D-optimal Designs for Factorial Experiments under Generalized Linear Models

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A motivating example: Hamada and Nelder (1997)

- Two-level factors: (A) poly-film thickness, (B) oil mixture ratio, (C) material of gloves, and (D) condition of metal blanks.
- Response: the windshield molding was good or not.

Row	A	B	C	D	Replicates	good molding
1	+	+	+	+	1000	338
2	+	+	−	−	1000	826
3	+	−	+	−	1000	350
4	+	−	−	+	1000	647
5	−	+	+	−	1000	917
6	−	+	−	+	1000	977
7	−	−	+	+	1000	953
8	−	−	−	−	1000	972

- **Question:** Can we do something better?

Preliminary setup

- Consider an experiment with m fixed and distinct design points:

$$X = \begin{pmatrix} \mathbf{x}_1' \\ \mathbf{x}_2' \\ \vdots \\ \mathbf{x}_m' \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1d} \\ x_{21} & x_{22} & \cdots & x_{2d} \\ \cdots & \cdots & \cdots & \cdots \\ x_{m1} & x_{m2} & \cdots & x_{md} \end{pmatrix}$$

  For example, a 2^k factorial experiment with main-effects model implies $m = 2^k$, $d = k + 1$, $x_{i1} = 1$, and $x_{i2}, \ldots, x_{id} \in \{-1, 1\}$.

- *Exact design problem:* Suppose n is given.
  Consider "optimal" n_i's such that $n_i \geq 0$ and $\sum_{i=1}^m n_i = n$.

- *Approximate design problem:* Let $p_i = n_i/n$.
  Consider "optimal" p_i's such that $p_i \geq 0$ and $\sum_{i=1}^m p_i = 1$.

Generalized linear model: single parameter

Consider independent univariate responses $Y_1, \ldots, Y_n$:

$$Y_i \sim f(y; \theta_i) = \exp\{yb(\theta_i) + c(\theta_i) + d(y)\}$$

For example,

$$\begin{array}{ll}
\exp\left\{y \log \frac{\theta}{1-\theta} + \log(1-\theta)\right\}, & \text{Bernoulli}(\theta) \\
\exp\{y \log \theta - \theta - \log y!\}, & \text{Poisson}(\theta) \\
\exp\left\{y \frac{-1}{\theta} - k \log \theta + \log \frac{y^{k-1}}{\Gamma(k)}\right\}, & \text{Gamma}(k, \theta),\ \text{fixed } k > 0 \\
\exp\left\{y \frac{\theta}{\sigma^2} - \frac{\theta^2}{2\sigma^2} - \frac{y^2}{2\sigma^2} - \frac{1}{2}\log(2\pi\sigma^2)\right\}, & N(\theta, \sigma^2),\ \text{fixed } \sigma^2 > 0
\end{array}$$

Generalized linear model (McCullagh and Nelder 1989, Dobson 2008): $\exists$ link function g and parameters of interest $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_d)'$, such that

$$E(Y_i) = \mu_i \text{ and } \eta_i = g(\mu_i) = \mathbf{x}_i' \boldsymbol{\beta}.$$

Information matrix and D-optimal design

Recall that there are m distinct predictor combinations $\mathbf{x}_1, \ldots, \mathbf{x}_m$ with numbers of replicates $n_1, \ldots, n_m$, respectively.

The maximum likelihood estimator of β has an asymptotic covariance matrix that is the inverse of the *information matrix*

$$\mathbf{I} = nX'WX$$

where $X = (\mathbf{x}_1, \ldots, \mathbf{x}_m)'$ is an $m \times d$ matrix, and $W = \mathrm{diag}(p_1 w_1, \ldots, p_m w_m)$ with $w_i = \frac{1}{\mathrm{var}(Y_i)} \left(\frac{\partial \mu_i}{\partial \eta_i}\right)^2$.

