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On perpendicularity in designed experiments

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Summary

The term of orthogonality is frequently used to describe some properties of experimental designs or referring to uncorrelated random variables. The spectrum of notions connected with the orthogonality concept in the theory of experimental designs contains such terms as geometrical orthogonality (Tjur, 1984), or strict and weak orthogonalities (Khatri and Shah, 1986). In all these cases the common notion of orthogonality was modified to describe some regularity in experimental plans. In this paper the geometrical interpretations of these properties are exhibited.

1. Decompositions of subspaces and perpendicularity

For a given matrix $\mathbf{A}$, let $R(\mathbf{A})$ and $R^{\perp}(\mathbf{A})$ be the range of $\mathbf{A}$ and the orthogonal complement of the $R(\mathbf{A})$, respectively. Moreover, let $\mathbf{P}_\mathbf{A}$ denote the orthogonal projector on $R(\mathbf{A})$ and $\mathbf{Q}_\mathbf{A} = \mathbf{I} - \mathbf{P}_\mathbf{A}$ the orthogonal projector on $R^{\perp}(\mathbf{A})$. Further, we recall that two subspaces $R(\mathbf{A})$ and $R(\mathbf{B})$ are said to be orthogonal if $R(\mathbf{A}) \subseteq R^{\perp}(\mathbf{B})$ or $R(\mathbf{B}) \subseteq R^{\perp}(\mathbf{A})$. Then we write $R(\mathbf{A}) \perp R(\mathbf{B})$.

The following lemma gives a basic decomposition which will be used in the sequel.

Lemma 1. For any two subspaces $R(\mathbf{A})$ and $R(\mathbf{B})$

$$R(\mathbf{A}) = \{R(\mathbf{A}) \cap R(\mathbf{B})\} \boxplus R(\mathbf{P}_\mathbf{A}\mathbf{Q}_\mathbf{B}) \ , \tag{1}$$

where the symbol $\boxplus$ is used to indicate the sum of orthogonal subspaces.

The proof of this result is postponed to the Appendix. In view of (1) the subspace $R(\mathbf{P}_\mathbf{A}\mathbf{Q}_\mathbf{B})$ is the orthogonal complement of $R(\mathbf{A}) \cap R(\mathbf{B})$ in $R(\mathbf{A})$. If this

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decomposition is applied to the subspaces R(**A**) and R(**B**) in the union R(**A** : **B**) = R(**A**) + R(**B**), then we obtain

$$R(\mathbf{A} : \mathbf{B}) = \{R(\mathbf{A}) \cap R(\mathbf{B})\} \boxplus \{R(\mathbf{P}_A\mathbf{Q}_B) \oplus R(\mathbf{P}_B\mathbf{Q}_A)\} \ , \tag{2}$$

where the symbol $\oplus$ indicates that the summands are disjoint subspaces. The property follows, since $\mathbf{u} = \mathbf{P}_A\mathbf{Q}_B\,\mathbf{a} = \mathbf{P}_B\mathbf{Q}_A\mathbf{b}$ for some **a** and **b**, implies $\mathbf{Q}_B\mathbf{P}_A\mathbf{Q}_B\mathbf{a} = \mathbf{Q}_B\mathbf{P}_B\mathbf{Q}_A\mathbf{b} = \mathbf{0}$, which gives $\mathbf{u} = \mathbf{0}$. Thus the only common vector of subspaces $R(\mathbf{P}_A\mathbf{Q}_B)$ and $R(\mathbf{P}_B\mathbf{Q}_A)$ is a zero vector.

The decomposition (2) forms the natural base for the concept of perpendicularity. Two subspaces are said to be perpendicular, in symbols R(**A**)][R(**B**), if the subspaces $R(\mathbf{P}_A\mathbf{Q}_B)$ and $R(\mathbf{P}_B\mathbf{Q}_A)$ are orthogonal, i.e. $R(\mathbf{P}_A\mathbf{Q}_B) \perp R(\mathbf{P}_B\mathbf{Q}_A)$. This definition is in full agreement with the geometrical intuition of perpendicularity, and means the orthogonality of such subspaces of R(**A**) and of R(**B**) which are orthogonal complements to their common part R(**T**) = R(**A**) ∩ R(**B**). Moreover, this property is closely connected with commutativity of orthogonal projectors.

