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On The Theory of Connected Designs: Characterization and Optimality

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Abstract

Connectedness is an important property which every block design must possess if it is to provide an unbiased estimator for all elementary treatment contrasts under the usual linear additive model. We have classified the family of connected designs into three subclasses: locally connected, globally connected and pseudo-globally connected designs. Basically, a locally connected design is one in which not all the observations participate in the estimation. A globally connected design is one in which all observations participate in the estimation. Finally, a pseudo-globally connected design is a compromise between locally and globally connected designs. Theorems and corollaries are given which characterize the different classes of connected designs.

In our discussion on the optimality of connected designs we show that there is much to be gained by partitioning the family of connected designs in the above fashion. Our optimality criteria are S-optimality suggested by Shah, which selects the design with minimum trace of the information matrix squared and (M,S)-optimality which selects the S optimal design from the class of designs with maximum trace of the information matrix.

Using these optimality criteria, we have been able to derive some new results which we hope to be of interest to the users and researchers in the field of optimum design theory. To be specific, let $BD\{v,b,(r_i),(k_u)\}$ denote a block design on a set of v treatments with b blocks of size k_u, $u = 1,2,\ldots,b$ and treatment i is replicated r_i times. Then we have shown that for the family of connected block designs $BD\{v,b,(r_i),k\}$ with (i) less than $k - 1$ treatments having replication equal to one and binary (0,1) the S-optimum design is pseudo-globally connected; (ii) the S-optimum design is globally connected if $r_i > 1$ and the designs are binary; and (iii) at least one treatment with replication greater than b, then the (M,S)-optimum design is pseudo-globally connected. In the final part of this paper we mention some unsolved problems in this area.

1. Introduction and Summary. The concept of connectedness in the theory of block designs is due to Bose (1947). Connectedness is an important property which every block design must possess if it is to provide an unbiased estimator for all elementary treatment contrasts under the usual linear additive model. While Bose has defined this concept in the form of chains between blocks and treatments, Chakrabarti (1963) has equivalently defined this concept in terms of the rank of the coefficient matrix or the information matrix of the design.

The notion of connectedness is not in general related to any optimality criteria, i.e., it is quite possible that, for the given v, b; $r_1, r_2, \ldots, r_v$; $k_1, k_2, \ldots, k_b$ the parameters of the design, an arbitrary connected design may happen to be the "worst" possible one. This means that one should study and classify the family of connected designs from an optimality point of view. This problem can be tackled in two different ways. (i) Search for the optimal design under the given optimality criterion. (ii) Decompose the family of connected designs into "meaningful" subclasses and study the optimality of each subclass. While approach (i) seems to be natural, it is certainly hard and in some cases formidable if not impossible, given our present mathematical machineries. Approach (ii) depends heavily on the way one might classify the family of connected designs. An arbitrary partition is certainly useless and will lead us nowhere. We will use the approach (ii) and the following considerations motivated our classifications. We observed that for some connected

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designs not every observation participates in the least squares estimation of contrasts. This consideration suggested to us the possibility that a connected design which has the property that every observation participates in such an estimation is "better" than one which lacks this property. Thus we classified the family of connected designs into three subclasses: locally connected, globally connected and pseudo-globally connected designs. Basically, a locally connected design is one in which not all the observations participate in the estimation. A globally connected design is one in which all the observations participate in the estimation. Finally, a pseudo-globally connected design is a compromise between locally and globally connected designs. In sections 2 and 3 the different classes of connected designs are defined and characterized. Some invariance properties and the problems of composing connected designs are discussed in section 4.

The optimality of connected designs is discussed in section 5. Our criteria are S-optimality and (M,S)-optimality both of which are defined in the section. We consider classes of designs for which no particular optimality results are known and show that the optimal design exhibits a specific type of connectedness. Thus the search for the optimal design need only concern designs with a specific connected nature. In general the widely known optimality results of Kiefer and others usually involve global or pseudo-global connected designs. This result also broadly applies to the wider class of designs which we consider.

2. Preliminaries and Definitions. Let $\Omega = \{1,2,\ldots,v\}$ be a set of v treatments assigned to b blocks of size k_u, $u = 1,2,\ldots,b$ and treatment i is replicated r_i times. Two different methods are used for denoting this general block design, $D = \{B_1, B_2, \ldots, B_b\}$ where B_u is the u-th block and $BD\{v, b, (r_i), (k_u)\}$. The statistical analysis of interest in this paper is the intrablock analysis with the model

$$E(y_{iu}) = \mu + t_i + \beta_u.$$

where y_{iu} is the observed response of the i-th treatment in the u-th block, μ = mean effect, t_i = the effect of treatment i, and β_u = the effect of the u-th block.

From the normal equations we have

$$\underline{C}\hat{\underline{t}} = \underline{Q} \tag{2.1}$$

where $\hat{\underline{t}}$ is a solution of (2.1) and called the vector of estimated treatment effects

$$\underline{C} = \text{diag}(r_1, r_2, \cdots, r_v) - \underline{N}\,\text{diag}(k_1^{-1}, k_2^{-1}, \cdots, k_b^{-1})\underline{N}'$$

(2.2) or

$$\underline{C} = \underline{R} - \underline{N}\underline{K}^{-1}\underline{N}' \ .$$

$\underline{N}'$ is the transpose of $\underline{N}$, the incidence matrix of the design

$$\underline{Q} = \underline{T} - \underline{N}\underline{K}^{-1}\underline{B}$$

$\underline{T}$ = column vector of treatment totals.

$\underline{B}$ = column vector of block totals.

