Exploring Best Practices in Design of Experiments

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Explorer Seminar – Module 1

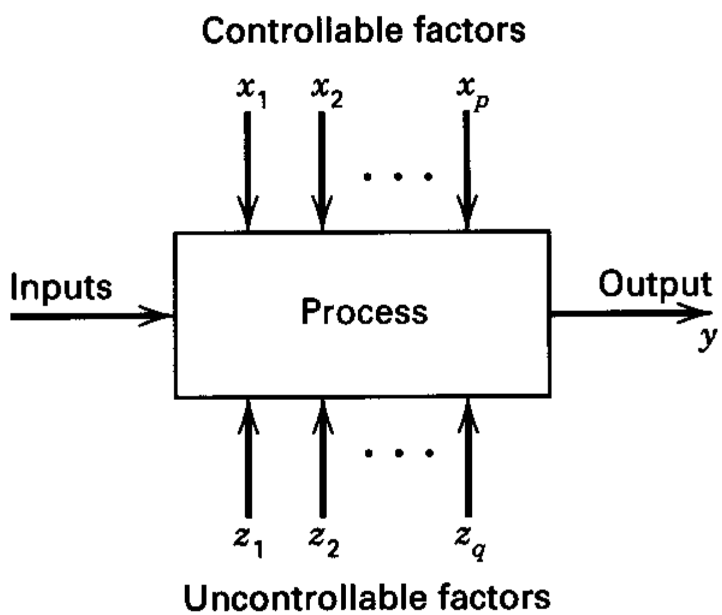
Introduction, Definitions and an Example

Goals

1. Introduce fundamental concepts
2. Introduce linear statistical models
3. Show the relationship of a model to a design
4. Introduce criteria for evaluating the goodness of a design

What Is a Designed Experiment?

a structured set of tests of a system or process



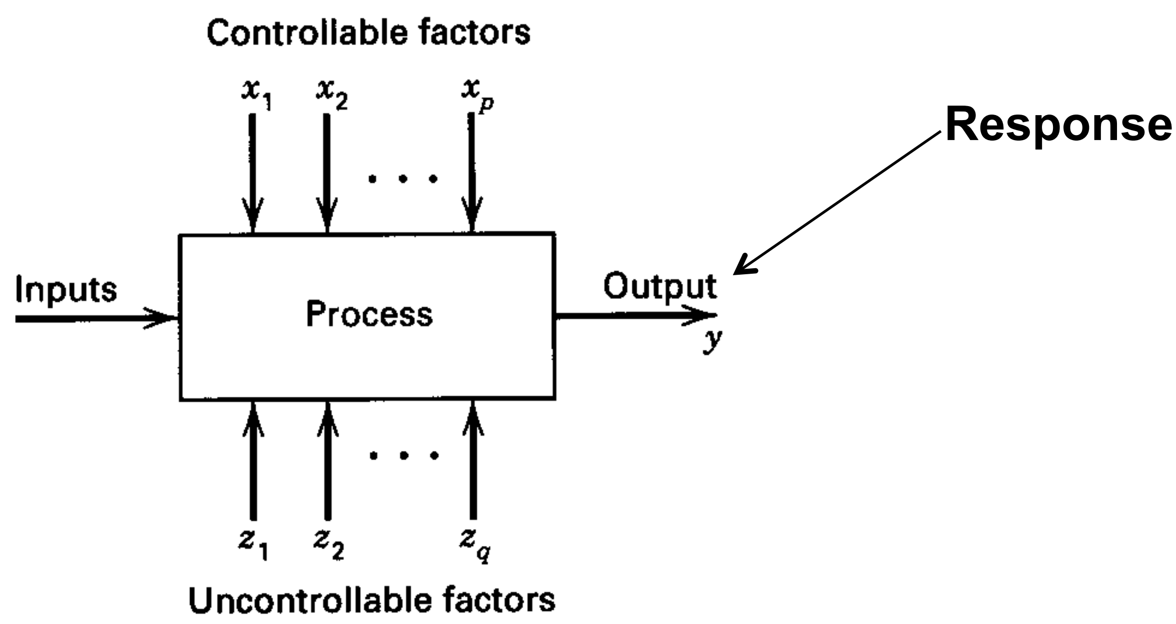
Integral to a designed experiment are…

1. Response(s)
2. Factor(s)
3. Model

What Is a Response?

