Analysis and Simulation of Definitive Screening Designs

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Outline

1. Introduction & Motivation
2. New Analytical Method
3. Simulation Studies
4. Recommendations

Notation and terminology

m factors, *n* runs

Linear main effect model (ME) – of primary interest in screening.

$$y_i = \beta_0 + \sum_{j=1}^{m} \beta_j x_{ij} + \varepsilon_i \qquad i = 1, \ldots, n$$

Full second order model – typical for RSM

$$y_i = \beta_0 + \sum_{j=1}^{m} \beta_j x_{ij} + \sum_{j=1}^{m-1} \sum_{k=j+1}^{m} \beta_{jk} x_{ij} x_{ik} + \sum_{j=1}^{m} \beta_{jj} x_{ij}^2 + \varepsilon_i \quad i = 1, \ldots, n$$

Two-factor interactions (2FIs)

Quadratic effects (Q)

The full second order (RSM) model

The response surface model (RSM) is the model consisting of:

1. The intercept term.
2. All main linear effects (for *m* factors, there are m of these)
3. All main quadratic (curvature) effects (*m* of these)
4. All two-factor interactions [there are $m(m-1)/2$ of these]

Number of terms in the full RSM:

$1 + 2m + m(m-1)/2 = (m+1)(m+2)/2$

Example: Six Factor RSM (m = 6)

1. Constant term
2. m = 6 main linear effects: $X_1, X_2, X_3, X_4, X_5, X_6$
3. m = 6 main quadratic effects: $X_1^2, X_2^2, X_3^2, X_4^2, X_5^2, X_6^2$
4. m = m(m-1)/2 = 15 two-factor interactions:

X_1X_2	X_1X_3	X_1X_4	X_1X_5	X_1X_6
	X_2X_3	X_2X_4	X_2X_5	X_2X_6
		X_3X_4	X_3X_5	X_3X_6
			X_4X_5	X_4X_6
				X_5X_6

Total is 1 + 6 + 6 + 15 = 28 model terms

Definitive Screening Design – minimum runs

Foldover Pair	Run (i)	Factor Levels				
		$x_{i,1}$	$x_{i,2}$	$x_{i,3}$	$\cdots$	$x_{i,m}$
1	1	0	±1	±1	$\cdots$	±1
	2	0	∓1	∓1	$\cdots$	∓1
2	3	±1	0	±1	$\cdots$	±1
	4	∓1	0	∓1	$\cdots$	∓1
3	5	±1	±1	0	$\cdots$	±1
	6	∓1	∓1	0	$\cdots$	∓1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
m	$2m-1$	±1	±1	±1	$\cdots$	0
	$2m$	∓1	∓1	∓1	$\cdots$	0
Centerpoint	$2m+1$	0	0	0	$\cdots$	0

Minimum design is saturated for the ME + Q effects.

Conference Matrix Definition

A conference matrix is an *mxm* matrix, C, with *0* for each diagonal element and *+1* or *–1* for each off diagonal element such that

$$\mathbf{C}^{T}\mathbf{C} = (m - 1)\mathbf{I}_{m\times m}$$

The columns of a conference matrix are orthogonal to each other.

A 6x6 conference matrix →

$$\begin{pmatrix} 0 & +1 & +1 & +1 & +1 & +1 \\ +1 & 0 & +1 & -1 & -1 & +1 \\ +1 & +1 & 0 & +1 & -1 & -1 \\ +1 & -1 & +1 & 0 & +1 & -1 \\ +1 & -1 & -1 & +1 & 0 & +1 \\ +1 & +1 & -1 & -1 & +1 & 0 \end{pmatrix}$$

Conference Matrix Construction

Let C be a conference matrix with *m* rows and *m* columns, then

$$\mathbf{D}_m = \begin{bmatrix} \mathbf{C}_m \\ -\mathbf{C}_m \\ \mathbf{0}' \end{bmatrix}$$

where D_m is a DSD with *m* factors and *2m+1* runs.

To construct a DSD with more than the minimal number of runs, use a conference matrix with $c > m$ columns and do not assign the last $c - m$ columns to factors.

