Exact D-optimal designs for response surface models on a circle

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Introduction

Model:

$$y(j,\mathbf{x}) = \alpha^T \mathbf{e}(j) + \beta^T f(\mathbf{x}) + \varepsilon, \qquad (1)$$

where $j \in \chi_J$ *and* $\mathbf{x} = (x_1, x_2)^T \in \mathbf{R}^2$, and

- $\chi_J = \{1, \cdots, J\}$: levels of the qualitative factor
- $\mathbf{e}(j) = (0, \cdots, 1, \cdots, 0)^T$: corresponding to the covariate of the jth qualitative level;
- $f(\mathbf{x}) = \left(x_1, x_2, x_1x_2, x_1^2, x_2^2\right)^T$: real function vector;
- $\alpha = (\alpha_1, \cdots, \alpha_J)^T$ and $\beta = (\beta_1, \beta_2, \beta_{12}, \beta_{11}, \beta_{22})^T$: unknown parameters for qualitative and quantitative factors,respectively;
- ε: a random variable with mean 0 and variance σ^2.

- Assume there is no interactive effect between quantitative and qualitative factors;
- The design region for quantitative factors at each qualitative level is $\chi = \left\{\mathbf{x} \in \mathbf{R}^2 : \mathbf{x}^T\mathbf{x} \leq 1\right\}$;
- Model with only one qualitative level, i.e. $J = 1$, can be reduced as

$$E(y) = \alpha + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2, \quad (2)$$

it is the same as the second order response surface model with only quantitative factors.

- An approximate design ζ:
  a probability measure with finite supports on $\chi_J \times \chi$;
- An exact design ζ_N:
  $N \times \zeta_N(j, \mathbf{x})$ is an integer $\forall (j, \mathbf{x}) \in \chi_J \times \chi$;
- The information matrix of a design ζ on design space $\chi_J \times \chi$:

$$M(\zeta) = \int_{\chi_J \times \chi} \begin{pmatrix} \mathbf{e}(j)\mathbf{e}^T(j) & \mathbf{e}(j) f^T(\mathbf{x}) \\ f(\mathbf{x})\mathbf{e}^T(j) & f(\mathbf{x}) f^T(\mathbf{x}) \end{pmatrix} d\zeta(j, \mathbf{x});$$

- The *D*-optimal design ζ^*:

$$\zeta^* = \arg\max_{\zeta} |M(\zeta)|;$$

Approximate *D*-optimal design:
-without qualitative factor, circular design region

- Kiefer (1960), Galil and Kiefer (1977),

Exact *D*-optimal designs:
-without qualitative factor, interval design region

- Gaffke and Krafft (1982), Gaffke (1987), Huang (1987), Chen and Huang (2000)

-with qualitative factor, square design region

- Atkinson and Donev (1989)

-without qualitative factor, circular design region

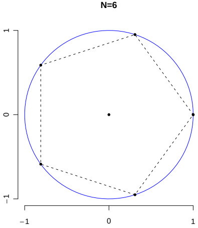
- Chang and Chen (2004)

Models with Quantitative Factors

Approximate D-optimal designs within a circular design region:

- Kiefer (1960): a design ξ^* is D-optimal iff
  - ξ^* is rotatable,
  - supported on the origin with weight $\frac{1}{6}$,
  - supported on the unit circle uniformly with weight $\frac{5}{6}$;
- If N is a multiple of 6, i.e. $N = 6p$, $p \geq 1$,
  an exact design consists of the origin and the vertices of a pentagon with p trials at each support is exact D-optimal;

pentagon



- N is not a multiple of 6,
  based on a kind of equiradial rotatable designs, symbolized by ξ_{N,n_0}, with n_0 central runs and a regular n-sided polygon on the unit circle, where $n_0 + n = N$, and $5 \le n \le N-1$ i.e.