A *D-optimal design* is the $\mathbf{p} = (p_1, \ldots, p_m)'$ which maximizes

$$|X'WX|$$

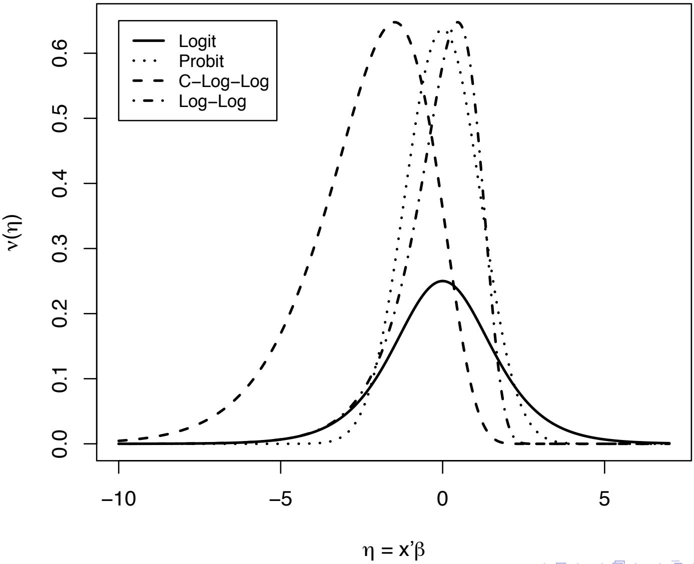
with given $w_1, \ldots, w_m$.

w as a function of β

Suppose the link function g is one-to-one and differentiable.
Suppose further μ_i itself determines $\mathrm{var}(Y_i)$.
Then $w_i = \nu(\eta_i) = \nu\left(\mathbf{x}_i{}'\beta\right)$ for some function ν.

- *Binary response, logit link:* $\nu(\eta) = \frac{1}{2+e^{\eta}+e^{-\eta}}$.
- *Poisson count, log link:* $w = \nu(\eta) = \exp\{\eta\}$.
- *Gamma response, reciprocal link:* $w = \nu(\eta) = k/\eta^2$.
- *Normal response, identity link:* $w = \nu(\eta) \equiv 1/\sigma^2$.

$w_i = \nu(\eta_i) = \nu(\mathbf{x}_i'\beta)$ for binary response



Example: 2^2 experiment with main-effects model

$$X = \begin{pmatrix} 1 & -1 & -1 \\ 1 & -1 & +1 \\ 1 & +1 & -1 \\ 1 & +1 & +1 \end{pmatrix}, W = \begin{pmatrix} w_1 p_1 & 0 & 0 & 0 \\ 0 & w_2 p_2 & 0 & 0 \\ 0 & 0 & w_3 p_3 & 0 \\ 0 & 0 & 0 & w_4 p_4 \end{pmatrix}$$

The optimization problem maximizing

$$|X'WX| = 16 w_1 w_2 w_3 w_4 L(\mathbf{p}),$$

where $v_i = 1/w_i$ and

$$L(\mathbf{p}) = v_4 p_1 p_2 p_3 + v_3 p_1 p_2 p_4 + v_2 p_1 p_3 p_4 + v_1 p_2 p_3 p_4$$

General case: order-d polynomial

For general case, X is an $m \times d$ matrix with distinct rows, $W = \mathrm{diag}(p_1 w_1, \ldots, p_m w_m)$.

Based on González-Dávila, Dorta-Guerra and Ginebra (2007) and Yang, Mandal and Majumdar (2012b), we have

Lemma

Let $X[i_1, i_2, \ldots, i_d]$ be the $d \times d$ sub-matrix consisting of the i_1th, ..., i_dth rows of the design matrix X. Then

$$f(\mathbf{p}) = |X'WX| = \sum_{1 \le i_1 < \cdots < i_d \le m} |X[i_1, \ldots, i_d]|^2 \cdot p_{i_1} w_{i_1} \cdots p_{i_d} w_{i_d}.$$

Characterization of locally D-optimal designs

For each $i = 1, \ldots, m$, $0 \le x < 1$, we define

$$\begin{aligned} f_i(x) &= f\left(\frac{1-x}{1-p_i}p_1, \ldots, \frac{1-x}{1-p_i}p_{i-1}, x, \frac{1-x}{1-p_i}p_{i+1}, \ldots, \frac{1-x}{1-p_i}p_m\right) \\ &= ax(1-x)^{d-1} + b(1-x)^d \end{aligned}$$

If $p_i > 0$, $b = f_i(0)$, $a = \frac{f(\mathbf{p}) - b(1-p_i)^d}{p_i(1-p_i)^{d-1}}$; otherwise, $b = f(\mathbf{p})$, $a = f_i\left(\frac{1}{2}\right) \cdot 2^d - b$.

