablock analysis was also the reason to consider the superblock effects as fixed. On the other hand, if block variance tends to be negligible in proportion to σ^2 the solution of (10) will tend to $\alpha = \mathbf{P}_A \mathbf{y} - \mathbf{P}_G \mathbf{y}$, i.e. simply ignoring block effects within superblocks with the minimal variance factor for treatment pair comparisons equal to 1/s.

6. Estimation of variance components in lattices

Now we address the problem of getting information on the two variances involved or their proportion. First we shall find preliminary estimates of both parameters by way of squares of orthogonal projections of y on well chosen subspaces whose expectations are linear combinations of the variances concerned. Those squares may lead to unbiased estimators of the parameters concerned. They may be used as initial values for an iterative procedure based on the method of maximum likelihood which in turn is based on the assumption of normality of the vector v in equation (8).

As far as the variance σ^2 is concerned an unbiased estimate is available as the ratio of the squared perpendicular from \mathbf{y} on the space $\langle A, B \rangle$ and the dimension of residual space, the orthogonal complement of $\langle A, B \rangle$ in R^n according to the intrablock analysis. This is an analysis under the condition that the random block effects have the values which they take. Under that condition the ratio above has expectation σ^2 . Since this expectation does not depend on the condition or more specifically on

the values of the block effects mentioned in the condition that expectation is also unconditionally correct.

For the variance between blocks within superblocks we consider the expectation of the square of the perpendicular from \mathbf{y} on $\langle A, S \rangle$. The contribution from $\boldsymbol{\mu}$ vanishes as $\boldsymbol{\mu} = \mathbf{P}_A \boldsymbol{\mu} + \mathbf{P}_S \boldsymbol{\mu} - \mathbf{P}_G \boldsymbol{\mu}$. The random part of $\mathcal{E} |\mathbf{y}|^2$ yields from (8) $(p\sigma_1^2 + \sigma^2)sp + \sigma^2(sp^2 - sp) = sp^2(\sigma_1^2 + \sigma^2)$, that of $\mathcal{E} |\mathbf{P}_S \mathbf{y}|^2$ gives $s(p\sigma_1^2 + \sigma^2)$ since $S \subset B$, and similarly $\mathcal{E} |\mathbf{P}_G \mathbf{y}|^2$ yields $p\sigma_1^2 + \sigma^2$ since $G \subset B$. Finally, the design is binary, i.e. each (super) block contains each treatment only once or not at all; hence the contribution 1/s times the squared sum of observations of any treatment to $\mathcal{E} |\mathbf{P}_A \mathbf{y}|^2$ will be $\sigma_1^2 + \sigma^2$ and thus $\mathcal{E} |\mathbf{P}_A \mathbf{y}|^2$ yields $p^2(\sigma_1^2 + \sigma^2)$. Hence $\mathcal{E}[|\mathbf{y}|^2 - |\mathbf{P}_A \mathbf{y}|^2 - |\mathbf{P}_S \mathbf{y}|^2 + |\mathbf{P}_G \mathbf{y}|^2] = (s-1)p^2(\sigma_1^2 + \sigma^2) - (s-1)(p\sigma_1^2 + \sigma^2) = (s-1)(p-1)[p\sigma_1^2 + (p+1)\sigma^2]$. Thus the ratio of the latter squared perpendicular and (p-1)(s-1) will be an unbiased estimator of $p\sigma_1^2 + (p+1)\sigma^2$. Subtraction of (p+1) times the previous estimate of σ^2 and division by p gives an unbiased estimator of σ_1^2 .