Design Properties

1. Small number of runs – $2m + 1$ at a minimum
2. Orthogonal main effects (MEs)
3. MEs orthogonal to 2FIs
4. 2FIs not confounded with other 2FIs
5. All the MEs and pure quadratic effects are estimable
6. DSDs with more than 5 factors project onto any 3 factors to allow fitting the full quadratic model

Citations

☐	A class of three-level designs for definitive screening in the presence of second-order effects B Jones, CJ Nachtsheim Journal of Quality Technology 43 (1), 1	112	2011

A Class of Three-Level Designs for Definitive Screening in the Presence of Second-Order Effects

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New Method

Since main effects and 2nd order effects are orthogonal to each other you can split the response (Y) into two new responses

- One response for identifying main effects – call it YME
- One response for identifying 2nd order effects – call it Y2nd
- And the two columns are orthogonal to each other

Computing the New Responses

1. Fit the main effects model (No Intercept) and save the predicted values (YME). These are the responses for the main effects model.

1. Save the residuals from the fit above – these residuals are the responses for the 2nd order effects (Y2nd).

Digression: Benefits of "Fake" Factors

Adding Fake Factors (factors you don't use) provides a way to estimate variance without repeating center runs!

Why?

Fake factors are orthogonal to the real factors

Fake factors are orthogonal to all the 2^{nd} order effects

Assuming the 3^{rd} and higher order effects are negligible, we can use the fake factor degrees of freedom to create an unbiased estimate of the error variance!

Note: Use both the real and fake factors when fitting the main effects model in step 1 of the previous slide.

Example: Six real factors and two fake factors

A	B	C	D	E	F	Fake 1	Fake 2	Y	Y2nd	YME
0	1	1	1	1	1	1	1	94.51	101.04	-6.53
0	-1	-1	-1	-1	-1	-1	-1	107.57	101.04	6.53
1	0	1	1	-1	1	-1	-1	94.36	101.175	-6.815
-1	0	-1	-1	1	-1	1	1	107.99	101.175	6.815
1	-1	0	1	1	-1	1	-1	91.80	90.525	1.275
-1	1	0	-1	-1	1	-1	1	89.25	90.525	-1.275
1	-1	-1	0	1	1	-1	1	93.70	94.485	-0.785
-1	1	1	0	-1	-1	1	-1	95.27	94.485	0.785
1	1	-1	-1	0	1	1	-1	89.55	88.71	0.84
-1	-1	1	1	0	-1	-1	1	87.87	88.71	-0.84
1	-1	1	-1	-1	0	1	1	94.58	95.235	-0.655
-1	1	-1	1	1	0	-1	-1	95.89	95.235	0.655
1	1	-1	1	-1	-1	0	1	93.23	89.58	3.65
-1	-1	1	-1	1	1	0	-1	85.93	89.58	-3.65
1	1	1	-1	1	-1	-1	0	98.11	95.815	2.295
-1	-1	-1	1	-1	1	1	0	93.52	95.815	-2.295
0	0	0	0	0	0	0	0	99.75	99.75	0

Adds 4 runs – 2 error df

YME
-6.53
6.53
-6.815
6.815
1.275
-1.275
-0.785
0.785
0.84
-0.84
-0.655
0.655
3.65
-3.65
2.295
-2.295
0

Examining the Main Effects Response (YME)

Note responses for each foldover pair sum to zero.

The response for the center run is zero.

There are 17 rows but only 8 independent values

(degrees of freedom – df)

There are 6 real factors but 8 df, so there are

$8 - 6 = 2$ df for estimating σ^2

Y2nd
101.04
101.04
101.175
101.175
90.525
90.525
94.485
94.485
88.71
88.71
95.235
95.235
89.58
89.58
95.815
95.815
99.75

Examining the 2^{nd} Order Response (Y2nd)

Responses for each foldover pair are the same.

There are 17 rows but only 9 independent values

(degrees of freedom – df)

After estimating the Intercept, there are 8 df left for estimating 2^{nd} order effects.

Analysis – Identify Active Main Effects

1. Recall that the residuals from fitting the Main Effects data (YME) to the real factors have 2 degrees of freedom.
2. To estimate σ^2, sum the squared residuals from this fit and divide the result by 2.
3. Using this estimate, do t-tests of each coefficient
4. If the resulting p-value for an effect is small, conclude that effect is active.

2^{nd} Digression: Model Heredity Assumption

The heredity assumption stipulates that 2^{nd} order effects only occur when the associated main effects are active.

