Screening for Simulation Experiments

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Main Effects Model:

Suppose there are K factors of interest with effect coefficients $\beta = \{\beta_1, \beta_2, \ldots, \beta_K\}$. The output of interest from a simulation replication is denoted by Y, and Y is represented as:

No Error

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots \beta_{k-1} x_{k-1}$$

$$\beta_i \geq 0 \quad \forall i$$

.

Sequential Bifurcation

$$\beta_i \geq 0 \quad \forall i$$

Threshold of Importance: 8 $\beta = \{1, 1, 2, 2, 1, 1, 30, 1, 2, 1\}$

- $<\beta_1 \ldots \beta_{10}>$ (42)
  - $<\beta_1 \ldots \beta_5>$ (7)
  - $<\beta_6 \ldots \beta_{10}>$ (35)
    - $<\beta_6 \ldots \beta_8>$ (32)
      - $<\beta_6, \beta_7>$ (31)
        - $<\beta_6>$ (1)
        - $<\beta_7>$ (30)
      - $<\beta_8>$ (1)
    - $<\beta_9, \beta_{10}>$ (3)

I	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+

$$\beta_i \geq 0 \quad \forall i$$

If and only if all factors have no effect, then this contrast will be zero.

I	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
+	+	+	+	+	+	+	+	-	-	-	-	-	-	-	-

If and only if A, B, C, D, E, F, & G all have no effect, then this contrast will be zero.

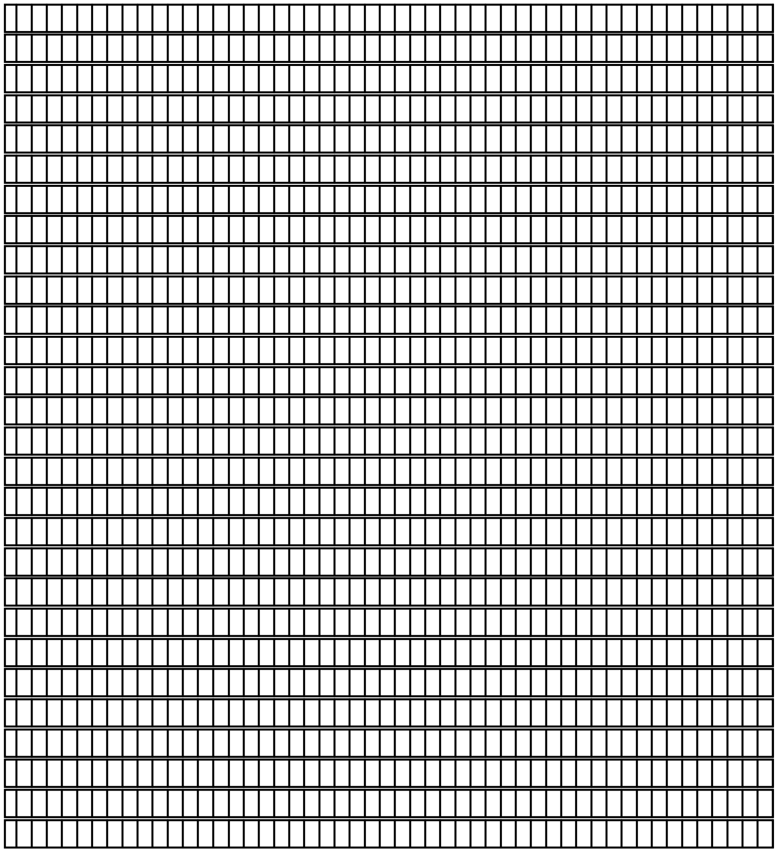
I	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
+	+	+	+	+	+	+	+	-	-	-	-	-	-	-	-
+	+	+	+	-	-	-	-	-	-	-	-	-	-	-	-

This process continues until all factor effects are either eliminated or estimated individually.

