New Three-Level Designs for Screening & Response Surface Exploration

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Response Surface Methods (RSM)

- Sequential RSM Strategy (Box and Wilson (1951))
  - 1. Initial small design to estimate linear main effects
  - 2. Exploration along path of steepest ascent
  - 3. Repeat step 1 in a new optimal location
  - 4. Augment to complete a 2^{nd}-order design (add axial runs and center point runs)
  - 5. Optimization based on fitted second-order model

One-Step RSM

- Cheng and Wu (2001) (CW) introduce response surface exploration using only one 3-level design
- Factor Screening from Design
  - Begin with 3-level regular or nonregular design in a large number of factors
  - CW suggests a main-effects only analysis
  - Interactions are not considered until after screening
    - Assumes strong effect heredity

One-Step RSM (cont.)

- Projection and Optimization from same Design
  - Project 3-level design onto the factors identified as important when screening
  - Projected design must be a second-order design (termed eligible) in order to explore the response surface
- CW and Xu, Cheng, and Wu (XCW) provides a set of optimal designs in terms of the proportion of eligible projections and D-efficiency

Example 1 – PVC Insulation

- Nine factors in 27-runs: 3^{9-6}
- Screening step identifies factors A, B, C, D, and G
- There is no eligible projected design of four or five factors in the 3^{9-6}
- CW finds an eligible projection in the three most significant factors

Run	A	B	C	D	E	F	G	H	J	Response1
1	0	0	0	0	0	0	0	0	0	5
2	0	0	0	0	1	1	1	1	1	2
3	0	0	0	0	2	2	2	2	2	8
4	0	1	1	1	0	0	0	2	2	-15
5	0	1	1	1	1	1	1	0	0	-6
6	0	1	1	1	2	2	2	1	1	-10
7	0	2	2	2	0	0	0	1	1	-28
8	0	2	2	2	1	1	1	2	2	-19
9	0	2	2	2	2	2	2	0	0	-23
10	1	0	1	2	0	1	2	0	1	-13
11	1	0	1	2	1	2	0	1	2	-17
12	1	0	1	2	2	0	1	2	0	-7
13	1	1	2	0	0	1	2	2	0	-23
14	1	1	2	0	1	2	0	0	1	-31
15	1	1	2	0	2	0	1	1	2	-23
16	1	2	0	1	0	1	2	1	2	-34
17	1	2	0	1	1	2	0	2	0	-37
18	1	2	0	1	2	0	1	0	1	-29
19	2	0	2	1	0	2	1	0	2	-27
20	2	0	2	1	1	0	2	1	0	-27
21	2	0	2	1	2	1	0	2	1	-30
22	2	1	0	2	0	2	1	2	1	-35
23	2	1	0	2	1	0	2	0	2	-35
24	2	1	0	2	2	1	0	1	0	-38
25	2	2	1	0	0	2	1	1	0	-39
26	2	2	1	0	1	0	2	2	1	-40
27	2	2	1	0	2	1	0	0	2	-41

Example 2 – XCW Recommended OA

- 3-level, 18-run Orthogonal Array (OA)
- Response is simulated from the following 'true' model
  - $Y = 10x_D + 9x_E + 8x_G + 5x_{DG} - 6x_{AD} - 6x_{AG} + 6x_D^2$
- Fit the following polynomial model:

$$y = \beta_0 + \sum_i x_i + \sum_i x_i^2$$

- Factors D, E, and G stand out as active
- Project the OA onto D, E, and G (this is eligible)
- Fit a second-order model in those three factors

Example (cont.)

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	1.3644249	5.362179	0.25	0.8056
D	10.711064	2.585872	4.14	0.0032*
E	10.91478	2.585872	4.22	0.0029*
G	8.6805705	2.585872	3.36	0.0100*
D*D	3.1981061	4.326992	0.74	0.4810
D*E	1.1719077	3.270899	0.36	0.7294
E*E	-2.137233	4.326992	-0.49	0.6346
D*G	5.6709758	3.270899	1.73	0.1212
E*G	1.2296474	3.270899	0.38	0.7167
G*G	2.6145559	4.326992	0.60	0.5624

Clearly, we have missed the opportunity to explore the large interactions involving factor A.