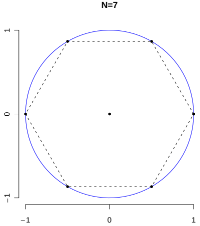
$$\xi_{N,n_0}(\mathbf{x}) \equiv \frac{n_0}{N}\xi_0(\mathbf{x}) + \frac{n}{N}P_n(\mathbf{x}), \qquad (3)$$

where

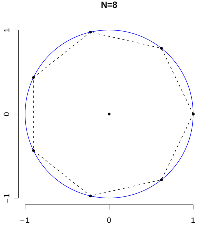
$$\xi_0(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{x} = \mathbf{0} \\ 0, & \text{otherwise} \end{cases}, \quad P_n(\mathbf{x}) = \begin{cases} \frac{1}{n}, & \text{if } \mathbf{x} \in V_n \\ 0, & \text{otherwise} \end{cases}, \qquad (4)$$

$$V_n = \left\{ \left(\cos\left(\frac{2\pi v}{n}\right), \sin\left(\frac{2\pi v}{n}\right) \right)^T, \ v = 0, \dots, n-1 \right\}.$$

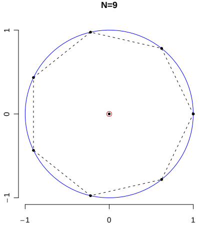
hexagon



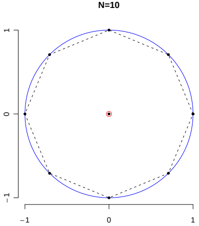
heptagon



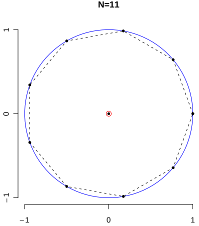
heptagon



octagon



nonagon



When N is not a multiple of 6,

- let $N = 6p + t$, $p \in \{1, 2, \cdots\}$ and $t \in \{1, \cdots, 5\}$;
- two candidate designs for each N among $\Xi_N = \{\xi_{N,n_0}, 1 \leq n_0 \leq N - 5\}$ are $\xi_{N,p}$ and $\xi_{N,p+1}$

Lemma (1)

$$|M(\xi_{N,p})| > |M(\xi_{N,p+1})|, \quad \textit{for } t \in \{1, 2\},$$

and

$$|M(\xi_{N,p})| < |M(\xi_{N,p+1})|, \quad \textit{for } t \in \{3, 4, 5\}.$$

Gaffke and Krafft (1982):
The arithmetic-geometric Inequality for matrices:

$$\frac{|M(\xi_N)|}{\left|M\left(\hat{\xi}_N\right)\right|} \leq \left(\frac{1}{k} tr\left(M(\xi_N)\, M^{-1}\left(\hat{\xi}_N\right)\right)\right)^k$$
$$= \left(\frac{1}{k}\frac{1}{N}\sum_{i=1}^N d\left(\mathbf{x}_i, \hat{\xi}_N\right)\right)^k$$

- ξ_N: a given design with design points $\{\mathbf{x}_i, i = 1, \cdots, N\}$;
- $\hat{\xi}_N$: a candidate exact design;
- k: the number of the model coefficients;
- $d\left(\mathbf{x}_i, \hat{\xi}_N\right)$: dispersion function of $\hat{\xi}_N$;

If $\frac{1}{N}\sum_{i=1}^N d\left(\mathbf{x}_i, \hat{\xi}_N\right) \leq k$, then $|M(\xi_N)| \leq \left|M\left(\hat{\xi}_N\right)\right|$.

Lemma (2)

If N is not a multiple of 6, then the following inequality holds for any exact design ξ_N on χ,

$$\min\left\{tr\left(M\left(\xi_N\right)M^{-1}\left(\xi_{N,p}\right)\right), tr\left(M\left(\xi_N\right)M^{-1}\left(\xi_{N,p+1}\right)\right)\right\} \leq 6.$$

The above inequality implies that

$$\left|M\left(\xi_N\right)\right| \leq \max\left\{\left|M\left(\xi_{N,p}\right)\right|, \left|M\left(\xi_{N,p+1}\right)\right|\right\}$$

Theorem

Let $N = 6p + t$, where $p \in \{1, 2, \cdots\}$ and $t \in \{1, \cdots, 5\}$, the exact D-optimal designs are $\xi_{N,p}$ for $t \in \{1, 2\}$ and $\xi_{N,p+1}$ for $t \in \{3, 4, 5\}$.

