Optimality in Designs of Experiment

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Abstract

Optimality for block designs have received much attention in the literature. Here we review these criteria and present results showing their A,D and E connection.Also we acquainted with the mathematical methods of designing optimal experiments.In this paper, we will to do work about optimality in experimental designs.

1. Introduction

Experimentation is an essential part of any problem of decision-making. Whenever one is faced with the necessity of acception one out of a set of alternative decisions , one has to undertake some experiments to collect observations on which the decision has to be based. In order that it may be possible to select an optimum decision procedure, the choice of the experiment must also be optimum in some sense. This is how the problem of optimal designing of experiments arises.

Let D(v,b,k,r) denote the set of connected, binary block designs that involve $v$treatments and b blocks such that each treatment is replicated r times and each blocksize is equal to k. The information matrix of any design d in D(v,b,r,k) is given by $C_d = rIv - k^{-1}NN'$, where N is the incidence matrix of the design.

Note that C is symmetric and nonnegative definite and that it arises from the reduced normal equation for the treatment effect alone.

The main purpose of this paper is to prove the relationship between A-optimality and any other optimalities.

2. Model and Preliminaries

Suppose that the model for a design is given by,

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$y_{ij\ell} = \mu + \tau_i + \beta_j + \epsilon_{ij\ell}$, $i = 1, \cdots, v$, $j = 1, \cdots, b$, $\ell = 1, \cdots, n_{ij}$, i.e.

$y = X\theta + \epsilon$,

where $y_{ij\ell}$ is an observation from the ith treatment and the jth block, μ is the overall mean , τ_i and $\beta_j$are the effects of the treatment and the jth block respectively. Then, it shows that

$$X^tX = (1_n | X_\tau | X_\beta)^t (1_n | X_\tau | X_\beta)$$
$$= \begin{pmatrix} 1_n^t \\ X_\tau^t \\ X_\beta^t \end{pmatrix} (1_n \ X_\tau \ X_\beta) = \begin{pmatrix} 1_n^t 1_n & 1_n^t X_\tau & 1_n^t X_\beta \\ X_\tau^t 1_n & X_\tau^t X_\tau & X_\tau^t X_\beta \\ X_\beta^t 1_n & X_\beta^t X_\tau & X_\beta^t X_\beta \end{pmatrix}$$
$$= \begin{pmatrix} n & r^t & k^t \\ r & R & N \\ k & N^t & K \end{pmatrix} \qquad \cdots\cdots \qquad (1)$$

The normal equation is given as the following :

$(X^tX)\hat{\theta} = X^t y$.More explicitly, it can be written as

$\begin{pmatrix} n & r^t & k^t \\ r & R & N \\ k & N^t & K \end{pmatrix} \begin{pmatrix} \hat{\mu} \\ \hat{\tau} \\ \hat{\beta} \end{pmatrix} = \begin{pmatrix} 1_n^t \\ X_\tau^t \\ X_\beta^t \end{pmatrix} y$,which is equivalent to

$$\begin{pmatrix} n\hat{\mu} + r^t\hat{\tau} + k^t\hat{\beta} \\ r\hat{\mu} + R\hat{\tau} + N\hat{\beta} \\ k\hat{\mu} + N^t\hat{\tau} + K\hat{\beta} \end{pmatrix} = \begin{pmatrix} 1_n^t y \\ X_\tau^t y \\ X_\beta^t y \end{pmatrix}.$$

Setting the corresponding terms equal, we obtain the following equations.

$$n\hat{\mu} + r^t\hat{\tau} + k^t\hat{\beta} = 1_n^t y = G \qquad \cdots\cdots \qquad (2)$$
$$r\hat{\mu} + R\hat{\tau} + N\hat{\beta} = X_\tau^t y = T \qquad \cdots\cdots \qquad (3)$$
$$k\hat{\mu} + N^t\hat{\tau} + K\hat{\beta} = X_\beta^t y = B \qquad \cdots\cdots \qquad (4)$$

To simplify the equations , we compute Let's be controled as the following, $(3) - (4) \times NK^{-1}$on both sides of (3) and (4).

Then, the following equality holds.

$(r - NK^{-1}k)\hat{\mu} + (R - NK^{-1}N^t)\hat{\tau} + (N - NK^{-1}K)\hat{\beta} = T - NK^{-1}B.$

Since it holds that

$r - NK^{-1}k = r - N1_b = r - r = 0$

$N - NK^{-1}K = N - N = 0$

If we set, $R - NK^{-1}N^t = C$, $T - NK^{-1}B = q$, then

we obtain the following reduced normal equation which illuminates the block effect $\hat{\beta}$.

$$C\hat{\tau} = q \qquad \cdots\cdots \qquad (5)$$

In (5), C is a $v \times v$ information matrix.

Denoting *G−inverse* of C by C^{-}, the following solution of (5) is obtained.

$\hat{\tau} = C^{-}q$ · · · · · · (6)

Using (4) and (6), the block effect $\hat{\beta}$ can be obtained as

$$\hat{\beta} = K^{-1}B - K^{-1}N^{t}\hat{\tau} - K^{-1}k\hat{\mu}$$

$$= K^{-1}B - K^{-1}N^{t}(C^{-}q) - 1_{b}\hat{\mu} \quad \cdots\cdots \quad (7)$$

Theorem 2.1 Let C_d be the information matrix for $d \in D(v,b,k,r)$. Then, it can be shown that

(*a*) C_d is a symmetric matrix.

(*b*) i) Sum of row and column of C_d equal to zero

ii) $rank(C_d) \leq v-1$.