Under the assumption of normality of \mathbf{y} in (7) equivalent to that in (8) with $\boldsymbol{\mu} \in \langle A, S \rangle$ and covariance matrix $\mathbf{V} = \sigma_1^2 \mathbf{J}_{p,ps} + \sigma_0^2 \mathbf{I}_n$ where $\mathbf{J}_{p,ps}$ consists of ps diagonal blocks $\mathbf{J}_p = \mathbf{1}_p \mathbf{1}_p'$, p of which belong to the same superblock, the provisional estimates of σ_0^2 and σ_1^2 may be improved by the application of the restricted or reduced maximum likelihood method. This requires using the residuals with respect to $\mathbf{P}_{\langle A,S\rangle}$ i.e. $\mathbf{y} - (\mathbf{P}_A \mathbf{y} + \mathbf{P}_S \mathbf{y} - \mathbf{P}_G \mathbf{y})$, striking out all elements belonging to one treatment and one superblock, thus s + p - 1 elements, in order to remove linear dependence and so continuing with $\mathbf{r} = \mathbf{C}\mathbf{y}$. Obviously, $\mathcal{E}\mathbf{r} = \mathbf{0}$ and $\mathbf{Cov} \ r = \mathbf{W} = \mathbf{CVC}' = \sigma_1^2 \mathbf{C} \mathbf{J}_{p,ps} \mathbf{C}' + \sigma_0^2 \mathbf{CC}'$.

Setting $\sigma_i^2 = \alpha_i (i = 0, 1)$, $CJ_{p,ps}C' = W_1$, $CI_nC' = W_0$ and thus $W_{\alpha} = \alpha_0 W_0 + \alpha_1 W_1$ one finds the likelihood equations $g(\alpha) = 0$ for the minimization of $-\ln L = \frac{1}{2} \ln \det W_{\alpha} + \frac{1}{2} r' W_{\alpha} r$ with respect to α_i , where

$$[g(\alpha)]_i = \frac{1}{2} \mathrm{tr}(\mathbf{W}_\alpha^{-1} \mathbf{W}_i) - \frac{1}{2} \mathbf{r}' \mathbf{W}_\alpha^{-1} \mathbf{W}_i \mathbf{W}_\alpha^{-1} \mathbf{r} \quad (i = 0, 1).$$

Successive iteration steps in a Gauss-Newton procedure with line search are given by

$$\alpha_{(j+1)} = \alpha_{(j)} - \rho_j \left[\frac{\partial g(\alpha)}{\partial \alpha} \right]_{\alpha = \alpha_{(j)}}^{-1} g(\alpha_{(j)}) \quad (j = 0, 1, 2...),$$

where $0 < \rho_j \le 1$ is chosen as the first non-negative integer power of $\frac{1}{2}$ such that $-\ln L(\alpha_{(j+1)}) < -\ln L(\alpha_{(j)})$ while $\partial g(\alpha)/\partial(\alpha)$ will be replaced by its expectation according to Fisher's scoring method $\mathcal{E}[g(\alpha_{(j)})g(\alpha_{(j)})']$. If α is the maximum likelihood solution this expectation is the information matrix equal to $\frac{1}{2}F(\alpha)$ with typical

element $\frac{1}{2}tr[\mathbf{W}_{\alpha}^{-1}\mathbf{W}_{i}\mathbf{W}_{\alpha}^{-1}\mathbf{W}_{i'}]$. Thus the iteration steps are given by

$$\alpha_{(j+1)} = \alpha_{(j)} - \rho_j \left[\frac{1}{2} F(\alpha_{(j)})\right]^{-1} g(\alpha_{(j)}) \quad (j = 0, 1, 2, \dots).$$

The two-component vector $\alpha_{(0)}$ may be provided by the previous estimates based on expected mean squares.

The present procedure is due to Kitanidis (1983) and was also discussed and given more detail by Corsten (1994) in a different context. It is essentially different from that by Nelder (1968) which involves a functional iteration procedure.

7. Lattice squares with fixed blocks

A lattice square design is a row by column arrangement of p^2 elements (treatments) in $s \geq 2$ superblocks or replicates, each superblock being a square consisting of p rows as well as p columns each of size p for the adjustment e.g. of level differences in fertility, the p^2 elements being arranged within a superblock in two pairwise orthogonal ways from the maximally p+1 possibilities.

