A note on mixed level supersaturated designs

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1. Introduction

In this paper, we consider mixed level supersaturated designs which are optimal with respect to the average $\chi^2$ statistic criterion of Yamada, Lin and Yausnari [3]. We propose a lower bound of the average $\chi^2$ 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 $S \subseteq R^n$, $\text{span}(S)$ denotes the linear subspace spanned by $S$. The inner product of two vectors $d$ and $d'$ are denoted by $\langle d, d' \rangle$.

We define the following families:

- $D_p^n \equiv \{ d \in \{0,1\}^n \mid d_1 + \cdots + d_n = n/p \}$
- $M_p^n \equiv \{ \langle d_1, \ldots, d_p \rangle \in D_p^n \mid \sum_{r=1}^{p} d_r = 1 \}$
- $M^n \equiv M_1^n \cup M_2^n \cup \cdots \cup M_p^n$

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

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

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

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

Clearly from the definition, we have the following.

Lemma 1 For any pair $(M, M') \in M_p^n \times M_p^n$, $\chi^2(M, M') = \left( \frac{pp'}{n} \right) \sum_{d \in M} \sum_{d' \in M'} \langle d, d' \rangle^2 .

3. Orthogonal Designs

When a mixed level design $F = \{M^1, M^2, \ldots, M^n\}$ satisfies the conditions that $1 \leq r < s \leq q$, $\chi^2(M^r, M^s) = 0$, we say that $F$ is orthogonal. An orthogonal design $F = \{M^1, M^2, \ldots, M^n\}$ satisfying $\dim(M^1 \cup M^2 \cup \cdots \cup M^n) = n - 1$ 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 $F = \{M^1, M^2, \ldots, M^n\}$ satisfies the inequality

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

**Theorem 2** Any design $F = \{M_1, \ldots, M_q\}$ satisfies $\chi^2(F) \geq (1/2)v(v-1)n(n-1)$ 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 $\{d_{r1}, d_{r2}, \ldots, d_{rp_r}\}$ 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 $X_r = [\sqrt{p_1}d_{r1}, \sqrt{p_2}d_{r2}, \ldots, \sqrt{p_{p_r}}d_{rp_r}]$. 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 $\lambda_1 = \lambda_{n+1} = \cdots = \lambda_{p^*} = 0$.

Since $Y$ is symmetric, we have

$$\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_{n-1}^2 = \text{tr}(Y^tY)$$

$$= 2n \sum_{r<s \leq q} \chi^2(M_r, M_s) + n^2v(n-1)$$

$$= 2n \chi^2(F) + n^2v(n-1).$$

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

**QP:** min $\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_{n-1}^2$

s.t. $\lambda_1 + \lambda_2 + \cdots + \lambda_{n-1} = \text{tr}(Y)$. Definition of $Y$ implies that $\text{tr}(Y) = \sum_{r=1}^q n(p_r - 1) = nv(n-1)$. The optimal value of QP is equal to $(nv)^2(n-1)$. The above results imply the desired inequality.

5. $\chi^2$-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 $f \in \text{spn}(M)$ satisfies

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

**Lemma 3** For any orthogonal base $F = \{M_1, M_2, \ldots, M_q\}$, 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 $F$ be a design and $\{F_1, F_2, \ldots, F_v\}$ a partition of $F$ such that each member of the partition is an orthogonal base. Then we have the equality $\chi^2(F) = (1/2)n(n-1)v(v-1)$.

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

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References