Equation (2.1) is known as the equation for estimating the treatment effects and the matrix defined by (2.2) is the well known coefficient matrix. Obviously, the C matrix plays a decisive role in the estimation of contrasts and hence the connectedness and optimality of designs.

Bose (1947) defined connectedness as follows:

"A treatment and block are said to be associated if the treatment is contained in the block. Two treatments, two blocks, or a treatment and a block may be said to be connected if it is possible to pass from one to the other by means of a chain consisting alternately of blocks and treatments such that any two members of a chair are associated. A design (or a portion of a design) is said to be a connected design (or a connected portion of a design) if every block or treatment of the design (or a portion of the design) is connected to every other."

Unbiased estimators of an elementary treatment contrast can be obtained directly from the chains connecting the treatments of the contrast. For example, consider a block design where block B_1 contains treatments (i, i_1), block B_2 contains treatments (i_1, i_2), $\cdots$, block B_h contains treatments (i_{h-1}, i_h) and block B_{h+1} contains treatments (i_h, j). Then treatments i and j are connected through the chain $iB_1 i_1 B_2 i_2 \cdots i_{h-1} B_h i_h B_{h+1} j$ and an unbiased estimator of $t_i - t_j$ is obtained from this chain by the following linear function of the corresponding observations $y_{i1} - y_{i_1 1} + y_{i_1 2} - y_{i_2 2} + \cdots + y_{i_{h-1} h} - y_{i_h h} + y_{i_{h+1} h+1} - y_{jh+1}$. Chains of the form $iB_u i$ are meaningless and should not appear as part of any chain between two treatments. It is interesting to note that if the design is connected with respect to treatments it is also connected with respect to blocks and all elementary contrasts between blocks are estimable, i.e., $\beta_u - \beta_{u'}$ is estimable for all $u, u' = 1, 2, \cdots, b$, $u \neq u'$. Chakrabarti (1963) defines a design to be connected if its $\underset{\sim}{C}$ matrix has rank $v - 1$, and has proved that his definition of connected designs is equivalent to that of Bose (1947).

The original definition of connectedness is extended and generalized to further classify connected designs as either locally, globally or pseudo-globally connected. Locally connected designs are defined the same as the connected designs of Bose (1947) and Chakrabarti (1963). However, two treatments are said to be globally connected if they satisfy the following definition.

<u>Definition 2.1</u>. Two treatments i and j, $i \neq j$, of a block design are said to be globally connected if each replicate of i is connected by a chain, as defined by Bose (1947) to each replicate of j.

Denote the x-th replicate of treatment i as i^x.

Example 2.1. Consider the following block design:

$$
D: \quad
\begin{array}{ccc}
B_1 & B_2 & B_3 \\
\boxed{\begin{array}{c} 1^1 \\ 2^1 \\ 3^1 \end{array}} &
\boxed{\begin{array}{c} 1^2 \\ 2^2 \\ 3^2 \end{array}} &
\boxed{\begin{array}{c} 1^3 \\ 2^3 \end{array}}
\end{array}
$$

The chains between the replicates of treatments 1 and 2 are:

$1^1 B_1 2^1$, $\quad 1^1 B_1 3 B_2 2^2$, $\quad 1^1 B_1 3 B_2 1 B_3 2^3$

$1^2 B^B 2^2$, $\quad 1^2 B_2 3 B_1 2^1$, $\quad 1^2 B_2 3 B_1 1 B_3 2^3$

$1^3 B_3 2^3$, $\quad 1^3 B_3 2 B_2 3 B_1 2^1$, $\quad 1^3 B_3 2 B_1 3 B_2 2^2$.

For treatments 1 and 3

$1^1 B_1 3^1$, $\quad 1^1 B_1 2 B_2 3^2$

$1^2 B_2 3^2$, $\quad 1^2 B_2 2 B_1 3^1$

$1^3 B_3 2 B_1 3^1$, $\quad 1^3 B_3 2 B_2 3^2$.

For treatments 2 and 3

$2^1 B_1 3^1$, $\quad 2^1 B_1 1 B_2 3^2$

$2^2 B_2 3^2$, $\quad 2^2 B_2 1 B_1 3^1$

$2^3 B_3 1 B_1 3^1$, $\quad 2^3 B_3 1 B_2 3^2$.

Each pair of treatments is globally connected.

Pseudo-global connectedness is defined as follows:

[illegible]

[illegible] connected if each replicate of i is connected by a chain, as defined by Bose, to at least one replicate of j and vice versa.

Example [illegible]. Consider the design in example [illegible] but with [illegible] differently.

	B_1	B_2	B_3
D:	1^1	1^2	2^3
	2^1	1^3	3^2
	2^2	3^1	

The chains between replicates of treatments 1 and 2 are:

$1^1 B_1 2^1, \qquad 1^1 B_1 2^1, \qquad 1^2 B_2 3 B_3 2^3, \qquad 1^3 B_2 3 B_3 2^3 \ .$

For treatments 1 and 3

$1^1 B_1 2 B_3 3^2, \qquad 1^2 B_2 3^1, \qquad 1^3 B_2 3^1 \ .$

For treatments 2 and 3

$2^1 B_1 1 B_2 3^1, \qquad 2^2 B_1 1 B_2 3^1, \qquad 2^3 B_3 3^2 \ .$

Each pair of treatments is pseudo-globally connected. Also it should be noted that no pair of treatments is globally connected.

In the following definition and lemma we use the term "x connected" where x can mean locally, globally or pseudo-globally.

<u>Definition 2.3</u>. A block design is said to be x connected if every pair of treatments is x connected.

