Generating and Assessing Exact *G*-Optimal Designs

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Design Optimality

- One of the truly great paradigm shifts in DOX
- Can create custom designs for almost any situation
- Modern software makes this easy for at least some optimality criteria
- What optimality criteria should we use?

Three Criteria:

The *D*-criteria: **M** = $\frac{\mathbf{X'X}}{N}$

$$D_{eff} = \left[\frac{|\mathbf{X'X}|}{Max[|\mathbf{X'X}|]} \right]^{1/p}$$

Maximize the determinant of **M**

The *G*-criteria: Maximize the *SPV* over *R*

$$G_{eff} = \frac{p}{\max_{x \in R}(SPV)}$$

$$SPV = \frac{NVar[\hat{y}(\mathbf{x})]}{\sigma^2} = N\mathbf{x}'^{(m)} \left(\mathbf{X'X}\right)^{-1} \mathbf{x}^{(m)}$$

The *I*-criteria: Minimize the average prediction variance over *R*

$$I = \frac{1}{A} \int_R \frac{NVar[\hat{y}(\mathbf{x})]}{\sigma^2} d\mathbf{x}$$

$$I_{eff} = \frac{Min(APV(D))}{APV(D)}$$

Which Criterion should I Use?

- First-order models, first-order models with interaction
  - Objective is usually factor screening
  - Parameter estimation is key
  - Use the *D*-criterion
- Second-order models, mixture models
  - Response estimation is usually of primary importance
  - Use the *G* or *I* criterion

Design Construction

- The coordinate exchange approach – candidate-free, very efficient
- Construction of *D* and *I*-optimal (or highly efficient) designs pretty easy
- Construction of *G*-optimal designs is more challenging
  - There's an ugly optimization problem to be solved at each step

G-Optimal Designs

- It's a combinatorial optimization problem
- Approaches:
  - Branch and bound
  - Simulated annealing
  - Genetic algorithms
  - see Borkowski (2003), Goldfarb, Borror, Montgomery, and Anderson-Cook (2005), Haines (1987), Hamada, Martz, Reese, and Wilson (2001), Heredia-Langner, Carlyle, Montgomery, Borror, and Runger (2003), Heredia-Langner, Montgomery, Carlyle, and Borror (2004), Ortiz, Simpson, and Pignatiello (2004), Park, Richardson, Montgomery, Ozol-Godfrey, Borror, and Anderson-Cook (2005), Welch (1984), and Zhou (2001).

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Cases Considered

- Second-order response surface models
- Cubodial region of interest
- Cases considered:
  - 2 factors; N = 6, 7, 8, 9, 10, 11, 12
  - 3 factors; N = 10, 11, 12, 13, 14, 15, 16
  - 4 factors; N = 15, 20, 24
  - 5 factors; N = 21, 26, 30

- We report the best designs produced by the optimality criteria *D*, *I*, and *G*.
- *D*-optimal and *I*-optimal designs were created using JMP Version 7.
- The *G*-optimal designs are created using the *G*-criterion and Brent's minimization algorithm* programmed in JSL.
- The starting designs or *parents* include *D*-optimal, *I*-optimal, completely random designs and sometimes a specific design.
- The execution time for the program is minimal (in seconds) and could easily be implemented in commercially available software.
- The JMP program used to create designs can be obtained from Myrta.

*Brent, R. P. (1973). *Algorithms for Minimization without Derivatives*. Englewood Cliffs, NJ: Prentice Hall.

Eye Chart!!

