

On connections between orthogonal arrays and D -optimal designs for certain generalized linear models with group effects

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Design and Analysis of Experiments in Healthcare
July 6-10, 2015

Joint work with Xijue Tan

Outline

- 1 Background
- 2 Smaller designs: Main-effects only
- 3 Adding interactions
- 4 Summary

Yang and S, 2009, Annals of Statistics

They considered generalized linear and nonlinear models with **two parameters**, $\theta = (\theta_1, \theta_2)' \dots$

... and **one design variable**, x , with values in an interval, possibly half-bounded or unbounded.

They used **approximate designs**: $\xi = \{(x_1, \omega_1), (x_2, \omega_2), \dots\}$, where $\omega_j > 0$, $\sum_j \omega_j = 1$.

They focused on **local optimality**, and aimed for **complete class results** under the Loewner ordering.

Thus, with $M_\xi(\theta)$ as the information matrix for θ with design ξ , the aim was to find a small class of designs Ξ so that for any design ξ_0 there is a design $\xi_0^* \in \Xi$ with $M_{\xi_0^*}(\theta) \geq M_{\xi_0}(\theta)$.

Many common optimality criteria adhere to the Loewner ordering.

Such classes always exist (all designs; Carathéodory).

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Among others, they showed the following:

Define $c = \theta_1 + \theta_2 x$, and let $c \in [L, U] \dots$

... then for the logistic or probit link with linear predictor c , a complete class (in terms of c) is formed by designs with at most two support points, where

- (i) one of them is U if $U \leq 0$;
- (ii) one of them is L if $L \geq 0$;
- (iii) the two points are symmetric if $-L = U$;
- (iv) the two points are symmetric or L is one of the points if $-L < U$;
- (v) the two points are symmetric or U is one of the points if $-L > U$.

Thus, the two points are symmetric, or one of them is the endpoint that is closest to 0.

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S and Yang, 2012, Statistica Sinica

What happens if we add **classificatory variables** (factors)?

With two factors at two levels each, a design consists of pairs $(x_{i_1 i_2 j}, \omega_{i_1 i_2 j})$, $i_1 = 1, 2$, $i_2 = 1, 2$, $j = 1, 2, \dots$, where $\omega_{i_1 i_2 j} > 0$ and $\sum_{i_1} \sum_{i_2} \sum_j \omega_{i_1 i_2 j} = 1$.

Could add **constraints for the cells** formed by the factors, such as $\sum_j \omega_{11j} = .30$, and so on.

We studied the problem without such constraints.

What is a reasonable family of models for problems of this nature?

What are parametric functions that might be of interest?

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For F factors and s_k levels for the k th factor, there are $\mathbf{s} = \mathbf{s}_1 \times \mathbf{s}_2 \times \dots \times \mathbf{s}_F$ cells.

For an exact design, let Y_{ij} be the j th binary response in the i th cell, and consider

$$Pr(Y_{ij} = 1) = P(\alpha_0 + \alpha_i + \beta x_{ij}),$$

where P is a cumulative distribution function.

Some observations and notation:

- * It is an overparametrized model.
- * Can use a slope parameter that depends on the cells, β_i .
- * Can model the α_i 's, e.g. using a main-effects model or main-effects and lower order interactions.
- * Will also write $i_1 i_2 \dots i_F$ instead of i .

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Let $\theta = (\alpha_0, \alpha_1, \dots, \alpha_s, \beta')'$, where β is either a scalar or the vector $(\beta_1, \dots, \beta_s)'$

Define $c_{ij} = \alpha_0 + \alpha_i + \beta x_{ij}$ or $c_{ij} = \alpha_0 + \alpha_i + \beta_i x_{ij}$, depending on which model is used

For cell i , let $[L_i, U_i]$ be the design space for c_{ij}

Then, for the logistic or probit link, a complete class is formed by all designs with at most two support points per cell, and with additional specifications for each cell as in the model without factors (i.e., in each cell the two points are symmetric or one is equal to one of the endpoints for that cell).

The proof uses a simple additivity property of the information matrix

The result remains true if the model is “simplified” by modeling the α_i 's (e.g. using only main-effects)

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With different slope parameters (β_i), will need at least two support points per cell if estimation of β_i 's is of interest

If α_j 's are not simplified, even with a common slope β , at least one observation per cell is needed if all $\alpha_0 + \alpha_j$'s are of interest

Will focus in the remainder on the **common slope model with simplifying assumptions for the α_j 's**

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$$\eta_1 = (\alpha_0 + \alpha_1^1 + \dots + \alpha_F^1, \alpha_1^2 - \alpha_1^1, \dots, \alpha_1^{s_1} - \alpha_1^1, \dots, \alpha_F^2 - \alpha_F^1, \dots, \alpha_F^{s_F} - \alpha_F^1, \beta)'$$

and let η_2 be obtained from η_1 by deleting its first entry.

Without restrictions on design space, D -optimal designs for η_1 and η_2 :

$$\xi^* = \left\{ (c_{i1} = c^*, \omega_{i1} = \frac{1}{2s}), (c_{i2} = -c^*, \omega_{i2} = \frac{1}{2s}) \right\},$$

where c^* maximizes

$$c^2 \Psi^{m+2}(c) \text{ and } c^2 \Psi^{m+1}(c),$$

respectively, $\Psi(c) = [P(c)']^2 / [P(c)(1 - P(c))]$, and $m = \sum_{k=1}^F (s_k - 1)$.

Results remain true with restrictions on the design space, provided that c^* and $-c^*$ are in the design space for each cell.