If we allow a treatment to be x connected to itself then the relation $R(x)$, treatments i and j are x connected, defines an equivalence relation on Ω. We now have the following lemma.

<u>Lemma 2.1</u>. <u>A design is</u> x <u>connected if and only if under the equivalence relation</u> $R(x)$ <u>there is only one equivalence class</u>.

3. <u>Characterization</u>.

A. <u>Locally Connected Designs</u>. In this section several new results for determining whether or not a design is locally connected are given. First, let us review some results from the literature.

Gateley (1962) and Weeks and Williams (1964) give conditions for an n-way crossed classification design with no interactions to be locally connected. Gateley's theorems involve the rank of the design matrix and for block designs ($n = 2$), it is equivalent to Chakrabarti's rank of $\underset{\sim}{C}$ definition. The procedure of Weeks and Williams is too lengthy to present here, and the reader is referred to their 1964 paper or Searle (1971). Lindstrom (1970) has generalized Gateley's (1962) and Weeks and Williams' (1964) results to n-way cross classification experiments with interactions, allowing unequal numbers of observations per cell. He proves that unbiased estimators of main effects and interactions can be constructed if and only if certain chains can be established among the non-empty cells of the design. An algorithm and a computer program to sort out the chains are also given by him. Birkes <u>et al</u> (1972a,1972b) have also recently obtained some relevant and useful results in this area.

One should note that Chakrabarti's 1963 paper contains many important results on the $\underline{C}$-matrix and is considered a major contribution to the theory of connected designs. From Lemma 2.1 we have the following necessary and sufficient condition for a design to be locally connected.

Theorem 3.1. Design D is locally connected if and only if its incidence matrix N cannot be partitioned as follows:

$$\underline{N} = \begin{bmatrix} N_1 & & & 0 \\ & N_2 & & \\ & & \ddots & \\ 0 & & & N_a \end{bmatrix}, \; 1 < a \le v, \; N_i \text{ are matrices}$$

N_i reflect the connected subsets of the set of treatments.

If $\underline{N}$ cannot be partitioned as above then there is only one equivalence class of the relationship of connectedness, and vice versa.

Corollary 3.1. NN' and N'N can be partitioned similar to N if and only if N can be partitioned as in theorem 3.1.

Remark 3.1. $\underline{N}$ can be replaced by $\underline{C}$ and theorem 3.1 still holds.

Theorem 3.2. D is locally connected if and only if there exists a set

$$D^* = \{B_1^*, B_2^*, \cdots, B_b^* \mid B_s^* \in D \ \forall \ s=1,2,\cdots,b \ \underline{\text{and there exists a}} \ q < p \ \underline{\text{such that}}$$

$$B_p^* \cap B_q^* \neq \phi \ \forall \ p=2,3,\cdots,b\} \ .$$

Proof:

(i) Sufficiency. The existence of D* implies that every treatment must appear in a block that contains at least two treatments. Thus each B_s^* must intersect with a B_r^* $r \neq s$, that contains at least two treatments and the union of all blocks containing two treatments contains Ω. Hence we can construct a chain that passes through all the blocks containing two or more treatments and thus pass through every treatment.

(ii) Necessity. If D* does not exist then there is a B_p^* for which no B_q^* exists such that $B_p^* \cap B_q^* \neq \phi$, $q < p$, and the B_s^*'s can be grouped into disjoint sets of B_s^*. Thus the treatments contained in these disjoint sets of B_s^* form subsets of connected treatments and D is not locally connected.

Corollary 3.2. A design is locally connected if and only if there exists a chain between two treatments that contain all the treatments or blocks.

Let us consider the set T_i, which has as elements the blocks that contain treatment i, and denote $\mathcal{T} = \{T_1, T_2, \cdots, T_v\}$.

Theorem 3.3. D is locally connected if and only if there exists a set

$$\mathcal{T}^* = \{T_1^*, T_2^*, \cdots, T_v^* \mid T_i^* \in \mathcal{T} \ \forall \ i=1,2,\cdots,v \ \underline{\text{and there exists a}} \ j < i \ \underline{\text{such that}}$$

$$T_i^* \cap T_j^* \neq \phi \ \forall \ i=2,3,\cdots,v\} \ .$$

Proof: This proof is analogous to that of theorem 3.2.

If treatment i and j are connected by a chain we write this as [ij]. Define the operator $\cdot$ (dot) by $[ij] \cdot [jk] = [ik]$; i.e., if i and j are connected and j and k are connected then, obviously, i and k are connected by a chain. Also, if i and j are connected by a chain then j and i are connected by a chain; i.e., $[ij] = [ji]$. It should be noted that if a design is locally connected then there are $v(v-1)$ chains excluding the chains of [ii]. We now have the following theorem:

Theorem 3.4. *D is locally connected if and only if there is a set, $\mathcal{U}$ with $v - 1$ elements each of the form $[ij] \epsilon D$, such that under the dot operator, as defined above, the $v(v-1)$ possible chains can be generated.*

The non-zero elements of $\underline{N}\underline{N}'$ represent the number of chains of the form iB_rj, which is the [ij] element. Thus $(\underline{N}\underline{N}')^2$ is in essence the result of the dot operation between the chains represented by non-zeros in $\underline{N}\underline{N}'$ and in general $(\underline{N}\underline{N}')^a, 2 \le a \le v-1$ is equivalent to the dot operation between the non-zero elements of $(\underline{N}\underline{N}')^{a-1}$ and those of $\underline{N}\underline{N}'$. The longest possible chain between any two treatments is one which contains all the treatments; such a chain could be constructed by the dot operation between $v - 1$ chains of the form iB_rj with distinct B_r's. Thus the non-zero elements of $(\underline{N}\underline{N}')^{v-1}$ represent those pairs of treatments that are locally connected. Obviously a similar argument will hold for $\underline{N}'\underline{N}$ to $(\underline{N}'\underline{N})^{b-1}$. We now have the following theorem:

Theorem 3.5. *A design is locally connected if and only if its incidence matrix $\underline{N}$ has the property that $(\underline{N}\underline{N}')^{v-1}$ or $(\underline{N}'\underline{N})^{b-1}$ has no zero entries.*

B. Globally Connected Designs. An advantage of globally connected designs is that when estimating the elementary contrast between the effects of treatments i and j every replicate participates to a maximum yielding $r_i \times r_j$ estimates of $t_i - t_j$ or $t_j - t_i$. In section 5 it is shown that this class of connected designs under certain restrictions and constraints contains the optimum design. The following theorem characterizes globally connected designs.

Theorem 3.6. A design D is globally connected if and only if the following conditions hold simultaneously:

(1) *D is locally connected.*

(2) *Every block of D contains at least two treatments that occur in more than one block; i.e., for all $B_s \in D$ there exists an i and $j \in B_s$ such that $i \in B_r$ and $j \in B_u$, $u \neq s$ and $r \neq s$.*

(3) *If any B_s contains exactly two treatments that occur in other blocks then these two treatments each occur in at least two other blocks.*

(4) *Any treatment, i say, that appears in two or more blocks (but not all blocks) must do so in blocks that contain*

(i) *a treatment that appears in two blocks containing i, and two not containing i. That is, $i \in B_r$ and B_s and there exists a $j \in B_r, B_s, B_m$, and B_n where $i \notin B_m$ and $i \notin B_n$,*

or

(ii) *two treatments each appearing in a block containing i, and a block not containing i. That is, i and $j \in B_r$, i and $k \in B_s$, then $j \in B_m$ and $k \in B_n$ with $i \notin B_m$ and $i \notin B_n$.*

Some of these conditions may seem redundant; however, with a few simple examples it can be shown that this is not the case, see Eccleston (1972). In the following proof by a singleton we mean a block containing exactly one treatment.

Proof of Theorem 3.6.

(i) Sufficiency: Consider any replicate of any treatment, say replicate x of treatment i, and denote as i^x. Then given that the conditions hold, can i^x be connected by a chain to any replicate of any other treatment, say m^y? Now by condition (2), if $i^x \in B_s$ then there exists a $j \in B_s$ such that we have $i^x B_s j$. Since the design is locally connected we can construct a chain between j and m. If j is connected to m^y, then we are finished. However, if j is connected to m^z, $z \neq y$, then since the blocks containing m^z and m^y satisfy the conditions (2), (3), and (4), a chain between m^z and m^y can be constructed.

(ii) Necessity: (i) Condition (1) is obvious. (ii) If condition (2) is violated then D has a singleton. The treatment belonging to the singleton cannot be connected by a chain to any other treatment and so it follows that D is not globally connected. (iii) If condition (3) is violated by i but not j of block B_s then i occurs in only one other block, B_r say. A chain between $j \in B_s$ and $i \in B_r$ cannot be constructed; consequently, the design is not globally connected. (iv) If condition (4)(i) is negated for treatment i say, then there is a treatment j which occurs in at least two blocks containing i, and exactly one not containing i, say B_r, or vice versa. It follows that one cannot construct chains between all the replications of j and i, namely the replicate of $j \in B_r$, and any replicate of i. If 4 (ii) is negated by j clearly it is impossible to connect any replicate of i to the replicate of k belonging to the block not containing i.

Corollary 3.5. If the same two treatments appear in every block, then the design is globally connected. (The design must have at least three blocks.)

Corollary 3.6. If N has no zero elements, then D is globally connected. (If N has no zero elements, then NN' and $N'N$ have no zero elements.)

Example 3.1. Consider the design

	B_1	B_2	B_3	B_4	B_5
	1	1	1	2	5
D:	2	2	4	3	4
			3	5	3

By inspecting D it is clear that the design satisfies theorem 3.6.

C. Pseudo-Globally Connected Designs. A pseudo-globally connected design assures one that in estimating elementary contrasts each replicate of the treatments involved is utilized. When estimating elementary treatment contrasts, globally connected designs maximize the use of all replicates of the treatments whereas pseudo-globally connected designs guarantee that no replicates are "wasted". That is, every replicate of each treatment in the contrast is involved at least once in the estimation. As mentioned before, this class of connected designs, under certain conditions, contains the optimum connected design. The following theorem characterizes pseudo-globally connected designs.

Theorem 3.7. A design D is pseudo-globally connected if and only if conditions (1), (2) and (4) of theorem 3.6 hold simultaneously.

The proof is analogous to that of theorem 3.6.

Example 3.2. Consider the design of example 3.1 but with treatment 2 of B_1 and treatment 4 of B_3 interchanged.

D:

B_1	B_2	B_3	B_4	B_5
1	1	1	2	3
4	2	2	3	4
		3	5	5

By inspection it is clear that D satisfies theorem 3.7 (i.e., fails only condition (3) of theorem 3.6).

Corollary 3.7. If a design D is locally connected and each replicate of treatment i is connected by a chain to every other replicate of i, for all $i \in \Omega$ then D is pseudo-globally connected. [Note: If, in addition to the above, condition (3) of theorem 3.6 holds then D is globally connected.]

Further corollaries, rules and examples are given by Eccleston (1972).