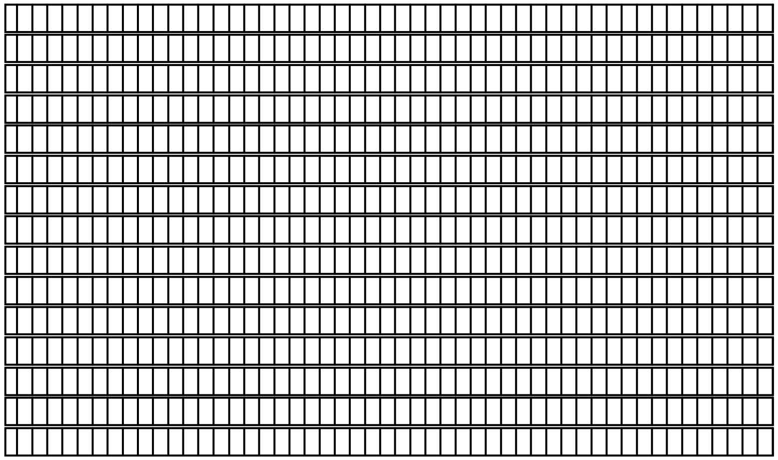
Current Research

- Using a FFD as a set of candidate points and attempting to run the design points in an order that allows for finding important effects without running the entire fractional factorial design. Uses the known direction of effects assumption.

Candidate Points



Selects design points sequentially until all effects are estimable.



If many factors have no effect, then the process finishes before the orthogonal array is finished.

Sequential Orthogonal Array

Using an orthogonal array as a set of candidate points and run the design points in an order that allows for finding important effects without running the entire design.

Uses the known direction of effects assumption. $\beta_i \geq 0 \quad \forall i$

A very small example with no noise.

Row	A	B	C	Y	
1	+	+	+	5	Sum of all coefficients=5
2	-	+	-	5	A & C have no effect.
3	+	-	-	1	B's coefficient is (5-1)/2 = 2
4	-	-	+		No need to run this trial.

Suppose that $\beta_0=3$, $\beta_1=0$, $\beta_2=2$, $\beta_3=0$

I	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
+	+	+	+	+	+	+	+	-	-	-	-	-	-	-	-
+	+	+	+	-	-	-	-	+	+	+	+	-	-	-	-
+	+	+	+	-	-	-	-	-	-	-	-	+	+	+	+
+	+	-	-	+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	-	-	+	+	-	-	+	+
+	+	-	-	-	-	+	+	+	+	-	-	-	-	+	+
+	+	-	-	-	-	+	+	-	-	+	+	+	+	-	-
+	-	+	-	+	-	+	-	+	-	+	-	+	-	+	-
+	-	+	-	+	-	+	-	-	+	-	+	-	+	-	+
+	-	+	-	-	+	-	+	+	-	+	-	-	+	-	+
+	-	+	-	-	+	-	+	-	+	-	+	+	-	+	-
+	-	-	+	+	-	-	+	+	-	-	+	+	-	-	+
+	-	-	+	+	-	-	+	-	+	+	-	-	+	+	-
+	-	-	+	-	+	+	-	+	-	-	+	-	+	+	-
+	-	-	+	-	+	+	-	-	+	+	-	+	-	-	+

Use an Orthogonal Array as a set of candidate points.

I	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
+	+	+	+	+	+	+	+	-	-	-	-	-	-	-	-

If and only if H, I, J, K, L, M, N & O all have no effect, then this contrast will be zero like sequential bifurcation.

I	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
+	+	+	+	+	+	+	+	-	-	-	-	-	-	-	-
+	+	+	+	-	-	-	-	+	+	+	+	-	-	-	-
+	+	+	+	-	-	-	-	-	-	-	-	+	+	+	+
+	+	-	-	+	+	-	-	+	+	-	-	+	+	-	-
+	+	-	-	+	+	-	-	-	-	+	+	-	-	+	+

If and only if B, C, F, & G all have no effect, then this contrast will be zero.

I	A	D	E	H	I	J	K	L	M	N	O
+	+	+	+	+	+	+	+	+	+	+	+
+	+	+	+	-	-	-	-	-	-	-	-
+	+	-	-	+	+	+	+	-	-	-	-
+	+	-	-	-	-	-	-	+	+	+	+
+	+	+	+	+	+	-	-	+	+	-	-
+	+	+	+	-	-	+	+	-	-	+	+

When B, C, F, & G are eliminated, then the design is closer to an orthogonal array in the remaining factors.

I	A	E	H	I	J	K
+	+	+	+	+	+	+
+	+	+	-	-	-	-
+	+	-	+	+	+	+
+	+	-	-	-	-	-
+	+	+	+	+	-	-
+	+	+	-	-	+	+
+	+	-	+	+	-	-
+	+	-	-	-	+	+
+	-	-	+	-	+	-
+	-	+	+	-	+	-
+	-	+	-	+	-	+
+	-	-	+	-	-	+

Eventually, when enough factors are eliminated, the remaining factor effects can be estimated and the process stops before all the candidate points are observed.

In the worst case, all candidate points will be run and we will have individual estimates of each factor effect.