Example 1: If main effects A and B are in the model you can consider the two-factor interaction AB

Example 2: B must be in the model before considering the quadratic effect B^2

While there is no physical law requiring that models exhibit heredity, there is empirical evidence that such models are much more probable in real systems.

Advantage of the Heredity Assumption

The set of possible models using the heredity assumption may be much smaller than allowing any 2^{nd} order effect to appear in the model

Example: Suppose your main effects analysis yields 3 active main effects (C, D, F say). Then the allowable 2^{nd} order terms are CD, CF, DF, C^2, D^2, F^2

We have 8 degrees of freedom and only 6 effects, so it is possible to identify all 6 if they are active.

If we allow consideration all 2^{nd} order effects, there are 15 two-factor interactions and 6 quadratic terms – or 21 terms in all.

There are 2^{21} or more 2 million possible models – a much harder model selection problem.

Analysis – Identifying 2nd Order Effects

Form all the 2nd order terms involving the active main effects

Do all subsets regression up to the point where the MSE of the best 2nd order model for a given number of terms is not significantly larger than your estimate of σ^2

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2. Three Ideas for Analysis
3. Simulation Studies
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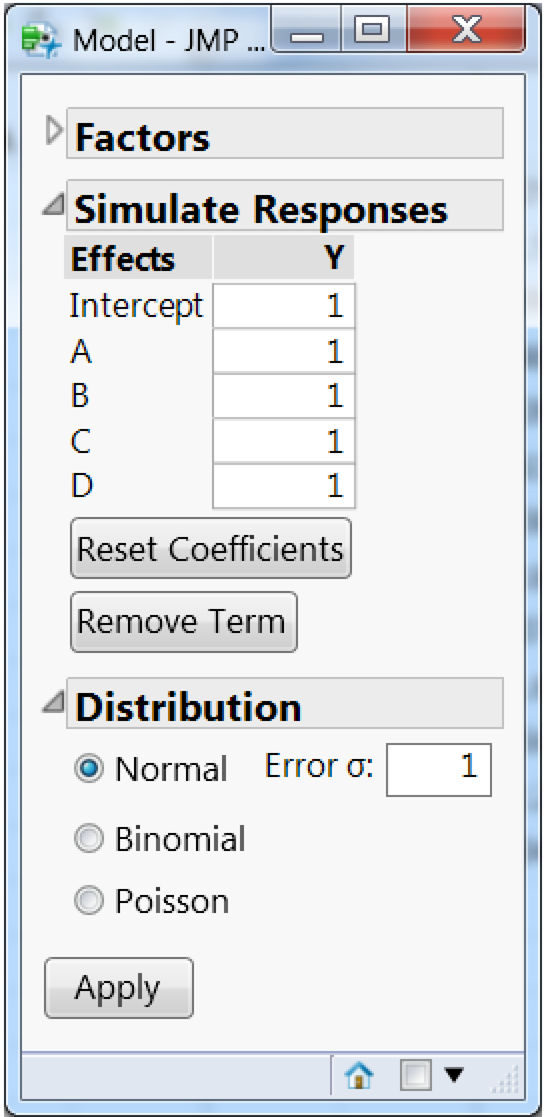
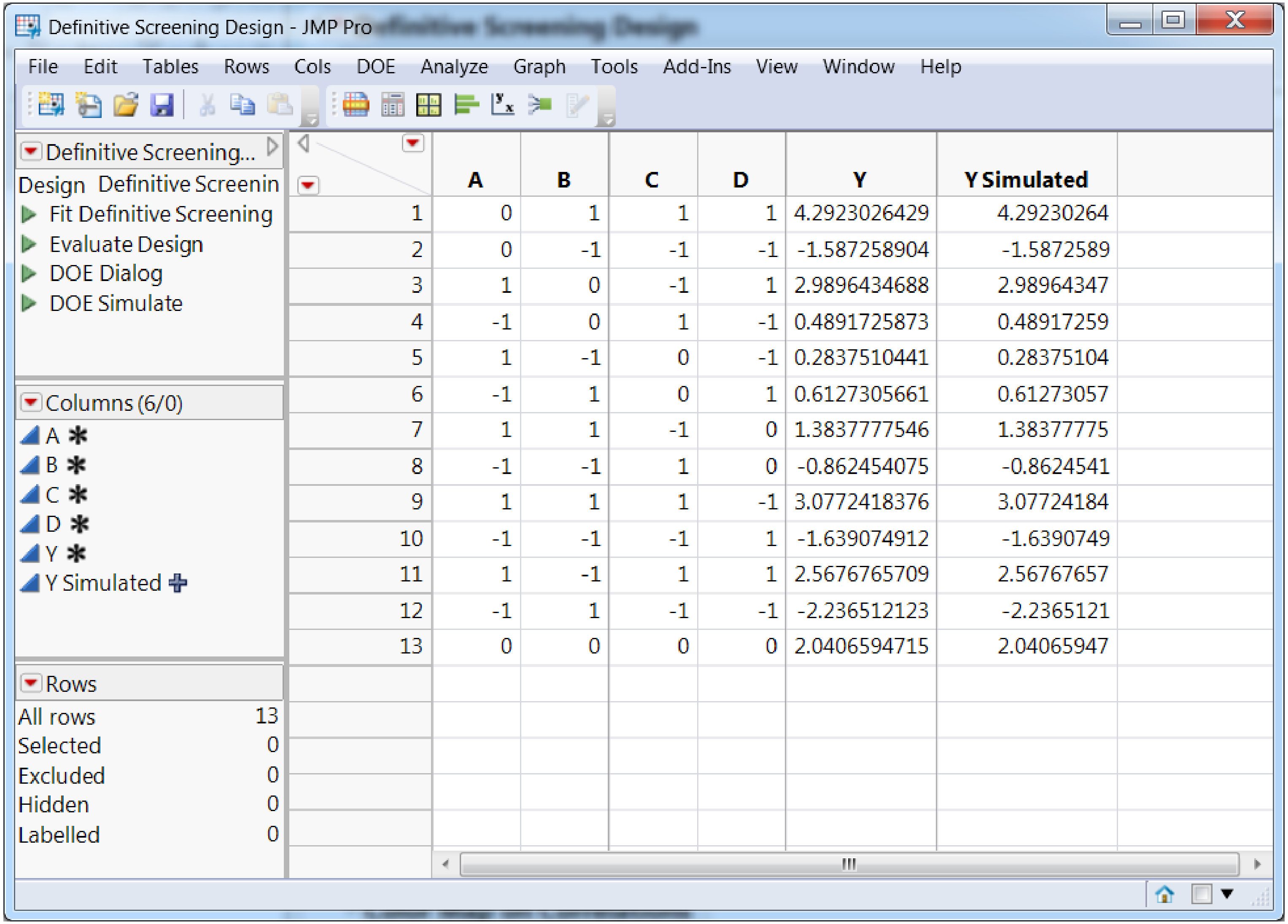
Simulate Responses User Interface