4. Invariance Properties and the Composition of Connected Designs.

A. Invariance Properties of Connected Designs. If a design D on Ω is locally (globally) connected then any of the following can occur and D will remain locally (globally) connected.

(a) For D locally connected: Any new block can be added to D so long as its elements belong to Ω.

(b) For D globally connected:

(i) any treatment belonging to Ω can be added to any block of D,

(ii) any new treatment(s) can be added to any block of D,

(iii) any block belonging to D can be repeated any number of times,

(iv) if a treatment appears in a block, it can be replicated any number of times within that block.

Recall that if a design is globally connected then it is pseudo-globally connected, which also implies that the design is locally connected. Thus the facts in (b) above apply to pseudo-globally and also locally connected designs.

B. The Composition of Connected Designs. Let us consider the proposition of composing two designs that are locally, globally and pseudo-globally connected.

(a) Compositions that yield locally connected designs:

(i) If D_1 and D_2 are locally connected designs on the sets of treatments Ω_1 and Ω_2, respectively, and $\Omega_1 \cap \Omega_2 = \phi$, then the design $\bar{D}_\ell = D_1 \cup D_2 \cup B$ is locally connected, where B is a block containing at least two treatments, i and j say, such that $i \in \Omega_1$ and $j \in \Omega_2$. The block B forms the link between the two designs D_1 and D_2. Since i is connected to all treatments in Ω_1 and j to all in Ω_2 then the chain iBj locally connects every pair of treatments of $\Omega_1 \cup \Omega_2$.

(ii) Let D_1 and D_2 be locally connected designs on Ω_1 and Ω_2, respectively, and if $\Omega_1 \cap \Omega_2 \neq \phi$, i.e., Ω_1 and Ω_2 have at least one element in common, then $D_1 \cup D_2$ is a locally connected design.

(b) Compositions that yield globally connected designs.

(i) Consider D_1 and D_2 to be globally connected designs on treatment sets Ω_1 and Ω_2, respectively, $\Omega_1 \cap \Omega_2 = \phi$. As before, $\bar{D}_g = D_1 \cup D_2 \cup B$ where B as above, is locally connected. However, if B contains four treatments i, j, k, and ℓ such that i and $j \in \Omega_1$ and k and $\ell \in \Omega_2$, also i and j each appear in at least two blocks of D_1 and similarly k and ℓ in D_2, then $\bar{D}_g$ is globally connected.

Moreover, if B contains three treatments of Ω_1 and three of Ω_2 then $\bar{D}_g$ is globally connected. It is easily shown that $\bar{D}_g$, with the above B's, satisfies theorem 3.6.

(ii) For $D_1 \cup D_2$ to be globally connected, it is sufficient for D_1 and D_2 each to be globally connected and one of the following:

(1) $\Omega_1 \cap \Omega_2 = \{i\}$ and i appears in two blocks of D_1 and two of D_2.

(2) $\Omega_1 \cap \Omega_2 = \{ij\}$ and i appears in at least one block of D_1 and two of D_2, while j appears in at least one block of D_2 and two of D_1.

(3) $\Omega_1 \cap \Omega_2 = \{i,j,k\}$.

(c) <u>Compositions that yield pseudo-globally connected designs</u>.

(i) Suppose D_1 and D_2 are pseudo-globally connected designs on treatment sets Ω_1 and Ω_2, respectively and $\Omega_1 \cap \Omega_2 = \phi$. As above $\bar{D}_{pg} = D_1 \cup D_2 \cup B$, where B is as in (a), locally connected. However, if i and j belong to two blocks of D_1 and D_2, respectively, then $\bar{D}_{pg}$ is pseudo-globally connected. Moreover, if B contains 3 treatments i, j and m where i and j $\epsilon\ \Omega$, and m belongs to two or more blocks of D_2, then $\bar{D}_{pg}$ is pseudo-globally connected.

(ii) For $D_1 \cup D_2$ to be pseudo-globally connected, it is sufficient that D_1 and D_2 each be pseudo-globally connected and one of the following:

(1) $\Omega_1 \cap \Omega_2 = \{i\}$ and i occurs in two blocks of D_1 and two of D_2.

(2) $\Omega_1 \cap \Omega_2 = \{i,j\}$.

It is interesting to note that two designs, D_1 and D_2, can each be not locally connected but their union $D_1 \cup D_2$ may be locally connected. This is obvious since given a locally connected design, D, one can often partition D into locally disconnected subsets. A similar remark is true for globally and pseudo-globally connected designs. The composition of more than two designs would follow along the lines of the above methods but be somewhat more complex.

5. Optimality: A - Background and our optimality criteria

The theory of optimum experiment and treatment designs is essentially the use of a well defined criterion to determine which in a specified class of legitimate or competing designs is the best. So far, almost all contributions to this field have been related to the optimality of non-randomized designs. This paper is also formulated in this framework. The first formal treatment of this subject was given about five decades ago by Smith (1918). It was revived after a 25-year pause by Wald (1943), Mood (1946), Elfving (1952), Chernoff (1953), Ehrenfeld (1955), Kiefer (1958, 1959), Kiefer and Wolfowitz (1959) and others. A voluminous literature has developed around the problem of finding optimal designs. The newly published book, Theory of Optimum Experiments, by V. V. Fedorov (1972) is a clear indication that this branch of statistics is growing fast and has attracted many leading mathematicians and statisticians around the world.