True model: $Y=10x_D + 9x_E + 8x_G + 5x_{DG} - 6x_{AD} - 6x_{AG} + 6x_D^2$

What have we learned?

- Two problems with CW's method:
  - Initial screening stage does not entertain the possibility of two-factor interactions – so we miss out on potentially important effects
  - Projection onto the factors of interest does not always yield a second-order design
- Let's consider a different initial design

Box-Behnken Designs

$$\begin{bmatrix} 1 & 6 & 7 \\ 1 & 3 & 5 \\ 1 & 2 & 4 \\ 4 & 5 & 6 \\ 3 & 4 & 7 \\ 2 & 5 & 7 \\ 2 & 3 & 6 \end{bmatrix} \Rightarrow \begin{bmatrix} \pm1 & 0 & 0 & 0 & 0 & \pm1 & \pm1 \\ \pm1 & 0 & \pm1 & 0 & \pm1 & 0 & 0 \\ \pm1 & \pm1 & 0 & \pm1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \pm1 & \pm1 & \pm1 & 0 \\ 0 & 0 & \pm1 & \pm1 & 0 & 0 & \pm1 \\ 0 & \pm1 & 0 & 0 & \pm1 & 0 & \pm1 \\ 0 & \pm1 & \pm1 & 0 & 0 & \pm1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{matrix} 2^3 \\ 2^3 \\ 2^3 \\ 2^3 \\ 2^3 \\ 2^3 \\ 2^3 \\ \\ \end{matrix}$$

Each set of 8 runs forms a 2^3.

$7*8+n_0$ runs

Fractional Box-Behnken Designs

$$
\begin{bmatrix}
1 & 6 & 7 \\
1 & 3 & 5 \\
1 & 2 & 4 \\
4 & 5 & 6 \\
3 & 4 & 7 \\
2 & 5 & 7 \\
2 & 3 & 6
\end{bmatrix}
\Rightarrow
\begin{bmatrix}
\pm1 & 0 & 0 & 0 & 0 & \pm1 & \pm1 \\
\pm1 & 0 & \pm1 & 0 & \pm1 & 0 & 0 \\
\pm1 & \pm1 & 0 & \pm1 & 0 & 0 & 0 \\
0 & 0 & 0 & \pm1 & \pm1 & \pm1 & 0 \\
0 & 0 & \pm1 & \pm1 & 0 & 0 & \pm1 \\
0 & \pm1 & 0 & 0 & \pm1 & 0 & \pm1 \\
0 & \pm1 & \pm1 & 0 & 0 & \pm1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{matrix}
~~\sout{2^3}~~ 2^{3-1} \\
~~\sout{2^3}~~ 2^{3-1} \\
~~\sout{2^3}~~ 2^{3-1} \\
~~\sout{2^3}~~ 2^{3-1} \\
~~\sout{2^3}~~ 2^{3-1} \\
~~\sout{2^3}~~ 2^{3-1} \\
~~\sout{2^3}~~ 2^{3-1} \\
\\
\end{matrix}
$$

~~Each set of 8 runs forms a 2^3.~~ **Each set of 4 runs forms a 2^{3-1}**

~~$7*8+n_0$ runs~~ **$7*4 + n_0$ runs**

Fractional Box-Behnken (or Box-Behnken like) Designs (FBBDs)

- Motivated by a Bayesian D-optimal Design search
- Assume a spherical design region – allows for wider ranges for each factor
- Constructed based on incomplete block designs
- Each subset of four runs is a resolution III 2^{3-1}
- Has a simpler aliasing structure than OA's