Lemma 2. Two subspaces R(**A**) and R(**B**) are perpendicular if and only if

$$\mathbf{P}_A\mathbf{P}_B = \mathbf{P}_B\mathbf{P}_A \ . \tag{3}$$

The proof of this result is also shown in the Appendix. The commutativity of orthogonal projectors plays a key role in many problems. A comprehensive collection of different commutativity criteria of projectors $\mathbf{P}_A$ and $\mathbf{P}_B$ with many applications to linear statistical inference can be found in Baksalary (1987), and Nordström and von Rosen (1987). The subspaces corresponding to commuting projectors are called commuting subspaces (see Birkhoff and von Neumann, 1936). In statistical literature some other terms are also used. Mostly they refer to the concept of orthogonality. For instance, Tjur (1984) in the context of the analysis of variance in linear models, have termed this property as geometrical orthogonality. It seems, however, that the term of perpendicularity is more relevant here as reflecting precisely the geometrical property of subspaces involved.

2. Perpendicularity in experimental designs

2.1. Block designs

The block design is an experiment, in which a given set of v treatments is distributed over units forming a set of b blocks. The sizes of blocks as well as the replicates of treatments are arbitrary. The assignment of treatments to units, and units to blocks, is commonly described with the use of two binary matrices $\mathbf{\Delta}'$ and $\mathbf{D}'$ of order $n{\times}v$ and $n{\times}b$, respectively, where n denotes the number of units in the experiment. The model for the expectation of the vector of observations $\mathbf{y} \in R^n$ can be expressed as

$$E(\mathbf{y}) \in R(\mathbf{\Delta}' : \mathbf{D}') \ .$$

We assume, as usually, that the dispersion matrix of $\mathbf{y}$ is proportional to the unit matrix of order n, i.e., $D(\mathbf{y}) = \sigma^2\mathbf{I}$, $\sigma^2 > 0$. In that way there is a direct correspondence between orthogonality, defined by the standard inner product, and the concept of uncorrelated random variables.

The block design is called orthogonal if $\mathbf{\Delta Q}_{\mathbf{D}'}\mathbf{Q}_{\mathbf{\Delta}'}\mathbf{D}' = \mathbf{0}$ or, equivalently,

$$\mathbf{N} = \mathbf{NK}^{-1}\mathbf{N}'\mathbf{R}^{-1}\mathbf{N} \ , \tag{4}$$

where $\mathbf{K} = \mathbf{DD}'$, $\mathbf{R} = \mathbf{\Delta\Delta}'$, and $\mathbf{N} = \mathbf{\Delta D}'$ is the incidence matrix. The condition (4) was formulated by Chakrabarti (1962). It ensures some simplicity of the analysis of the block experiment. On the other way, the question arises what is geometrical interpretation of the property (4). To this aim observe that (4) can equivalently be written as

$$\mathbf{\Delta D}' = \mathbf{\Delta P}_{\mathbf{D}'}\mathbf{P}_{\mathbf{\Delta}'}\mathbf{D}' \ , \tag{5}$$

since for any full column rank $\mathbf{A}$, $\mathbf{P}_{\mathbf{A}} = \mathbf{A}(\mathbf{A}'\mathbf{A})^{-1}\mathbf{A}'$. But (5) is equivalent to the commutativity of $\mathbf{P}_{\mathbf{D}'}$ and $\mathbf{P}_{\mathbf{\Delta}'}$ which takes place if and only if the subspaces $R(\mathbf{\Delta}')$ and $R(\mathbf{D}')$ are perpendicular, i.e. $R(\mathbf{D}')$][$R(\mathbf{\Delta}')$. In result the orthogonal block design is a design having the treatment subspace, $R(\mathbf{\Delta}')$, perpendicular to the block subspace, $R(\mathbf{D}')$.