Kiefer, in 1958 and subsequent papers discusses the three most used and well-known optimality criteria, namely A, D and E optimality. The optimality criteria involve functions of the non-zero eigen values, $\{\lambda_i,\ i = 1,2,\ldots\}$, of the information matrix of the design. In general these criteria are not related and need not agree in comparing given designs. Only in restricted settings such as designs with equal replication and block size or designs with λ_i constant for all i have the above criteria offered readily tractable solutions. Since we discuss designs restricted only by their degree of connectedness a different criterion is necessary. In addition we compare only designs with the same parameter set $\left\{v,b,(r_i),\ (k_i)\right\}$ and do not consider interblock information. Some of these ideas, together with other reasons led Shah (1960) to introduce an optimality criteria which will hereafter be called S-optimality.

S-Optimality. Minimize $\sum_i \lambda_i^2$ if the trace of information matrices of the competing designs are identical. The corresponding optimum design will be referred to as S-optimum.

We now introduce an optimality criterion which is a useful and somewhat hybrid of the preceding optimality criteria. The corresponding optimization is carried in two stages and is formally defined as follows:

(M,S)-Optimality. First, form a subclass of designs whose information matrices have maximum trace. Then, select a design from this subclass such that its square of the information matrix has minimum trace. The resulting design is called the (M,S)-optimum design.

S-optimality and (M,S)-optimality will be our optimality criteria in this paper. Using these optimality criteria, we have been able to derive some new results which we hope to be of interest to the users and researchers in the field of optimum design theory. To be specific, we have shown that for the family of connected block designs $BD\{v,b,(r_i),k\}$ with (i) less than k - 1 treatments having replication equal to one and binary (0,1) the S-optimum design is pseudo-globally connected; (ii) the S-optimum design is globally connected if $r_i > 1$ and the designs are binary; and (iii) at least one treatment with replication greater than b, then the (M,S)-optimum design is pseudo-globally connected.

B - S-Optimality and (M,S)-Optimality of Connected Designs.

Let Δ denote the family of all connected designs with the parameter set $\{v,b,(r_i),(k_u)\}$. Let also $\Delta_1 \subset \Delta$ denote the set of those designs in Δ which are pseudo-globally connected. Note that the cardinality of Δ_1 ranges from zero to the cardinality of Δ depending on the given set of parameters.

Definition 5.1. Let D_1 and D_2 be two designs in Δ. Then we say D_1 is S-better than D_2 if D_1 has a smaller trace of $\underline{C}$ squared than D_2.

Consider a situation where the connected designs in Δ are binary with $n_{iu} = 0$ or 1 and proper, i.e., $k_u = k$. These designs constitute most of the well-known classical designs. Then we have the following theorem.

Theorem 5.1. *Corresponding to any design in $\Delta_2 = \Delta - \Delta_1$ there is a pseudo-globally connected design in Δ_1 which is S-better if less than $k - 1$ of the r_i's are equal to one.*

Proof. Let $D \in \Delta_2$. Then by the conditions imposed on Δ the design D satisfies conditions (1) and (2) of theorem 3.7. Therefore, condition (3) must be violated by one or more treatments in D. We shall devise an algorithm which involves the rearrangement of the experimental units in D in a manner such that the resulting design $\bar{D}$ is pseudo-globally connected and is S-better than D.

Suppose treatment i fails to satisfy condition (3) of theorem 3.7 but since the design is locally connected there exists a treatment ℓ that

(a) belongs to only one block containing i and at least one not containing i, or

(b) belongs to at least one block containing i and only one not containing i.

The design can be divided into two parts, T_i the set of blocks which contain i, and $D - T_i$ the set of blocks which do not contain i. We discuss (a) only, but an analogous proof holds for (b). For the designs we are considering there exists a replicate of treatment $z \in B_r \in T_i$, $r_z > 1$, $z \neq \ell$ and a replicate of treatment $p \in B_t \in D - T_i$, $r_p > 1$, $p \neq \ell$ which can be interchanged to yield a design in which treatment i satisfies condition (3). Such a z and p always exist since there are less than k - 1 treatments with $r_i = 1$. Whether or not the interchange yields a smaller trace of $\underset{\sim}{C}^2$ depends on the change in the elements of $\underset{\sim}{C}$, in particular, the elements of the row corresponding to treatment ℓ. The possibilities are as follows:

(i) Suppose $\ell \in B_r$ and $\ell \in B_t$. The elements of $\underset{\sim}{C}$ that are changed are as follows (recall that all diagonal elements are fixed for all designs of this theorem).

Before interchange		After interchange
c_{zi}	$\longrightarrow$	$c_{zi} + \frac{1}{k}$
c_{zm}	$\longrightarrow$	$c_{zm} + \frac{1}{k}$ where $m \in B_r$ $m \neq \ell$, $m \neq z$, $m \neq i$
c_{pw}	$\longrightarrow$	$c_{pw} + \frac{1}{k}$ where $w \in B_t$ $w \neq \ell$, $w \neq p$
$c_{zw}(= 0)$	$\longrightarrow$	$-\frac{1}{k}$ for all w of which there are k - 3
$c_{pm}(= 0)$	$\longrightarrow$	$-\frac{1}{k}$ for all m of which there are k - 2.

