

Fast Computation of Exact G-Optimal Designs Via I_λ -Optimality

Chris Nachtsheim
Carlson School of Management
University of Minnesota

Fall Technical Conference, West Palm Beach
October 4, 2018

Joint work with Lucia Hernandez:

**Assistant Professor
School of Economics and Statistics
National University of Rosario
Rosario, Argentina**

- **My former PhD student**
- **Carried out her dissertation research at Minnesota on Fulbright grant**



My Fulbright Trip to Argentina October, 2017

**Studying off
line quality
control of
wines in the
Mendoza
wine region
with Lucia**



**And now---for those with suspicious minds in
this time of the “Me Two” movement...**

**And now---for those with suspicious minds in
this time of the “Me Two” movement...**

My wife took that picture!

Here we are in the Andies near Chilean border

Same trip



Here we are in the Andies near Chilean border

**My wife
Maureen
and two of
our best
friends**



Here we are in the Andies near Chilean border

**Lucia and
her sister
and
parents**



First, a little bit of optimal design theory

- In our first submission, we skipped this
- Editor: add a primer!!!

First, a little bit of optimal design theory

- In our first submission, we skipped this
- Editor: add a primer!!!

So here we go ...

Basic notation

- **Standard linear model:**

$$y = X\beta + \epsilon$$

- **X is n by p , β is p by 1, and the i th row of X is:**

$$\mathbf{f}'(\mathbf{x}_i)$$

- **So that the i th observation can be written:**

$$y_i = \mathbf{f}'(\mathbf{x}_i)\beta + \epsilon_i$$

- **Assume constant error variance, and, WLOG: $\sigma^2 = 1$**

What is an approximate design?

- An approximate design is a probability measure ξ on a design space χ
- Design problem: Quadratic regression on $\chi = [-1, 1]$, and we can take **$n = 16$ runs**
- **Example design measure ξ :**

Place 1/3 weight at -1	$16/3 = 5.333$ runs
Place 1/3 weight at 0	$16/3 = 5.333$ runs
Place 1/3 weight at +1	$16/3 = 5.333$ runs
- **Can only implement “approximately.”**

Information matrix of approximate design ξ

- **Information matrix:**

$$M(\xi) = \int_{\mathcal{X}} \mathbf{f}(\mathbf{x})\mathbf{f}'(\mathbf{x})d\xi(\mathbf{x})$$

- **By Caratheodory's theorem, any continuous measure can be discretized:**

$$M(\xi) = \sum_{i=1}^s \mathbf{f}(\mathbf{x}_i)\mathbf{f}'(\mathbf{x}_i)\xi(\mathbf{x}_i)$$

- **So, we can focus on discrete probability measures**

Discretization example

- Approximate design ξ is given by the uniform probability measure on $\chi = [-1, 1]$.
- Model is quadratic: $\mathbf{f}^T(\mathbf{x}) = (1, x, x^2)$

$$\begin{aligned}\mathbf{M}(\xi) &= \int_{\chi} \mathbf{f}(\mathbf{x}) \mathbf{f}'(\mathbf{x}) d\xi(\mathbf{x}) = \int_{-1}^1 \begin{pmatrix} 1 \\ x \\ x^2 \end{pmatrix} (1, x, x^2) f(x) dx \\ &= \int_{-1}^1 \begin{pmatrix} 1 & x & x^2 \\ x & x^2 & x^3 \\ x^2 & x^3 & x^4 \end{pmatrix} \frac{1}{2} dx = \begin{pmatrix} 1 & 0 & 1/3 \\ 0 & 1/3 & 0 \\ 1/3 & 0 & 1/5 \end{pmatrix}\end{aligned}$$

- The discrete design placing 5/18 weight at $\pm \sqrt{3/5}$ and 4/9 weight at 0 yields the same \mathbf{M}

What is an exact design?

- Assume n a positive integer and for ξ a discrete design measure on χ .
- ξ a an exact n -point design if $n\xi(x)$ is a positive integer $\forall x \in \chi$
- Example: $n = 3$ (or 6 or 9 or 12 ...)

$x:$	-1	0	1
$\xi_3(x):$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$

M matrix for exact design and some notation

- Assume n (not necessarily distinct) points $\mathbf{x}_1, \dots, \mathbf{x}_n$.
- Information matrix is:

$$\mathbf{M}(\xi_n) = \sum_{i=1}^n \mathbf{f}(\mathbf{x}_i) \mathbf{f}'(\mathbf{x}_i) \frac{1}{n} = \mathbf{X}'\mathbf{X}/n$$

- Notation: Sets of possible designs

Ξ = set of all approximate designs

Ξ_n = set of all n -point exact designs

D-Optimal designs

Definition: The D-optimal design maximizes the determinant of the information matrix:

$$\xi^D = \arg \max_{\xi \in \Xi} |\mathbf{M}(\xi)| \quad \text{(Approximate case)}$$

$$\xi_n^D = \arg \max_{\xi_n \in \Xi_n} |\mathbf{M}(\xi_n)| \quad \text{(Exact case)}$$

Why D?

- D-optimal designs minimize the volume of the confidence region for β .
- D-optimal designs best for estimation of β .

D-optimal approximate design

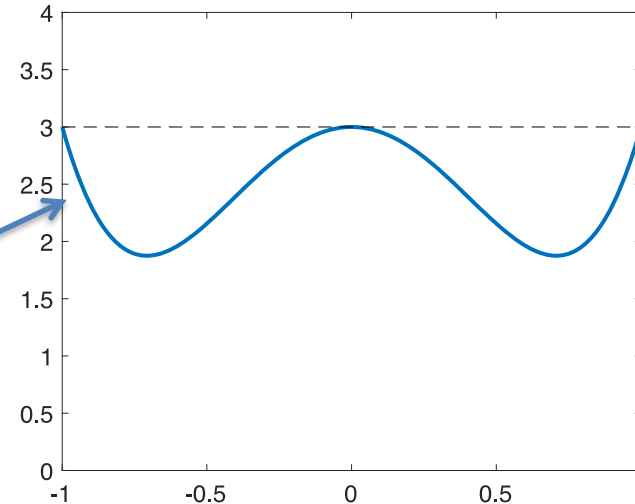
$$\xi^D = \arg \max_{\xi \in \Xi} |\mathbf{M}(\xi)|$$

Example: Quadratic regression on $\chi = [-1,1]$

$$\xi^D = \left\{ \begin{array}{ccc} -1 & 0 & 1 \\ 1/3 & 1/3 & 1/3 \end{array} \right\}$$

$$|\mathbf{M}| = 4/27$$

Variance of prediction



What if prediction is of primary interest?

- **Normalized variance of prediction:**

$$v(\mathbf{x}, \xi) = \begin{cases} \mathbf{f}'(\mathbf{x})\mathbf{M}^{-1}(\xi)\mathbf{f}(\mathbf{x}) & \text{if } \mathbf{M}(\xi) \text{ is not singular} \\ \infty & \text{if } \mathbf{M}(\xi) \text{ is singular} \end{cases}$$

- **Pick the design to minimize the maximum variance of prediction (G-optimality)**
- **Pick the design to minimize the average variance of prediction (I-optimality)**

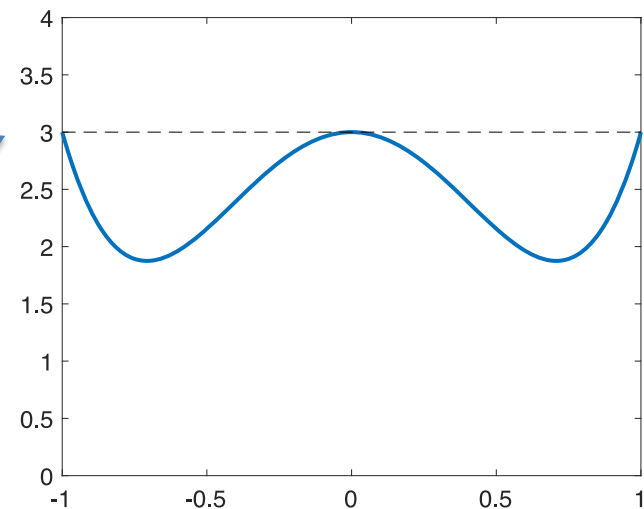
G-optimal (minimax) design

$$\xi^G = \arg \min_{\xi \in \Xi} \max_{\mathbf{x} \in \chi} v(\mathbf{x}, \xi)$$

Example: Quadratic regression on $\chi = [-1, 1]$

$$\xi^G = \left\{ \begin{array}{ccc} -1 & 0 & 1 \\ 1/3 & 1/3 & 1/3 \end{array} \right\}$$

Minimax $v(\mathbf{x}) = 3$
Average $v(\mathbf{x}) = 2.4$



Wait! That G-optimal design looked just like the D-optimal design

$$\xi^D = \begin{Bmatrix} -1 & 0 & 1 \\ 1/3 & 1/3 & 1/3 \end{Bmatrix}$$

$$\xi^G = \begin{Bmatrix} -1 & 0 & 1 \\ 1/3 & 1/3 & 1/3 \end{Bmatrix}$$

Kiefer-Wolfowitz Equivalence Theorem (1959)

The following conditions are equivalent:

1. ξ is D-optimal.
2. ξ is G-optimal.
3. $\max_{\mathbf{x} \in \chi} v(\mathbf{x}, \xi) = p$

K-W does NOT hold for exact designs

- D-optimal and G-optimal designs are not necessarily the same for finite n
- Fast algorithms exist for D-optimal designs
- Fast algorithms **do not** exist for G-optimal designs

OK, so why is G-optimality hard?