3. Optimal Criteria

Let *Bvo* be a set of all $v \times v$ nonnegative definite matrices of which sum of row is zero. Let, $\lambda_1,\cdots,\lambda_{v-1}(\lambda_1 \geq \lambda_2 \geq,\cdots,\geq \lambda_{v-1})$ be the eigenvalues of $C_d \in Bvo$ for $d \in D(v,b,k,r)$.

A function $\phi_A : Bvo \rightarrow R$ is defined by $\phi_A(C_d) = Tr(C_d^{-}) = \sum_{i=1}^{v-1}\frac{1}{\lambda_i}$.

Then $\phi_A : A$ −optimal criteria are follows.

Definition 3.1. $d^{*} \in D(v,b,k,r)$ is A−optimal if and only if

$$\min_{d \in D} \phi_A(C_d) = \phi_A(C_d^{*}).$$

If $\phi_P : Bvo \rightarrow R$ is defined by

$$\phi_P(C_d) = \left\{\frac{1}{v-1} Tr(C_d^{-P})\right\}^{\frac{1}{P}},$$

then ϕ_F is an optimal criteria.

Definition 3.2. $d^{*} \in D(v,b,k,r)$ is ϕ_F−optimal if and only if

$$\min_{d \in D} \phi_P(C_d) = \phi_P(C_{d^{*}}).$$

Definition 3.3. $d^{*} \in D(v,b,k,r)$ is D−optimal if and only if

$$\min_{d \in D} \phi_D(C_d) = \phi_D(C_{d^{*}}) = det(C_{d^{*}}^{-}).$$

Definition 3.4. $d^* \in D(v,b,k,r)$ is type 1-optimal if and only if

$$\min_{d \in D} \phi_f(C_d) = \phi_f(C_{d^*}).$$

where $f : (0,\infty) \to R$ is a function satisfying

$$f(0) = \lim_{x \to 0+} f(x) = +\infty$$

$$f'(x) < 0, \quad f''(x) > 0, \quad f'''(x) < 0,$$

and $\phi_f(C_d) = \sum_{i=1}^{v-1} f(\lambda_i)$.

Definition 3.5. $d^* \in D(v,b,k,r)$ is E-optimal if and only if
d^* maximizes the smallest eigenvalue of any information matrix
C_d for $d \in D(v,b,k,r)$.

It is important to study the interrelationships among the various criteria because
if a class of optimality criteria is included in a larger class, a design which is
optimal with respect to each criterion in the larger class is optimal w.r.t. each
criterion in the smaller class.

It can be verified that all the criteria considered so far satisfy D, A, E-optimality criteria.

If $\lambda_i (\neq 0), i = 1, 2, \cdots, v-1$ are the eigenvalues of the information matrix $C_d \in Bvo$ for $d \in D(v,b,k,r)$, then the average efficiency E_d can be written by $E_d = \frac{v-1}{\sum_i^{v-1} e_i^{-1}}$, where $e_i = \frac{\lambda_i}{r}$.

Theorem 3.1. Suppose the information matrix C_{d^*} has $v-1$ nonzero eigenvalues that are all equal for $d^* \in D(v,b,k,r)$.

(a) If d^* is D-optimal in $D(v,b,k,r)$, then d^* is A-optimal in $D(v,b,k,r)$

(b) If d^* is A-optimal in $D(v,b,k,r)$, then d^* is E-optimal in $D(v,b,k,r)$.

Theorem 3.3. If $d^* \in D(v,b,k,r)$ is ϕ_1-optimal, then d^* is A-optimal.

Theorem 3.4. Let $f:(0,\infty)\rightarrow R$ be a function defined by $f(x)=\frac{1}{x}$. Then ϕ_f−criteria is type 1−criteria, and also ϕ_f−criteria is A−optimal.

Theorem 3.5. For $d^* \in D(v,b,k,r)$, let $\lambda_i=\left(\frac{1}{v-1}\right)^{\frac{1}{v-2}}$ $(i=1,\cdots,v-1)$ be the eigenvalues of the information matrix C_{d^*}.Then d^* is D−optimal if and only if d^* is A−optimal.

References

[1] Chernoff, H. (1953). Locally optimum designs for estimation parameters. *Ann. Math. Statist.* 24 586−602.

[2] Eccleston, J. A. (1972). On the theory of connected designs. Ph. D. thesis, Cornell Univ.

[3] Young Nam Son (2002). Balanced and Orthogonal Block Designs for Diallel Cross, the Journal of Korean Data Analysis Society, Vol.4, No.3, pp. 307−314

[4] Elfving, G. (1952). Optimum allocation in linear regression theory. *Ann. Math. Statist.* 23 255−262.

[5] Yung Nam Son, Jang−Jae Lee (2004) Construction of A−Optimal Block Design for Comparing a set of Test Inbred Lines with a set of Contro,2004 Proceedings of the Spring Conference , Korea Statistical Society(2004), Chonbuk University, 1 261−269.

[6] Kuey Chung Choi, Young Nam Son (2002), Optimal Designs for Complete Diallel Cross two Sources of Nuisance Variability, the Journal of Korean Data Analysis Society, Vol. 2, No.4, pp. 529−534

[7] Kiefer, J. (1958). On the nonrandomized optimality and randomized nonoptimality of symmetrical designs. *Ann. Math. Statist.* 29 675−699.

[8] Kiefer, J. (1959). Optimum experimental designs (with discussion). *J. Roy. Statist. Soc. Ser. B* 21 272−319.