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ON THE BASIC CONTRASTS IN PBIB DESIGNS

Abstract. The notion of an association scheme for the basic contrasts is introduced. A necessary and sufficient condition is given for the basic contrasts to determine a certain association scheme.

1. Introduction. This paper presents a new approach to the problem of basic contrasts in a PBIB design. The novelty consists in defining an association scheme by the basic contrasts. In the literature the basic contrasts have been discussed only in the analysis of variance corresponding to the design.

The main results are contained in Section 3. They are: Definition 1 of an association scheme of the basic contrasts, and Theorem 1. This theorem provides a necessary and sufficient condition for given basic contrasts to determine a certain association scheme. This yields very interesting corollaries, given in Sections 3 and 4.

2. Preliminaries. Let $v, n_i, p_{jk}^i, i, j, k = 1, \dots, m$, be the parameters of an association scheme with association matrices $\mathbf{A}_0, \mathbf{A}_1, \dots, \mathbf{A}_m$, where m is the number of associate classes. The above matrices are all symmetric, linearly independent and satisfy the following conditions:

$$(1) \quad \mathbf{A}_0 = \mathbf{I}, \quad \sum_{i=0}^m \mathbf{A}_i = \mathbf{1}\mathbf{1}', \quad \mathbf{A}_i\mathbf{1} = n_i\mathbf{1}, \quad \mathbf{A}_j\mathbf{A}_k = \sum_{i=0}^m P_{jk}^i \mathbf{A}_i,$$

where \mathbf{I} and $\mathbf{1}$ are the unit $v \times v$ matrix and the column vector of v ones, respectively.

Let $\mathbf{N} = (n_{ij})$ be the incidence matrix of a PBIB design in which each of v treatments ($i = 1, \dots, v$) occurs r times and each of b blocks ($j = 1, \dots, b$)

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is of size k . Then the matrix NN' can be expressed as

$$(2) \quad NN' = \sum_{i=0}^m \lambda_i \mathbf{A}_i,$$

where the λ_i are called the *coincidence numbers* of the PBIB design.

It is known (see, for example, [1]) that NN' can be equivalently expressed as

$$(3) \quad NN' = \sum_{i=0}^m \varrho_i \mathbf{A}_i^{\#},$$

where $\mathbf{A}_i^{\#}$ and ϱ_i are orthogonal idempotent matrices and the latent roots of NN' with multiplicities $\alpha_i = \text{tr}(\mathbf{A}_i^{\#})$, respectively.

It is also known that there is a relation between $\mathbf{A}_i^{\#}$ and \mathbf{A}_i given by

$$(4) \quad \mathbf{A}_i^{\#} = \sum_{j=0}^m z^{ji} \mathbf{A}_j, \quad i = 0, 1, \dots, m,$$

where the $(m+1) \times (m+1)$ matrix of real coefficients z^{ji} is nonsingular.

3. Main results. Let

$$(5) \quad \mathbf{p}_{ij}, \quad i = 1, \dots, m; \quad j = 1, \dots, \alpha_i,$$

be $v-1 = \sum_{i=1}^m \alpha_i$ orthonormal column vectors satisfying the condition $\mathbf{p}'_{ij} \mathbf{1} = 0$ for every i, j . We introduce

DEFINITION 1. We say that the vectors \mathbf{p}_{ij} in (5) *determine an association scheme with m associate classes* if there exist symmetric binary matrices $\tilde{\mathbf{A}}_j$, $j = 0, \dots, m$, which satisfy (1) and

$$(6) \quad \sum_{j=1}^{\alpha_i} \mathbf{p}_{ij} \mathbf{p}'_{ij} = \sum_{j=0}^m \tilde{z}^{ji} \tilde{\mathbf{A}}_j, \quad i = 1, \dots, m,$$

where \tilde{z}^{ji} are scalar constants.

Note that the matrices $\tilde{\mathbf{A}}_j$ in (6) are the association matrices of the above scheme.

Let γ be the column vector of the treatment parameters; then the functions $\mathbf{p}'_{ij} \gamma$ will be called the *basic contrasts*.

It can be seen that if $c_i = r - \varrho_i/k \neq 0$, then the contrasts $\mathbf{p}'_{ij} \gamma$ are estimable with the same variance $\text{Var}(\widehat{\mathbf{p}'_{ij} \gamma}) = \sigma^2/c_i$ for $j = 1, \dots, \alpha_i$, where σ^2 denotes the error variance of the intra-block analysis.

Now we are going to give a method for finding matrices $\tilde{\mathbf{A}}_j$ satisfying (6) for given \mathbf{p}_{ij} , which is useful in practical applications of Definition 1.

