A Comparison of Three Approaches for Constructing Robust Experimental Designs

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Outline

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1. Introduction and Motivation

- Main criticism of optimal designs: Model dependency
- In most applications: true model not necessary known
- Assumption: true model unknown element of a known set of models
- This is the general approach for model robust optimal designs
- Model robust optimal designs: gaining popularity recently
- Main objective: Find designs that are efficient over a class of models
- Introduction of a new Bayesian model robustness (BMR) criterion that use aspects model robust design of LN (LN) and Bayesian criterion of DJ

2. Three Approaches to design robustness

- Notation:
  - $\mathbf{X}(d) = [\mathbf{x}_1, \ldots, \mathbf{x}_n]'$: Design matrix where the ith row of $\mathbf{X}(d)$ is $(x_{i1}, \ldots, x_{im})$
  - $\mathcal{F} = \{\mathbf{f}_1, \ldots, \mathbf{f}_L\}$: Set of models under consideration
  - $n \times p_l$ model matrix $\mathbf{X}$ for model l is:

    $$\mathbf{X}_l(d) = [\mathbf{f}_l(\mathbf{x}_1), \ldots, \mathbf{f}_l(\mathbf{x}_n)]'$$

    $\mathbf{f}_l$ indicates which effects are present in model l
  - Linear model assumption: $\mathcal{F}$:

    $$\mathbf{y} = \mathbf{X}_T \beta_T + \varepsilon$$

$$\mathrm{SS}_{n,m} = \{\text{all possible models having } n-1 \text{ or fewer main effects}\}, \quad (1)$$

where $n \leq m$

2. Three Approaches to design robustness

2.1. Model Robust Design of LN: Criterion and Model Space

- The Approach:
  - $\mathcal{F}$: Set of models having g two-factor interactions
  - ξ^* is robust for $\mathcal{F}$ if $\xi^*(n) = arg\max \sum w_i e_i(\xi(n))$
  - For Estimation Capacity (EC_g-Optimality)

    $$e_i = \begin{cases} 1 & \text{if } f_i \text{ is estimable,} \\ 0 & \text{otherwise.} \end{cases}$$
  - For Information Capacity (IC_g-Optimality)

    $e_i = (\frac{D_i(\xi(n))}{D_i(\xi_i^*(n))})^{\frac{1}{p_i}}$

    where $\xi_i^*(n)$ is the D-optimal design for model f_i and $D_i(\xi(n)) = | \mathbf{X}_i' \mathbf{X}_i |$

2. Three Approaches to design robustness

2.2. DuMouchel-Jones Design

- Main idea:
  - Primary terms: Assumed to be present in the true model (p_1)
  - Potential terms: May/may not be present in the model (p_2)
- Prior distribution: variance of parameters $\mathbf{R} = \frac{\mathbf{K}}{\tau^2}$ where

$$\mathbf{K} = \begin{pmatrix} \mathbf{0}_{p_1 \times p_1} & \mathbf{0}_{p_1 \times p_2} \\ \mathbf{0}_{p_2 \times p_1} & \mathbf{I}_{p_2 \times p_2} \end{pmatrix}$$

- Criterion: Maximize

$$\phi(\xi) = \left| \mathbf{X}'_\xi \mathbf{X}_\xi + \frac{\mathbf{K}}{\tau^2} \right|$$

2. Three Approaches to design robustness

2.3. Bayesian Model Robust Design (BMR)

- X_i:design matrix for the model f_i with dimension k_i
- $p(i) = w_i$: prior probability for model f_i
- Prior distribution: $\boldsymbol{\theta} \; |i \sim N(\boldsymbol{\theta}_{0i}, \, \sigma^2 \mathbf{R}_i^{-1})$
- Assumption: $p(i)$ independent of $p(\mathbf{y}, \boldsymbol{\theta} \mid i, \xi)$

$$
\begin{aligned}
U(\xi) &= \int \int \int \log p(\boldsymbol{\theta} \mid \mathbf{y}, i, \xi)\} p(\mathbf{y}, \boldsymbol{\theta}, i \mid \xi) d\boldsymbol{\theta} d\mathbf{y} c(di) \\
&= \int \int \int \log p(\boldsymbol{\theta} \mid \mathbf{y}, i, \xi)\} p(\mathbf{y}, \boldsymbol{\theta} \mid i, \xi) p(i) d\boldsymbol{\theta} d\mathbf{y} c(di) \\
&= \sum_{i=1}^{d} \int \int \log p(\boldsymbol{\theta} \mid \mathbf{y}, i, \xi) p(\mathbf{y}, \boldsymbol{\theta} \mid i, \xi) p(i) d\boldsymbol{\theta} d\mathbf{y}
\end{aligned}
$$