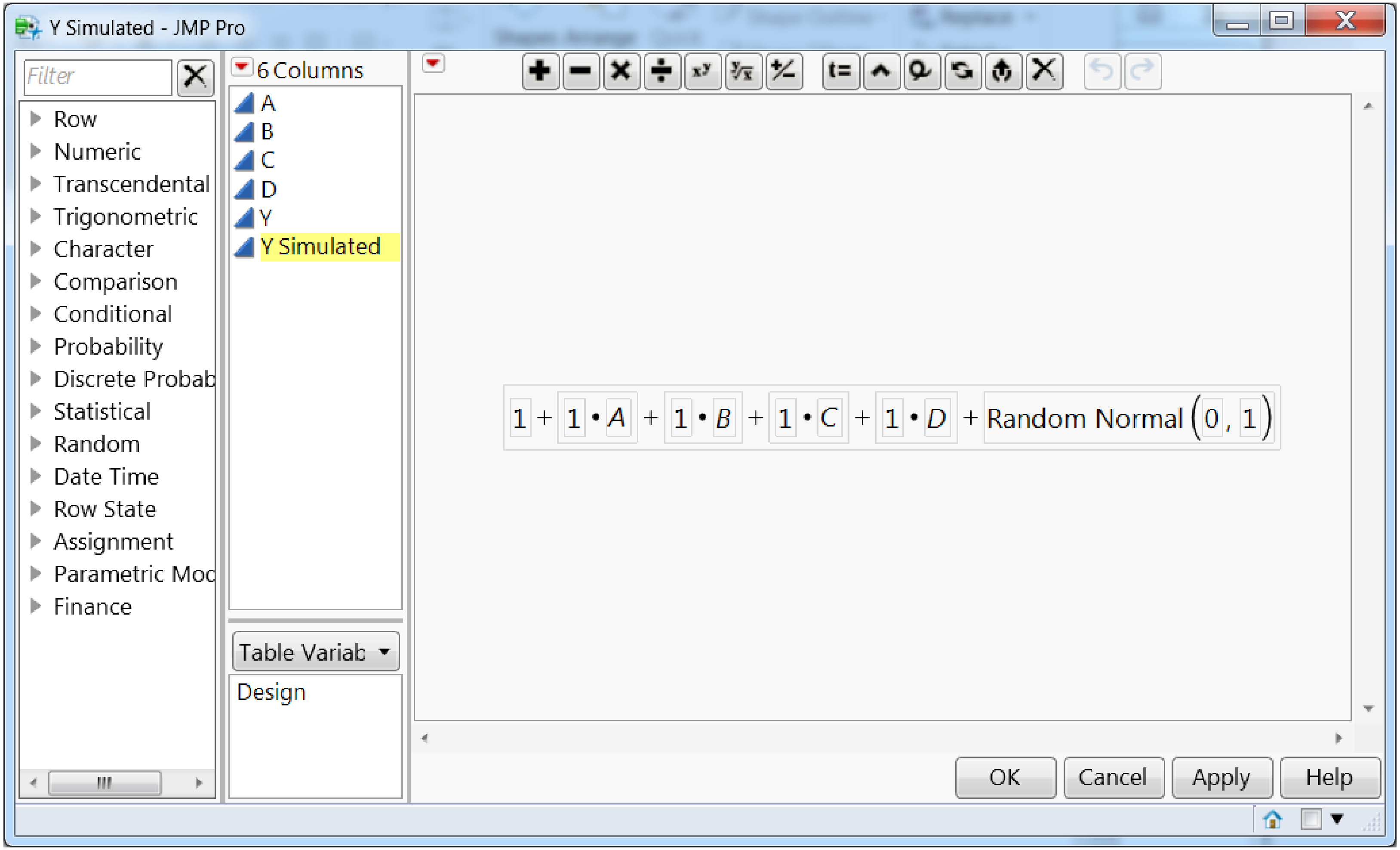


Resulting Table



	A	B	C	D	Y	Y Simulated
1	0	1	1	1	4.2923026429	4.29230264
2	0	-1	-1	-1	-1.587258904	-1.5872589
3	1	0	-1	1	2.9896434688	2.98964347
4	-1	0	1	-1	0.4891725873	0.48917259
5	1	-1	0	-1	0.2837510441	0.28375104
6	-1	1	0	1	0.6127305661	0.61273057
7	1	1	-1	0	1.3837777546	1.38377775
8	-1	-1	1	0	-0.862454075	-0.8624541
9	1	1	1	-1	3.0772418376	3.07724184
10	-1	-1	-1	1	-1.639074912	-1.6390749
11	1	-1	1	1	2.5676765709	2.56767657
12	-1	1	-1	-1	-2.236512123	-2.2365121
13	0	0	0	0	2.0406594715	2.04065947

Formula Column with Random Numbers



JMP Demonstration of New Method

TABLE 2. Three-Level Definitive Screening Design for Six Factors with a Simulated Response Vector

Run (i)	$x_{i,1}$	$x_{i,2}$	$x_{i,3}$	$x_{i,4}$	$x_{i,5}$	$x_{i,6}$	y_i
1	0	1	−1	−1	−1	−1	21.04
2	0	−1	1	1	1	1	10.48
3	1	0	−1	1	1	−1	17.89
4	−1	0	1	−1	−1	1	10.07
5	−1	−1	0	1	−1	−1	7.74
6	1	1	0	−1	1	1	21.01
7	−1	1	1	0	1	−1	16.53
8	1	−1	−1	0	−1	1	20.38
9	1	−1	1	−1	0	−1	8.62
10	−1	1	−1	1	0	1	7.80
11	1	1	1	1	−1	0	23.56
12	−1	−1	−1	−1	1	0	15.24
13	0	0	0	0	0	0	19.91

Stage 1 - Main Effect Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
x1	3.408	0.1873	18.196	0.0030*
x2	2.748	0.1873	14.672	0.0046*
x3	-1.309	0.1873	-6.989	0.0199*
x4	-0.851	0.1873	-4.544	0.0452*