The solution of the estimation problem of the additive treatment and non-random block effects is analogous to the previous situation where A is again the p^2 -dimensional space of treatment effects, but B is now the space generated by the space B_r spanned by the ps row blocks, as well as B_c spanned by the ps column blocks. It will be given by (1) and (2) with $\mathbf{d} = \mathbf{P}_A(\mathbf{y} - \mathbf{P}_B\mathbf{y})$ orthogonal to the intersection G of A and B. Here $\mathbf{P}_B = \mathbf{P}_{B_r} + \mathbf{P}_{B_c} - \mathbf{P}_S$ where S is the intersection of B_r and B_c , the space of superblock effects.

In looking for canonical vectors and values of $\mathbf{P}_A\mathbf{P}_B$ one considers the p-dimensional subspace A_k of A constant within each class of the classification k. The subspace of A_k orthogonal to G satisfies $\sum_{j=1}^p a_j = 0$. Obviously, that subspace is also orthogonal to S. Some of the classes of A_k will coincide with those according to row blocks or to column blocks while each remaining row or column block contains all elements $a_1, ..., a_p$. Let the number of superblocks whose row blocks correspond with the classification A_k be equal to s_{kr} , and that for column blocks to s_{kc} . We make this distinction since we need it in later developments. As row and column classification k will never be equal within any superblock, application of \mathbf{P}_{B_r} to the defined subspace of A_k which leaves the row blocks generated by A_k unchanged, while the elements in all other row blocks will vanish, may simply be added to \mathbf{P}_{B_c} which leaves the elements generated by A_k in essentially different superblocks unchanged while those in all other column blocks will vanish. Hence the effect of \mathbf{P}_B is here equivalent to $\mathbf{P}_{B_r} + \mathbf{P}_{B_c}$ which also follows from the mentioned orthogonality of the relevant subspaces to S. Subsequent application of \mathbf{P}_A assigns $(s_{kr} + s_{kc})a_j/s$ to all elements corresponding to

treatments occurring in class j of A_k . Consequently, $(s_{kr} + s_{kc})/s$ is canonical value of $\mathbf{P}_A\mathbf{P}_B$ for the orthogonal complement of G in A_k . Note that $\sum_k (s_{kr} + s_{kc}) = 2s$. Let for convenience $s_{kr} + s_{kc}$ be denoted as s_k . The m orthogonal canonical spaces span a subspace of dimension m(p-1). Let the orthogonal complement of $A_1, ..., A_m$ in A be called A_{m+1} of dimension (p-1)(p+1-m), vanishing for m=p+1. Each vector in A_{m+1} which is not void has vanishing row and column block sums due to the orthogonality of A_{m+1} to the generators of B_r and B_c consisting of vectors whose elements in one specific block are 1, and zero elsewhere.

Hence the solutions for m = p + 1 and m will again be (3) and (4), respectively, although for the same <math>p, s, and similar ratios between s_1 up to s_m the coefficients of $\mathbf{P}_{A_k}\mathbf{d}$ will be larger, i.e. closer to 1, than for lattice designs. Further, \mathbf{d} is now $\mathbf{P}_A(\mathbf{y} - \mathbf{P}_{B_r}\mathbf{y} - \mathbf{P}_{B_c}\mathbf{y} + \mathbf{P}_S\mathbf{y})$. Although the variance factors (5) and (6) have the same appearance as before, their values for the same p, s, and similar ratios between s_1 up to s_m will be larger than for lattices. This will, hopefully, be outweighed by a smaller residual variance (estimate).

8. Lattice square with random row and column effects within replicates

Now we turn to the model with fixed treatment and superblock effects, but with row and column block effects within superblocks being random uncorrelated variables with variance σ_r^2 and σ_c^2 , respectively, and with expectation zero. The counterpart of (7) will be:

$$\mathbf{y} = \boldsymbol{\mu} + \sigma_r \sqrt{p} \mathbf{P}_{B_r} \mathbf{v} + \sigma_c \sqrt{p} \mathbf{P}_{B_c} \mathbf{v} + \sigma \mathbf{v}$$
 (11)

with $\mu \in E = \langle A, B \rangle$. On the introduction of B_r^* and B_c^* as orthogonal complements of S in B_r and B_c respectively, (11) can be decomposed into

