1998年度日本オペレーションズ・リサーチ学会
秋季研究発表会

A note on mixed level supersaturated designs

01605000 Univ. of Tokyo MATSUI Tomomi

1. Introduction

In this paper, we consider mixed level supersaturated designs which are optimal with respect to the average χ^2 statistic criterion of Yamada, Lin and Yausnari [3]. We propose a lower bound of the average χ^2 statistic of a design and show a property which indicates a construction method of optimal designs.

Our results are extensions of that in the paper [2] by Tang and Wu on two-level supersaturated designs.

2. Notations and Definitions

Throughout this paper, we consider mixed level supersaturated designs with n runs. For any $S \subseteq R^n$, spn(S) denotes the linear subspace spanned by S. The inner product of two vectors $\boldsymbol{d}$ and $\boldsymbol{d}'$ are denoted by $\langle \boldsymbol{d}, \boldsymbol{d}' \rangle$.

We define the following families:

$\mathcal{D}_p^n \equiv \{\boldsymbol{d} \in \{0,1\}^n \mid d_1 + \cdots + d_n = n/p\}$

$\mathcal{M}_p^n \equiv \{\{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_p\} \subseteq \mathcal{D}_p^n \mid \sum_{r=1}^p \boldsymbol{d}_r = \boldsymbol{1}\}$

$\mathcal{M}^n \equiv \mathcal{M}_1^n \cup \mathcal{M}_2^n \cup \cdots \cup \mathcal{M}_n^n$.

Any element M in $\mathcal{M}^n$ is called a *column* and $p(M)$ denotes the integer p satisfying $M \in \mathcal{M}_p^n$. A multiset of columns is called a (*mixed level*) *design.* For any pair of columns $(M, M') \in \mathcal{M}_p^n \times \mathcal{M}_{p'}^n$, $\chi^2(M, M')$ denotes the value

$$\sum_{\boldsymbol{d} \in M} \sum_{\boldsymbol{d}' \in M'} \left(\langle \boldsymbol{d}, \boldsymbol{d}' \rangle - \frac{n}{pp'} \right)^2 \Big/ \left(\frac{n}{pp'} \right).$$

For any design $\mathcal{F} = \{M^1, M^2, \ldots, M^q\}$, $\chi^2(\mathcal{F}) \equiv \sum \{\chi^2(M^r, M^s) \mid 1 \le r < s \le q\}$.

When the design $\mathcal{F}$ consists of two-level columns, $\chi^2(\mathcal{F})$ is equivalent to the average squared inner products of $\mathcal{F}$ defined by Booth and Cox [1].

The linear subspace $\{\boldsymbol{x} \in \mathbf{R}^n \mid \boldsymbol{1}^T \boldsymbol{x} = 0\}$ is denoted by H. For any vector $\boldsymbol{d} \in \mathcal{D}_p^n$, we denote $\boldsymbol{d} - (1/p)\boldsymbol{1}$ by $\overline{\boldsymbol{d}}$. For any column $M \in \mathcal{M}^n$, we denote the vector set $\{\overline{\boldsymbol{d}} \mid \boldsymbol{d} \in M\}$ by $\overline{M}$.

Clearly from the definition, we have the following.

Lemma 1 For any pair $(M, M') \in \mathcal{M}_p^n \times \mathcal{M}_{p'}^n$,
$\chi^2(M, M') = (pp'/n) \sum_{\boldsymbol{d} \in M} \sum_{\boldsymbol{d}' \in M'} \left\langle \overline{\boldsymbol{d}}, \overline{\boldsymbol{d}'} \right\rangle^2.$

3. Orthogonal Designs

When a mixed level design $\mathcal{F} = \{M^1, M^2, \ldots, M^q\}$ satisfies the conditions that $1 \le \forall r < \forall s \le q$, $\chi^2(M^r, M^s) = 0$, we say that $\mathcal{F}$ is *orthogonal.* An orthogonal design $\mathcal{F} = \{M^1, M^2, \ldots, M^q\}$ satisfying $\dim \left(\overline{M^1} \cup \overline{M^2} \cup \cdots \cup \overline{M^q} \right) = n - 1$ is called an *orthogonal base.*

The following theorem provides an upper bound of the number of columns of an orthogonal design.

Theorem 1 Any orthogonal design $\mathcal{F} = \{M^1, M^2, \ldots, M^q\}$ satisfies the inequality

$$\sum_{r=1}^{q} (p(M^r) - 1) \le n - 1.$$

Proof. From the definition, spn$\left(\overline{M^r}\right) \subseteq H$. When $r \neq s$, the orthogonality implies that spn$\left(\overline{M^r}\right) \perp$ spn$\left(\overline{M^s}\right)$. Thus, we have the inequality.//

When a given design is an orthogonal base, then the above equality holds. A mixed level design which violates the above formula is called a *supersaturated* design.