D-optimal exchange algorithms

1. Generate a random starting design
2. Cycle through the n points in the design:
 - For point i , find the point in the the design space x^* , such that when x^* is exchanged for x_i , we get a maximal increase in the determinant.
3. Repeat step 2 until no further improvements

An optimization over c is required for every design point -- function to be evaluated is the determinant

OK, so why is G-optimality hard?

G-optimal exchange algorithms

1. Generate a random starting design
2. Cycle through the n points in the design:
 - For point i , find the point in the the design space x^* , such that when x^* is exchanged for x_i , we get a maximal decrease in the maximum variance.
3. Repeat step 2 until no further improvements

An optimization over c is required for every design point – but to evaluate the criterion must do another maximization of the variance function

Now, let's beat a dead dog:

Coordinate exchange is really bad with G-optimality.

- 1) The criterion is the maximum variance over the design space. Algorithms that attempt to do minimax are very expensive!!!!**
- 2) The algorithm fails regularly to find the global optimum.**

Example: Quadratic regression, $n = 6$

We know the G-optimal design places two observations at the each of the endpoints and two at the center.

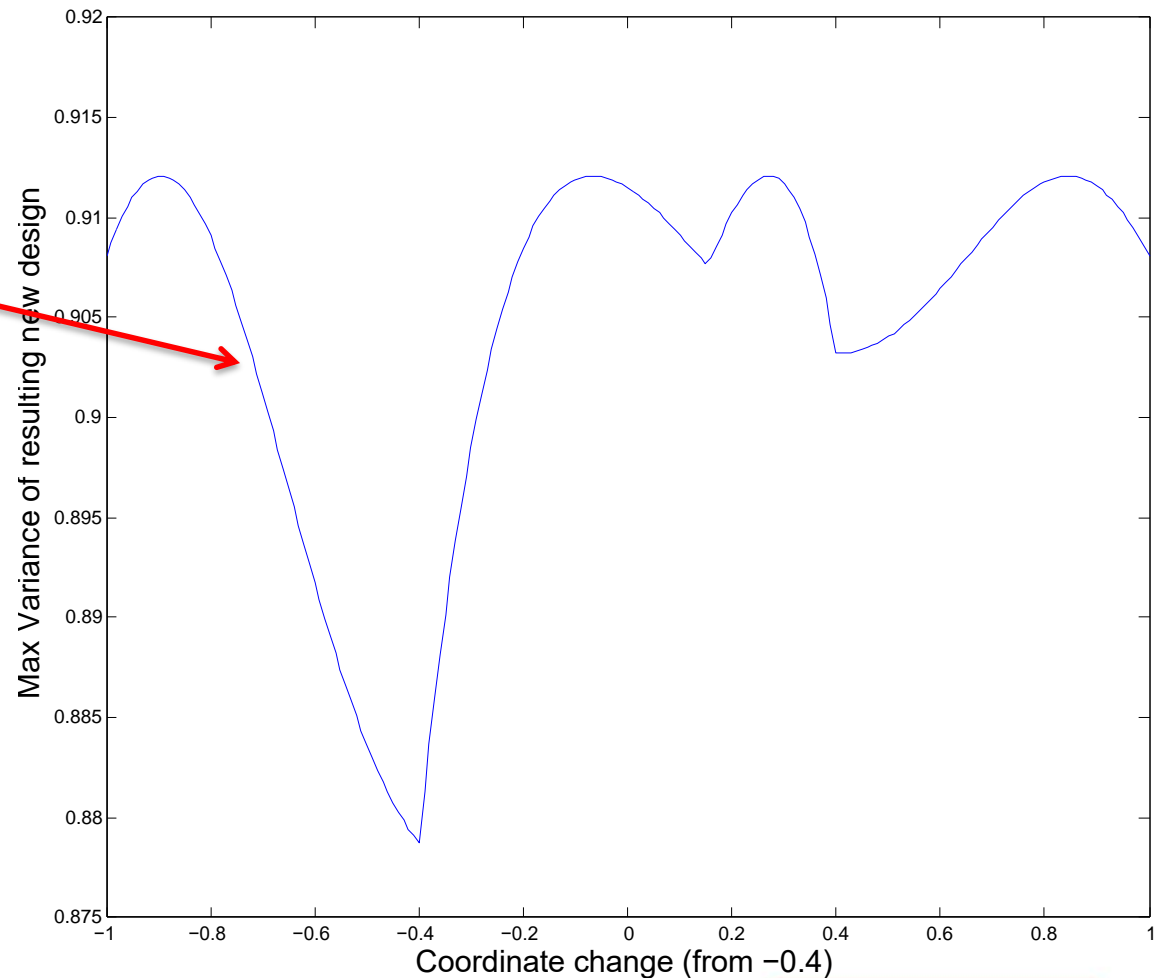
Consider this starting design:

-1 -0.4 0 0 0.4 1

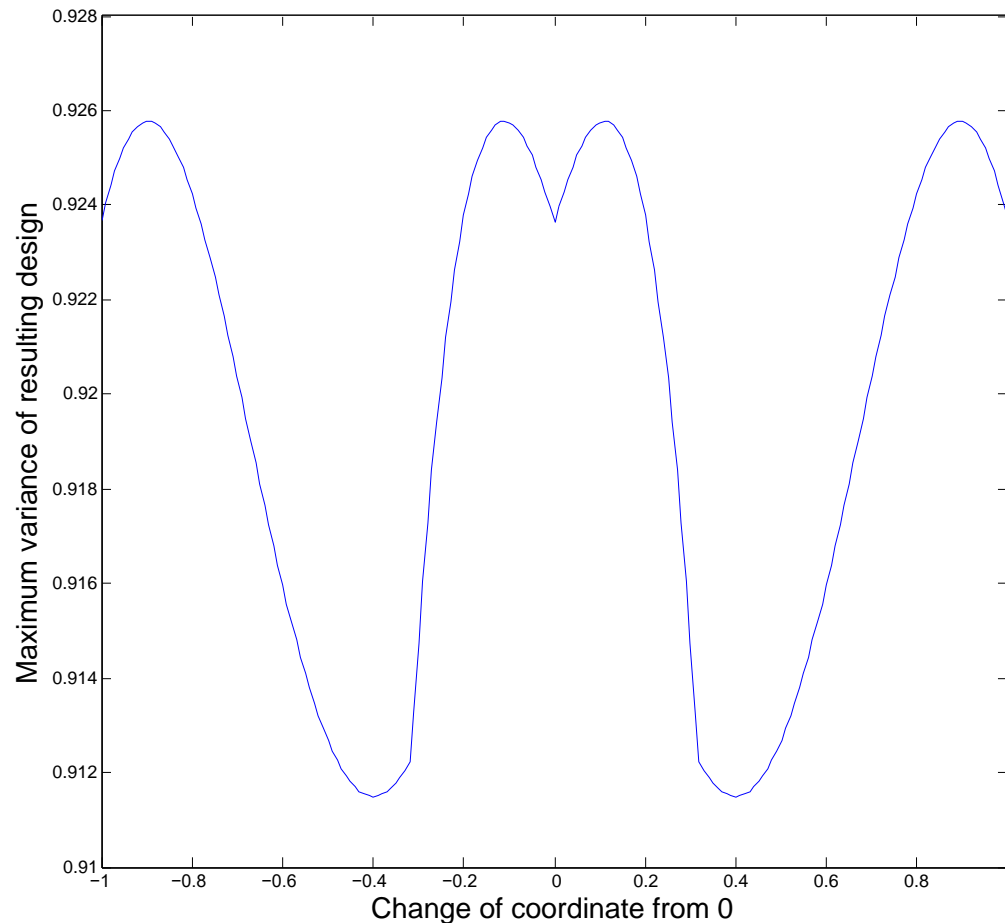
Seems clear we want to move 0.4 to 1 and -0.4 to -1.