2.2. Row and column designs

The row and column design is defined when a given set of v treatments is allocated on the units arranged in a given number, say b_1, of rows and, simultaneously, in a given number, say b_2, of columns. Rows and columns form a desired structure for eliminating two directions of heterogeneity in the set of experimental units. The space of the expectation of an observation vector $\mathbf{y} \in R^n$ is now spanned by three binary matrices – a matrix for treatments, $\mathbf{\Delta}'$, a matrix for rows, $\mathbf{D}_1'$, and a matrix for columns $\mathbf{D}_2'$. In consequence, we have

$$E(\mathbf{y}) \in R(\mathbf{\Delta}' : \mathbf{D}_1' : \mathbf{D}_2') \ .$$

To complete the model, let us assume that the dispersion matrix of $\mathbf{y}$, $D(\mathbf{y})$, is proportional to the $n \times n$ identity matrix, as in the case of block designs.

If in the row and column design

$$\mathrm{Cov}(\mathbf{D}_1\mathbf{Q}_{(\mathbf{\Delta}' : \mathbf{D}_2')}\mathbf{y}) \ , \ \mathbf{D}_2\mathbf{Q}_{(\mathbf{\Delta}' : \mathbf{D}_1')}\mathbf{y}) = 0 \ , \tag{6}$$

then it is called orthogonal (see Chakrabarti, 1962) or weakly orthogonal (see Khatri and Shah, 1986), Following Siatkowski (1993, Theorem 2.2), the condition (6) can be rewritten equivalently as

$$\mathbf{P_A P_B} = \mathbf{P_B P_A} \ ,$$

where $\mathbf{A} = \mathbf{Q}_{\Delta'}\mathbf{D}'_1$ and $\mathbf{B} = \mathbf{Q}_{\Delta'}\mathbf{D}'_2$. Thus the row and column design is weakly orthogonal if and only if

$$R(\mathbf{Q}_{\Delta'}\mathbf{D}'_1) \,][\, R(\mathbf{Q}_{\Delta'}\mathbf{D}'_2) \ . \tag{7}$$

If the condition (7) can be replaced by the stronger condition of orthogonality of the subspaces involved, i.e. by the condition

$$R(\mathbf{Q}_{\Delta'}\mathbf{D}'_1) \perp R(\mathbf{Q}_{\Delta'}\mathbf{D}'_2) \ , \tag{8}$$

then the row and column design is called strongly orthogonal (see Khatri and Shah, 1986). In the view of the discussion above the conditions (7) and (8) have clear geometrical interpretation. It is seen directly when the space of the expectation of $\mathbf{y}$ is decomposed to the form

$$R(\mathbf{\Delta}' : \mathbf{D}'_1 : \mathbf{D}'_2) = R(\mathbf{\Delta}') \boxplus \{R(\mathbf{Q}_{\Delta'}\mathbf{D}'_1) + R(\mathbf{Q}_{\Delta'}\mathbf{D}'_2)\} \ .$$

Since $R\{\mathbf{Q}_{\Delta'}(\mathbf{D}'_1 : \mathbf{D}'_2)\} = R(\mathbf{Q}_{\Delta'}\mathbf{D}'_1) + R(\mathbf{Q}_{\Delta'}\mathbf{D}'_2)$ represents the subspace of $R(\mathbf{\Delta}' : \mathbf{D}'_1 : \mathbf{D}'_2)$ after eliminating treatments, the weak orthogonality of row and column design geometrically means the perpendicularity of the subspace of rows to the subspace of columns, both adjusted with respect to the subspace of treatments. When these two subspaces are perpendicular and disjoint, which is equivalent to their orthogonality, then the design possesses strong orthogonality property. In this light, it seems justified to link the concept of perpendicularity with a design satisfying (7), and reserve the term of orthogonality for a design satisfying condition (8). This observation can be simply extended on the multi-factor designs by adopting the approach of Khatri and Shah (1986).