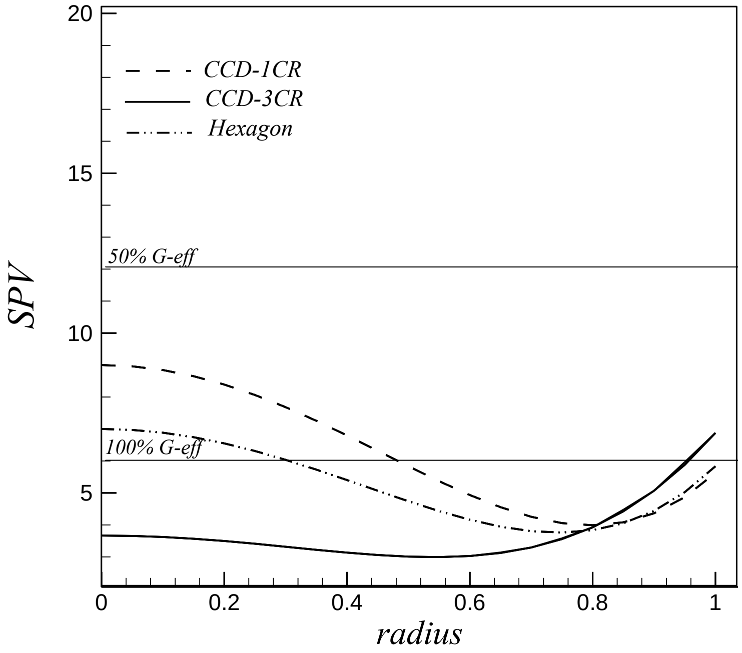
n	Optimal Design	*G*-eff.	*D*-eff.	*I*-eff.	*n*	Optimal Design	*G*-eff.	*D*-eff.	*I*-eff.
2 Factors					**3 Factors**				
6	G	100.00	94.60	92.40	10	G	100.00	91.40	79.06
	D	71.82	100.00	93.67		D	77.40	100.00	96.84
	I	57.96	91.17	100.00		I	69.38	97.56	100.00
7	G	100.00	88.06	75.10	11	G	100.00	93.27	74.97
	D	78.29	100.00	86.93		D	78.30	100.00	70.97
	I	56.41	85.11	100.00		I	63.67	91.51	100.00
8	G	100.00	97.55	81.05	12	G	100.00	93.04	69.39
	D	75.61	100.00	88.45		D	69.33	100.00	70.38
	I	64.94	89.70	100.00		I	59.91	87.66	100.00
9	G	100.00	93.86	81.28	13	G	100.00	98.50	68.90
	D	95.87	100.00	94.76		D	95.78	100.00	72.77
	I	70.44	90.71	100.00		I	65.17	86.80	100.00
10	G	100.00	94.31	75.45	14	G	100.0	99.95	98.21
	D	88.40	100.00	84.29		D	93.28	100.00	76.78
	I	87.54	97.37	100.00		I	53.08	86.10	100.00
11	G	100.00	93.93	70.88	15	G	100.00	99.57	90.17
	D	82.25	100.00	78.14		D	93.16	100.00	72.63
	I	79.77	92.81	100.00		I	99.65	97.14	100.00
12	G	100.00	89.21	73.90	16	G	100.00	96.94	95.39
	D	78.30	100.00	75.78		D	92.14	100.00	71.03
	I	74.39	87.56	100.00		I	98.97	93.65	100.00
4 Factors					**5 Factors**				
15	G	100.00	98.01	75.89	21	G	100.00	98.89	65.20
	D	98.28	100.00	78.23		D	92.86	100.00	63.04
	I	76.44	87.01	100.00		I	54.35	78.26	100.00
20	G	100.00	93.75	73.40	26	G	93.08	99.34	80.86
	D	95.18	100.00	65.63		D	86.41	100.0	61.06
	I	82.11	85.48	100.00		I	64.50	82.69	100.00
24	G	99.97	96.59	87.00	30	G	100.00	99.93	60.04
	D	90.71	100.00	61.82		D	98.65	100.00	60.15
	I	55.38	87.79	100.00		I	71.06	87.08	100.00

Results

- We found designs that were identical to published *G*-optimal designs
  - $k = 2, 3$ factors
- There are cases where our designs are better than published designs
  - $K = 4, N = 15; k = 5, N = 21$
- There are cases for which no published designs were available for comparison
  - $K = 4, N = 20; k = 5, N = 30$

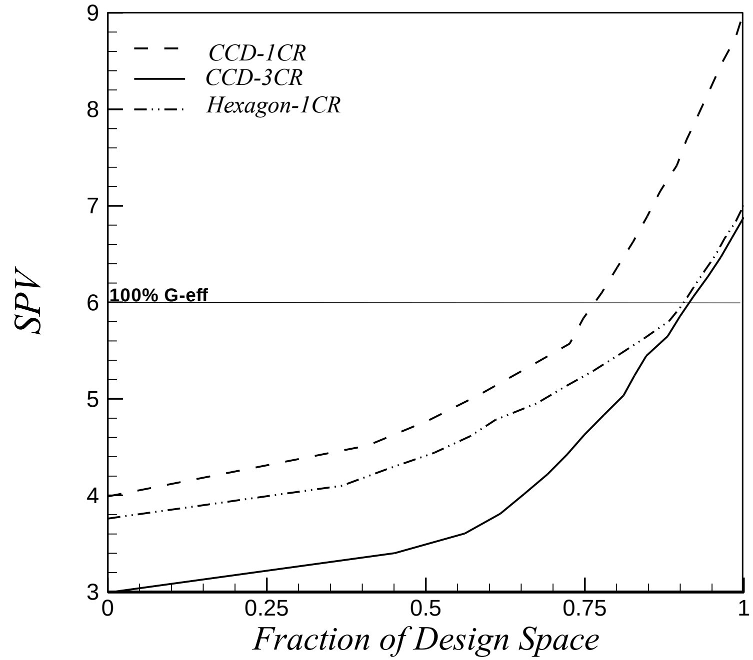
Looking at Efficiencies can be Misleading