When you try to change the -.4 coordinate, you can't

**Resulting
maximum
variance from
exchange of -
0.4**

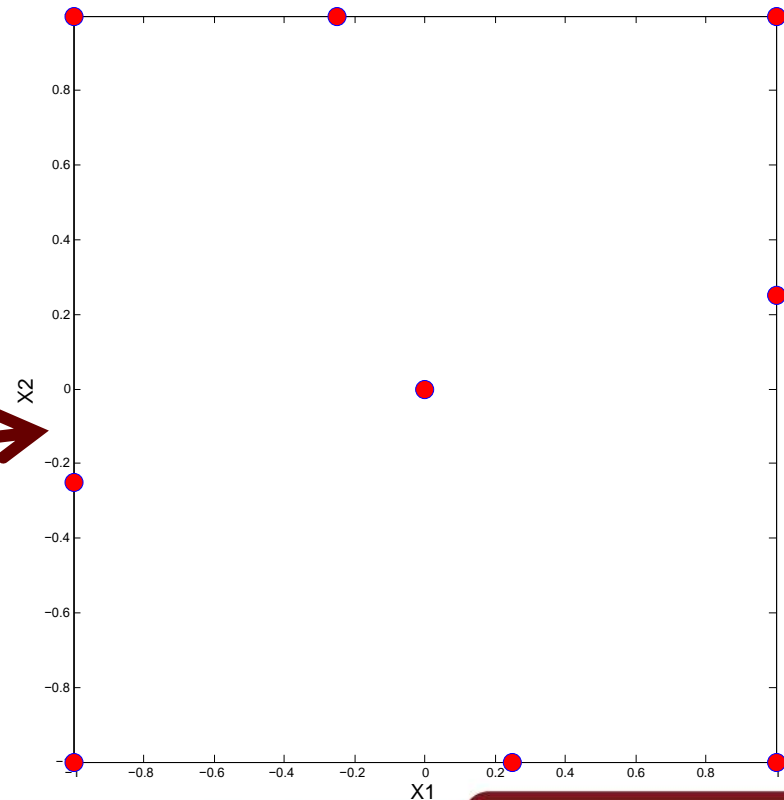


When you try to change the 0 coordinate, your best move is to change it to ± 0.4 ...and then you're stuck



G-optimal algorithm success rates are bad using random starting designs

1. One factor, $n = 6$,
86% success rate
2. Two factors, $n = 9$,
0% success rate.
Best design



I_λ -optimal (minimum average variance) Design

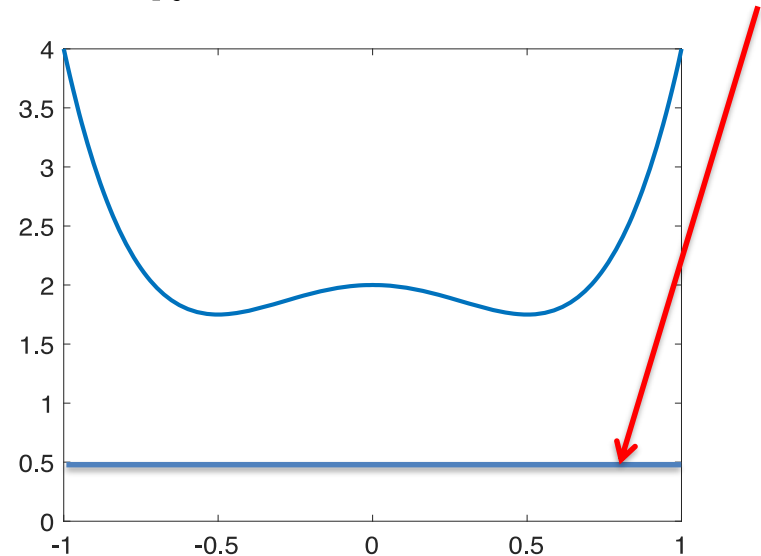
$$\xi^{I_\lambda} = \arg \min_{\xi \in \Xi} \int_{\chi} v(\mathbf{x}, \xi) \lambda(\mathbf{x}) d\mathbf{x}$$

Example: Quadratic regression on $\chi = [-1, 1]$; $\lambda(\mathbf{x})$ uniform

$$\xi^{I_\lambda} = \left\{ \begin{array}{ccc} -1 & 0 & 1 \\ 1/4 & 1/2 & 1/4 \end{array} \right\}$$

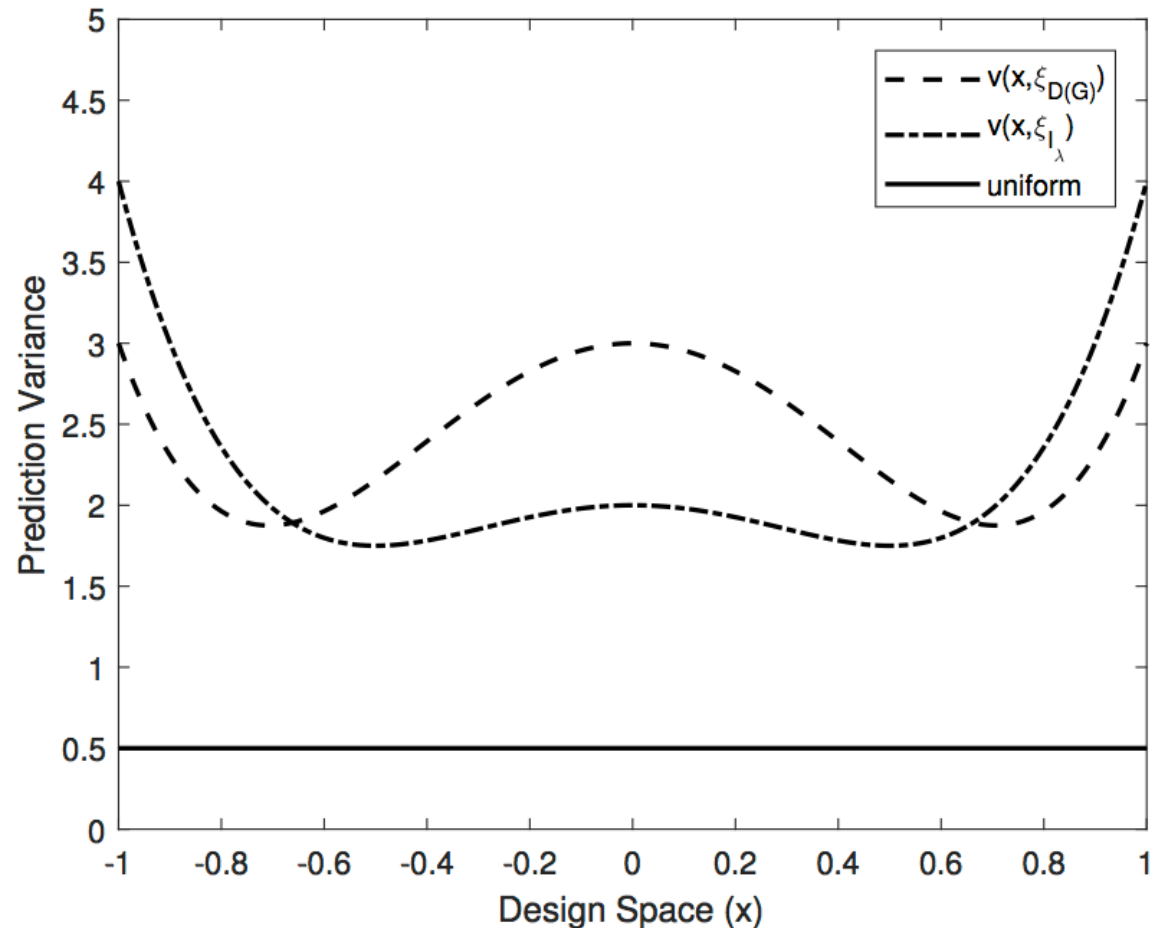
Minimax $v(\mathbf{x}) = 4$

Average $v(\mathbf{x}) = 2.133$



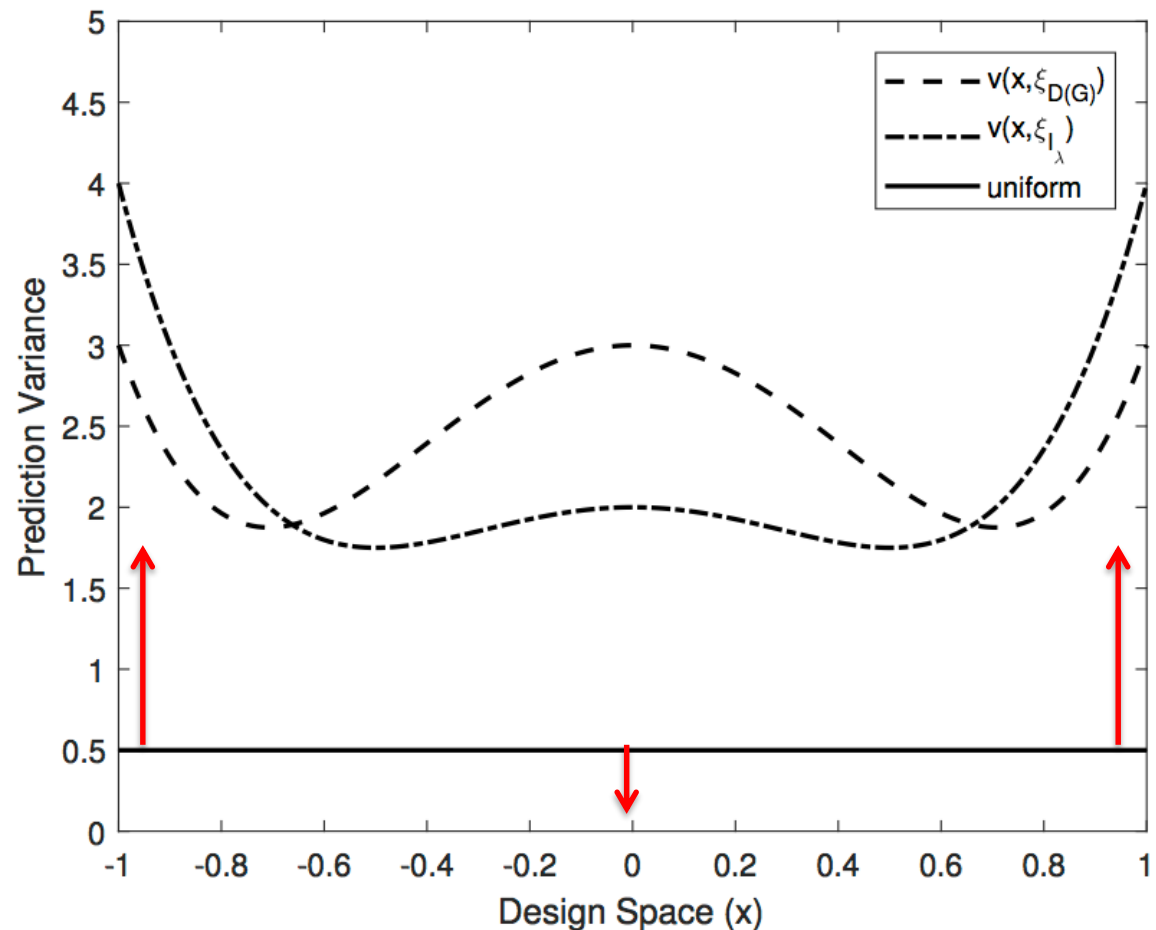
Superimpose G and I_λ optimal variance functions

What if we increased $\lambda(x)$ near the boundaries and reduced it in the center?