Aliasing of 29-run FBBD (7-factors)

Linear Main Effect	Aliasing
G	+ C*D + B*E + A*F
F	+ B*C + D*E + A*G
E	+ A*C + D*F + B*G
D	+ A*B + E*F + C*G
C	+ A*E + B*F + D*G
B	+ A*D + C*F + E*G
A	+ B*D + C*E + F*G

Aliasing of XCW 27-run OA (7-factors)

Intercept = - 0.83333*A - 0.16667*C + 0.33333*D - 0.5*E - 0.33333*F + G + 1.16667*A*A - 1.33333*A*B
+ 0.33333*B*B - A*C - 1.33333*B*C + 0.16667*C*C - 0.66667*A*D - 0.66667*B*D - 0.66667*C*D - 0.33333*A*E
+ 0.33333*B*E + C*E + 1.33333*D*E - 0.16667*E*E - 0.66667*A*F + 1.33333*B*F + 0.33333*C*F + 1.33333*D*F
= - 0.16667*A - 0.66667*B - 0.16667*C - 0.33333*D + 0.16667*E - 0.33333*F + G + 0.5*A*A - 0.33333*B*B - A*C
- 1.33333*B*C + 0.16667*C*C - 0.66667*A*D - 0.66667*B*D - 0.66667*C*D + 0.66667*D*D - 0.33333*A*E
+ 0.33333*B*E + C*E + 0.5*E*E + 0.66667*A*F + 0.33333*C*F + 1.33333*E*F
= - 0.16667*A - 0.66667*B - 0.16667*C + 0.33333*D + 0.16667*E - 0.33333*F + 0.33333*G + 0.5*A*A - 0.33333*B*B
- A*C + 0.16667*C*C - 0.66667*B*D - 0.66667*C*D + 0.66667*D*D - 0.33333*A*E + 0.33333*B*E + C*E
+ 0.5*E*E + 0.66667*A*F + 0.33333*C*F - 0.66667*A*G
= - 0.83333*A - 0.66667*B - 0.16667*C + 0.33333*D + 0.16667*E - 0.33333*F + G + 1.16667*A*A - 1.33333*A*B
- 0.33333*B*B - A*C - 1.33333*B*C + 0.16667*C*C - 0.66667*A*D - 0.66667*B*D - 0.66667*C*D - 0.33333*A*E
+ 0.33333*B*E + C*E + 1.33333*D*E + 0.5*E*E - 0.66667*A*F + 1.33333*B*F + 0.33333*C*F + 1.33333*C*G
= - 0.16667*A - 0.66667*B - 0.16667*C + 0.33333*D + 0.16667*E - 0.33333*F + 0.33333*G + 1.16667*A*A
- 0.33333*B*B - A*C + 0.16667*C*C - 0.66667*B*D - 0.66667*C*D - 0.33333*A*E + 0.33333*B*E + C*E
+ 0.5*E*E + 0.66667*A*F + 0.33333*C*F - 0.66667*D*G
= - 0.16667*A - 0.66667*B - 0.16667*C + 0.33333*D + 0.16667*E - 0.33333*F + 0.33333*G + 0.5*A*A - 0.33333*B*B
- A*C + 0.16667*C*C - 0.66667*A*D - 0.66667*B*D - 0.66667*C*D - 0.33333*A*E + 0.33333*B*E
+ C*E + 0.5*E*E + 0.66667*A*F + 0.33333*C*F + 0.66667*G*G

B = C + E - F + 2*A*B - B*B - 2*A*C + C*C - 2*A*E + 2*C*E + E*E + 2*A*F - 2*B*F - F*F
= E + 2*A*B - B*B - 2*A*C - 2*A*E + 2*C*E - 2*D*E + E*E + 2*A*F - 2*B*F + 2*B*G
= E - B*B - 2*A*C - 2*B*D + 2*C*E + E*E + 2*A*F - 2*B*F + 2*E*G
= E - B*B - 2*A*C - 2*C*D + E*E + 2*A*F + 2*F*G