Table 1. Exact D-optimal designs for $6 \leq N \leq 11$ on $\chi = \{\mathbf{x} \in \mathbf{R}^2 | \mathbf{x}^T \mathbf{x} \leq 1\}$.

sample size N	(quotient, remainder) (p, t)	center runs n_0	regular polygon	vertices $n = N - n_0$
6	$(1, 0)$	1	pentagon	5
7	$(1, 1)$	1	hexagon	6
8	$(1, 2)$	1	heptagon	7
9	$(1, 3)$	2	heptagon	7
10	$(1, 4)$	2	octagon	8
11	$(1, 5)$	2	nonagon	9

Minimal Supports

Lemma (3)

Given an exact design P_n, if $n \geq 10$, then there exists an exact design $\left(\frac{n_1}{n}P_{n_1} + \frac{n_2}{n}P_{n_2}\right)$ such that

$$M\left(\frac{n_1}{n}P_{n_1} + \frac{n_2}{n}P_{n_2}\right) = M\left(P_n\right),$$

with $n_1 + n_2 = n$, $n_1 \geq 5$ and $n_2 \geq 5$.

- Recall that

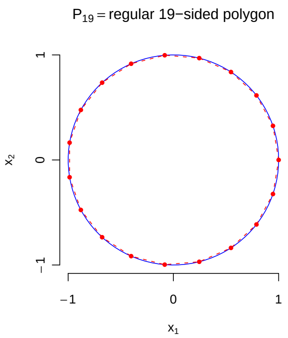
$$P_n\left(\mathbf{x}\right) = \begin{cases} \frac{1}{n}, & \text{if } \mathbf{x} \in V_n \\ 0, & \text{otherwise} \end{cases},$$

$$V_n = \left\{\left(\cos\left(\frac{2\pi v}{n}\right), \sin\left(\frac{2\pi v}{n}\right)\right)^T, \quad v = 0, \ldots, n-1\right\}$$

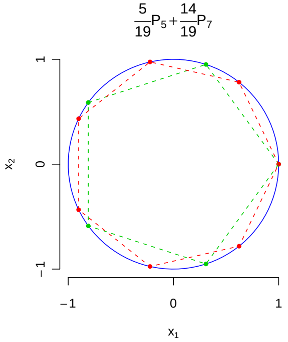
Table 2. Illustration of the procedure in reducing supports for P_{19}.

Step 1 (n_1, n_2)	Step 2 (n_1, n_{21}, n_{22})	number of distinct supports
$(5, 14)$	$(5, 5, 9)$	13
	$(5, 6, 8)$	18
	$(5, 7, 7)$	11
$(6, 13)$	$(6, 5, 8)$	18
	$(6, 6, 7)$	12
$(7, 12)$	$(7, 5, 7)$	11
	$(7, 6, 6)$	12
$(8, 11)$	$(8, 5, 6)$	18
$(9, 10)$	$(9, 5, 5)$	13

original



minimal supports



Lemma (4)

Let n_1 *and* n_2 *be relatively prime positive integers. If*

$$n \geq (n_1 - 1)(n_2 - 1),$$

then there exist nonnegative integers u_1 *and* u_2 *such that*

$$n_1 u_1 + n_2 u_2 = n.$$

Procedure for obtaining minimal supports exact D-optimal designs

Step 1 : if n is a multiple of $m \in \{5, \cdots, 9\}$, choose P_m to replace P_n with weight $\frac{m}{n}$;

Step 2 : if n is not a multiple of $m \in \{5, \cdots, 9\}$ and $n \geq 20$, then use a convex combination of P_5 and P_6 to replace P_n;

Step 3 : the remaining cases of n are listed at the Table 3.

