Supplementary Materials for "Incorporating Minimum Variances into Weighted Optimality Criteria"

Katherine Allen-Moyer
Department of Statistics, North Carolina State University*
and
Jonathan Stallrich†
Department of Statistics, North Carolina State University

June 20, 2021

1 Approximate $c_{\mathcal{E}}$-Optimal CRDs

An approximate CRD is represented by its proportional replication vector $\boldsymbol{p}_d$ where $p_{di} \in [0, 1]$ such that $\sum_i p_{di} = 1$. To ensure estimability of all contrasts, we must have $p_{di} \in (0, 1)$. If the traditional c-optimal design for a contrast has p_{di} in this range, obviously it will also be $c_{\mathcal{E}}$-optimal. Otherwise, at least one $p_{di} = 0$. If all non-zero p_{di} of the traditional c-optimal design were reduced by an arbitrarily small amount, ϵ, that is redispersed among the zero p_{di}, the resulting approximate design would have the desired estimability. However, decreasing ϵ will always lead to a decrease in the targeted contrast's variance, so there can be no $c_{\mathcal{E}}$-optimal design. To reconcile this issue, we propose a hybrid approach between the exact and approximate design theory.

Note, we can refer to an approximate CRD's replication vector as $\boldsymbol{r}_d = N\boldsymbol{p}_d$ which places the exact and approximate design approaches on a similar scale. If $N\boldsymbol{p}_d$ is comprised of integers, the approximate design is equivalent to an exact design. Just like in the exact

*The authors want to thank the reviewers and the editors for their insights and feedback.
†Title: Assistant Professor; Employer: Department of Statistics, North Carolina State University, 2311 Stinson Drive, Raleigh, NC 27695-8203; Email: jwstalli@ncsu.edu.

design case, we ensure estimability of all contrasts by requiring $r_{di} \geq 1$. In the approximate case, we have $r_{di} \in [1, N-t+1]$. The approximate $c_{\mathcal{E}}$-optimal design is the set of such r_{di} that minimize

$$\sum_i \frac{h_i^2}{r_{di}} + \lambda(\sum_i j r_{di} - 1 - N + t) \ . \tag{1}$$

Let $2 \leq t_h \leq t$ be the number of treatments with nonzero coefficients in the desired contrast $\boldsymbol{h}^T\boldsymbol{\tau}$. The approximate $c_{\mathcal{E}}$-optimal design then has

$$r_{di}^* = \begin{cases} 1 & \text{if } h_i = 0 \\ (N - t + t_h)\frac{|h_i|}{\sum_i j|h_i|} & \text{otherwise} \ . \end{cases} \tag{2}$$

2 Proof of Theorem 1

By induction The $c_{\mathcal{E}}$-criterion minimizes $\text{Var}(\widehat{\boldsymbol{h}^T\boldsymbol{\tau}}) = \sum_i \frac{h_i^2}{r_{i,N}}$ subject to $r_{di} \geq 1$ to ensure estimability. The base case has $N = t$ so $r_{di,N} = 1$. Thus, for d_{N+1}^*, there is an $\tilde{i}$ such that $r_{\tilde{i},N+1} = r_{\tilde{i},N} + 1$, otherwise estimability no longer holds. Now suppose d_N^* is a $c_{\mathcal{E}}$-optimal exact design with $N > t$ runs. The $c_{\mathcal{E}}$-optimal design for $N+1$ runs, d_{N+1}^*, must have a treatment $\tilde{i}$ where $r_{\tilde{i},N+1} \geq 1 + r_{\tilde{i},N}$, otherwise $\sum_i r_{\tilde{i},N+1} < N + 1$. This gives us two cases to consider.

Case 1: $r_{\tilde{i},N+1} = r_{\tilde{i},N} + 1$. We now show this forces $r_{i,N+1} = r_{i,N}$ for all $i \neq \tilde{i}$. Clearly $\sum_{i \neq \tilde{i}} r_{i,N+1} = \sum_{i \neq \tilde{i}} r_{i,N} = N - r_{\tilde{i},N}$, implying both d_N^* and d_{N+1}^* minimize $\sum_{i \neq i'} \frac{h_i^2}{r_{i,N}}$ given the sum equality constraints. The two designs therefore assign the same replication numbers to all treatments except $\tilde{i}$ up to permutation among the $r_{i,N}$ with the same value for h_i^2.

Case 2: $r_{\tilde{i},N+1} = r_{\tilde{i},N} + a$ for an integer $a \geq 2$. Then $\sum_{i \neq \tilde{i}} r_{i,N+1} = \sum_{i \neq \tilde{i}} r_{i,N} - (a-1)$. Relative to d_N^*, the design d_{N+1}^* is found by increasing the replication of treatment $\tilde{i}$ by a, and decreasing the total replication for all other treatments by $a - 1$. This implies adding a replicates to $\tilde{i}$ and removing a total of $(a-1)$ replicates from the other treatments decreases $\sum_i \frac{h_i^2}{r_{i,N+1}}$ more than adding one replicate to treatment $\tilde{i}$ and maintaining the same replication sum for the other $t-1$ treatments. Following the same logic, d_N^* is improved by adding $a-1$ replicates to treatment $\tilde{i}$ and, in some fashion, removing $a-1$ replicates from among the other $t-1$ treatments. This contradicts the fact that d_N^* is $c_{\mathcal{E}}$-optimal.