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Results remain true with restrictions on the design space, provided that c^* and $-c^*$ are in the design space for each cell.

Outline

- 1 Background
- 2 Smaller designs: Main-effects only**
- 3 Adding interactions
- 4 Summary

Tan and S, 2015a

Each cell has two support points; algorithms also gave designs with many support points, both for D -optimality and other criteria.

Modest goal: For a main-effects model, can we reduce the number of support points by using an orthogonal array (OA)?

An $OA(N, s_1 \times \dots \times s_F, t)$ of strength t is an $N \times F$ array with s_k symbols in the k th column, so that for any t columns, all combinations that can appear as a row in the induced $N \times t$ subarray appear equally often.

If we can select 2 points in each cell corresponding to an $OA(N, s_1 \times \dots \times s_F, t)$, then the number of support points is $2N$ rather than $2s$; so we want an array with $N < s$.

This idea works for a main-effects model and the logistic or probit links with an OA of strength 2.

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Statement of result: For the logistic or probit link, with a main-effects model and η_1 and η_2 as before, a design that places weight $\frac{1}{2N}$ on each of c^* and $-c^*$, which are defined as before, for the cells that correspond to an $OA(N, s_1 \times \dots \times s_F, 2)$ is D -optimal.

Outline of proof: It suffices to check that the information matrices for these designs agree with those for the known D -optimal designs.

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$\sum_i \sum_j \omega_{ij} \Psi(c_{ij})$ over all cells i and $j \leq 2$

$\sum_i \sum_j \omega_{ij} \Psi(c_{ij})$ over all cells i with factor k at level i_k and $j \leq 2$

$\sum_i \sum_j \omega_{ij} \Psi(c_{ij})$ over all cells i with factors $k \neq k'$ at levels i_k and $i_{k'}$ and $j \leq 2$

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Using that Ψ is an even function, it can be shown that the OA-based designs give the same values for these expressions as the D -optimal designs that use all cells.

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Some benefits of the OA-based designs . . .

. . . simpler because of smaller support size ($2N$ points vs $2s$ points)

. . . correspond to more exact designs (weights $\frac{1}{2N}$ vs $\frac{1}{2s}$)

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Still assuming the main-effects model, if there is an $OA(N, s_1 \times \dots \times s_F \times 2, 2)$, then there are designs that use **only N support points, each with weight $\frac{1}{N}$** , that have the same information matrix for θ as the D -optimal designs.

How to obtain such designs? Use c^* in the $N/2$ cells corresponding to the first F columns for which the last factor is at level 1, say; use $-c^*$ for the other $N/2$ cells.

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Example: Let $F = s_1 = s_2 = 2$, and consider the following $OA(4, 2 \times 2 \times 2, 2)$:

1	1	1
1	2	2
2	1	2
2	2	1

The first two columns denote the cells, while the last column is used to select c^* or $-c^*$:

1	1	c^*
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In this toy example, we still need to use all 4 cells (in general this number is reduced), but only a single support point in each cell.

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... if there is an $OA(N, s_1 \times \dots \times s_F \times (2u + 1), 2)$, then there is a design that matches the information matrix and that has $(2u + 2)N/(2u + 1)$ support points; it has 2 support points in $N/(2u + 1)$ cells and 1 support point in the other $N - N/(2u + 1)$ cells

Do not take it to be uniform on its support: For cells with 2 points, use the weight $\frac{1}{2N}$, but for cells with 1 point use $\frac{1}{N}$...

... thus the total weight for points in each of the N cells is $\frac{1}{N}$

Can show that a single point per cell can be used if this OA has additional structure (e.g. if it is of strength 3)

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Tan and S, 2015b

What if the α_i 's in the linear predictor are modeled using **main-effects and interactions**?

Will **keep it simple**: add all two-factor interactions, or all two- and three-factor interactions, and so on; still using the logistic or probit link.

Consider finding a D -optimal design for $\eta = B\theta$, a **“maximal” vector of estimable functions**.

Unlike the main-effects model, S and Yang (2012) do not present a D -optimal design for this problem.

Information matrix becomes very complicated though, and we were not able to maximize the determinant of the information matrix for η directly.

But their complete class result still holds; so we can focus on designs with no more than 2 support points per cell.

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Guessed the form for a D -optimal design, using all cells.

Theoretically verified that the guess is correct using the generalized equivalence theorem.

Conclusion: D -optimal designs have the same form as for the main-effects model, but now with c^* as the maximizer of $c^2 \Psi^r(c)$, where $r = \text{rank}(B)$.

Requires again that c^* and $-c^*$ are in the design region for every cell.

And as for the main-effects model, orthogonal arrays (of high enough strength) can be used to reduce the number of support points . . .

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If such an OA exists with an additional 2-symbol column, then a D -optimal design can be obtained that uses only a singly support point in each of the cells corresponding to the rows of the OA.

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Summary

OA-based designs can help to reduce the number of support points, correspond to larger families of exact designs, and reduce requirements on the design space for the existence of D -optimal designs.

Algorithms seem to have a hard time to find optimal designs, especially “small” designs, for these types of problems.

We focused on D -optimality . . .

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Models tend to have a large number of parameters, which reduces the appeal of using local optimality . . .

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Summary

OA-based designs can help to reduce the number of support points, correspond to larger families of exact designs, and reduce requirements on the design space for the existence of D -optimal designs.

Algorithms seem to have a hard time to find optimal designs, especially “small” designs, for these types of problems.

We focused on D -optimality . . .

. . . with no constraints on the cells.

Models tend to have a large number of parameters, which reduces the appeal of using local optimality . . .

. . . but other approaches also face challenges.