$$\begin{array}{lll} \boldsymbol{\mu} + \boldsymbol{\sigma_r}\sqrt{p}\mathbf{P}_S\mathbf{v} & + \boldsymbol{\sigma_c}\sqrt{p}\mathbf{P}_S\mathbf{v} & + \boldsymbol{\sigma}\mathbf{P}_S\mathbf{v} \\ + \boldsymbol{\sigma_r}\sqrt{p}\mathbf{P}_{B_r^*}\mathbf{v} & + \boldsymbol{\sigma}\mathbf{P}_{B_r^*}\mathbf{v} \\ & + \boldsymbol{\sigma_c}\sqrt{p}\mathbf{P}_{B_c^*}\mathbf{v} & + \boldsymbol{\sigma}\mathbf{P}_{B_r^*}\mathbf{v} \\ & + \boldsymbol{\sigma}\mathbf{P}_{B_r^\perp}\mathbf{v} \end{array}$$

where B^{\perp} is the orthogonal complement of B in \mathbb{R}^n .

This can be reduced to

$$\mu + \sqrt{p\sigma_r^2 + p\sigma_c^2 + \sigma^2} \mathbf{P}_S \mathbf{v} + \sqrt{p\sigma_r^2 + \sigma^2} \mathbf{P}_{B_c^*} \mathbf{v} + \sqrt{p\sigma_c^2 + \sigma^2} \mathbf{P}_{B_c^*} \mathbf{v} + \sigma \mathbf{P}_{B^{\perp}} \mathbf{v}.$$
(11a)

Without loss of essentials the second term can be incorporated into μ as a component of S. So we find

$$\mu + \sqrt{p\sigma_r^2 + \sigma^2} \mathbf{P}_{B_r^*} \mathbf{v} + \sqrt{p\sigma_c^2 + \sigma^2} \mathbf{P}_{B_c^*} \mathbf{v} + \sigma \mathbf{P}_{B^{*\perp}} \mathbf{v}, \tag{12}$$

where $\mu \in \langle A, S \rangle$ and $B^{*\perp}$ is the orthogonal complement of $\langle B_r^*, B_c^* \rangle$ in \mathbb{R}^n , as the counterpart of (8).

Setting $g_r = \sigma^2/(\sigma^2 + p\sigma_r^2)$ and $g_c = \sigma^2/(\sigma^2 + p\sigma_c^2)$ one sees that best estimation of μ requires $\mathbf{m} = \alpha + \gamma \in E = \langle A, S \rangle$, $\alpha \in A$ and $\gamma \in S$ such that $\mathbf{P}_E[g_r\mathbf{P}_{B_r^*}(\mathbf{y} - \mathbf{m}) + g_c\mathbf{P}_{B_c^*}(\mathbf{y} - \mathbf{m}) + \mathbf{P}_{B^{*\perp}}(\mathbf{y} - \mathbf{m})] = \mathbf{0}$. Application of \mathbf{P}_S on the form in square brackets leads to vanishing of the first two terms, and since $S \subset B^{*\perp}$ to $\mathbf{P}_S(\alpha + \gamma) = \mathbf{P}_S\mathbf{y}$. Setting α orthogonal to G and thus to S leads to $\gamma = \mathbf{P}_S\mathbf{y}$ as before. Next, projection on A of the same expression where γ vanishes in the first two terms while in the third term it can be replaced with $\gamma = \mathbf{P}_S\mathbf{y}$ leads to the counterpart of (9b):

$$(\mathbf{I} - w_r \mathbf{P}_A \mathbf{P}_{B_c^*} - w_c \mathbf{P}_A \mathbf{P}_{B_c^*}) \alpha = \mathbf{P}_A [\mathbf{y} - \mathbf{P}_S \mathbf{y} - w_r \mathbf{P}_{B_c^*} \mathbf{y} - w_c \mathbf{P}_{B_c^*} \mathbf{y}], \tag{13}$$

where $w_r = 1 - g_r$ and $w_c = 1 - g_c$.