Theorem

Suppose $f(\mathbf{p}) > 0$. Then $\mathbf{p}$ is D-optimal if and only if for each $i = 1, \ldots, m$, one of the two conditions below is satisfied:

(i) $p_i = 0$ *and* $f_i\left(\frac{1}{2}\right) \le \frac{d+1}{2^d} f(\mathbf{p})$;

(ii) $0 < p_i \le \frac{1}{d}$ *and* $f_i(0) = \frac{1 - p_i d}{(1-p_i)^d} f(\mathbf{p})$.

Saturated designs

Theorem

Let $\mathbf{I} = \{i_1, \ldots, i_d\} \subset \{1, \ldots, m\}$ *satisfying* $|X[i_1, \ldots, i_d]| \neq 0$. *Then* $p_{i_1} = p_{i_2} = \cdots = p_{i_d} = \frac{1}{d}$ *is D-optimal if and only if for each* $i \notin \mathbf{I}$,

$$\sum_{j \in \mathbf{I}} \frac{|X[\{i\} \cup \mathbf{I} \setminus \{j\}]|^2}{w_j} \leq \frac{|X[i_1, i_2, \ldots, i_d]|^2}{w_i}.$$

- 2^2 *main-effects model:* $p_1 = p_2 = p_3 = 1/3$ is D-optimal if and only if $v_1 + v_2 + v_3 \leq v_4$, where $v_i = 1/w_i$.
- 2^3 *main-effects model:* $p_1 = p_4 = p_6 = p_7 = 1/4$ is D-optimal if and only if $v_1 + v_4 + v_6 + v_7 \leq 4\min\{v_2, v_3, v_5, v_8\}$.

Saturated designs: more example

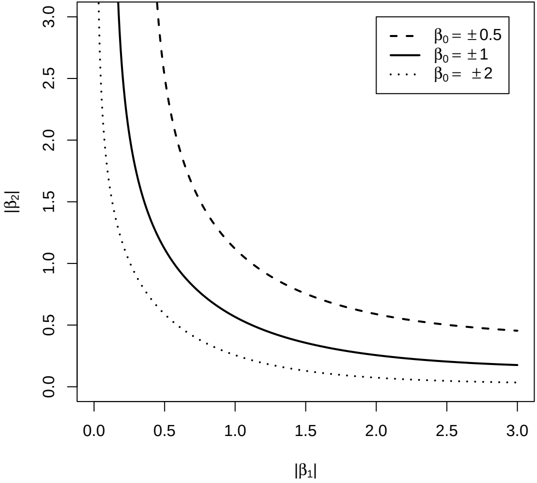
2×3 *factorial design:* Suppose the design matrix

$$X = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & -2 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & -1 & 0 & -2 \\ 1 & -1 & -1 & 1 \end{pmatrix}.$$

- $p_1 = p_2 = p_3 = p_4 = 1/4$ is D-optimal if and only if $v_1 + v_2 + v_4 \le v_5$ and $v_1 + v_3 + v_4 \le v_6$.
- $p_2 = p_3 = p_4 = p_5 = 1/4$ is D-optimal if and only if $v_2 + v_4 + v_5 \le v_1$ and $v_2 + v_3 + v_5 \le v_6$.
- $p_3 = p_4 = p_5 = p_6 = 1/4$ is D-optimal if and only if $v_3 + v_4 + v_6 \le v_1$ and $v_3 + v_5 + v_6 \le v_2$.

Saturation condition in terms of β: logit link, 2^2 design

For fixed β_0, a pair (β_1, β_2) satisfies the saturation condition if and only if the corresponding point is above the curve labelled by β_0.