Statistic	Value
RMSE	0.5923
DF	2

Stage 2 - Even Order Effect Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	20.058	0.291	68.926	<.0001*
x2*x3	5.595	0.2	27.979	0.0001*
x1*x1	-7.271	0.3325	-21.87	0.0002*
x4*x4	1.2235	0.3325	3.6798	0.0348*

Statistic	Value
RMSE	0.3999
DF	3

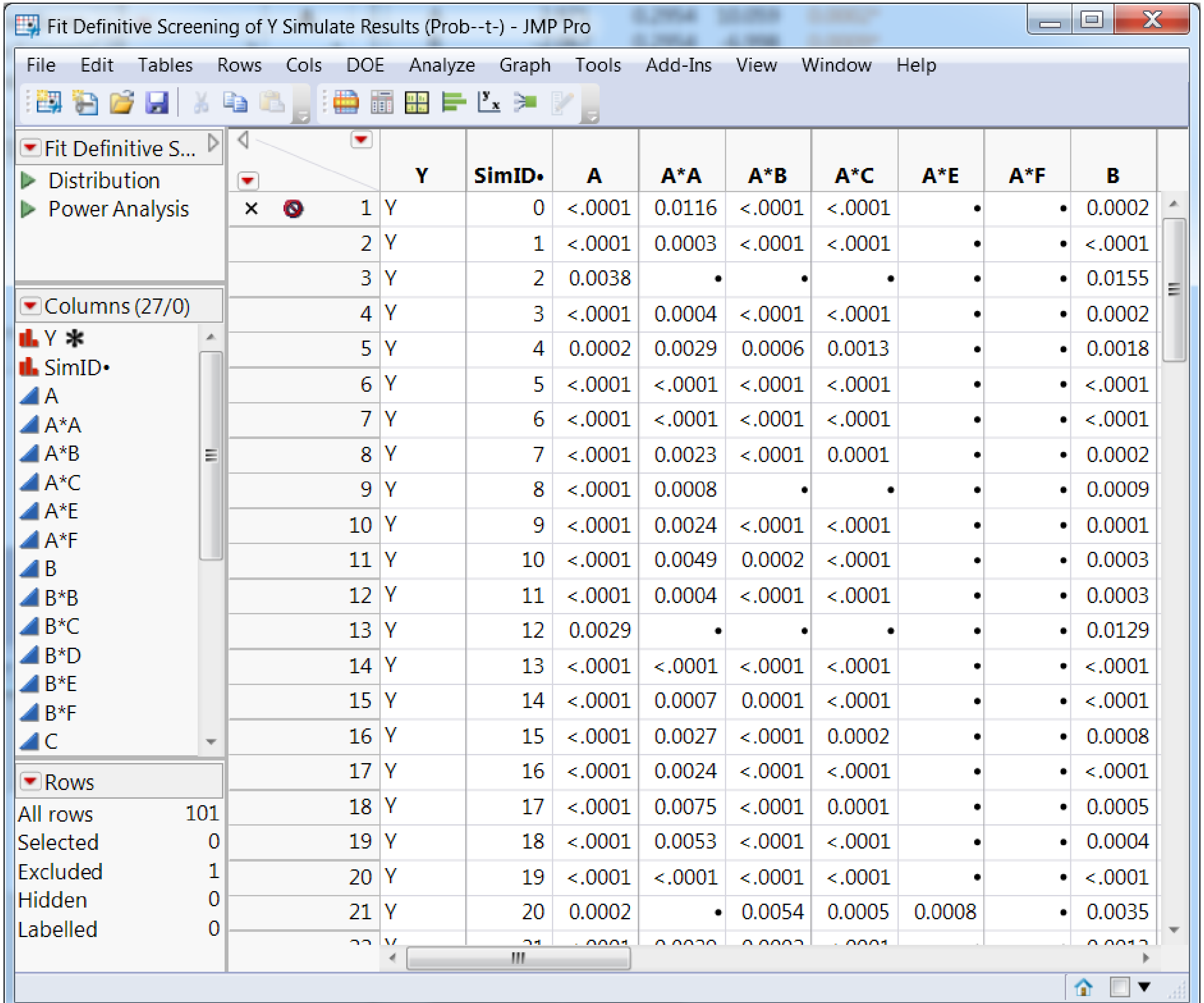
Combined Model Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	20.058	0.3537	56.71	<.0001*
x1	3.408	0.1537	22.17	<.0001*
x2	2.748	0.1537	17.877	<.0001*
x3	-1.309	0.1537	-8.516	0.0004*
x4	-0.851	0.1537	-5.536	0.0026*
x2*x3	5.595	0.243	23.02	<.0001*
x1*x1	-7.271	0.4041	-17.99	<.0001*
x4*x4	1.2235	0.4041	3.0276	0.0292*