Table 3. Exact D-optimal designs with minimal supports.

sample size N	center runs n_0	vertices of P_n $n = N - n_0$	partitions for n (n_1, n_2)	(u_1, u_2)	number of supports
13	2	11	$(5, 6)$	$(1, 1)$	11
16	3	13	$(6, 7)$	$(1, 1)$	13
20	3	17	$(5, 6)$	$(1, 2)$	11
21	4	17	$(5, 6)$	$(1, 2)$	11
23	4	19	$(5, 7)$	$(1, 2)$	12

Models with Both Qualitative and Quantitative Factors

- Recall the model

$$y(j,\mathbf{x}) = \alpha^T \mathbf{e}(j) + \beta^T f(\mathbf{x}) + \varepsilon$$

- When $J \geq 2$, we restrict our attentions to the exact designs in the class Ξ^* defined as

$$\Xi^* = \left\{ \zeta_N : \zeta_N(j,\mathbf{x}) = \frac{N_j}{N} \times \xi_{N_j,n_{0j}}(\mathbf{x}),\ 1 \leq n_{0j} \leq N_j - 5, \sum_j N_j = N, N_j \geq 6 \right\}$$

- Here, we assume that the sample size $N \geq 2J$

For any $\zeta_N \in \Xi^*$, the information matrix of ζ_N is

$$M(\zeta_N) = \begin{pmatrix} M_\alpha(\zeta_N) & M_{\alpha\beta}(\zeta_N) \\ M_{\alpha\beta}^T(\zeta_N) & M_\beta(\zeta_N) \end{pmatrix},$$

where

$$M_\alpha(\zeta_N) = \frac{1}{N} Diag(N_1, \cdots, N_J),$$

$$M_{\alpha\beta}(\zeta_N) = \frac{1}{2N}(0,0,0,1,1) \otimes \begin{pmatrix} N_1 - n_{01} \\ \vdots \\ N_J - n_{0J} \end{pmatrix},$$

$$M_\beta(\zeta_N) = \frac{s_J}{8N} \begin{pmatrix} 4 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 3 & 1 \\ 0 & 0 & 0 & 1 & 3 \end{pmatrix}, and \;\; s_J = \sum_{j=1}^{J} (N_j - n_{0j}).$$

Table 4. Exact D-optimal designs for model (1) with 2 qualitative levels within Ξ^*. Assume that $N_j = 6p + t_j,\ n_{oj} = p + u_j,\ j = 1, 2$.

(t_1, t_2)	(u_1, u_2)	(t_1, t_2)	(u_1, u_2)
$(0, 0)$	$(0, 0)$	$(1, 0)$	$(0, 0)$
$(1, 1)$	$(0, 0)$	$(2, 1)$	$(0, 0)$
$(2, 2)$	$(1, 0)$	$(3, 2)$	$(1, 0)$
$(3, 3)$	$(1, 0)$	$(4, 3)$	$(1, 0)$
$(4, 4)$	$(1, 1)$	$(5, 4)$	$(1, 1)$
$(5, 5)$	$(1, 1)$	$(6, 5)$	$(1, 1)$

Table 5. Exact D-optimal designs for model (1) with 3 qualitative levels within Ξ^*. Assume that $N_j = 6p + t_j,\ n_{oj} = p + u_j,\ j = 1, 2, 3.$

(t_1, t_2, t_3)	(u_1, u_2, u_3)	(t_1, t_2, t_3)	(u_1, u_2, u_3)	(t_1, t_2, t_3)	(u_1, u_2, u_3)
(0, 0, 0)	(0, 0, 0)	(1, 0, 0)	(0, 0, 0)	(1, 1, 0)	(0, 0, 0)
(1, 1, 1)	(0, 0, 0)	(2, 1, 1)	(0, 0, 0)	(2, 2, 1)	(1, 0, 0)
(2, 2, 2)	(1, 0, 0)	(3, 2, 2)	(1, 0, 0)	(3, 3, 2)	(1, 0, 0)
(3, 3, 3)	(1, 1, 0)	(4, 3, 3)	(1, 1, 0)	(4, 4, 3)	(1, 1, 0)
(4, 4, 4)	(1, 1, 0)	(5, 4, 4)	(1, 1, 0)	(5, 5, 4)	(1, 1, 1)
(5, 5, 5)	(1, 1, 1)	(6, 5, 5)	(1, 1, 1)	(6, 6, 5)	(1, 1, 1)

Construction method of Exact D-optimal designs for $J \geq 4$

step 1 Choose $N_1, \cdots, N_J$ to be as equal as possible, i.e. $|N_i - N_j| \leq 1$, $\forall i, j \in \{1, \cdots, J\}$.