Lift-one algorithm (Yang, Mandal and Majumdar, 2012b)

Given X and $w_1, \ldots, w_m$, search for $\mathbf{p} = (p_1, \ldots, p_m)'$ maximizing $f(\mathbf{p}) = |X'WX|$:

1° Start with arbitrary $\mathbf{p}_0 = (p_1, \ldots, p_m)'$ satisfying $0 < p_i < 1$, $i = 1, \ldots, m$ and compute $f(\mathbf{p}_0)$.

2° Set up a random order of i going through $\{1, 2, \ldots, m\}$.

3° For each i, determine $f_i(z)$. In this step, either $f_i(0)$ or $f_i\left(\frac{1}{2}\right)$ needs to be calculated.

4° Define
$$\mathbf{p}_*^{(i)} = \left(\frac{1-z_*}{1-p_i}p_1, \ldots, \frac{1-z_*}{1-p_i}p_{i-1}, z_*, \frac{1-z_*}{1-p_i}p_{i+1}, \ldots, \frac{1-z_*}{1-p_i}p_{2^k}\right)',$$
where z_* maximizes $f_i(z)$, $0 \le z \le 1$. Here $f(\mathbf{p}_*^{(i)}) = f_i(z_*)$.

5° Replace $\mathbf{p}_0$ with $\mathbf{p}_*^{(i)}$, $f(\mathbf{p}_0)$ with $f(\mathbf{p}_*^{(i)})$.

6° Repeat 2° $\sim$ 5° until convergence, that is, $f(\mathbf{p}_0) = f(\mathbf{p}_*^{(i)})$ for each i.

Comments on lift-one algorithm

- The basic idea of the lift-one algorithm is that, for randomly chosen $i \in \{1, \ldots, m\}$, we update p_i to p_i^* and all the other p_j's to $p_j^* = p_j \cdot \frac{1-p_i^*}{1-p_i}$.
- The major advantage of the lift-one algorithm is that in order to determine an optimal p_i^*, we need to calculate $|X'WX|$ only once.
- This algorithm is motivated by the *coordinate descent algorithm* (Zangwill, 1969).
- It is also in spirit similar to the idea of one-point correction in the literature (Wynn, 1970; Fedorov, 1972; Müller, 2007), where design points are added/adjusted one by one.

Convergence of lift-one algorithm

Modified lift-one algorithm:

(1) For the $10m$th iteration and a fixed order of $i = 1, \ldots, m$ we repeat steps $3^\circ \sim 5^\circ$. If $\mathbf{p}_*^{(i)}$ is a better allocation found by the lift-one algorithm than the allocation $\mathbf{p}_0$, instead of updating $\mathbf{p}_0$ to $\mathbf{p}_*^{(i)}$ immediately, we obtain $\mathbf{p}_*^{(i)}$ for each i, and replace $\mathbf{p}_0$ with the best $\mathbf{p}_*^{(i)}$ only.

(2) For iterations other than the $10m$th, we follow the original lift-one algorithm update.

Theorem

When the lift-one algorithm or the modified lift-one algorithm converges, the converged allocation $\mathbf{p}$ *maximizes* $|X'WX|$ *on the set of feasible allocations. Furthermore, the modified lift-one algorithm is guaranteed to converge.*

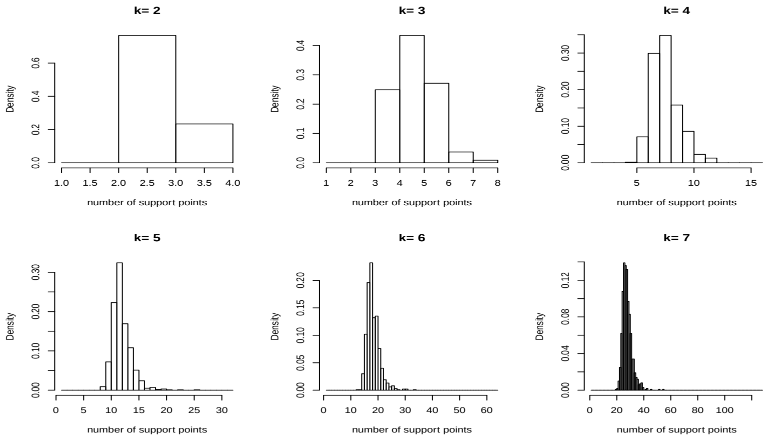
Performance of lift-one algorithm: comparison