The Hexagon and the CCD-3CR have about the same *G*-efficiency (86%)



Variance Dispersion Graph

The CCD-3CR is uniformly superior in the sense that for a given *SPV*, it has the largest fraction of design space at or below this level



Fraction of Design Space Plot

Variance Ratio Fraction of Design Space Plot (VRFDS)

At a specific design point **x** the prediction variance of design *i* is compared to the prediction variance of a reference design:

$$VR_i = \frac{PV_i(\mathbf{x})}{PV_{\text{Ref}}(\mathbf{x})}$$

If $VR_i < 1$ the reference design predicts worse than design *i*; if $VR_i > 1$ the reference design predicts better than design *i*

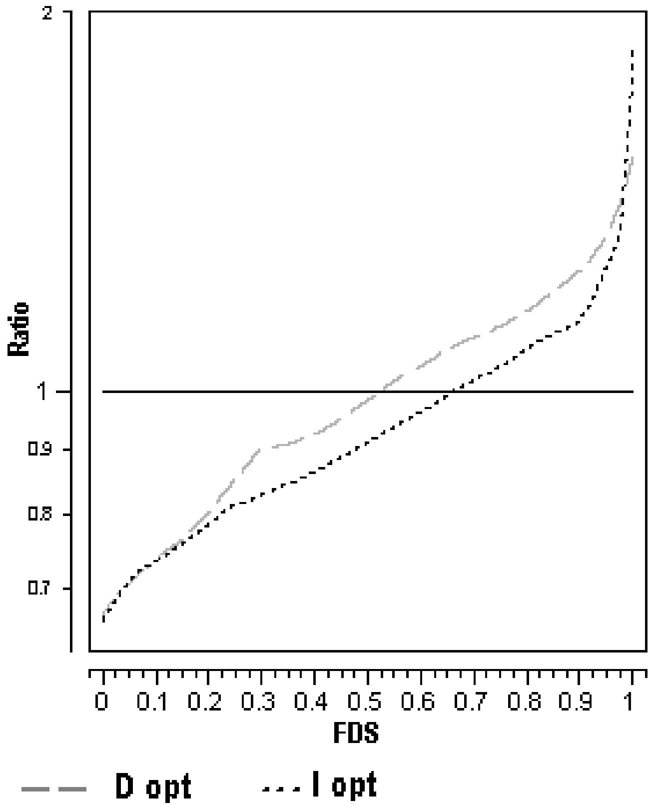
$$VR_D = \frac{PV_D(\mathbf{x})}{PV_G(\mathbf{x})} \qquad VR_I = \frac{PV_I(\mathbf{x})}{PV_G(\mathbf{x})}$$

We used the VRFDS plots to compare the *D* and *I*-optimal designs to the *G*-optimal designs:

$$VR_D = \frac{PV_D(\mathbf{x})}{PV_G(\mathbf{x})} \qquad VR_I = \frac{PV_I(\mathbf{x})}{PV_G(\mathbf{x})}$$