- W.l.o.g., we assume that $N_1 = \cdots = N_r = 6p + t + 1$, $N_{r+1} = \cdots = N_J = 6p + t$, where $r \in \{1, \cdots, J-1\}$, $p \in \{1, 2, \cdots\}$ and $t \in \{0, \cdots, 5\}$.

step 2 An exact design $\zeta_N \in \Xi^*$ with $n_{0j} = p$ or $p + 1$, $j = 1, \cdots, J$, is a candidate for exact D-optimal designs.

Construction method of Exact D-optimal designs for $J \geq 4$

step 3 Choose the design ζ_N^* among these 2^J candidates s.t.

$$\begin{aligned} \zeta_N^* &= \arg\max |\zeta_N| \\ &= \arg\max \frac{N_1 \cdots N_J}{N^{(J+5)}} \left[s_J^4 \left(s_J - \sum_{j=1}^{J} \frac{(N_j - n_{0j})^2}{N_j} \right) \right] \end{aligned}$$

where $s_J = \sum_{j=1}^{J} (N_j - n_{0j})$.

Then ζ_N^* is an exact D-optimal design within the subclass.

References

- Atkinson, A. C. and Donev, A. N. (1989). The construction of exact *D*-optimum experimental designs with application to blocking response surface designs. *Biometrika*, 76, 515-26
- Chang, F. C. and Chen, Y. H. (2004). *D*-optimal designs for multivariate linear and quadratic polynomial regression. *Journal of the Chinese Statistical Association*, 42, 383-402.
- Chen, R. B. , and Huang, M.-N. L. (2000). Exact *D*-optimal designs for weighted polynomial model. *Computational Statistics and Data Analysis*, 33, 137-149.

References

- Gaffke, N. and Krafft, O. (1982). Exact *D*-optimum designs for quadratic regression. *J. Roy. Statist. Soc. Ser.B*, 44, 394-397.
- Gaffke, N. (1987). On *D*-optimality of exact linear regression designs with minimum support. *Journal of Statistical Planning and Inference*, 15, 189-204.
- Galil, Z. and Kiefer, J. (1977). Comparison of rotatable designs for regression on balls, I (Quadratic). *Journal of Statistical Planning and Inference*, 1, 27-40.
- Huang, M.-N. L. (1987). Exact *D*-optimal designs for polynomial regression. *Bulletin of the Institute of Mathematics, Academia Sinica*, 15, 59-71.

References

- Kiefer, J. (1960). Optimum experimental designs V, with applications to systematic and rotatable designs. In *Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, Berkeley, CA 1960, Volume 1*, 381-405.

Properties of ξ_{N,n_0}:

- The information matrix is identical as long as $n = N - n_0 \geq 5$:

$$M\left(\xi_{N,n_0}\right) = \begin{pmatrix} 1 & 0 & 0 & 0 & \frac{n}{2N} & \frac{n}{2N} \\ 0 & \frac{n}{2N} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{n}{2N} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{n}{8N} & 0 & 0 \\ \frac{n}{2N} & 0 & 0 & 0 & \frac{3n}{8N} & \frac{n}{8N} \\ \frac{n}{2N} & 0 & 0 & 0 & \frac{n}{8N} & \frac{3n}{8N} \end{pmatrix}; \qquad (5)$$

- The determinant of $M\left(\xi_{N,n_0}\right)$:

$$\left|M\left(\xi_{N,n_0}\right)\right| = \left(\frac{1}{2}\right)^8 \left(\frac{n_0}{N}\right)\left(\frac{n}{N}\right)^5; \qquad (6)$$