Table: CPU time in seconds for 100 simulated β

	Algorithms				
	Nelder-Mead	quasi-Newton	conjugate gradient	simulated annealing	lift-one
2^2 Designs	0.77	0.41	4.68	46.53	0.17
2^3 Designs	46.75	63.18	925.5	1495	0.46
2^4 Designs	125.9	NA	NA	NA	1.45

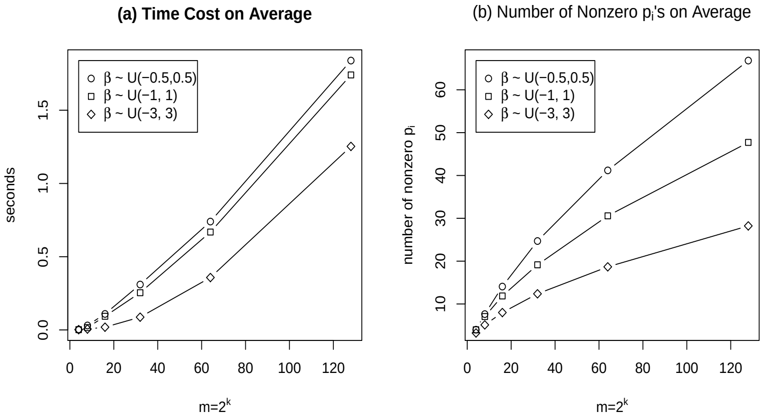
Performance of lift-one algorithm: number of nonzero p_i's

Under 2^k main-effects model, binary response, logit link, β_i's iid from Uniform(-3,3):



Performance of lift-one algorithm: time cost

Under 2^k main-effects model, binary response, logit link, we simulate β_i's iid from a uniform distribution and check the time cost in seconds by lift-one algorithm:



EW D-optimal designs

- For experiments under generalized linear models, we may need to specify the β_i's, which gives us the w_i's, to get D-optimal designs, known as *local D-optimality*.
- An *EW D-optimal* design is an optimal allocation of **p** that maximizes $|X'E(W)X|$. It is one of several alternatives suggested by Atkinson, Donev and Tobias (2007).
- EW D-optimal designs are often approximately as efficient as Bayesian D-optimal designs.
- EW D-optimal designs can be obtained easily using the lift-one algorithm.
- In general, EW D-optimal designs are robust.

EW D-optimal design and Bayesian D-optimal design

Theorem

For any given link function, if the regression coefficients $\beta_0, \beta_1, \ldots, \beta_d$ are independent with finite expectation, and $\beta_1, \ldots, \beta_d$ all have a symmetric distribution about 0 (not necessarily the same distribution), then the uniform design is an EW D-optimal design.

A Bayes D-optimal design maximizes $E(\log|X'WX|)$ where the expectation is taken over the prior distribution of β_i's. Note that, by Jensen's inequality,

$$E\left(\log|X'WX|\right) \leq \log|X'E(W)X|$$

since $\log|X'WX|$ is concave in $\mathbf{w}$. Thus an EW D-optimal design maximizes an upper bound to the Bayesian D-optimality criterion.

Example: 2^2 main-effects model

Suppose $\beta_0, \beta_1, \beta_2$ are independent, $\beta_0 \sim U(-1, 1)$, and $\beta_1, \beta_2 \sim U[0, 1)$.

- Under the logit link, the EW D-optimal design is $\mathbf{p}_e = (0.239, 0.261, 0.261, 0.239)'$.
- The Bayes optimal design, which maximizes $\phi(\mathbf{p}) = E \log |X'WX|$ is $\mathbf{p}_o = (0.235, 0.265, 0.265, 0.235)'$. The relative efficiency of $\mathbf{p}_e$ with respect to $\mathbf{p}_o$ is

$$\exp\left\{\frac{\phi(\mathbf{p}_e) - \phi(\mathbf{p}_o)}{k+1}\right\} \times 100\% = 99.99\%$$

  for logit link, or 99.94% for probit link, 99.77% for log-log link, and 100.00% for complementary log-log link.
- The time cost for EW is 0.11 sec, while it is 5.45 secs for maximizing $\phi(\mathbf{p})$.
- It should also be noted that the relative efficiency of the uniform design $\mathbf{p}_u = (1/4, 1/4, 1/4, 1/4)'$ with respect to $\mathbf{p}_o$ is 99.88% for logit link, and is 89.6% for complementary log-log link.