Proposed FBBDs

Design	t	Design Structure	Number of Parameters (Second-Order Model)	Number of Runs
4.1	4	BIBD: $4 \times 2^{3-1}$	15	17
5.1	5	RG: $5 \times 2^{3-1}$	21	21
6.1	6	RG: $6 \times 2^{3-1}$ (Cyclic)	28	25
7.1	7	BIBD: $7 \times 2^{3-1}$ (Cyclic)	36	29
9.1	9	BIBD: $12 \times 2^{3-1}$	55	49
10.1	10	RG: $20 \times 2^{3-1}$ (Cyclic)	66	81
11.1	11	RG: $22 \times 2^{3-1}$ (Cyclic)	78	89
12.1	12	RG: $24 \times 2^{3-1}$	91	97
13.1	13	BIBD: $26 \times 2^{3-1}$	105	105

Design Comparisons

- FBBDs either outperform or are comparable to the 18 and 27-run OAs as well as D-optimal designs of the same run size in terms of the number of eligible projections and D-efficiency
- Simulation results indicate that FBBDs are able to better identify important factors using the main effects only analysis strategy vs. the OAs proposed by CW and XCW
- Since, Box-Behnken designs are often D-optimal for second-order models in a spherical region, it makes sense that fractions of these designs perform well

Analysis Strategy

- What do we assume?
  - Effect Hierarchy
  - Effect Sparsity (not necessarily factor sparsity)
  - Weak Effect Heredity
- Structure of FBBDs allows us to obtain r=3,4,6 independent estimates of each factor's linear main effect

Analysis Strategy Illustrated (Simulated Data)

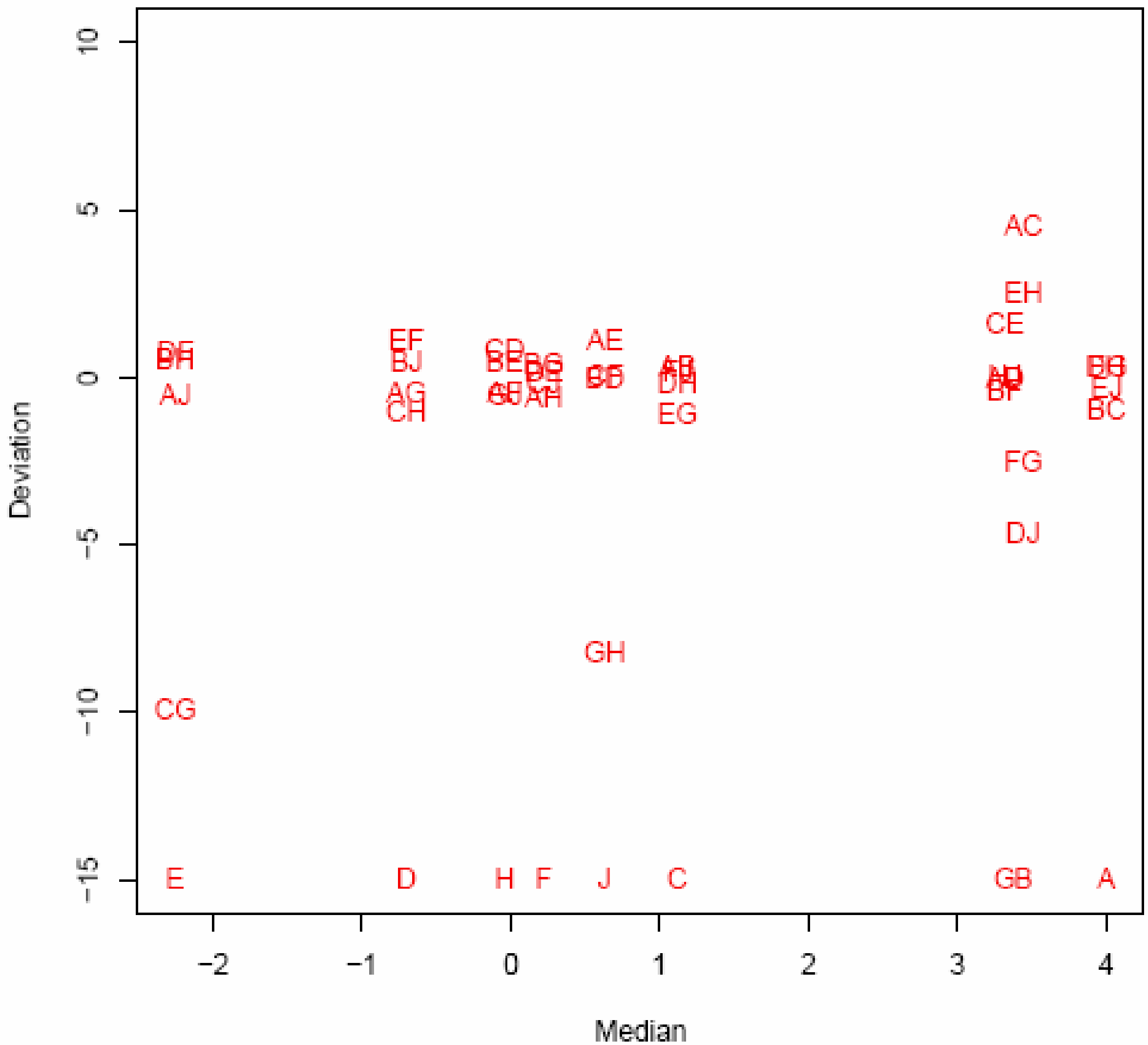
- 9-factor, 49-run FBBD, r=4
- Simulate from:

$$Y = 2x_A - 1.5x_E + 2x_G + 2.5x_{E^2} - 3x_{H^2} + 4x_{AC} - 5x_{CG} + 3.5x_{EH} - 4x_{GH} + \epsilon$$

- Aliasing:

Linear Main Effect	Aliasing
J	+ B*D + A*E + C*F + G*H
E	+ D*F + C*G + B*H + A*J
D	+ E*F + A*G + C*H + B*J
F	+ D*E + B*G + A*H + C*J
B	+ A*C + F*G + E*H + D*J
A	+ B*C + D*G + F*H + E*J
C	+ A*B + E*G + D*H + F*J
H	+ C*D + B*E + A*F + G*J
G	+ A*D + C*E + B*F + H*J

Analysis Graphic



Analysis Example (cont.)

Factor Group	s_j	U_j
A	0.600	0.620
B	4.291	4.433
C	0.653	0.674
D	0.948	0.979
E	5.108	5.277
F	0.447	0.462
G	0.880	0.909
H	0.690	0.713
J	4.329	4.472

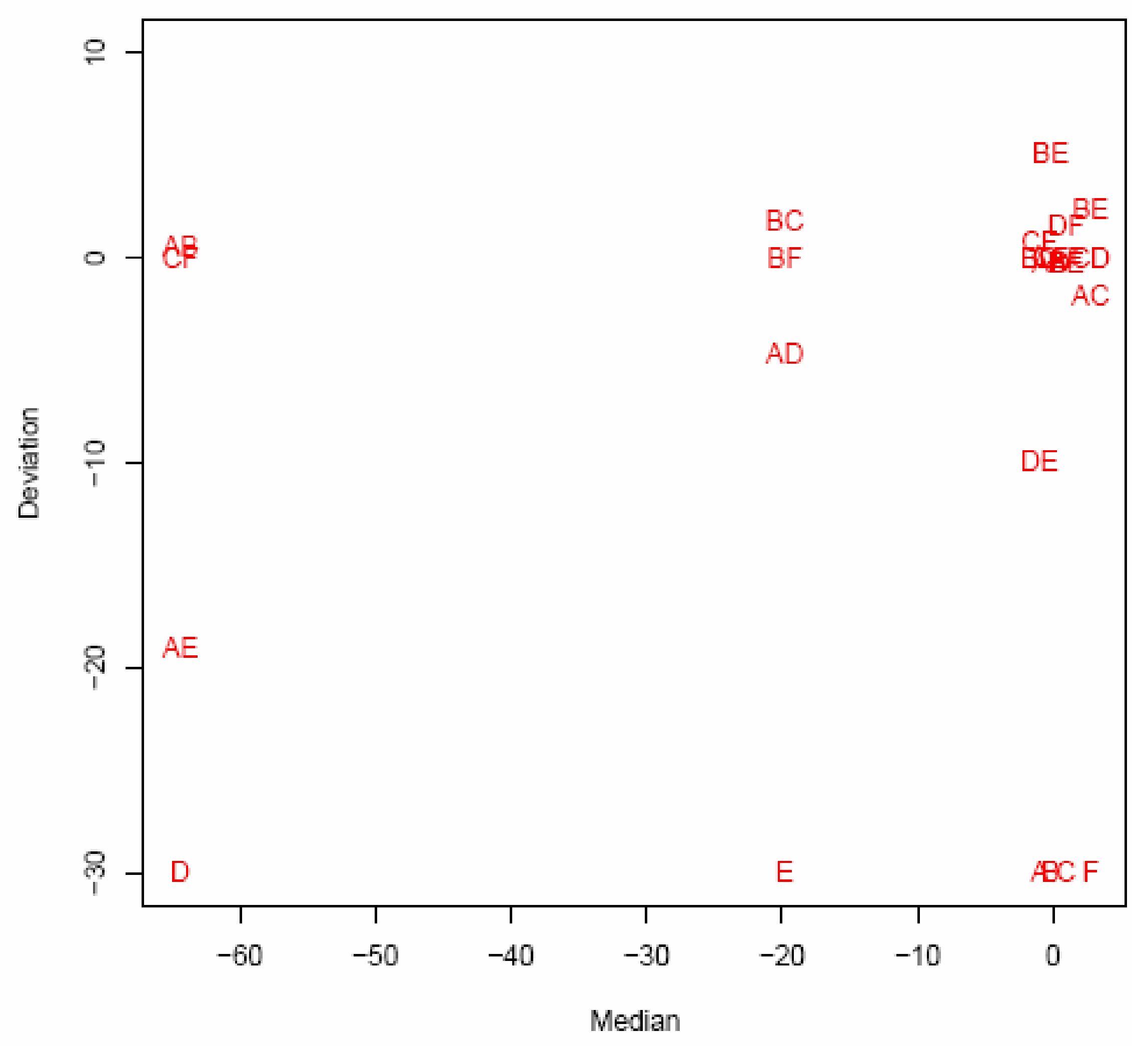
t	$U_{0.01}$	$U_{0.05}$	$U_{0.1}$
4	5.41	2.80	2.02
5	4.95	2.60	1.92
6	4.29	2.44	1.85
7	3.89	2.34	1.81
9	3.18	2.13	1.74
10	2.34	1.77	1.53
11	2.28	1.74	1.51
12	2.25	1.72	1.50
13	2.19	1.70	1.49

- Compare U_j's to critical values
- Interactions aliased with B, E, and J are most likely at $\alpha=0.05$
- NOTE: Using the 27-run OA of XCW, no linear or quadratic effects were detected at 10% using the CW analysis strategy
- Now project onto A, B, C, E, F, G, H (which is eligible)

Real Data Example

- Experiment conducted to optimize a very-large-scale-integrated (VLSI) process, device, and circuit design
- They use a 50-run, 6 factor Box-Behnken design
- Authors identify all terms in a second-order model involving factors D and E to be important
- We use only half their Box-Behnken design (FBBD with 25-runs and 6-factors)