Superimpose G and I_λ optimal variance functions

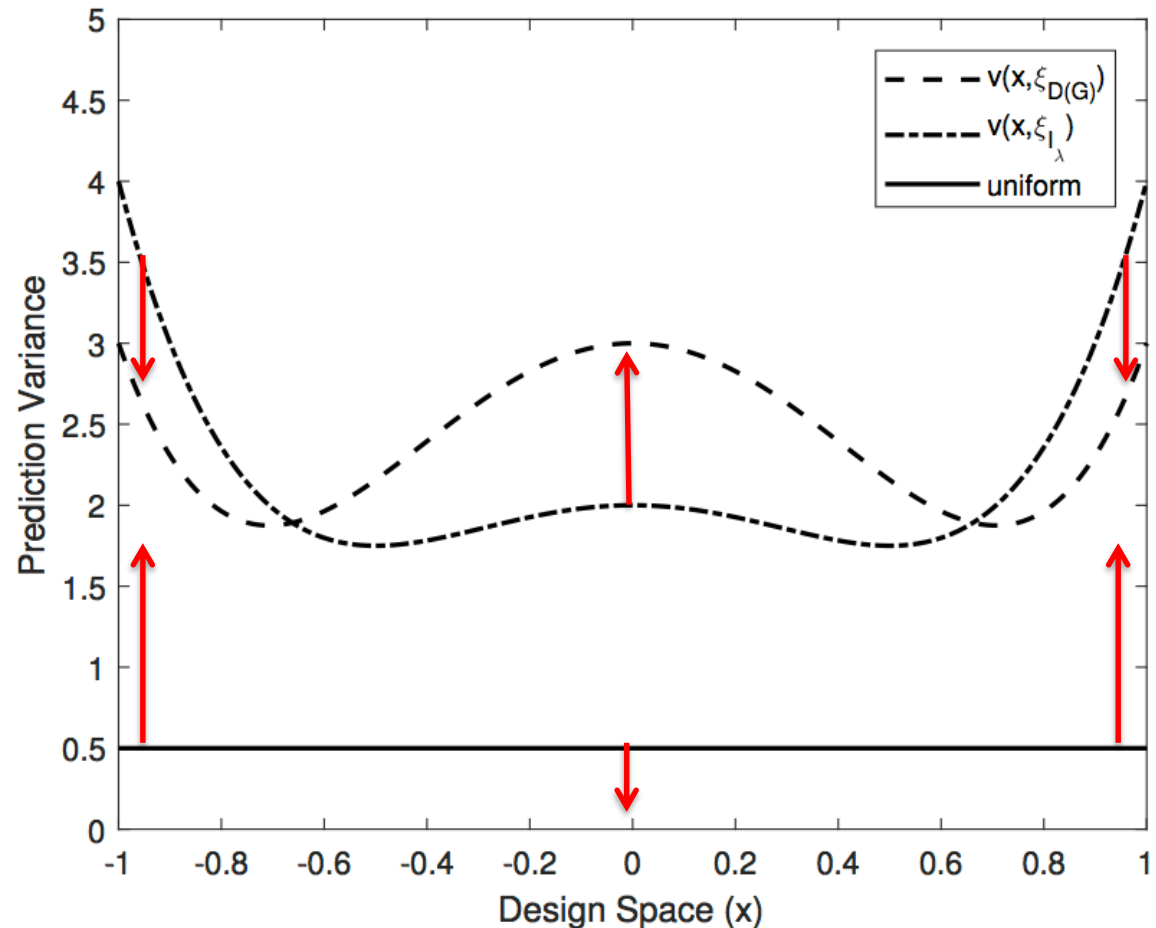
What if we increased $\lambda(x)$ near the boundaries and reduced it in the center?



Superimpose G and I_λ optimal variance functions

What if we increased $\lambda(x)$ near the boundaries and reduced it in the center?

That should bring down the maximum variance of prediction at the boundaries



Research Question

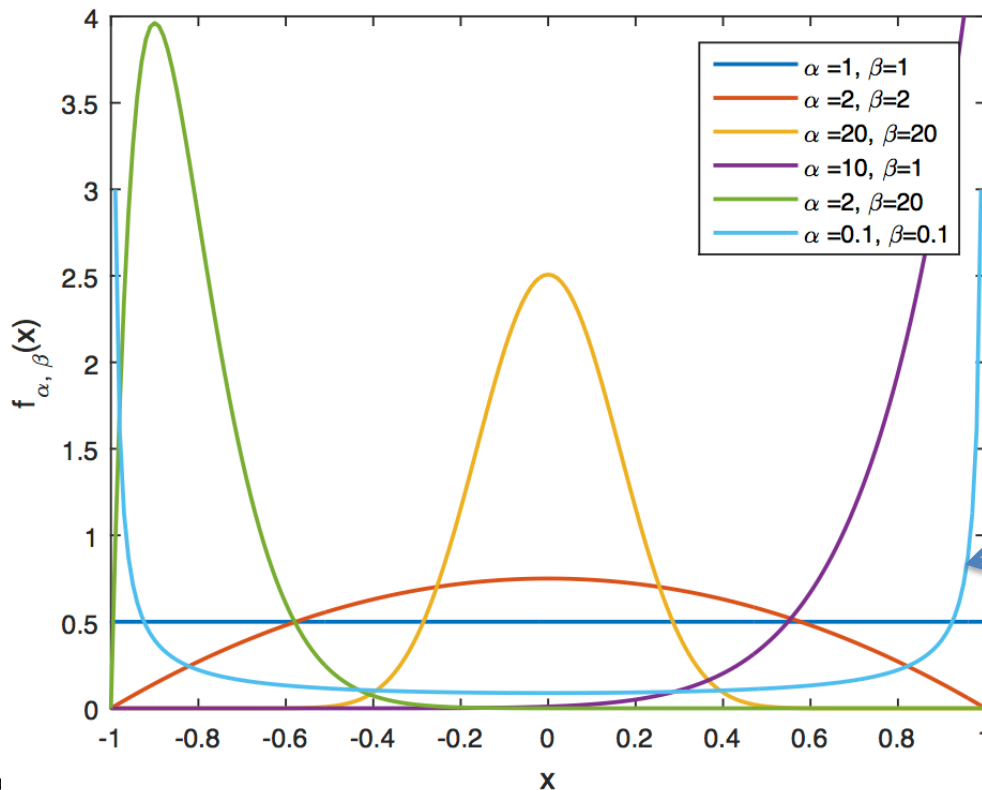
Can a clever choice of the weight function λ yield:

$$\xi^{G(D)} \approx \xi^{I_\lambda}$$

If so, we can use standard, fast exchange algorithms (with no minimax search) to find the G-optimal design

Try $\lambda(x)$ = beta density on $[-1,1]$

$$f_{\alpha,\beta} = \left(\frac{1}{2}\right)^{\alpha+\beta-1} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} (1+x)^{\alpha-1} (1-x)^{\beta-1} \quad -1 \leq x \leq 1, \alpha, \beta > 0$$