- The Bayesian Model Robust Optimal design maximizes:

$$
\phi_{BR}(\xi) = \sum_{i=1}^{d} w_i \log \mid (\mathbf{X}'_{i,\xi} \mathbf{X}_{i,\xi} + \mathbf{R}_i) \mid
$$

3. Empirical Comparison

3.1. MEPI$_g$ model space

Table 1: Comparison of designs for $n = 8$, $m = 5$, and $g = 1$ (BMR values are for $(c_1, c_2) = (1, 1)$)

Design	EC	IC	BMR	DJ	balance
FFD	.40	.40	14.44	18.14	yes
BMR-optimal	1.00	.84	14.49	18.13	no
(EC,IC)-optimal	1.00	.84	14.49	18.13	no
DJ-optimal	.40	.40	14.44	18.14	yes

Table 2: Comparison of designs using BMR and DJ criteria (BMR values are for $(c_1, c_2) = (1, 1)$)

(n, m, g)	Design criterion	EC	IC	BMR	DJ
(8,4,2)	BMR	.80	.80	15.07	18.90
	(EC,IC)	1.00	.85	14.59	17.72
	DJ	.80	.80	15.07	18.90
(8,5,2)	BMR	.82	.60	15.96	18.13
	(EC,IC)	.82	.60	15.96	18.13
	DJ	.09	.09	15.63	18.14
(12,8,2)	BMR	.89	.73	26.46	34.13
	(EC,IC)	.97	.76	26.23	33.64
	DJ	.89	.73	26.46	34.13
(16,8,2)	BMR	.89	.89	30.92	54.17
	(EC,IC)	1.00	.88	29.99	50.80
	DJ	.89	.89	30.92	54.17

3. Bayesian Model Discrimination Design Criteria

Supersaturated design model space SS$_{n,m}$

Table 3: Comparison of designs using BMR and DJ criteria ($c = .2$ for both BMR and DJ)

(n, m)	Design criterion	EC	IC	BMR	DJ
(6,8)	BMR	.9312	.3521	7.5054	8.1341
	(EC,IC)	.9862	.3627	7.3342	7.8883
	DJ	.7385	.2821	7.3025	8.1630
(6,10)	BMR	.8352	.2840	7.9436	6.2517
	(EC,IC)	.9686	.3134	7.6332	5.9326
	DJ	.8352	.2840	7.9436	6.2517
(8,10)	BMR	.9535	.3276	11.1821	14.0843
	(EC,IC)	.9990	.3216	10.6364	13.0006
	DJ	.9535	.3276	11.1821	14.0843
(8,12)	BMR	.9727	.2940	11.7981	12.1850
	(EC,IC)	.9897	.2900	11.4679	11.6356
	DJ	.9476	.2872	11.7963	12.2285
(10,12)	BMR	.9674	.3094	15.0353	20.5695
	(EC,IC)	1.0000	.3047	15.8523	19.5698
	DJ	.9589	.3048	15.0137	20.6209
(10,15)	BMR	.9904	.2700	16.3986	17.8790
	(EC,IC)	.9960	.2611	15.8523	16.9605
	DJ	.9904	.2700	16.3986	17.8790

6. Conclusion

- In this presentation: New criterion for Bayesian model robust (BMR) design proposed
- Empirical evaluation of the performance of three approaches for constructing robust experimental designs in presence of model uncertainty
- Model spaces included MEPI$_g$ and supersaturated model space SS$_{n,m}$.
- Use of model robust paradigm (LN) leads substantial improvements in EC compared to DJ.
- In many instances, these seemingly disparate approaches produce the same designs.

6. Conclusion: continued

- The BMR approach: similar to (EC, IC) approach but flexible with use of prior probabilities.
- the DJ approach has clear advantages in terms of computational efficiency.
- Recommendation: Use of model robust designs when computing time not an issue.
- In other circumstances, the DJ approach provides a very fast and effective alternative.

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