2.3 Orthogonality in the analysis of variance

Finally, let us consider the general linear model in a parameter-free approach formulation. For the vector $\mathbf{y}$ of n observations we then have

$$E(\mathbf{y}) = \mathbf{0} \in \Omega \subseteq R^n \ , \quad D(\mathbf{y}) = \sigma^2\mathbf{I} \ ,$$

where Ω is a proper subspace of R^n. In this general framework, Darroch and Silvey (1963) have considered the problem of testing the hypotheses $H_i : \mathbf{0} \in \omega_i$, $i = 1,2,\ldots,k$, where ω_i are some subspaces of Ω. The experimental design such that

$$\omega_i^{\perp} \cap \Omega \perp \omega_j^{\perp} \cap \Omega, \quad i,j = 1,2,\ldots,k, \quad i \neq j\,, \tag{9}$$

is called orthogonal. The condition (9) ensures desirable properties, when the problem of testing hypotheses $H_i : \mathbf{0} \in \omega_i$, $i = 1,2,\ldots,k$, is regarded. In the light of the equality $R^{\perp}(\mathbf{C}) \cap R(\mathbf{A}) = R(\mathbf{Q}_C\mathbf{A})$ fulfilled for any $R(\mathbf{C}) \subseteq R(\mathbf{A})$, the condition (9) can be replaced by

$$R(\mathbf{Q}_i\mathbf{X}) \perp R(\mathbf{Q}_j\mathbf{X}), \quad i,j = 1,2,\ldots,k, \quad i \neq j\,, \tag{10}$$

where $\mathbf{X}$ is such a matrix that $R(\mathbf{X}) = \Omega$ and $\mathbf{Q}_i$ is the orthogonal projector on the orthogonal complement of ω_i. Since $\omega_i \subseteq \Omega$, for $i = 1, 2, \ldots, k$, then (10) is equivalent to the commutativity of projectors $\mathbf{P}_i\mathbf{P}_j = \mathbf{P}_j\mathbf{P}_i$ for $i,j = 1,2,\ldots,k$, $i \neq j$, and thus the experimental design is orthogonal if and only if the set of hypotheses $H_i : \mathbf{0} \in \omega_i$, $i = 1,2,\ldots,k$, is related to pairwise perpendicular linear subspaces, i.e. if and only it ω_i][ω_j $i,j = 1,2,\ldots,k$, $i \neq j$.

Appendix

Proof of Lemma 1. Let $R(\mathbf{T}) = R(\mathbf{A}) \cap R(\mathbf{B})$. Since $R(\mathbf{P_A}) = R(\mathbf{A})$ and $R(\mathbf{T}) \subseteq R(\mathbf{A})$, the sum on the right hand side of (1) is contained in $R(\mathbf{A})$. To show the reverse inclusion, we use the orthogonal projectors on $R(\mathbf{S}) = R(\mathbf{A} : \mathbf{B})$ and on $R(\mathbf{T})$, given by Ben-Israel and Greville (1974, p.198,199) (see also Anderson and Duffin, 1969, or Rao and Mitra, 1971, p. 189). These projectors have the following forms

$$\mathbf{P_S} = \mathbf{KK}^+\,, \tag{A1}$$

$$\mathbf{P_T} = 2\mathbf{P_A}\mathbf{K}^+\mathbf{P_B} = 2\mathbf{P_B}\mathbf{K}^+\mathbf{P_A}\,, \tag{A2}$$

where $\mathbf{K}^+$ is the Moore-Penrose inverse of $\mathbf{K} = \mathbf{P_A} + \mathbf{P_B}$. In view of (A1), (A2) and the relation $R(\mathbf{A}) \subseteq R(\mathbf{S})$, we have