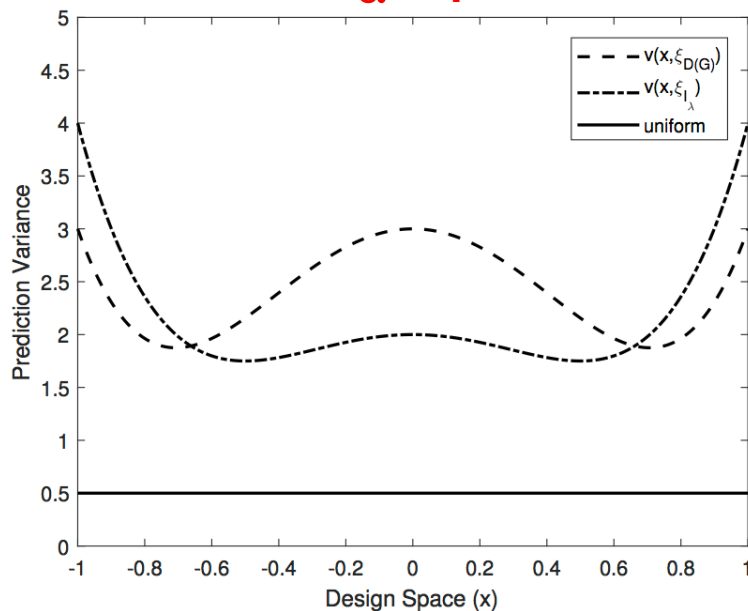


Blue guy has $\alpha = \beta < 1$, bathtub shape—what we want

Find $\alpha = \beta$ so that designs are the same

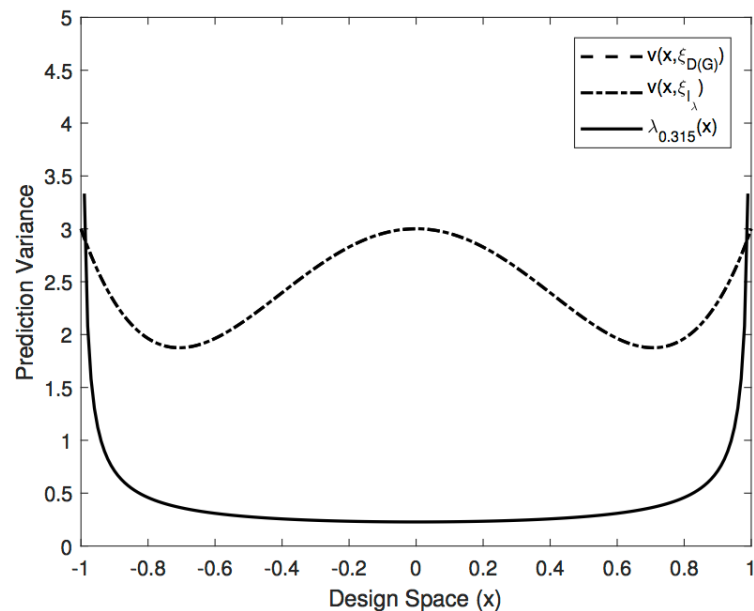
$$\alpha^* = \arg \min_{\alpha} \int_{\mathcal{X}} [d(x, \xi^{G(D)}) - d(x, \xi^{I_{\lambda}})]^2 d\lambda_{\alpha}(x)$$

$\alpha = 1$



(a) Uniform weight function (λ)

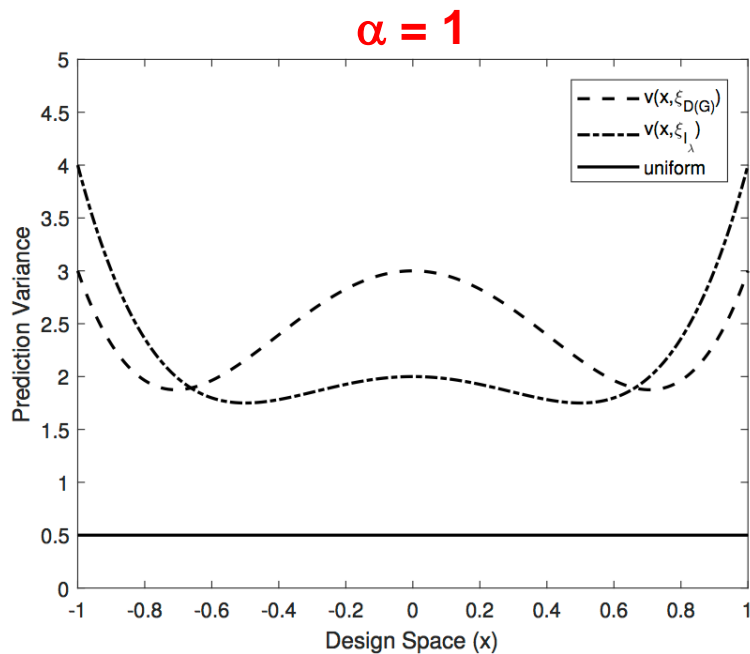
$\alpha^* = 0.315$



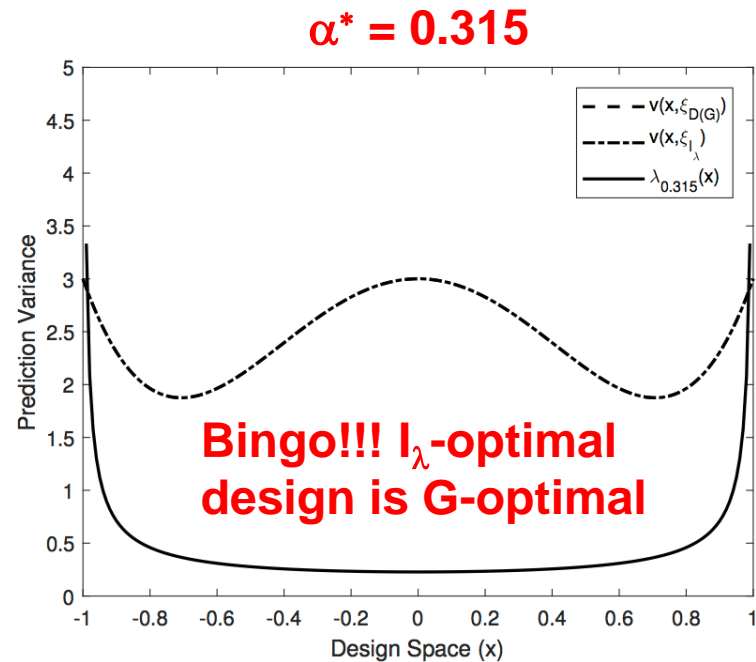
(b) Bathtub-shaped weight function (λ)

Find $\alpha = \beta$ so that designs are the same

$$\alpha^* = \arg \min_{\alpha} \int_{\mathcal{X}} [d(x, \xi^{G(D)}) - d(x, \xi^{I_{\lambda}})]^2 d\lambda_{\alpha}(x)$$



(a) Uniform weight function (λ)



(b) Bathtub-shaped weight function (λ)

OK, how about more factors

- **Need multidimensional gamma density for weight function**
- **Assume independence, product of gammas?**

OK, how about more factors

- Need multidimensional gamma density for weight function
- Assume independence, product of gammas?

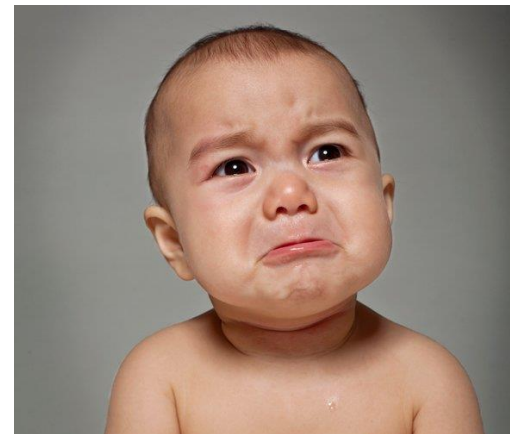
**Failure! Dead end.
Abandon ship..**

OK, how about more factors

- Need multidimensional gamma density for weight function
- Assume independence, product of gammas?

**Failure! Dead end.
Abandon ship..**

Lucia was sad



But wait!

- Think about the I_λ criterion:

$$\int_{\chi} v(\mathbf{x}, \xi) \lambda(\mathbf{x}) d\mathbf{x} = \text{tr}[\mathbf{M}^{-1}(\xi) \int_{\chi} \mathbf{f}'(\mathbf{x}) \mathbf{f}(\mathbf{x}) \lambda(\mathbf{x}) d\mathbf{x}] = \text{tr}[\mathbf{M}^{-1}(\xi) \mathbf{W}]$$

where:

$$\mathbf{W} = \int_{\chi} \mathbf{f}'(\mathbf{x}) \mathbf{f}(\mathbf{x}) \lambda(\mathbf{x}) d\mathbf{x}$$

- Only purpose of the λ density is to produce \mathbf{W}
- **So skip choosing λ – try choosing \mathbf{W} directly**

But \mathbf{W} has $p(p+1)/2$ entries---daunting?

$$\begin{aligned}\mathbf{W} &= \int_{\chi} \mathbf{f}(x) \mathbf{f}'(x) d\lambda_{\alpha}(x) = \int_{\chi} \begin{pmatrix} 1 & x & x^2 \\ x & x^2 & x^3 \\ x^2 & x^3 & x^4 \end{pmatrix} \lambda_{\alpha}(x) d(x) \\ &= \begin{pmatrix} 1 & E_{\lambda}(x) & E_{\lambda}(x^2) \\ E_{\lambda}(x) & E_{\lambda}(x^2) & E_{\lambda}(x^3) \\ E_{\lambda}(x^2) & E_{\lambda}(x^3) & E_{\lambda}(x^4) \end{pmatrix} = \begin{pmatrix} 1 & w_1 & w_2 \\ w_1 & w_2 & w_3 \\ w_2 & w_3 & w_4 \end{pmatrix}\end{aligned}$$

But W has $p(p+1)/2 - 1$ entries---daunting?

$$\begin{aligned} \mathbf{W} &= \int_{\chi} \mathbf{f}(x) \mathbf{f}'(x) d\lambda_{\alpha}(x) = \int_{\chi} \begin{pmatrix} 1 & x & x^2 \\ x & x^2 & x^3 \\ x^2 & x^3 & x^4 \end{pmatrix} \lambda_{\alpha}(x) d(x) \\ &= \begin{pmatrix} 1 & E_{\lambda}(x) & E_{\lambda}(x^2) \\ E_{\lambda}(x) & E_{\lambda}(x^2) & E_{\lambda}(x^3) \\ E_{\lambda}(x^2) & E_{\lambda}(x^3) & E_{\lambda}(x^4) \end{pmatrix} = \begin{pmatrix} 1 & w_1 & w_2 \\ w_1 & w_2 & w_3 \\ w_2 & w_3 & w_4 \end{pmatrix} \end{aligned}$$