A general Linear Programming method for finding the null effects with no noise.

$$\mathbf{y} = \mathbf{X}\beta$$

Let D be the Design matrix at some particular stage (*m* rows) of the experiment. D will have more columns than rows if the OA is not complete.

$$\mathbf{y} = \mathbf{D}\boldsymbol{\beta}$$

Any solution, say $\tilde{\boldsymbol{\beta}}$, can be written as

$$\tilde{\boldsymbol{\beta}} = \mathbf{G}\mathbf{D}\boldsymbol{\beta} + (\mathbf{I}_{n\times n} - \mathbf{G}\mathbf{D})\mathbf{z}$$

where G is a generalized inverse of D and **z** is an *n* - dimensional column vector of arbitrary 'spanning' variables

.

(see Searle, 1971)

Since we know that y = Dβ and all betas are positive, then the constraints on **z** become

$$\tilde{\boldsymbol{\beta}} = \mathbf{Gy} + (\mathbf{I}_{n\times n} - \mathbf{GD})\mathbf{z} \geq \mathbf{0}$$

Partition D as

$$\mathbf{D} = [\mathbf{D}_1 \; \mathbf{D}_2]$$

where $\mathbf{D}_1$ is the square matrix formed from the first *m* rows and *m* columns. We assume that the columns are sorted so that $\mathbf{D}_1$ is nonsingular and so has inverse $\mathbf{D}_1^{-1}$.

A convenient generalized inverse **G** of **D** is:

$$\mathbf{G} = \begin{bmatrix} \mathbf{D}_1^{-1} \\ \mathbf{0}_{(n-m)\times m} \end{bmatrix} \begin{matrix} \}m \\ \}n-m \end{matrix}$$

$$\mathbf{GD} = \begin{bmatrix} \mathbf{D}_1^{-1} \\ \mathbf{0}_{(n-m)\times m} \end{bmatrix} [\mathbf{D}_1 \ \mathbf{D}_2] = \begin{bmatrix} \mathbf{I}_{\mathrm{m}\times\mathrm{m}} & \mathbf{D}_1^{-1}\mathbf{D}_2 \\ \mathbf{0}_{(\mathrm{n}-\mathrm{m})\times\mathrm{m}} & \mathbf{0}_{(\mathrm{n}-\mathrm{m})\times(n-\mathrm{m})} \end{bmatrix}$$

$$\mathbf{z} = \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \begin{matrix} \}m \\ \}n-m \end{matrix}$$

$$\begin{aligned} \tilde{\boldsymbol{\beta}} &= \mathbf{Gy} + (\mathbf{I}_{\mathrm{n}\times\mathrm{n}} - \mathbf{GD})\mathbf{z} \\ &= \mathbf{Gy} + \left(\mathbf{I}_{\mathrm{n}\times\mathrm{n}} - \begin{bmatrix} \mathbf{I}_{\mathrm{m}\times\mathrm{m}} & \mathbf{D}_1^{-1}\mathbf{D}_2 \\ \mathbf{0}_{(\mathrm{n}-\mathrm{m})\times\mathrm{m}} & \mathbf{0}_{(\mathrm{n}-\mathrm{m})\times(n-\mathrm{m})} \end{bmatrix} \right) \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \end{aligned}$$

This simplifies to

$$\tilde{\boldsymbol{\beta}} = \begin{pmatrix} \mathbf{D}_1^{-1}\mathbf{y} - \mathbf{D}_1^{-1}\mathbf{D}_2\mathbf{v} \\ \mathbf{v} \end{pmatrix} \begin{matrix} \}m \\ \}n-m \end{matrix}$$

which now has only *n*-*m* arbitrary positive variables.

If we can show that the *i*th component of

$$\tilde{\boldsymbol{\beta}} = \begin{pmatrix} \mathbf{D}_1^{-1}\mathbf{y} - \mathbf{D}_1^{-1}\mathbf{D}_2\mathbf{v} \\ \mathbf{v} \end{pmatrix}$$

is fixed, then β_i is fixed, if it is fixed at zero then β_i can be eliminated from the design.