$$\begin{aligned} \mathbf{A} = \mathbf{P_S}\mathbf{A} = (\mathbf{P_A} + \mathbf{P_B})\mathbf{K}^+\mathbf{A} &= \mathbf{P_A}\mathbf{K}^+\mathbf{A} + \mathbf{P_B}\mathbf{K}^+\mathbf{P_A}\mathbf{A} \\ &= \mathbf{P_A}\mathbf{K}^+\mathbf{A} - \mathbf{P_A^2}\mathbf{K}^+\mathbf{P_B}\mathbf{A} + 2\mathbf{P_B}\mathbf{K}^+\mathbf{P_A}\mathbf{A} \\ &= \mathbf{P_A}\mathbf{K}^+\mathbf{A} - \mathbf{P_A}\mathbf{P_B}\mathbf{K}^+\mathbf{P_A}\mathbf{A} + 2\mathbf{P_B}\mathbf{K}^+\mathbf{P_A}\mathbf{A} \\ &= \mathbf{P_A}\mathbf{Q_B}\mathbf{K}^+\mathbf{A} + 2\mathbf{P_B}\mathbf{K}^+\mathbf{P_A}\mathbf{A}\,, \end{aligned}$$

which implies that $R(\mathbf{A}) \subseteq R(\mathbf{T}) + R(\mathbf{P_A}\mathbf{Q_B})$. Finally observe that if $\mathbf{u} \in R(\mathbf{T})$, then $\mathbf{u} = \mathbf{P_A}\mathbf{u} = \mathbf{P_B}\mathbf{u}$ and thus $\mathbf{u}'\mathbf{P_A}\mathbf{Q_B} = \mathbf{u}'\mathbf{P_B}\mathbf{Q_B} = \mathbf{0}$, which shows that $R(\mathbf{T}) \subseteq R^{\perp}(\mathbf{P_A}\mathbf{Q_B})$, i.e. $R(\mathbf{T}) \perp R(\mathbf{P_A}\mathbf{Q_B})$. ❑

Proof of Lemma 2. The condition (3) is equivalent with the equation

$$\mathbf{P_A P_B} = \mathbf{P_A P_B P_A P_B} \tag{A3}$$

by the use of results given, with the other 44 equivalent conditions, by Baksalary (1987). Thus the proof reduces to showing that (3) and (A3) are equivalent with perpendicularity of R(**A**) and R(**B**). Consider the product $\mathbf{W} = \mathbf{Q_B P_A P_B Q_A}$. If the condition (3) is fulfilled, then $\mathbf{W} = \mathbf{0}$ and $R(\mathbf{P_A Q_B}) \perp R(\mathbf{P_B Q_A})$ i.e. R(**A**)][R(**B**). Conversely, if $\mathbf{W} = \mathbf{0}$, then $\mathbf{P_A P_B Q_A} = \mathbf{P_B P_A P_B Q_A}$ and, in consequence, $\mathbf{P_A P_B} - \mathbf{P_A P_B P_A} = \mathbf{P_B P_A P_B} - \mathbf{P_B P_A P_B P_A}$. On account of symmetry of $\mathbf{P_A P_B P_A}$ and $\mathbf{P_B P_A P_B}$, the equality above implies the symmetry of $\mathbf{P_A P_B} + \mathbf{P_B P_A P_B P_A}$. Thus $\mathbf{P_A P_B} + \mathbf{P_B P_A P_B P_A} = \mathbf{P_B P_A} + \mathbf{P_A P_B P_A P_B}$, or, equivalently,

$$\mathbf{P_A P_B} - \mathbf{P_A P_B P_A P_B} = \mathbf{P_B P_A} - \mathbf{P_B P_A P_B P_A}\ (= \mathbf{F})\ .$$

But the product $\mathbf{FF'}$ is a zero matrix, which implies (A3). ❑

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O prostopadłości w układach eksperymentalnych

Streszczenie

Ortogonalność jest pojęciem często używanym do opisu własności układów doświadczalnych lub odwołującym się do nieskorelowania zmiennych losowych. W teorii układów eksperymentalnych, wśród pojęć nawiązujących do ortogonalności spotkać można takie określenia jak ortogonalność geometryczna (Tjur, 1984) lub ortogonalność ścisła albo słaba (Khatri i Shah, 1986). W każdym z tych przypadków zwykłą ortogonalność stosownie zmodyfikowano w celu podkreślenia pewnych szczególnych własności planów eksperymentalnych. W prezentowanej pracy własności te uwypuklono nadając im w pełni geometryczną interpretację.

Słowa kluczowe: przestrzenie przemienne, przestrzenie prostopadłe, układy ortogonalne.