Each VRFDS plot has a horizontal reference line at unity

$K = 2$, $N = 6$

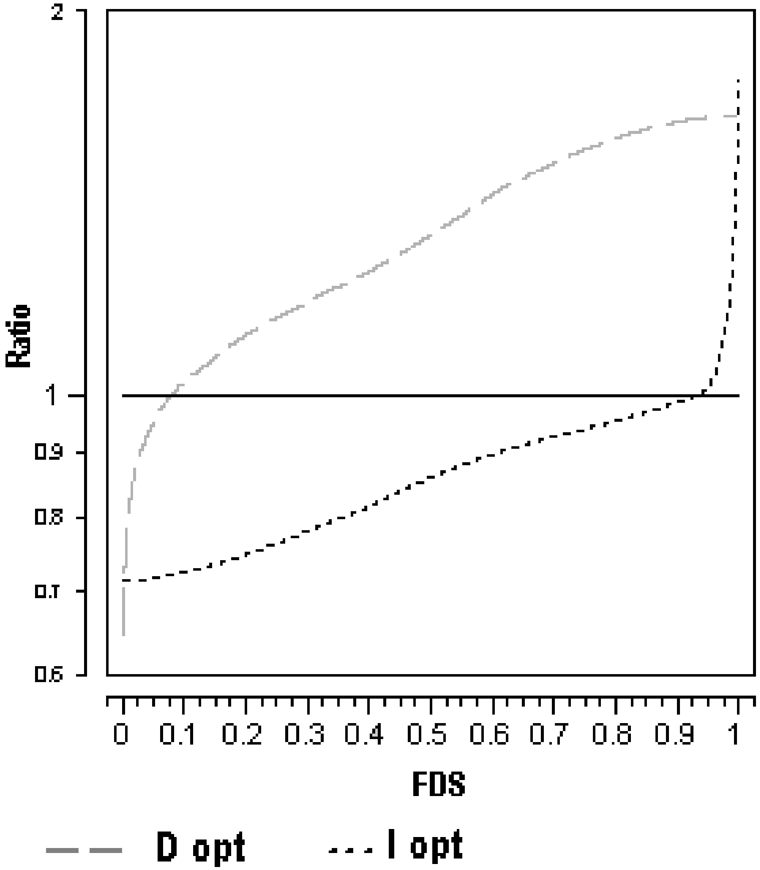


The *I*-optimal design outperforms the *D*-optimal design

The *D*-optimal design outperforms the *G*-optimal design over about 50% of the design space

The *I*-optimal design outperforms the *G*-optimal design over about 2/3 of the design space

$K = 3, N = 15$



Both the *D* and *I*-optimal designs have similar *G*-efficiencies

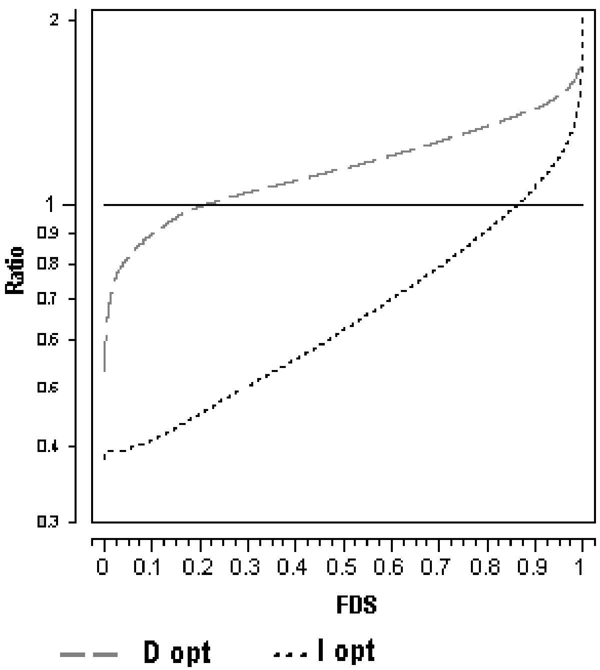
The *I*-optimal design outperforms the *D*-optimal design

The *D*-optimal design is worse than the *G*-optimal design over about 90% of the design space

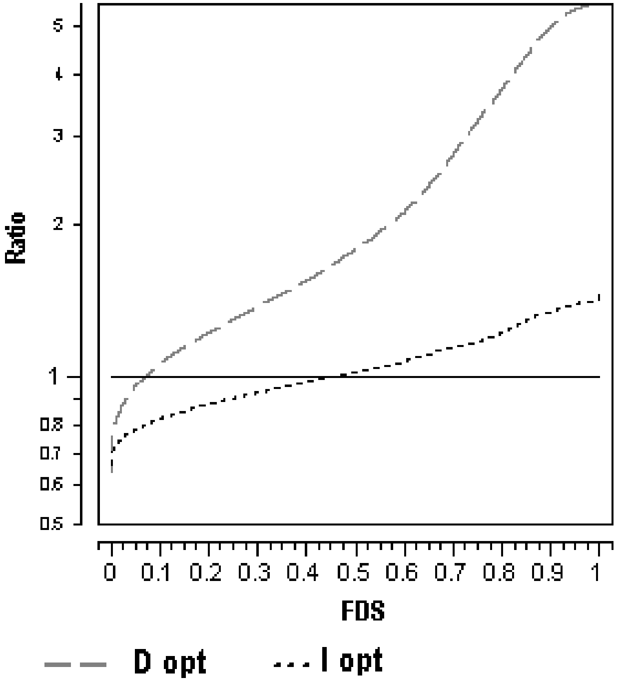
The *I*-optimal design outperforms the *G*-optimal design over about 93% of the design space

As design size increases, generally the *D*-optimal designs result in poorer prediction variance than the *G*-optimal designs