Statistic	Value
RMSE	0.4861
DF	5

Make Model | Run Model

Monte Carlo Simulation in JMP 13



	Y	SimID•	A	A*A	A*B	A*C	A*E	A*F	B
1	Y	0	<.0001	0.0116	<.0001	<.0001	•	•	0.0002
2	Y	1	<.0001	0.0003	<.0001	<.0001	•	•	<.0001
3	Y	2	0.0038	•	•	•	•	•	0.0155
4	Y	3	<.0001	0.0004	<.0001	<.0001	•	•	0.0002
5	Y	4	0.0002	0.0029	0.0006	0.0013	•	•	0.0018
6	Y	5	<.0001	<.0001	<.0001	<.0001	•	•	<.0001
7	Y	6	<.0001	<.0001	<.0001	<.0001	•	•	<.0001
8	Y	7	<.0001	0.0023	<.0001	0.0001	•	•	0.0002
9	Y	8	<.0001	0.0008	•	•	•	•	0.0009
10	Y	9	<.0001	0.0024	<.0001	<.0001	•	•	0.0001
11	Y	10	<.0001	0.0049	0.0002	<.0001	•	•	0.0003
12	Y	11	<.0001	0.0004	<.0001	<.0001	•	•	0.0003
13	Y	12	0.0029	•	•	•	•	•	0.0129
14	Y	13	<.0001	<.0001	<.0001	<.0001	•	•	<.0001
15	Y	14	<.0001	0.0007	0.0001	<.0001	•	•	<.0001
16	Y	15	<.0001	0.0027	<.0001	0.0002	•	•	0.0008
17	Y	16	<.0001	0.0024	<.0001	<.0001	•	•	<.0001
18	Y	17	<.0001	0.0075	<.0001	0.0001	•	•	0.0005
19	Y	18	<.0001	0.0053	<.0001	<.0001	•	•	0.0004
20	Y	19	<.0001	<.0001	<.0001	<.0001	•	•	<.0001
21	Y	20	0.0002	•	0.0054	0.0005	0.0008	•	0.0035

Empirical Power Analysis

x1

Simulation Results

Simulated Power

Alpha	Rejection Count	Rejection Rate	Lower 95%	Upper 95%
0.01	387	0.9675	0.9452	0.98091
0.05	398	0.995	0.98196	0.99863
0.10	400	1	0.99049	1
0.20	400	1	0.99049	1

x1*x1

Simulation Results

Simulated Power

Alpha	Rejection Count	Rejection Rate	Lower 95%	Upper 95%
0.01	369	0.9225	0.8921	0.94487
0.05	369	0.9225	0.8921	0.94487
0.10	369	0.9225	0.8921	0.94487
0.20	369	0.9225	0.8921	0.94487

Analyzing DSDs Conclusion

JUST DO IT.

Recommendations

Prefer using fake factors to repeated center runs.

Assume model heredity unless there is substantial scientific evidence to the contrary.

Model main effects separately from 2^{nd} order effects by breaking the response into two responses.

And one last thing…

You can use the two response decomposition idea for any foldover design.

References

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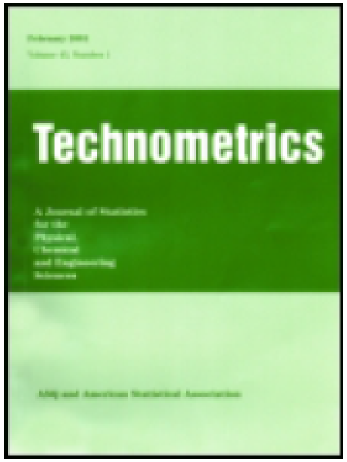

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Effective Design-Based Model Selection for Definitive Screening Designs

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