But W has $p(p+1)/2 - 1$ entries---daunting?

$$\begin{aligned} \mathbf{W} &= \int_{\chi} \mathbf{f}(x) \mathbf{f}'(x) d\lambda_{\alpha}(x) = \int_{\chi} \begin{pmatrix} 1 & x & x^2 \\ x & x^2 & x^3 \\ x^2 & x^3 & x^4 \end{pmatrix} \lambda_{\alpha}(x) d(x) \\ &= \begin{pmatrix} 1 & E_{\lambda}(x) & E_{\lambda}(x^2) \\ E_{\lambda}(x) & E_{\lambda}(x^2) & E_{\lambda}(x^3) \\ E_{\lambda}(x^2) & E_{\lambda}(x^3) & E_{\lambda}(x^4) \end{pmatrix} = \begin{pmatrix} 1 & w_1 & w_2 \\ w_1 & w_2 & w_3 \\ w_2 & w_3 & w_4 \end{pmatrix} \end{aligned}$$

All we know is that $-1 \leq w_i \leq 1$

W-entries for full quadratic—Yes, daunting

Factors	p	W-entries
1	3	5
2	6	20
3	10	54
4	15	119
5	21	230
6	28	405

Why is this a problem?

I need to find the W matrix that leads the I_λ -optimality (coord exch) algorithm to find the minimax design

1. Fix W
2. Now use coordinate exchange to find $\xi_n|W$.
 - This is (pretty) FAST
3. OK, now evaluate $\xi_n|W$ using the minimax criterion
 - This is SLOW
4. Change W (move toward optimality), go to 2.

This is a minimax algorithm in W

Why is this a problem?

I need to find the W matrix that leads the I_λ -optimality (coord exch) algorithm to find the minimax design

1. Fix W
2. Now use coordinate exchange to find $\xi_n|W$.
 - This is (pretty) FAST
3. OK, now evaluate $\xi_n|W$ using the minimax criterion
 - This is SLOW
4. Change W (move toward optimality), go to 2.

NOOOOOO!!



Is there a way to guess at W^* in advance?

Little Theorem (Nachtsheim, 1979).

Let $\xi^{G(D)}$ denote the $G(D)$ -optimal design for model f in design space χ , and let ξ^λ denote the I_λ -optimal design. Then:

$$\xi^{G(D)} = \lambda \Rightarrow \xi^\lambda = \xi^{G(D)}$$

Is there a way to guess at W^* in advance?

Little Theorem (Nachtsheim, 1979).

Let $\xi^{G(D)}$ denote the $G(D)$ -optimal design for model f in design space χ , and let ξ^λ denote the I_λ -optimal design. Then:

$$\xi^{G(D)} = \lambda \Rightarrow \xi^\lambda = \xi^{G(D)}$$

Translated: Use the approximate $G(D)$ -optimal design as the weight function λ . Then the I_λ -optimal design is the $G(D)$ -optimal design

Implication:

Really good guess for the optimal W :

$$W^* \approx \int_{\mathcal{X}} \mathbf{f}(\mathbf{x}) \mathbf{f}^T(\mathbf{x}) d\xi^{G(D)}(\mathbf{x})$$

That is: a really good guess at the best W , is the information matrix for the $G(D)$ -optimal design!

OK, we have a starting value for W

- But we still have the dimensionality problem, no?
- Well, turns out that goes away too!
- Why? The information matrix for the $G(D)$ -optimal designs for full second-order models have only two unique values, w_1 and w_2
- Upshot: Dimensionality in W is 2!

Example: Two-factor RSM model

$$W = \begin{pmatrix} 1 & 0 & 0 & 0 & 0.744 & 0.744 \\ 0 & 0.744 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.744 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.583 & 0 & 0 \\ 0.744 & 0 & 0 & 0 & 0.744 & 0.583 \\ 0.744 & 0 & 0 & 0 & 0.583 & 0.744 \end{pmatrix}$$

Example: Two-factor RSM model

$$\mathbf{W} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0.744 & 0.744 \\ 0 & 0.744 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.744 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.583 & 0 & 0 \\ 0.744 & 0 & 0 & 0 & 0.744 & 0.583 \\ 0.744 & 0 & 0 & 0 & 0.583 & 0.744 \end{pmatrix}$$

Example: Two-factor RSM model

$$W = \begin{pmatrix} 1 & 0 & 0 & 0 & 0.744 & 0.744 \\ 0 & 0.744 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.744 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.583 & 0 & 0 \\ 0.744 & 0 & 0 & 0 & 0.744 & 0.583 \\ 0.744 & 0 & 0 & 0 & 0.583 & 0.744 \end{pmatrix}$$

Amazingly, this is always true

$$W_{ij} = \begin{cases} 1 : & i = j = 1 \\ w_1 : & i = j = 2, \dots, m+1; \quad i = j = m(m+1)/2 + 2, \dots, p; \\ & i = 1, \quad j = m(m+1)/2 + 2, \dots, p; \quad j = 1, \quad i = m(m+1)/2 + 2, \dots, p; \\ w_2 : & i = j = m+2, \dots, m(m+1)/2 + 1; \\ & i = m(m+1)/2 + 2, \dots, p, \quad j = m(m+1)/2 + 2, \dots, p, \text{ and } i \neq j; \\ 0 : & \text{elsewhere} \end{cases}$$

From Atkinson, Donev, Tobias Optimal Design Book (2007)

m	Approximate G(D)-optimal design point weights			s	Non-zero \mathbf{W} entries	
	Center point	Edge Centers	Corner Points		w_1	w_2
1	0.333 (1)	-	0.333 (2)	3	0.667	0.667
2	0.096 (1)	0.080 (4)	0.146 (4)	9	0.744	0.583
3	0.066 (1)	0.035 (12)	0.064 (8)	21	0.793	0.651
4	0.047 (1)	0.016 (32)	0.028 (16)	49	0.828	0.702
5	0.036 (1)	0.007 (80)	0.013 (32)	113	0.852	0.739

Amazingly, this is always true

$$W_{ij} = \begin{cases} 1 : & i = j = 1 \\ w_1 : & i = j = 2, \dots, m+1; \quad i = j = m(m+1)/2 + 2, \dots, p; \\ & i = 1, \quad j = m(m+1)/2 + 2, \dots, p; \quad j = 1, \quad i = m(m+1)/2 + 2, \dots, p; \\ w_2 : & i = j = m+2, \dots, m(m+1)/2 + 1; \\ & i = m(m+1)/2 + 2, \dots, p, \quad j = m(m+1)/2 + 2, \dots, p, \text{ and } i \neq j; \\ 0 : & \text{elsewhere} \end{cases}$$

- **At least for number of factors up to five. We haven't looked further**

Finally, the algorithm

1. Obtain the approximate $G(D)$ -optimal design, its information matrix, and the two starting w values
2. Use the coordinate exchange algorithm to find the optimal w_1 and w_2 values in a neighborhood of the starting values
 1. To evaluate w_1 and w_2 , obtain the I_λ -optimal design given W and evaluate the maximum variance
 2. If the new maxvar is less than the best maxvar found, save the new maxvar and the new w_1 and w_2 values, and continue with the coordinate exchange algorithm on the w values until convergence

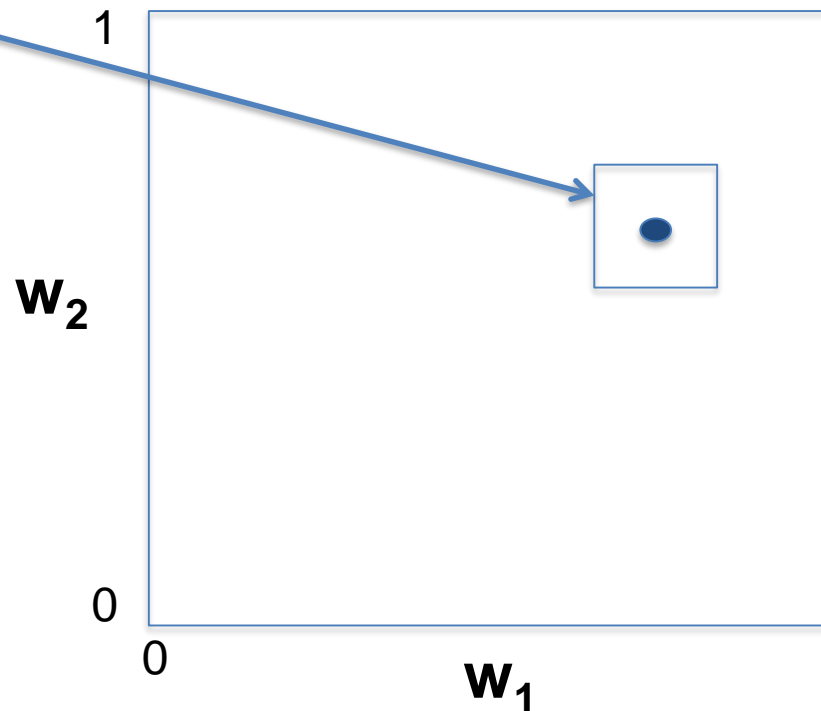
The “neighborhood” of w_1 and w_2 values

$$\mathcal{W} = [w_1^{G(D)} - \Delta, w_1^{G(D)} + \Delta] \times [w_2^{G(D)} - \Delta, w_2^{G(D)} + \Delta]$$

The “neighborhood” of w_1 and w_2 values

$$\mathcal{W} = [w_1^{G(D)} - \Delta, w_1^{G(D)} + \Delta] \times [w_2^{G(D)} - \Delta, w_2^{G(D)} + \Delta]$$

- We use $\Delta = 0.1$



Performance

We have to do a 2D minimax search over a small space

- We might predict that the standard G-optimal algorithm based on the coordinate exchange will do better in one and two dimensions.
- But for three or more factors, this algorithm should be better

Competitors (But only consider 1 – 3 factors)

1. Genetic programming

- Borkowski, J. J. (2003). “Using a genetic algorithm to generate small exact response surface designs”. *Journal of Probability and Statistical Science* 1(1), 65–88.