Example: 2^3 main-effects model

Suppose $\beta_0, \beta_1, \beta_2, \beta_3$ are independent, and the experimenter has the following prior information for the parameters: $\beta_0 \sim U(-3, 3)$, and $\beta_1, \beta_2, \beta_3 \sim U[0, 3)$.

- For the logit link the uniform design is not EW D-optimal.
- In this case, EW solution is $\mathbf{p}_e = (0, 1/6, 1/6, 1/6, 1/6, 1/6, 1/6, 0)'$, while

  $$\mathbf{p}_o = (0.004, 0.165, 0.166, 0.165, 0.165, 0.166, 0.165, 0.004)'$$

  which maximizes $\phi(\mathbf{p})$.
- The relative efficiency of $\mathbf{p}_e$ with respect to $\mathbf{p}_o$ is 99.98%.
- On the other hand, the relative efficiency of the uniform design with respect to $\mathbf{p}_o$ is 94.39%.
- It takes about 2.39 seconds to find an EW solution while it takes 121.73 seconds to find $\mathbf{p}_o$. The difference in computational time is even more prominent for 2^4 case (24 seconds versus 3147 seconds).

Robustness for misspecification of w

- Denote the D-criterion value as

$$\psi(\mathbf{p}, \mathbf{w}) = |X'WX|$$

for given $\mathbf{w} = (w_1, \ldots, w_m)'$ and $\mathbf{p} = (p_1, \ldots, p_m)'$.

- Define the relative loss of efficiency of $\mathbf{p}$ with respect to $\mathbf{w}$ as

$$R(\mathbf{p}, \mathbf{w}) = 1 - \left(\frac{\psi(\mathbf{p}, \mathbf{w})}{\psi(\mathbf{p}_w, \mathbf{w})} \right)^{\frac{1}{d}},$$

where $\mathbf{p}_w$ is a D-optimal allocation with respect to $\mathbf{w}$.

- Define the maximum relative loss of efficiency of a given design $\mathbf{p}$ with respect to a specified region $\mathcal{W}$ of $\mathbf{w}$ by

$$R_{\max}(\mathbf{p}) = \max_{\mathbf{w} \in \mathcal{W}} R(\mathbf{p}, \mathbf{w}).$$

Robustness of uniform design: 2^2 main-effects model

- Yang, Mandal and Majumdar (2012a) showed that under 2^2 experiment with main-effects model, if $w_i \in [a, b]$, $i = 1, 2, 3, 4$, $0 < a \leq b$, then the uniform design $\mathbf{p}_u = (1/4, 1/4, 1/4, 1/4)'$ is the most robust one in terms of the maximum of relative loss of efficiency.

- On the other hand, if the experimenter has some prior knowledge about the model parameters, for example, if one believes that $\beta_0 \sim \text{Uniform}(-1, 1)$, $\beta_1, \beta_2 \sim \text{Uniform}[0, 1)$ and $\beta_0, \beta_1, \beta_2$ are independent, then the theoretical $R_{\max}$ of uniform design is 0.134, while the theoretical $R_{\max}$ of design given by $\mathbf{p} = (0.19, 0.31, 0.31, 0.19)'$ is 0.116. That is, uniform design may not be the most robust one.

Robustness of uniform design: 2^4 main-effects model

Simulate $\beta_0, \ldots, \beta_4$ for 1000 times and calculate the corresponding $\mathbf{w}$'s. For each $\mathbf{w}_s$, we obtain a D-optimal allocation $\mathbf{p}_s$.