By solving a single linear program, we can find all the betas fixed at zero.

$$\mathbf{D}_1^{-1}\mathbf{y} - \mathbf{D}_1^{-1}\mathbf{D}_2\mathbf{v} \geq \mathbf{0}$$

$$\mathbf{v} \geq \mathbf{0}$$

is equivalent to

$$\mathbf{A}\mathbf{v} \geq \mathbf{0}$$

$$\mathbf{A} = \begin{pmatrix} \mathbf{D}_1^{-1}\mathbf{y} - \mathbf{D}_1^{-1}\mathbf{D}_2 \\ \mathbf{I}_{(n-m)x(n-m)} \end{pmatrix}$$

Consider the linear program:

$$\max_{\mathbf{x},\mathbf{y}} \mathbf{1}^{\mathrm{T}}\mathbf{w} \quad \text{subject to} \quad \begin{array}{c} \mathbf{Av}+\mathbf{w} \leq \mathbf{0} \\ \mathbf{0} \leq \mathbf{w} \leq \mathbf{1} \end{array}$$

For any (optimal) solution, $(\mathbf{x}^*, \mathbf{y}^*)$,

if $y_i^* = 0$, then the *i*th constraint in

$$\mathbf{Av} \leq \mathbf{0}$$

is always active (=0).

see Freund, Roundy and Todd (1985)

For each beta that is not fixed at zero, two separate linear programs must be solved to prove that the beta is fixed.

Let $\mathbf{a}_i$ be the ith row of $\mathbf{A}$.

Suppose that $\mathbf{a}_i\mathbf{v} = \theta$ and $\theta > 0$

LP #1

Replace the ith constraint in $\mathbf{Av}$ with $\mathbf{a}_i\mathbf{v} - \theta$.

LP #2

Replace the ith constraint in $\mathbf{Av}$ with $-\mathbf{a}_i\mathbf{v} + \theta$.

If both constraints are always active, then β_i is fixed at θ.

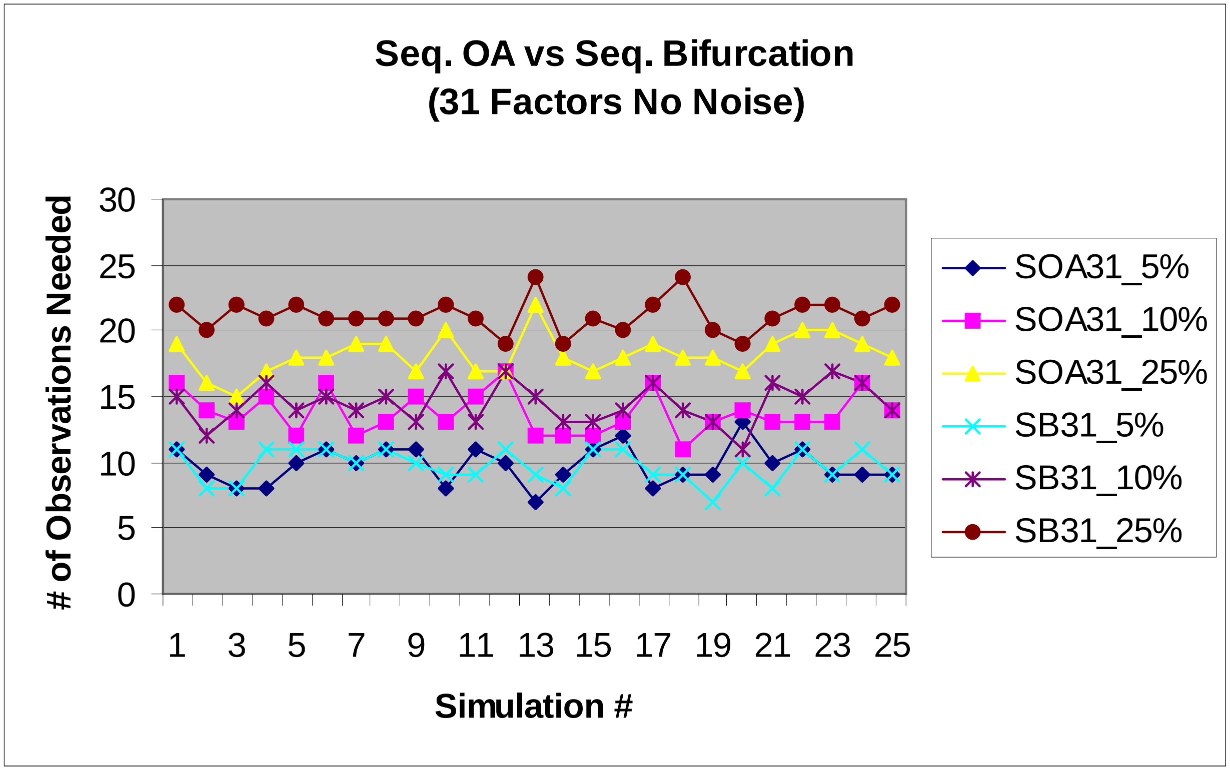
Simulations with No Noise

25 random sets of 31 factor effects were generated for three cases:

5% of the factors important (2 factors important)

10% of the factors important (4 factors important)

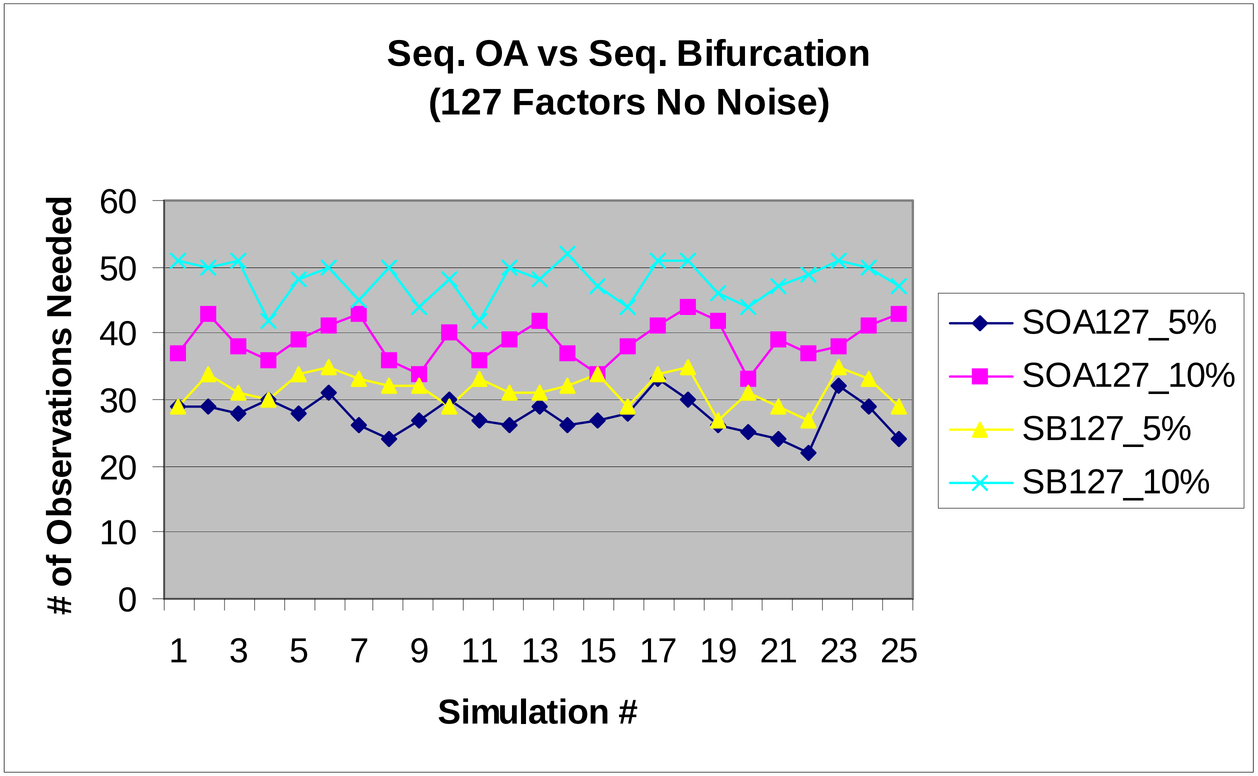
25% of the factors important (8 factors important)



25 random sets of 31 factor effects were generated for two cases:

5% of the factors important (7 factors important)

10% of the factors important (13 factors important)



Both methods use prior ranking of the factor effects to increase efficiency so an additional run was made with the factor effects clustered at the beginning of the factor set (the best position for both algorithms). The results for the clustered factor effects were identical for both methods and are shown below:

7 observations when 5% of the factors important
9 observations when 10% of the factors important
13 observations when 25% of the factors important

Sequential Bifurcation with Replicates

Kleijnen, J. P. C., Bettonvil, B. and Persson, F. (2006) Screening for the important factors in large discrete-event simulation models: sequential bifurcation and its applications. In *Screening: methods for experimentation in industry, drug discovery and genetics*. Eds. A. M. Dean and S. M. Lewis. New York: Springer.

Future Research

- Sequential Orthogonal Array with Replicates
- Sequential Orthogonal Array with Error and Power control.
- Sequential Orthogonal Array screening for dispersion effects.

Dispersion Effects

Since replicates are needed to guarantee Type 1 error and Power, there is information about the dispersion effects of the factors, so screening can run tests for both location and dispersion effects.

This would allow for robust design of the system.

Questions?