All other elements of $\underset{\sim}{C}$ are unchanged. Thus trace of $\underset{\sim}{C}^2$ before the interchange can be written as

$$(5.1) \qquad \text{tr } \underset{\sim}{C}^2 = c_{zi}^2 + \sum_m c_{zm}^2 + \sum_w c_{zw}^2 + \sum_m c_{pm}^2 + \sum_w c_{pw}^2 + \text{Remainder.}$$

After the interchange

$$(5.2) \qquad \text{tr } \underset{\sim}{C}^2 = (c_{zi} + \frac{1}{k})^2 + \sum_m (c_{zm} + \frac{1}{k})^2 + \sum_w \frac{1}{k^2} + \sum_m (\frac{1}{k})^2 + \sum_w (c_{pw} + \frac{1}{k})^2 + \text{Remainder.}$$

The remainder term is the same for both equations (5.1) and (5.2); therefore, their difference is

$$(5.3 \qquad (5.1) - (5.2) = -2c_{zi}\,\frac{1}{k} - \frac{2}{k^2} - 2\sum_m c_{zm}\,\frac{1}{k} - \frac{2(k-3)}{k^2} - 2\sum_w c_{pw}\,\frac{1}{k} - 2(\frac{k-3}{k^2}).$$

We know that $c_{mn} \leq 0$ for $m \neq n$; therefore, $-c_{mn} \geq 0$. Since $-c_{zi} > \frac{1}{k}$, $-c_{zm} \geq \frac{1}{k}$ for all m, $-c_{p\ell} \geq \frac{1}{k}$, and $-c_{z\ell} = \frac{1}{k}$. Therefore (5.3) > 0. Thus the design is S-better after the interchange.

(ii) Suppose $\ell \notin B_r$ and $\ell \in B_t$, then

Before interchange		After interchange
$c_{p\ell}$	$\longrightarrow$	$c_{p\ell} + \frac{1}{k}$
$c_{z\ell} (= \frac{-1}{k})$	$\longrightarrow$	$c_{z\ell} - \frac{1}{k}$.

All other elements of $\underset{\sim}{C}$ are as in (i). Thus the difference between the trace of $\underset{\sim}{C}^2$ before and after interchange is the same as in (i) except for the $c_{p\ell}$ and $c_{z\ell}$ terms. Therefore, before interchange

$$(5.4) \qquad \operatorname{tr} \underset{\sim}{C}^2 = c_{p\ell}^2 + c_{z\ell}^2 + [(5.1) - c_{p\ell}^2 - c_{z\ell}^2]$$

and after interchange

$$(5.5) \qquad \operatorname{tr} \underset{\sim}{C}^2 = (c_{p\ell} + \frac{1}{k})^2 + (c_{z\ell} - \frac{1}{k})^2 + [(5.2) - c_{p\ell}^2 - c_{z\ell}^2].$$

From (i) we have

$$(5.4) - (5.5) > \frac{2c_{p\ell}}{k} - \frac{4}{k^2} .$$

If $c_{p\ell} = -\frac{1}{k}$ then (5.4) - (5.5) may not be greater than zero. But recall that ℓ belongs to only one block in T_i, namely B_r, and since $r_z > 1$ there exists a replicate of $z \in B_s$ and $\ell \in B_s$ which can be used for the interchange rather than $z \in B_r$. The interchange between $z \in B_s$ and $p \in B_t$ is equivalent to (i).

(iii) Suppose $\ell \notin B_r$ and $\ell \notin B_t$. This is analogous to (i) and the design after the interchange is S-better.

(iv) Suppose $\ell \in B_r$ and $\ell \notin B_t$, then

Before interchange		After interchange
$c_{z\ell}(= \frac{-1}{k})$	$\longrightarrow$	$c_{z\ell} + \frac{1}{k}(= 0)$
$c_{p\ell}$	$\longrightarrow$	$c_{p\ell} - \frac{1}{k}.$

All other elements of $\underset{\sim}{C}$ are as in (i). As in (ii) we have that before the interchange

$$(5.6) \qquad \text{tr } \underset{\sim}{C}^2 = c^2_{z\ell} + c^2_{p\ell} + [(5.1) - c^2_{z\ell} - c^2_{p\ell}]$$

and after the interchange

$$(5.7) \qquad \text{tr } \underset{\sim}{C}^2 = (c_{z\ell} + \frac{1}{k})^2 + (c_{p\ell} - \frac{1}{k})^2 + [(5.2) - c^2_{z\ell} - c^2_{p\ell}].$$

From (i) we have

$$(5.6) - (5.7) > \frac{2c_{p\ell}}{k}.$$

We know that $c_{p\ell} \leq \frac{-1}{k}$; thus (5.6) - (5.7) may not be greater than zero. But recall that ℓ belongs to only one block in T_i, namely B_r, and since $r_z > 1$ there exists a replicate of $z \in B_s \in T_i$, $s \neq r$, which can be used for the interchange. The interchange is now between $z \in B_s$ and $p \in B_t$ with $\ell \notin B_s$ and $\ell \notin B_t$ which is equivalent to (ii).

If now there exists another treatment, q say, that fails to satisfy condition (3) it can be corrected so that the interchange for i is not negated. Reversing the interchange between z and p is the only way to negate the correction for i. Let treatment m be to treatment q as ℓ was to treatment i, $\ell \neq m$ otherwise the correction for i would be sufficient for q (see example 5.1). Suppose the correction for q reverses the interchange between z and p. This implies

(a') either $q \in B_r \in T_q$ and $B_t \in D - T_q$ or $q \in B_t \in T_q$ and $B_r \in D - T_q$ but $\ell \in B_r$ and B_t; therefore q does not fail condition (3). This is a contradiction.

Or

(b') q, i and p ϵ B_r ϵ T_q and z ϵ D - T_q. Then all blocks containing z must belong to D - T_q, but z and i belong to the same block at least once and similarly if B_r ϵ D - T_q and B_t ϵ T_q. This implies that q satisfies condition (3), which is a contradiction.

So, in general, any treatments which fail condition (3) of theorem 3.7 can be corrected to yield a pseudo-globally connected design which is S-better. This completes the proof.