	Percentages											
	$\beta_0 \sim U(-3,3)$			$U(-1,1)$			$U(-3,0)$			$N(0,5)$		
	$\beta_1 \sim U(-1,1)$			$U(0,1)$			$U(1,3)$			$N(0,1)$		
	$\beta_2 \sim U(-1,1)$			$U(0,1)$			$U(1,3)$			$N(2,1)$		
	$\beta_3 \sim U(-1,1)$			$U(0,1)$			$U(-3,-1)$			$N(-.5,2)$		
	$\beta_4 \sim U(-1,1)$			$U(0,1)$			$U(-3,-1)$			$N(-.5,2)$		
	(I)	(II)	(III)	(I)	(II)	(III)	(I)	(II)	(III)	(I)	(II)	(III)
R_{99}	.35	.35	.35	.15	.11	.11	.50	.27	.30	.65	.86	.73
R_{95}	.30	.30	.30	.13	.09	.09	.50	.25	.26	.62	.79	.67
R_{90}	.27	.27	.27	.12	.08	.09	.49	.24	.23	.59	.74	.63

Note: (I) $= R_{100\alpha}(\mathbf{p}_u)$, uniform design;

(II) $= \min_{1\le s\le 1000} R_{100\alpha}(\mathbf{p}_s)$, best among 1000;

(III) $= R_{100\alpha}(\mathbf{p}_e)$, EW design.

Windshield experiment: revisited (Yang, Mandal and Majumdar, 2012b)

- Based on the data presented in Hamada and Nelder (1997), $\hat{\beta} = (1.77, -1.57, 0.13, -0.80, -0.14)'$ under logit link.
- The efficiency of the original 2_{III}^{4-1} design $\mathbf{p}_{HN}$ is 78% of the locally D-optimal design if $\hat{\beta}$ were the true value.
- It might be reasonable to consider an initial guess of $\beta = (2, -1.5, 0.1, -1, -0.1)'$. This will lead to the locally D-optimal half-fractional design $\mathbf{p}_a$ with relative efficiency 99%.
- Another reasonable option is to consider a range, for example, $\beta_0 \sim \text{Unif}(1,3)$, $\beta_1 \sim \text{Unif}(-3,-1)$, $\beta_2, \beta_4 \sim \text{Unif}(-0.5, 0.5)$, and $\beta_3 \sim \text{Unif}(-1, 0)$, the relative efficiency of the EW D-optimal half-fractional design $\mathbf{p}_e$ is 98%.

Windshield experiment: optimal half-fractional design

Row	A	B	C	D	η	π	$\mathbf{p}_{HN}$	$\mathbf{p}_a$	$\mathbf{p}_e$
5	+1	−1	+1	+1	-0.87	0.295		0.044	0.184
1	+1	+1	+1	+1	-0.61	0.352	0.125	0.178	0.011
6	+1	−1	+1	−1	-0.59	0.357	0.125	0.178	0.011
2	+1	+1	+1	−1	-0.33	0.418		0.059	0.184
7	+1	−1	−1	+1	0.73	0.675	0.125	0.163	
3	+1	+1	−1	+1	0.99	0.729			0.195
8	+1	−1	−1	−1	1.01	0.733			0.195
4	+1	+1	−1	−1	1.27	0.781	0.125	0.147	
13	−1	−1	+1	+1	2.27	0.906	0.125	0.158	0.111
9	−1	+1	+1	+1	2.53	0.926			
14	−1	−1	+1	−1	2.55	0.928			
10	−1	+1	+1	−1	2.81	0.943	0.125	0.074	0.110
15	−1	−1	−1	+1	3.87	0.980			
11	−1	+1	−1	+1	4.13	0.984	0.125		
16	−1	−1	−1	−1	4.15	0.984	0.125		
12	−1	+1	−1	−1	4.41	0.988			

Conclusions

- We consider the problem of obtaining locally D-optimal designs for experiments with fixed finite set of design points under generalized linear models.
- We obtain a characterization for a design to be locally D-optimal.
- Based on this characterization, we develop efficient numerical techniques to search for locally D-optimal designs.
- We suggest the use of EW D-optimal designs. These are much easier to compute and still highly efficient compared with Bayesian D-optimal designs.
- We investigate the properties of fractional factorial designs (not presented here, see Yang, Mandal and Majumdar, 2012b).
- We also study the robustness of the D-optimal designs.

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