VLSI Data Graphic



VLSI Data Example

Factor Group	s_j	U_j
A	5.942	2.358
B	3.014	1.196
C	0.991	0.393
D	11.116	4.411
E	3.303	1.311
F	2.117	0.840

Linear Main Effect	Aliasing
A	-B*D -D*E -C*F
C	-B*E -A*F -D*F
B	-A*D -C*E -E*F
D	-A*B -C*F -A*E
E	-B*C -A*D -B*F
F	-C*D -B*E -A*C

- Interactions partially aliased with A and D are likely
- Same effects stand out in graphic
- All interactions satisfy weak effect heredity

VLSI Data – Second-order Model

- Project onto factors A, B, D, E
- R^2 = 0.9977
- We identify the same effects as the authors (plus a few others)

Term	Estimate	Std Error	t Ratio	P-value
Intercept	62.780968	0.974543	64.42	< .0001
A	-0.11	1.025423	-0.11	0.9167
B	1.39375	0.661908	2.11	0.0615
D	-32.185	1.025423	-31.39	< .0001
E	-9.68125	0.661908	-14.63	< .0001
A*A	1.4522043	0.908496	1.6	0.141
A*B	-0.2725	1.450167	-0.19	0.8547
B*B	-2.466962	0.908496	-2.72	0.0217
A*D	2.08375	0.888042	2.35	0.0409
B*D	0.4075	1.450167	0.28	0.7844
D*D	14.857204	0.908496	16.35	< .0001
A*E	9.4875	1.450167	6.54	< .0001
B*E	-1.4425	0.725083	-1.99	0.0747
D*E	5.3375	1.450167	3.68	0.0042
E*E	14.633038	0.908496	16.11	< .0001

Comments Regarding FBBDs

- Provide a useful alternative to the OAs of CW and XCW
- More real case studies involving Box-Behnken designs would be useful
- What properties to FBBDs of smaller run sizes have?
- Develop critical values based on center point replication
- Investigate the Bayesian approach to analysis of FBBDs

Thank you!

Any Questions?

Design Comparisons

FBBDs

t	Run Size	Projection	Number of Projections	Number of Eligible Projections	$\overline{D}$
4	17	2	6	6	0.728
		3	4	4	0.588
		4	1	0	*
5	21	3	10	10	0.664
		4	5	5	0.582
		5	1	0	*
6	25	3	20	20	0.668
		4	15	15	0.521
		5	6	6	0.616
7	29	3	35	35	0.632
		4	35	35	0.558
		5	21	21	0.563
		6	7	7	0.639

18-run OA

t	Projection	Number of Projections	Number of Eligible Projections	$\overline{D}$
4	2	6	6	0.725
	3	4	4	0.589
	4	1	1	0.465
5	3	10	10	0.589
	4	5	5	0.465
	5	1	0	*
6	3	20	20	0.589
	4	15	15	0.465
	5	6	0	*
7	3	35	34	0.579
	4	35	31	0.445
	5	21	0	*

Design Comparisons (cont.)

FBBDs

t	Run Size	Projection	Number of Projections	Number of Eligible Projections	$\overline{D}$
4	17	2	6	6	0.728
		3	4	4	0.588
		4	1	0	*
5	21	3	10	10	0.664
		4	5	5	0.582
		5	1	0	*
6	25	3	20	20	0.668
		4	15	15	0.521
		5	6	6	0.616
7	29	3	35	35	0.632
		4	35	35	0.558
		5	21	21	0.563
		6	7	7	0.639
9	49	3	84	84	0.507
		4	126	126	0.503
		5	126	126	0.436
		6	84	84	0.519
		7	36	36	0.599
		8	9	9	0.655