From theorem 5.1 we have the following corollary:

Corollary 5.1. Within the family of connected designs BD$\{v,b,(r_i),k\}$ with $n_{iu} = 0$ or 1 the S-optimal design is pseudo-globally connected if there are less than k - 1 treatments with $r_i = 1$.

If Δ_1 contains a globally connected design then we have the following theorem and corollary:

Theorem 5.2. Corresponding to any design in $\Delta_2 = \Delta - \Delta_1$ there is a globally connected design which is S-better if all $r_i > 1$ and $k \geq 3$.

The proof is analogous to that of theorem 5.1.

Corollary 5.2. Within the family of connected designs BD$\{v,b,(r_i),k\}$ with $n_{iu} = 0$ or 1 the S-optimal design is globally connected if all $r_i > 1$ and $k \geq 3$.

Instead of $r_i > 1$ and $k \geq 3$ it is sufficient if all $r_i \geq 2$ for theorem 5.2. and corollary 5.2. to be true.

Example 5.1. Let D be the following locally connected design in BD$\{9,6,(2,2,3,1,2,6,2,2,1),3\}$.

	B_1	B_2	B_3	B_4	B_5	B_6
	1	1	3	3	6	6
D:	2	2	4	5	7	7
	9	3	5	6	8	8

trace of $\underline{C} = 12$ and trace $\underline{C}^2 = 24$

Treatments 1, 2, 7 and 8 fail to satisfy condition (3) of theorem 3.7. In the notation of the proof of theorem 5.1 for treatments 1 and 2, $\ell = 3$ and for treatments 7 and 8, $\ell = 6$. Therefore, a correction for treatments 1 and 7 will be sufficient for treatments 2 and 8 respectively. By interchanging $2 \in B_2$ with $5 \in B_3$ and $8 \in B_5$ with $3 \in B_4$ results in

	B_1	B_2	B_3	B_4	B_5	B_6
	1	1	3	8	6	6
$\bar{D}$:	2	5	4	5	7	7
	9	3	2	6	3	8

trace of $\underline{C} = 12$ and trace $\underline{C}^2 = 68/3$

is globally connected and S-better.

If the condition of theorem 5.1 and corollary 5.1 is relaxed so as to include designs with more than $k - 1$ treatments with $r_i = 1$ then the lemma and theorem no longer hold in general. A counterexample which is too lengthy to present here can be found in Eccleston (1972).

Recall that the procedure for determining the (M,S)-optimal design is to first find the class of designs with maximum trace of $\underline{C}$ and then within that class determine those with minimum trace of $\underline{C}$ squared. Let Δ, Δ_1 and Δ_2 be as defined in the first paragraph of this section; then we have:

Theorem 5.3. Any design in Δ_2 can be transformed into a design in Δ_1 with the same trace of $\underset{\sim}{C}$.

Proof. For design BD$\{v, b, (r_i), (k_u)\}$ to be locally but not pseudo-globally connected either or both conditions (2) and (3) of theorem 3.7 fail to be satisfied. Each can be corrected by an interchange(s) as described in theorem 5.1. Suppose $z \in B_r$ and $p \in B_t$ are interchanged to correct either condition (2) or (3). The only diagonal elements of $\underset{\sim}{C}$ affected by the interchange are c_{zz} and c_{pp}. Block B_r is of size k_r and B_t is of size k_t:

$$c_{zz} \text{ becomes } c_{zz} - \frac{1}{k_t} + \frac{1}{k_r}$$

and

$$c_{pp} \text{ becomes } c_{pp} - \frac{1}{k_r} + \frac{1}{k_t}.$$

therefore, the trace of $\underset{\sim}{C}$ after interchange remains invariant. The same argument follows no matter how many interchanges are performed.

Theorem 5.4. For the family of designs BD$\{v, b, (r_i), k\}$ the (M,S)-optimal design is pseudo-globally connected if there is one $r_i = \alpha b + \beta$, $\alpha > 0$ and integer $\beta \geq 0$ and less than $k - (\alpha + 1)$ treatments with replication equal to one.

Proof. Given $r_i = \alpha b + \beta$

$$\max \operatorname{tr} \underset{\sim}{C} = \sum_i \max c_{ii}$$

where

$$c_{ii} = r_i - \sum_u n_{iu}^2/k.$$

Maximising c_{ii} is equivalent to minimising n_{iu} for all u. This implies that all n_{iu} should be as close to equal as possible, i.e.,

$$|n_{iu} - n_{iu'}| \leq 1 \qquad \text{for } u,u'$$

and

$$n_{iu} = \alpha \text{ or } \alpha + 1 \qquad \text{for all } u,\ u = 1,2,\ldots,b.$$

Such a design satisfies theorem 3.7. Therefore the design with max tr $\underline{C}$ is pseudo-globally connected and trivially it follows that the same design is (M,S)-optimal.

Corollary 5.3. For the family of connected designs $BD\{v,b,(r_i),k\}$ the (M,S)-optimal design is globally connected if there exists two $r_i \geq b$.

6. Concluding Remarks:

Results analogous to theorem 5.2, and corollary 5.1 for nonproper designs (i.e., designs with $k_u \neq k$ for all u) have not been proved as yet. The (M,S) optimality of the family of nonproper connected designs remains unsolved. Perhaps some method of generating pseudo-globally connected designs other than considered here may yield better optimality results. However, by partitioning the family of connected designs as we have done, many new results have been obtained. Virtually nothing is known about the optimality of nonproper designs, thus there remains a vast and challenging area of optimum design theory open to research.

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