4. Lower Bound Theorem

The following theorem gives a lower bound of the average χ^2 statistic.

Theorem 2 Any design $\mathcal{F} = \{M^1, \ldots, M^q\}$ satisfies $\chi^2(\mathcal{F}) \geq (1/2)v(v-1)n(n-1)$ where $v = (\sum_{r=1}^{q}(p(M^r)-1))/(n-1)$.

Outline of a proof. For any index r, we denote $p(M^r)$ by p_r, M^r by $\{\boldsymbol{d}_1^r, \boldsymbol{d}_2^r, \ldots, \boldsymbol{d}_{p_r}^r\}$ and $p_1 + \cdots + p_q$ by p^*. Let X be an $n \times p^*$ matrix defined by $X = [X_1, X_2, \ldots, X_q]$ where $X_r = \left[\sqrt{p_r}\overline{\boldsymbol{d}_1^r}, \sqrt{p_r}\overline{\boldsymbol{d}_2^r}, \ldots, \sqrt{p_r}\overline{\boldsymbol{d}_{p_r}^r}\right]$. We denote the positive semidefinite matrix X^tX by Y and the ordered eigenvalues of Y by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{p^*} \geq 0$. Since the rank of Y is less than or equal to $n-1$. we have $\lambda_n = \lambda_{n+1} = \cdots = \lambda_{p^*} = 0$.

Since Y is symmetric, we have

$$\begin{aligned}\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_{n-1}^2 &= \mathrm{tr}(Y^tY) \\ &= 2n\textstyle\sum_{1\leq r<s\leq q}\chi^2(M^r, M^s) + n^2v(n-1) \\ &= 2n\chi^2(\mathcal{F}) + n^2v(n-1).\end{aligned}$$

A lower bound of $\lambda_1^2 + \cdots + \lambda_{n-1}^2$ is obtained as the optimal value of the convex quadratic programming problem;

$$\begin{aligned}\text{QP: min.} \quad & \lambda_1^2 + \lambda_2^2 + \cdots + \lambda_{n-1}^2 \\ \text{s.t.} \quad & \lambda_1 + \lambda_2 + \cdots + \lambda_{n-1} = \mathrm{tr}(Y).\end{aligned}$$

Definition of Y implies that $\mathrm{tr}(Y) = \sum_{r=1}^{q} n(p_r - 1) = nv(n-1)$. The optimal value of QP is equal to $(nv)^2(n-1)$. The above results imply the desired inequality.//

5. χ^2-Optimal Supersaturated Designs

Lastly, we consider the properties of mixed level supersaturated designs which attains the lower bound obtained in the previous section.

Lemma 2 For any column $M \in \mathcal{M}^n$, every vector $\boldsymbol{f} \in \mathrm{spn}\left(\overline{M}\right)$ satisfies

$$\sum_{\boldsymbol{d}\in M} \left\langle \overline{\boldsymbol{d}}, \boldsymbol{f} \right\rangle \overline{\boldsymbol{d}} = \frac{n}{p(M)} \boldsymbol{f}.$$

Lemma 3 For any orthogonal base $\mathcal{F} = \{M^1, M^2, \ldots M^q\}$, every column $M \in \mathcal{M}^n$ satisfies the equality

$$\sum_{r=1}^{q} \chi^2(M, M^r) = n(p(M)-1).$$

Theorem 3 Let $\mathcal{F}$ be a design and $\{\mathcal{F}_1, \mathcal{F}_2, \ldots, \mathcal{F}_v\}$ a partition of $\mathcal{F}$ such that each member of the partition is an orthogonal base. Then we have the equality $\chi^2(\mathcal{F}) = (1/2)n(n-1)v(v-1)$.

Above theorem indicates that we can obtain a χ^2-optimal mixed level super saturated design by merging orthogonal bases.

This research owes much to the thoughtful and helpful comments of Shu Yamada.

References

[1] K.H.V. Booth and D.R. Cox, Some systematic supersaturated designs, *Technometrics*, 4 (1962), 489–495.

[2] B. Tang and C.F.J. Wu, A method of constructing supersaturated designs and its ε_{s^2} optimality, *Canadian Journal of Statistics*, 25 (1997), 191–201.

[3] S. Yamada, D.K.J. Lin and Y. Yasunari, Three-level supersaturated design, *Memoirs of Tokyo Metropolitan Institute of Technology*, 11 (1997).