2. Standard minimax coordinate exchange algorithm

- Rodriguez, M., Jones, B., Borrer, C. M. and Montgomery, D. C. (2010). “Generating and assessing exact G-optimal designs.” *Journal of Quality Technology* 42(1), 1–18.

Borkowski (2003): Genetic Algorithm (GA)

1. John Borkowski's paper was first, and well done.
2. Identified the following test problems

Factors	Run Sizes (n)						
1	3	4	5	6	7	8	9
2	6	7	8	9	10	11	12
3	10	11	12	13	14	15	16

3. Found some very good designs (tough to beat)

Borkowski (2003): Genetic Algorithm (GA)

1. John Borkowski's paper was first, and well done.
2. Identified the following test problems

Factors	Run Sizes (n)						
1	3	4	5	6	7	8	9
2	6	7	8	9	10	11	12
3	10	11	12	13	14	15	16

3. Found some very good designs (tough to beat)
4. Takes forever!

Rodriguez, Jones, Borrer, Montgomery

- **Used standard coordinate exchange where the objective is to minimize the maximum variance**
- **Used same test problems**
- **Mixed results – but did find a design or two that was better than the GP designs**
- **Faster than GP**

Comparisons: Quality of Design

Efficiencies of our designs relative to G-CEXCH and GA

One factor			Two factors			Three factors		
n	G-CEXCH	GA	n	G-CEXCH	GA	n	G-CEXCH	GA
3	100.0%	100.0%	6	97.5%	96.1%	10	102.0%	95.4%
4	97.4%	96.2%	7	97.6%	95.5%	11	103.2%	96.9%
5	98.3%	97.0%	8	95.0%	94.7%	12	99.6%	93.7%
6	100.0%	100.0%	9	98.8%	95.8%	13	106.6%	99.1%
7	99.1%	98.8%	10	95.6%	93.2%	14	114.2%	100.0%
8	95.3%	94.7%	11	103.2%	97.0%	15	101.7%	100.1%
9	111.8%	100.0%	12	94.0%	95.1%	16	100.1%	103.9%

Comparisons: Efficiency of Design

Efficiencies of our designs relative to G-CEXCH and GA

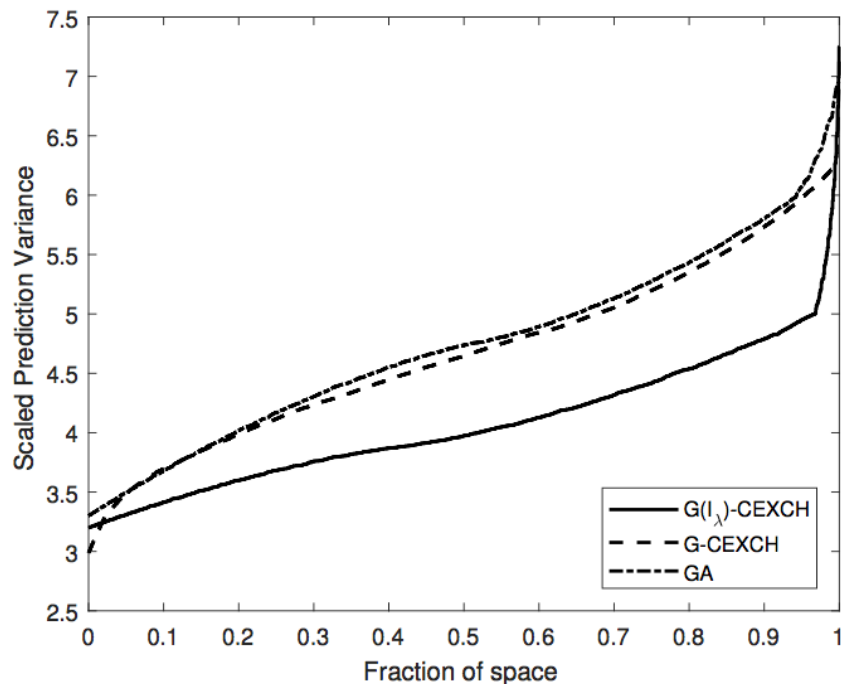
One factor			Two factors			Three factors		
<i>n</i>	G-CEXCH	GA	<i>n</i>	G-CEXCH	GA	<i>n</i>	G-CEXCH	GA
3	100.0%	100.0%	6	97.5%	96.1%	10	102.0%	95.4%
4	97.4%	96.2%	7	97.6%	95.5%	11	103.2%	96.9%
5	98.3%	97.0%	8	95.0%	94.7%	12	99.6%	93.7%
6	100.0%	100.0%	9	98.8%	95.8%	13	106.6%	99.1%
7	99.1%	98.8%	10	95.6%	93.2%	14	114.2%	100.0%
8	95.3%	94.7%	11	103.2%	97.0%	15	101.7%	100.1%
9	111.8%	100.0%	12	94.0%	95.1%	16	100.1%	103.9%

**G-CEXCH and
GA comparable**

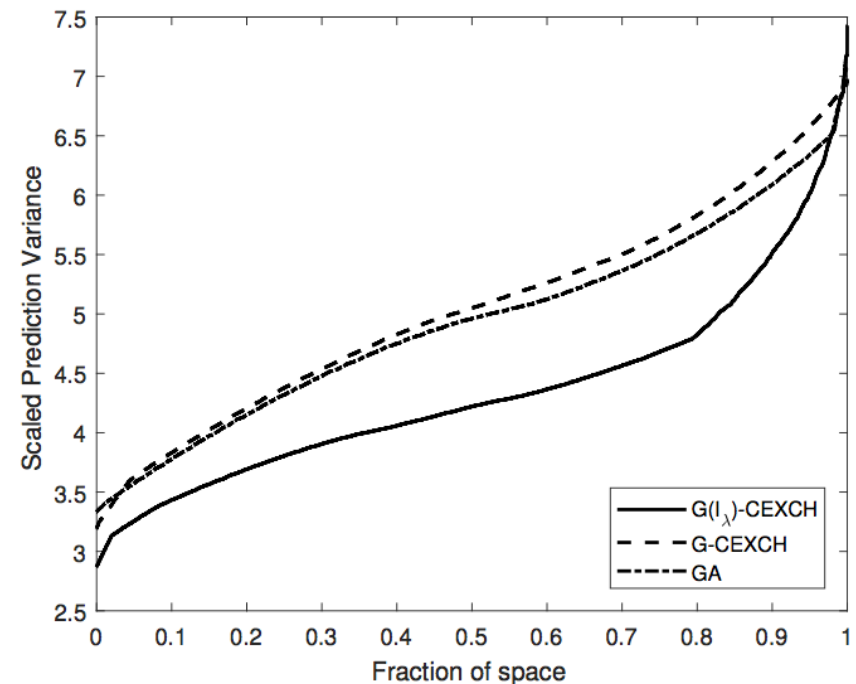
**G-CEXCH and
GA comparable**

**We're now beating G-
CEXCH, sometimes GA**

But these results are undersell our designs --
Consider the FDS plots – here 2D examples