Note that the right hand side of (13) to be denoted as d_{13} is orthogonal to S. On the other hand, it can be replaced with

$$\mathbf{d}_{13} = \mathbf{P}_A[\mathbf{y} - \mathbf{P}_G\mathbf{y} - w_r(\mathbf{P}_{B_r}\mathbf{y} - \mathbf{P}_G\mathbf{y}) - w_c(\mathbf{P}_{B_c}\mathbf{y} - \mathbf{P}_G\mathbf{y})$$

since $\mathbf{P}_A \mathbf{P}_S = \mathbf{P}_G$.

Further, the orthogonal complements of G in $A_1, ..., A_m$ will be canonical with respect to $w_r \mathbf{P}_A \mathbf{P}_{B_r^*} + w_c \mathbf{P}_A \mathbf{P}_{B_c^*}$ and the canonical values will be $\lambda_k = (w_r s_{kr} + w_c s_{kc})/s$ for k = 1, ..., m, while that for A_{m+1} , if it is not void, will be zero again. The solution for α follows accordingly:

$$\sum_{k=1}^{m} (1 - \lambda_k)^{-1} \mathbf{P}_{A_k} \mathbf{d}_{13} \quad \text{for} \quad m = p + 1$$

and

$$\mathbf{d}_{13} + \sum_{k=1}^{m} \lambda_k (1 - \lambda_k)^{-1} \mathbf{P}_{A_k} \mathbf{d}_{13}$$
 for $m .$

Similarly, the estimation variance factors of σ^2 for effect difference between a pair of treatments occurring together in blocks according to A_k , will be analogously to (5) and (6)

$$\sum_{\substack{k=1\\k\neq k'}}^{m} (1-\lambda_k)^{-1}/ps \quad \text{for} \quad m=p+1$$

and

$$\sum_{\substack{k=1\\k \neq k'}}^{m} \lambda_k (1 - \lambda_k)^{-1} / ps + 1/s \quad \text{for} \quad m$$

The restriction $k \neq k'$ is omitted from the last equation if the pair of treatments does not occur together in any block.

9. Variance components estimation in lattice squares

Finally, the provisional estimation of σ_r^2 and σ_c^2 will be considered which may be followed by the application of the maximum likelihood method sketched before under the normality assumption in order to improve the three variance component estimates together.

First an alternative method of obtaining an unbiased estimate of σ_1^2 for the lattice with model $\mathbf{y} = \boldsymbol{\mu} + \sqrt{p\sigma_1^2 + \sigma^2} \mathbf{P}_B \mathbf{v} + \sigma \mathbf{P}_{B^\perp} \mathbf{v}$ where $\boldsymbol{\mu} \in \langle A, S \rangle$ will be presented. Obviously, $\mathcal{E} |\mathbf{y}|^2 = |\boldsymbol{\mu}|^2 + p^2 s \sigma_1^2 + p^2 s \sigma_1^2$. If R is the residual space in R^n orthogonal to $\langle A, S \rangle$ we have $\mathcal{E}[|\mathbf{y}|^2 - |\mathbf{P}_R \mathbf{y}|^2] = |\boldsymbol{\mu}|^2 + p^2 s \sigma_1^2 + (p^2 - 1 + ps)\sigma^2$. Since $\mathcal{E}[|\mathbf{P}_S \mathbf{y}|^2] = s(p\sigma_1^2 + \sigma^2)$ we have $\mathcal{E} |\mathbf{y}|^2 - \mathcal{E} |\mathbf{P}_R \mathbf{y}|^2 - \mathcal{E} |\mathbf{P}_S \mathbf{y}|^2 = |\boldsymbol{\mu}|^2 - |\mathbf{P}_S \boldsymbol{\mu}|^2 + (p^2 s - ps)\sigma_1^2 + (p^2 - 1 + ps - s)\sigma^2$ pertaining the projection of y on the space spanned by effects of A^* and those of blocks within S.