From (4) and (6) we have

$$(7) \quad \mathbf{A}_i^\# = \sum_{j=1}^{\alpha_i} \mathbf{p}_{ij} \mathbf{p}'_{ij}, \quad i = 1, \dots, m.$$

Of the matrices $\mathbf{A}_i^\#$, let $\mathbf{A}_l^\#$ be one with the greatest number, say l^* , of different elements.

If $l^* > m+1$ then the vectors \mathbf{p}_{ij} cannot determine an association scheme with m associate classes.

If $l^* = m+1$ then the matrix $\mathbf{A}_l^\#$ has $m+1$ different elements $\tilde{z}^{0l}, \dots, \tilde{z}^{ml}$. We construct matrices $\tilde{\mathbf{A}}_j$ by putting one in the place where z^{jl} occurs, and zero in the remaining places.

If $l^* < m+1$ then we first construct l^* matrices $\tilde{\mathbf{A}}_j^1$ as above. If one of the matrices $\mathbf{A}_i^\#$ has $s \geq 2$ different elements in places of ones in $\tilde{\mathbf{A}}_j^1$, then we divide $\tilde{\mathbf{A}}_j^1$ into s matrices corresponding to those s elements. If it is not possible to construct $m+1$ matrices $\tilde{\mathbf{A}}_j$ in this way, then the vectors \mathbf{p}_{ij} cannot determine an association scheme with m associate classes.

After determining the matrices $\tilde{\mathbf{A}}_j$ we must check the conditions (1), according to Definition 1. It turns out that satisfying the first two conditions implies the fulfilment of the other ones, which is expressed in Theorem 1.

THEOREM 1. *The vectors (5) determine an association scheme with m associate classes if and only if there exist binary matrices $\tilde{\mathbf{A}}_i$, $i = 0, \dots, m$, which satisfy*

$$(a) \quad \tilde{\mathbf{A}}_0 = \mathbf{I}, \quad \sum_{i=0}^m \tilde{\mathbf{A}}_i = \mathbf{1}\mathbf{1}',$$

$$(b) \quad \mathbf{A}_i^\# = \sum_{j=0}^m \tilde{z}^{ji} \tilde{\mathbf{A}}_j, \quad i = 1, \dots, m,$$

where $\mathbf{A}_i^\#$ are defined by (7) and \tilde{z}^{ji} are scalar constants. The matrices $\tilde{\mathbf{A}}_i$ are the association matrices of the above scheme.

Proof. The necessity is obvious: take $\mathbf{A}_i = \tilde{\mathbf{A}}_i$.

Sufficiency. According to Definition 1 we must prove that the matrices $\tilde{\mathbf{A}}_i$ are symmetric and satisfy the third and fourth conditions of (1). We first represent the matrices $\tilde{\mathbf{A}}_i$ as linear combinations of the matrices $\mathbf{A}_i^\#$ and $\mathbf{A}_0^\# = \mathbf{1}\mathbf{1}'/v$. Since these matrices are linearly independent, the matrix $\tilde{\mathbf{Z}}^{-1} = (\tilde{z}^{ji})$, where \tilde{z}^{ji} denotes the j th element of $\mathbf{A}_i^\#$, is nonsingular. Hence $\tilde{\mathbf{A}}_i = \sum_{l=0}^m \tilde{z}_{li} \mathbf{A}_l^\#$, where \tilde{z}_{li} is the (l, i) th element of $\tilde{\mathbf{Z}}$. It follows that

$\tilde{\mathbf{A}}'_i = \tilde{\mathbf{A}}_i$, $\tilde{\mathbf{A}}_i \mathbf{1} = \tilde{n}_i \mathbf{1}$ and $\tilde{\mathbf{A}}_j \tilde{\mathbf{A}}_k = \sum_{i=0}^m \tilde{p}_{jk}^i \tilde{\mathbf{A}}_i$, where $\tilde{n}_i = \tilde{z}_{0i}$ and

$$(8) \quad \tilde{p}_{jk}^i = \sum_{l=0}^m \tilde{z}_{lj} \tilde{z}_{lk} \tilde{z}^{il}, \quad i, j, k = 0, 1, \dots, m.$$

This completes the proof.

This useful theorem gives criteria for the vectors (5) to determine an association scheme. The following corollaries are also helpful:

COROLLARY 1. Let $\mathbf{p}_{ij} = (f_{ij}^1, \dots, f_{ij}^v)'$ for $i = 1, \dots, m$; $j = 1, \dots, \alpha_i$. If there exist i, s and s' such that either

- (i) $f_{ij}^s = 0$ for $j = 1, \dots, \alpha_i$, or
- (ii) $|f_{ij}^s| \geq |f_{ij}^{s'}|$ for $j = 1, \dots, \alpha_i$ and $|f_{ij}^s| > |f_{ij_0}^{s'}|$ for some $j_0 \in \{1, \dots, \alpha_i\}$, or
- (iii) $\alpha_i = 1$ and $|f_{i1}^s| \neq |f_{i1}^{s'}|$,

then the vectors (5) do not determine an association scheme with m associate classes.