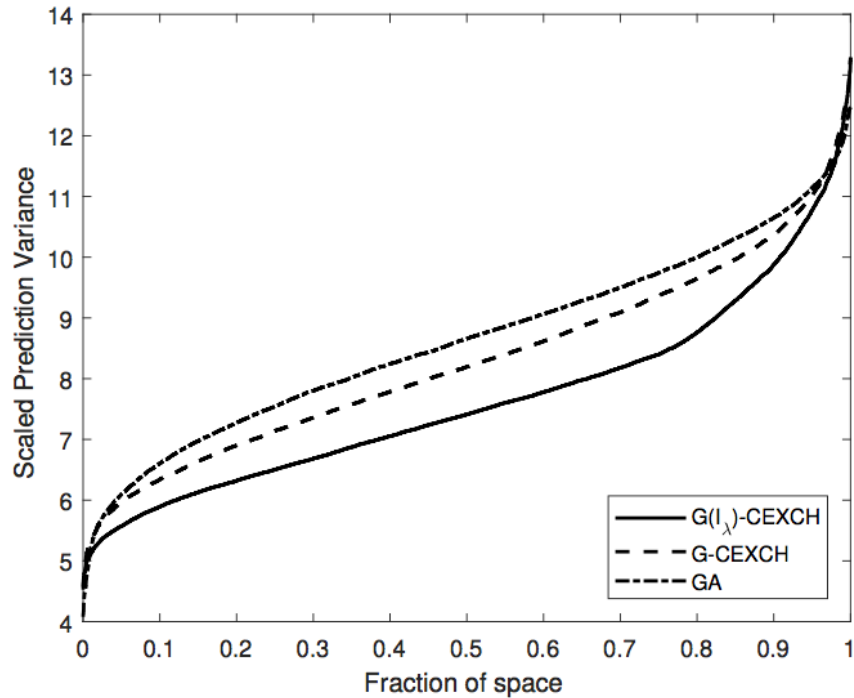


(c) $m=2, n=9$

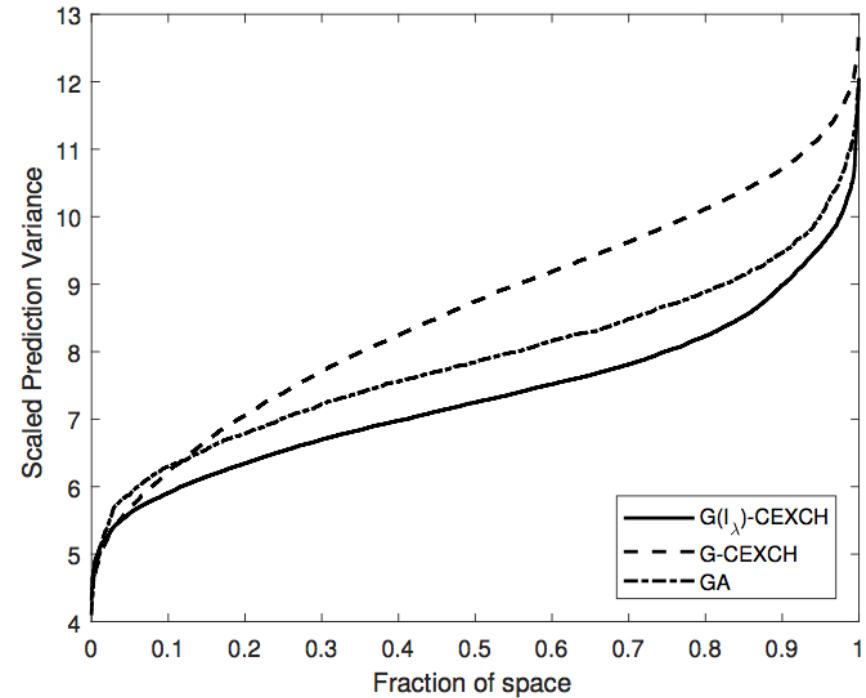


(d) $m=2, n=12$

FDS plots – 3D Examples



(e) $m=3$, $n=12$



(f) $m=3$, $n=13$

Now consider relative computing time

One factor				Two factors				Three factors			
n	$G(I_\lambda)$ -CEXCH	G-CEXCH	GA	n	$G(I_\lambda)$ -CEXCH	G-CEXCH	GA	n	$G(I_\lambda)$ -CEXCH	G-CEXCH	GA
3	1.00	0.12	6.18	6	1.00	1.15	16.18	10	1.00	6.33	47.26
4	1.00	0.06	2.92	7	1.00	0.72	10.75	11	1.00	6.27	42.85
5	1.00	0.05	2.40	8	1.00	1.43	18.96	12	1.00	6.69	45.21
6	1.00	0.14	5.18	9	1.00	3.19	39.30	13	1.00	4.97	34.53
7	1.00	0.07	2.36	10	1.00	1.42	18.56	14	1.00	8.96	56.16
8	1.00	0.05	2.28	11	1.00	1.54	20.09	15	1.00	8.14	51.02
9	1.00	0.06	2.50	12	1.00	0.77	9.79	16	1.00	9.30	57.07

One factor:

Best: G-CEXCH
Good: $G-I_\lambda$ (us)
Bad!: GA

Two factors:

Best: $G-I_\lambda$ (us)
Good: G-CEXCH
Bad!!!: GA

Three factors:

Best: $G-I_\lambda$ (us)
Good: G-CEXCH
BAD!!!!: GA

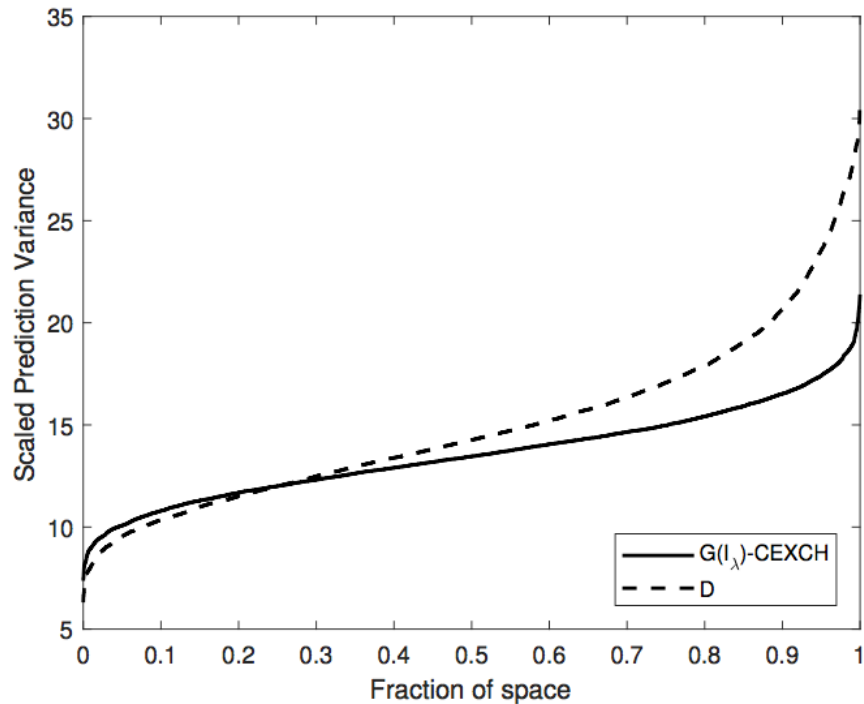
What about four and five factors?

- G-CEXCH: **Forget it**
 - Predicted time for five factors: 166 days
- GA: **Forget it**
 - Predicted time for five factors: Hell freezes over
- Our algorithm: **not a problem**

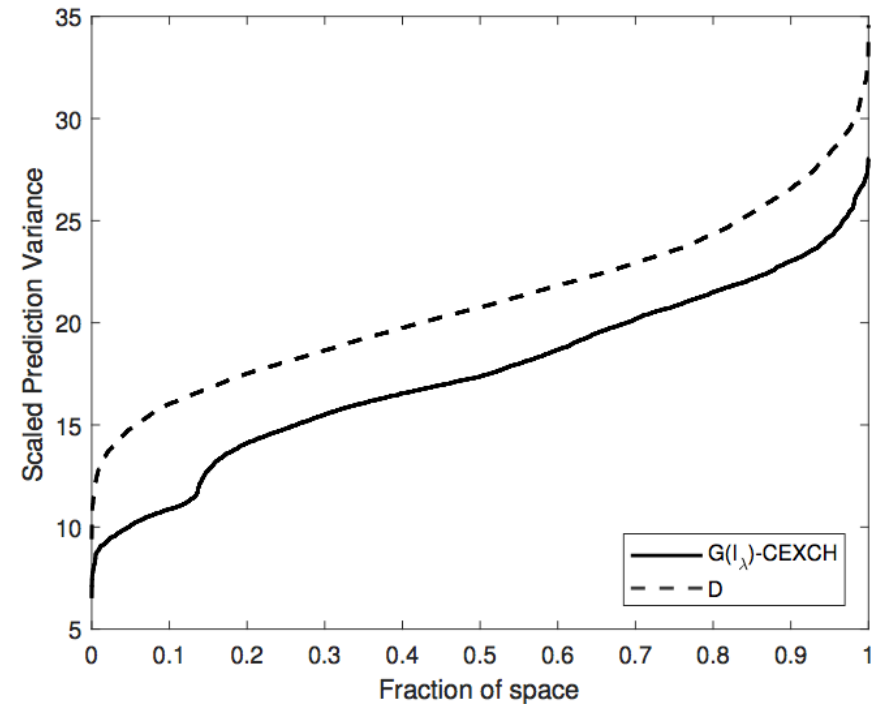
What about four and five factors?

- **G-CEXCH: Forget it**
 - Predicted time for five factors: 166 days
- **GA: Forget it**
 - Predicted time for five factors: Hell freezes over
- **Our algorithm: not a problem, but still 24 hours for 200 random starts---7 minutes per random start**

Our G-optimal designs vs D-optimal designs



(a) $m=4, n=17$



(b) $m=5, n=23$

Conclusions

- **Developed a (relatively) fast algorithm for computing G-optimal designs for quadratic models**
 - **Idea: Choose the W (moment) matrix for I-optimality such that the solution is G-optimal**
- **Much to be done:**
 - **Other models will present more complex W matrices**
 - **That means more w_i entries, more computing**
 - **Similarly for irregular design spaces**
 - **But--algorithm is linear in the number of w_i entries**

Thank you!

- **Compliments, congratulations:**
 - nacht001@umn.edu
- **Criticisms, complaints:**
 - lucianhernandez@gmail.com