27-run OA

t	Projection	Number of Projections	Number of Eligible Projections	$\overline{D}$
4	2	6	6	0.725
	3	4	4	0.616
	4	1	1	0.555
5	3	10	10	0.607
	4	5	5	0.527
	5	1	1	0.445
6	3	20	20	0.601
	4	15	15	0.512
	5	6	6	0.408
7	3	35	35	0.598
	4	35	35	0.505
	5	21	21	0.407
8	3	56	56	0.597
	4	70	70	0.502
	5	56	56	0.402
9	3	84	84	0.596
	4	126	126	0.501
	5	126	126	0.401

Simulation Study

$$Y = 57.3 + 1.5X_1 - 2.1X_2 + 1.8X_3 - 4.7X_1^2 - 6.3X_2^2 - 5.2X_3^2 - 7.1X_1X_2 - 3.3X_1X_3 - 2.7X_2X_3 + \epsilon$$

		18-run OA		27-run OA		FBBD	
		PCF	MEA	PCF	MEA	PCF	MEA
t	NCF	$\sigma = 1/2/3$	$\sigma = 1/2/3$	$\sigma = 1/2/3$	$\sigma = 1/2/3$	$\sigma = 1/2/3$	$\sigma = 1/2/3$
4	3	0.003/0.029/0.047	1.113/1.146/1.145	0.284/0.244/0.177	2.124/1.997/1.829	0.053/0.095/0.105	3.076/2.652/2.414
	2	0.341/0.288/0.247		0.555/0.461/0.411		0.296/0.267/0.258	
	1	0.405/0.409/0.401		0.161/0.273/0.346		0.602/0.462/0.410	
	0	0.251/0.274/0.305		0.000/0.022/0.066		0049/0.176/0.227	
5	3	0.000/0.015/0.026	0.398/0.665/0.785	0.255/0.204/0.197	2.182/2.040/1.952	0.227/0.203/0.123	2.900/2.676/2.126
	2	0.066/0.128/0.158		0.578/0.514/0.423		0.191/0.220/0.211	
	1	0.263/0.337/0.324		0.162/0.240/0.293		0.452/0.377/0.384	
	0	0.671/0.520/0.492		0.005/0.042/0.087		0.130/0.200/0.282	
6	3	0.000/0.001/0.009	0.010/0.171/0.397	0.231/0.227/0.169	2.399/2.402/2.159	0.867/0.607/0.431	4.390/3.857/3.273
	2	0.000/0.024/0.056		0.599/0.495/0.435		0.101/0.279/0.318	
	1	0.010/0.118/0.223		0.166/0.253/0.311		0.032/0.100/0.191	
	0	0.990/0.857/0.712		0.004/0.025/0.085		0.000/0.014/0.060	
7	3	0.379/0.318/0.318	3.764/3.421/3.390	0.272/0.214/0.193	2.622/2.416/2.355	0.997/0.881/0.662	4.910/4.444/3.866
	2	0.122/0.151/0.121		0.464/0.440/0.378		0.003/0.103/0.235	
	1	0.015/0.056/0.122		0.235/0.273/0.332		0.000/0.016/0.083	
	0	0.484/0.475/0.439		0.029/0.073/0.097		0.000/0.000/0.020	
9	3	-	-	0.156/0.144/0.134	2.240/2.233/2.262	1.000/0.996/0.914	6.504/6.020/5.440
	2	-		0.426/0.388/0.358		0.000/0.004/0.074	
	1	-		0.351/0.363/0.346		0.000/0.000/0.012	
	0	-		0.067/0.105/0.162		0.000/0.000/0.000	
12	3	-	-	0.348/0.332/0.284	4.642/4.307/4.050	1.000/1.000/0.988	7.220/7.160/6.930
	2	-		0.154/0.146/0.160		0.000/0.000/0.012	
	1	-		0.149/0.132/0.156		0.000/0.000/0.000	
	0	-		0.349/0.390/0.400		0.000/0.000/0.000	