3 Elfving Theorem for the Quadratic Model

The proofs in this section follow from Chapter 2 of Pukelsheim (2006) and concern c-optimality, not $c_{\mathcal{E}}$-optimality. For the one-factor quadratic polynomial model with $x_i \in [-1, 1]$ the model is,

$$y_i = \tau_0 + \tau_1 x_i + \tau_{11} x_i^2 + e_i = \boldsymbol{x}_i^T \boldsymbol{\tau} + e_i \ .$$

The regression range $\mathcal{X}$ is comprised of all vectors $(1, x_i, x_i^2)$. The Elfving set $\mathcal{R} = \text{conv}(\mathcal{X} \cup -\mathcal{X})$ is the convex hull of the set $\mathcal{X} \cup -\mathcal{X}$ where $-\mathcal{X}$ multiplies all vectors in $\mathcal{X}$ by -1. A coefficient vector, $\boldsymbol{h}$, for an estimable function $\boldsymbol{h}^T\boldsymbol{\tau}$ can be constructed using a linear combination of vectors in $\mathcal{R}$. Each coefficient vector requires multiplication by a scaling factor to lie on the boundary of $\mathcal{R}$. The minimum variance for $\widehat{\boldsymbol{h}^T\boldsymbol{\tau}}$, with respect to an approximate design, is the square of the scaling factor. The coefficient vector for the linear term τ_1, $\boldsymbol{h}^T = (0, 1, 0)$, defines a supporting hyperplane to $\mathcal{R}$ and so must lie on its boundary. Hence the minimum variance of $\hat{\tau}_1$ is 1 in terms of the approximate design. The variance in terms of its corresponding exact design is then $1/N$. The approximate c-optimal design, written as proportions of N, is represented by

$$\xi = \begin{Bmatrix} -1 & 1 \\ 0.5 & 0.5 \end{Bmatrix} ,$$

where ± 1 are the two x_i in the design and are equally-replicated $0.5N$ times. Clearly this design will be unable to estimate the quadratic effects and so cannot be $c_{\mathcal{E}}$-optimal.

The quadratic term has coefficient vector $\boldsymbol{h}^T = (0, 0, 1)$, which does not lie on the boundary of $\mathcal{R}$. However, $(0, 0, \frac{1}{2})$ is on the boundary since it intersects the supporting hyperplane defined by $\boldsymbol{v}^T = (-1, 0, 2)$. Hence, scaling $\mathcal{R}$ by 2 puts this $\boldsymbol{h}$ on the boundary. The approximate design's minimum variance for the quadratic term is $2^2 = 4$ so the exact design's variance is $4/N$. The approximate c-optimal design is the three-point design

$$\xi = \begin{Bmatrix} 0 & -1 & 1 \\ 0.5 & 0.25 & 0.25 \end{Bmatrix} .$$

This design can also estimate τ_1 and so is also $c_{\mathcal{E}}$-optimal.

If we added an additional factor, $u_i \in [-1, 1]$, and include its main and quadratic effect as well as its interaction effect with x and u, the previous minimum variances for the main effect and and quadratic terms remain the same in x, with $u_i = 0$. Any number of factors could be added to the model in this manner, establishing the c-optimality of the main effect and quadratic effect for the larger models.

Concerning c-optimality for the two-factor interaction we need only consider the two-factor model

$$y_i = \tau_0 + \tau_1 x_i + \tau_2 u_i + \tau_{12} x_i u_i + \tau_{11} x_i^2 + \tau_{22} u_i^2 + e_i = \boldsymbol{x}_i^T \boldsymbol{\tau} + e_i \ .$$

The coefficient vector for τ_{12} is $\boldsymbol{h}^T = (0, 0, 0, 1, 0, 0)$ which is a supporting hyperplane for the Elfving set and so shares the same minimum variance as the main effects. Its approximate c-optimal design, with supports expressed as coordinates (x_i, u_i), is

$$\xi = \begin{Bmatrix} (-1,-1) & (-1,1) & (1,-1) & (1,1) \\ 0.25 & 0.25 & 0.25 & 0.25 \end{Bmatrix} \ .$$

This design will be simultaneously c-optimal for τ_1 and τ_2, but is clearly unable to estimate the quadratic effects. Hence it fails to be $c_{\mathcal{E}}$-optimal.

References

Pukelsheim, F. (2006), *Optimal Design of Experiments*, SIAM.