The square of the component orthogonal to A-effect requires subtraction of the square of the orthogonal projection of \mathbf{y} on A^* , and hence equals $|\mathbf{y}|^2 - |\mathbf{P}_R \mathbf{y}|^2 - |\mathbf{P}_S \mathbf{y}|^2 - |\mathbf{P}_A \mathbf{y}|^2 + |\mathbf{P}_G \mathbf{y}|^2$ with expectation

$$p(p-1)(s-1)\sigma_1^2 + (p-1)s\sigma^2,$$
 (14)

i.e. the expectation of the square of the perpendicular on treatments from the vector of block effects within superblocks. Division of this observable square equal to $(\alpha, \mathbf{d}) + |\mathbf{P}_B \mathbf{y}|^2 - |\mathbf{P}_S \mathbf{y}|^2 - |\mathbf{P}_A \mathbf{y}|^2 - |\mathbf{P}_G \mathbf{y}|^2|$ by the corresponding dimension yields a mean square with expectation $\sigma_1^2 p(s-1)/s + \sigma^2$. Subtraction of the previous estimate of σ^2 and division by p(s-1)/s gives an unbiased estimate of σ_1^2 .

It follows easily that this procedure leads to a result equivalent to the previous one: the present sum of squares is an amount of $|\mathbf{P}_R \mathbf{y}|^2$ or $|\mathbf{y}|^2 - [(\alpha, \mathbf{d}) + |\mathbf{P}_B \mathbf{y}|^2]$ less than the previous one, causing merely a change of the coefficient of σ^2 in the expectation to the amount of the dimension of R. Although the previous one is more convenient the alternative method has its merits in what follows.

In order to get information on σ_c^2 in the lattice square model (11a):

$$\mathbf{y} = \boldsymbol{\mu} + \sqrt{p\sigma_r^2 + p\sigma_c^2 + \sigma^2} \mathbf{P}_S \mathbf{v} + \sqrt{p\sigma_r^2 + \sigma^2} \mathbf{P}_{B_r^*} \mathbf{v} + \sqrt{p\sigma_c^2 + \sigma^2} \mathbf{P}_{B_c^*} \mathbf{v} + \mathbf{P}_{B^{\perp}} \mathbf{v},$$

where $\mu \in \langle A, S \rangle$ and B^{\perp} is the orthogonal complement of $\langle B_r, B_c \rangle$ in \mathbb{R}^n , we have $\mathcal{E} |\mathbf{y}|^2 = p^2 s \sigma_r^2 + p^2 s \sigma_c^2 + p^2 s \sigma_c^2 + |\mu|^2$ and $\mathcal{E} |\mathbf{P}_R \mathbf{y}|^2 = \sigma^2 [p^2 s - p^2 + 1 - s - 2s(p-1)]$ so that $\mathcal{E}[|\mathbf{y}|^2 - |\mathbf{P}_R \mathbf{y}|^2] = p^2 s \sigma_r^2 + p^2 s \sigma_c^2 + (p^2 - 1 + 2ps - s)\sigma^2 + |\mu|^2$.

Further $\mathcal{E} |\mathbf{P}_S \mathbf{y}|^2 = (p\sigma_r^2 + p\sigma_c^2 + \sigma^2)s + |\mathbf{P}_S \boldsymbol{\mu}|^2$. Hence $\mathcal{E}[|\mathbf{y}|^2 - |\mathbf{P}_R \mathbf{y}|^2 - |\mathbf{P}_S \mathbf{y}|^2] = |\boldsymbol{\mu}|^2 - |\mathbf{P}_S \boldsymbol{\mu}|^2 + p(p-1)s(\sigma_r^2 + \sigma_c^2) + (p^2 - 1 + 2ps - 2s)\sigma^2$.

Joint information on σ_r^2 and σ_c^2 is provided by the square of the perpendicular on treatment space from the vector sum of row and column effects, i.e. by subtraction, from the latter squared projection of \mathbf{y} on the space of treatment effects together with all block effects within replicates, of $|\mathbf{P}_A\mathbf{y}|^2 - |\mathbf{P}_G\mathbf{y}|^2$ with expectation $p^2(\sigma_r^2 + \sigma_c^2 + \sigma^2) + |\mathbf{P}_{A^*}\boldsymbol{\mu}|^2 - (p\sigma_r^2 + p\sigma_c^2 + \sigma^2)$ leading to $(\boldsymbol{\alpha}, \mathbf{d}) + |\mathbf{P}_{B_r^*}\mathbf{y}|^2 + |\mathbf{P}_{B_c^*}\mathbf{y}|^2 - |\mathbf{P}_A\mathbf{y}|^2 + |\mathbf{P}_G\mathbf{y}|^2$ with expectation

$$p(p-1)(s-1)(\sigma_r^2 + \sigma_c^2) + 2(p-1)s\sigma^2.$$
 (15)