Proof. Assume that (5) determines an association scheme. Then from (7) we have $\mathbf{A}_i^\# = (z_i^{ss'})$, where $z_i^{ss'} = \sum_{j=1}^{\alpha_i} f_{ij}^s f_{ij}^{s'}$ and, in particular,

$$(9) \quad z_i^{ss} = \sum_{j=1}^{\alpha_i} (f_{ij}^s)^2.$$

Conditions (a) and (b) of Theorem 1 imply that z_i^{ss} are all equal, for $s = 1, \dots, v$. From this and (i) it follows that \mathbf{p}_{ij} , $j = 1, \dots, \alpha_i$, are the null vectors, which is impossible. In cases (ii) and (iii) the values z_i^{ss} defined by (9) are not equal for fixed i , which is also impossible. This completes the proof.

From condition (iii) we get a very interesting conclusion:

COROLLARY 2. If, in a PBIB design, $\alpha_i = 1$ for some $i \in \{1, \dots, m\}$, then the number of treatments v must be even.

4. Examples

4.1. Let

$$\begin{aligned} \mathbf{w}_0^{(i)} &= \mathbf{1}, & \mathbf{w}_1^{(i)} &= (s_i - 1, -1, \dots, -1)', \\ \mathbf{w}_2^{(i)} &= (0, s_i - 2, -1, \dots, -1)', \dots, & \mathbf{w}_{s_i-1}^{(i)} &= (0, \dots, 0, 1, -1)' \end{aligned}$$

be $s_i \times 1$ vectors, where $s_i \geq 2$ for $i = 1, \dots, p$. Assume there are $m = 2^p - 1$ associate classes, which are denoted by (c_1, \dots, c_p) , where c_i is 0 or 1 and $\sum_{i=1}^p c_i > 0$.

We define $W_{c_1 \dots c_p}$ as the set of all vectors of the form

$$(10) \quad \mathbf{w} = (\mathbf{w}_{e_1}^{(1)} \otimes \dots \otimes \mathbf{w}_{e_p}^{(p)}) / \|\mathbf{w}_{e_1}^{(1)} \otimes \dots \otimes \mathbf{w}_{e_p}^{(p)}\|,$$

where $\|\mathbf{w}\| = \sqrt{\mathbf{w}'\mathbf{w}}$, $e_i = 0$ if $c_i = 0$ and e_i is one of $1, \dots, s_i - 1$ if $c_i = 1$. The operator " \otimes " always denotes the Kronecker product of some matrices or vectors. Let

$$W = \left\{ \mathbf{w} \in W_{c_1 \dots c_p} : c_i = 0 \text{ or } 1, i = 1, \dots, p, \sum_{i=1}^p c_i > 0 \right\}$$

be the same vectors as in (5) with $m = 2^p - 1$.

COROLLARY 3. *The vectors $\mathbf{w} \in W$ determine an association scheme with $2^p - 1$ associate classes. The association matrices of the above scheme are of the form*

$$(11) \quad \mathbf{A}_{a_1 \dots a_p} = \bigotimes_{i=1}^p \mathbf{A}_{a_i}^{(i)},$$

where $a_i = 0$ or 1 , $i = 1, \dots, p$, $\mathbf{A}_0^{(i)} = \mathbf{I}$ and $\mathbf{A}_1^{(i)} = \mathbf{1}\mathbf{1}' - \mathbf{I}$ are $s_i \times s_i$ matrices.

Proof. Substituting $\mathbf{w} \in W_{c_1 \dots c_p}$ in place of \mathbf{p}_{ij} on the left hand side of formula (6) we get

$$(12) \quad \mathbf{A}_{c_1 \dots c_p}^{\#} = \sum_{\mathbf{w} \in W_{c_1 \dots c_p}} \mathbf{w}\mathbf{w}' = \bigotimes_{i=1}^p \mathbf{A}_{c_i}^{\#(i)},$$

where $\mathbf{A}_0^{\#(i)} = \mathbf{1}\mathbf{1}'/s_i$ and $\mathbf{A}_1^{\#(i)} = \mathbf{I} - \mathbf{1}\mathbf{1}'/s_i$ are $s_i \times s_i$ matrices. Note that $\mathbf{A}_0^{\#(i)} = (\mathbf{A}_0^{(i)} + \mathbf{A}_1^{(i)})/s_i$ and $\mathbf{A}_1^{\#(i)} = ((s_i - 1)\mathbf{A}_0^{(i)} - \mathbf{A}_1^{(i)})/s_i$, thus

$$\mathbf{A}_{c_1 \dots c_p}^{\#} = \sum_{a_1, \dots, a_p} z^{a_1 \dots a_p, c_1 \dots c_p} \mathbf{A}_{a_1 \dots a_p},$$

where

$$z^{a_1 \dots a_p, c_1 \dots c_p} = v^{-1} \prod_{i: c_i=1} \{(1 - a_i)(s_i - 1) - a_i\}, \quad v = \prod_{i=1}^p s_i;$$

on the other hand, the matrices $\mathbf{A}_{a_1 \dots a_p}$ are defined by (11). In this way we have proven that each of the matrices (12) is a linear combination of the matrices (11). Thus the matrices (11) satisfy condition (b) of Theorem 1. Since (a) is clear, this ends the proof.