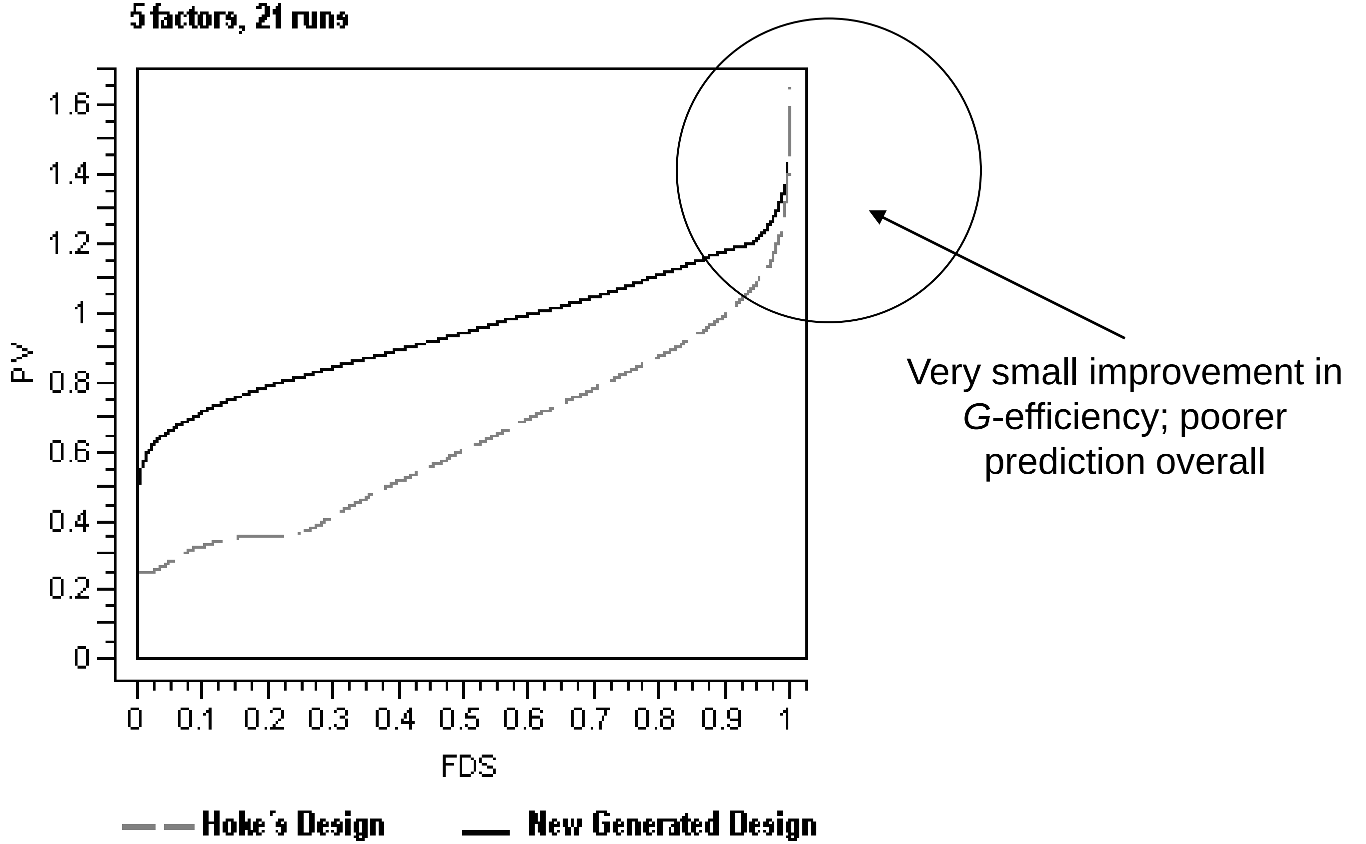
K = 4, *N* = 20



K = 5, *N* = 26



The difference between the new designs and standard designs can be subtle:



Conclusions

- The maximum PV for the *I*-optimal design is always worse that the maximum PV for the *G*-optimal design
- The *I*-optimal designs have smaller PV over most of the design region
- For 60% of the cases considered, the PV for the *I*-optimal design is less than the PV for the *G*-optimal design over 85% of the design space

Conclusions

- The new algorithm produces G-optimal designs in commercially-feasible times (seconds)
- Many *G*-optimal designs are not competitive in PV over a large portion of the design space
- This may be a big price to pay for protection near the boundaries of the region
- So, is it worth it?
- Probably not

Possibly the performance of the *I*-optimal design could be improved near the region boundary by using a weighted objective function:

$$I = \frac{1}{A}\int_R \frac{N w(\mathbf{x}) Var[\hat{y}(\mathbf{x})]}{\sigma^2}\, d\mathbf{x}$$