The square of the perpendicular on $\langle A^*, B_r^* \rangle$ from the vector of column effects will be obtained as the difference between the latter squared perpendicular on A^* from the sum of row and column effects on the one hand and, on the other hand, the squared perpendicular on A^* from the row effects vector obtainable from the procedure above where block effects from columns within superblocks are ignored, and the procedure for lattices with block effects from rows only within superblocks will be recognized.

The difference is equal to

$$(\boldsymbol{\alpha}, \mathbf{d}) + \left| \mathbf{P}_{B_r^*} \mathbf{y} \right|^2 + \left| \mathbf{P}_{B_c^*} \mathbf{y} \right|^2 - \left| \mathbf{P}_A \mathbf{y} - \mathbf{P}_G \mathbf{y} \right|^2 +$$

$$-[(\boldsymbol{\alpha}_r, \mathbf{d}_r) + \left| \mathbf{P}_{B_r^*} \mathbf{y} \right|^2 - \left| \mathbf{P}_A \mathbf{y} - \mathbf{P}_G \mathbf{y} \right|^2],$$
(16)

where (α, \mathbf{d}) is the sum of squares for treatments adjusted for row and column effects as obtained by means of the quantities s_k in the canonical values, while (α_r, \mathbf{d}_r) is the sum of squares for treatments adjusted for row effects belonging to a model where column effects are ignored and thus obtainable by means of quantities s_{kr} in the canonical values. The latter difference (16) is numerically equal to

$$(\boldsymbol{lpha},\mathbf{d})+\left|\mathbf{P}_{B_{c}^{*}}\mathbf{y}\right|^{2}-(\boldsymbol{lpha}_{r},\mathbf{d}_{r}),$$

although the squared projections of y on A^* have different expectations under the general model and the previous restricted model.

It follows that the expectation of the difference will be the difference between the couple of expectations of squared perpendiculars (15) and (14), that is

$$p(p-1)(s-1)\sigma_c^2 + (p-1)s\sigma^2$$
.

Now, an estimate of σ_c^2 is obtained by subtracting the estimate of σ^2 from the corresponding mean square and dividing the difference again by p(s-1)/s.

On interchanging the role of row and column effects the difference providing information on σ_r^2 is equal to

$$(\boldsymbol{lpha},\mathbf{d})+\left|\mathbf{P}_{B_{r}^{*}}\mathbf{y}\right|^{2}-(lpha_{c},\mathbf{d}_{c}),$$

where the last inner product (or sum of squares for treatments adjusted for column effects) will be obtained by using the quantities s_{kc} in the canonical values.

Comparison with Williams et al. (1986) may show how much our approach in Sections 7, 8 and 9 is more general, more direct, e.g. in avoiding the cumbersome estimation of block effects, and less algebraic.

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Ogólna analiza krat niezrównoważonych i krat kwadratowych z odzyskiwaniem informacji międzyblokowej

STRESZCZENIE

Praca traktuje o analizie układów kratowych i układów krat kwadratowych w sposób bardziej geometryczny niż czyni się to w podejściach macierzowych. Omówione są najlepsze estymatory efektów obiektowych w analizie wewnątrzbłokowej, jak również czynniki związane z wariancją resztową. Proponowane jest zastosowanie metody REML, zmodyfikowanej przez Kitanidisa na iteracyjną procedurę Gaussa-Newtona, dla eksploracji ilorazu wariancji blokowych i wariancji resztowej przy założeniu normalności.

SLOWA KLUCZOWE: układ kratowy, wartości i przestrzenie kanoniczne, odzyskiwanie informacji międzyblokowej, estymacja REML komponentów wariancyjnych, metoda Gaussa-Newtona, układ kraty kwadratowej.