Assume now that there are $v = \prod_{i=1}^p s_i$ treatments, and p factors at s_1, \dots, s_p levels, respectively. The treatments are denoted by $\phi(\beta_1, \dots, \beta_p)$, where $\beta_i = 0, 1, \dots, s_i - 1$; $i = 1, \dots, p$. In the literature (see [4], p. 197)

the following notion of association scheme is called an F_p type association scheme with $2^p - 1$ associate classes:

DEFINITION 2. Two treatments $\phi(\beta_1, \dots, \beta_p)$ and $\phi(\beta'_1, \dots, \beta'_p)$ are (a_1, \dots, a_p) -th associates when $\beta_i = \beta'_i$ if $a_i = 0$, and $\beta_i \neq \beta'_i$ if $a_i = 1$.

After numbering the v treatments in lexicographical order, we find that the association matrices occurring in the above definition of association scheme are the same as in (11). In this way Corollary 3 is a new definition of an F_p type association scheme. It is worth noticing that $\mathbf{w} \in W_{c_1 \dots c_p}$ are the contrasts belonging to the interaction between the factors i_1, \dots, i_q , where $c_{i_1} = \dots = c_{i_q} = 1$ and $\sum_{i=1}^p c_i = q$. If in the above $q = 1$ then we call these vectors the contrasts of the main effects of the factor i_1 .

4.2. Let $W_i = \bigcup_i W_{c_1 \dots c_p}$, where \bigcup_i denotes the sum over all c_1, \dots, c_p with $c_1 + \dots + c_p = i$, and $W_{c_1 \dots c_p}$ is defined by (10). Let W^* be the set $\{\mathbf{w} \in W_i : i = 1, \dots, p\}$ with $s_1 = \dots = s_p = s$.

COROLLARY 4. The vectors $\mathbf{w} \in W^*$ determine an association scheme with p associate classes. The association matrices of this scheme are of the form

$$(13) \quad \mathbf{A}_0 = \mathbf{I}, \quad \mathbf{A}_i = \sum_i' \mathbf{A}_{a_1 \dots a_p},$$

where \sum_i' is the sum over all a_1, \dots, a_p satisfying $a_1 + \dots + a_p = i$.

Proof. Substituting $\mathbf{w} \in W_i$ in place of \mathbf{p}_{ij} on the left hand side of (6) we get

$$\mathbf{A}_i^\# = \sum_{\mathbf{w} \in W_i} \mathbf{w}\mathbf{w}' = \sum_i'' \mathbf{A}_{c_1 \dots c_p}^\#,$$

where \sum_i'' is the sum over all c_1, \dots, c_p with $c_1 + \dots + c_p = i$. Hence, and from (12), we get $\mathbf{A}_i^\# = \sum_{j=1}^m z^{ji} \mathbf{A}_j$, where \mathbf{A}_j is defined by (13), $z^{ji} = v^{-1} \sum_i \{(s-1)^q (-1)^{i-q}\}$ for every a_1, \dots, a_p with $a_1 + \dots + a_p = j$, q is the number of zeros in $\{a_i : c_i = 1, i = 1, \dots, p\}$ and $v = s^p$. So, condition (b) of Theorem 1 is satisfied by the matrices in (13). Since (a) is clear, this ends the proof.

In the literature (see [4], p. 203, [2], p. 572, and [3]) a C_p type association scheme or hypercubic association scheme is known as a special case of an F_p type association scheme. If we assume that there are $v = s^p$ treatments $\phi(\beta_1, \dots, \beta_p)$, $\beta_i = 0, 1, \dots, s-1$; $i = 1, \dots, p$, then a C_p association scheme among these treatments with $m = p$ associate classes is defined as follows:

DEFINITION 3. Two treatments $\phi(\beta_1, \dots, \beta_p)$ and $\phi(\beta'_1, \dots, \beta'_p)$ are i -th associates if $\sum_{k=1}^p \varepsilon(\beta_k - \beta'_k) = i$, where $\varepsilon(x) = 0$ if $x = 0$ and $\varepsilon(x) = 1$ otherwise.

After numbering the s^p treatments in lexicographical order, we find that the association matrices occurring in the above definition are the same as in (13). Therefore Corollary 4 is another definition of a C_p association scheme.

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