A *response* is a **measurable** result.

- yield of a chemical reaction (chemical process)
- deposition rate (semiconductor)
- gas mileage (automotive)



What Is a Factor?

A *factor* is any **variable** that you think may affect a response of interest. We begin by considering three types of factors – continuous, categorical and blocking

continuous factors take any value on an interval

e.g. octane rating [89 93]

categorical factors have a discrete number of levels

e.g. brand [BP, Shell, Exxon]

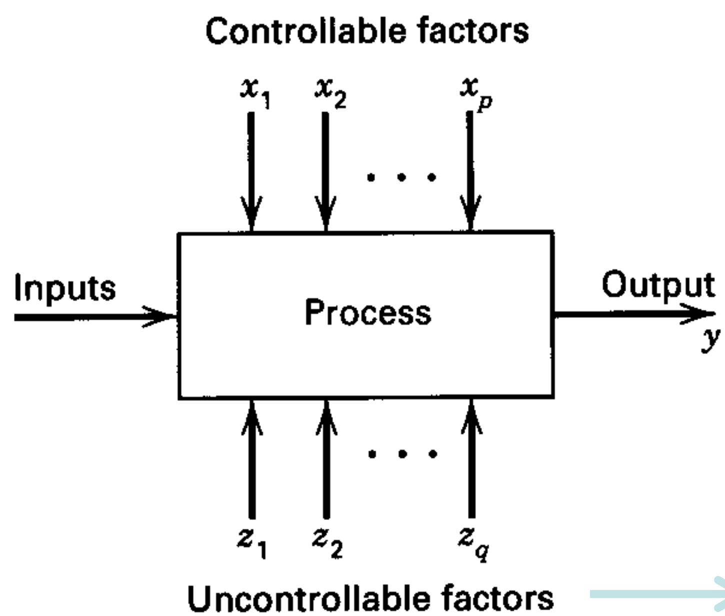
blocking factors are categorical but not generally reproducible

e.g. driver to driver variability

What is a model?

a simplified mathematical surrogate for the process

Factor(s) ⟶ Model ⟶ Response(s)



⟶ *Candidates for blocking*

Examples of Models

Comparing three brands of gasoline using an ANOVA model:

$$Y_{ij} = \mu + \alpha_i + \epsilon_{ij}$$

Finding the effect of octane rating using a regression model:

$$Y_i = \beta_0 + \beta_1 X_1 + \epsilon_i$$

Y (the response) is the mileage of a car in miles per gallon.

ANOVA and regression models are equivalent…

$$Mileage_i = \begin{cases} \mu + \alpha_1 + \epsilon_i & \text{if } Brand = BP; \\ \mu + \alpha_2 + \epsilon_i & \text{if } Brand = Shell; \\ \mu + \alpha_3 + \epsilon_i & \text{if } Brand = Exxon. \end{cases}$$

Replace μ with β_0 and α_1 and α_2 with β_1 and β_2.

$$Mileage_i = \begin{cases} \beta_0 + \beta_1 1 + \beta_2 0 + \epsilon_i & \text{if } Brand = BP; \\ \beta_0 + \beta_1 0 + \beta_2 1 + \epsilon_i & \text{if } Brand = Shell; \\ \beta_0 + \beta_1(-1) + \beta_2(-1) + \epsilon_i & \text{if } Brand = Exxon. \end{cases}$$

$$Mileage_i = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon_i$$

ANOVA/Regression Model – Matrix Notation

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & -1 & -1 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \end{bmatrix}$$

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

$$\mathrm{Var}(\boldsymbol{\varepsilon}) = \sigma^2 \mathbf{I}$$

The Model/Design Relationship – Parameter Estimates

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \qquad \mathrm{Var}(\boldsymbol{\varepsilon}) = \sigma^2\mathbf{I}$$

The matrix, **X**, is called the design matrix. The least-squares estimator of β is:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

The variance of the least-squares estimator of β is:

$$\mathrm{Var}(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$$

σ is inherent to the system but we choose the design matrix, **X**.

The Model/Design Relationship – Predicted Responses

The predicted values of the response are contained in the vector:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \mathbf{H}\mathbf{y}$$

Where the so-called, “hat” matrix, H, is: $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$

The variance matrix of the predicted responses is:

$$Var(\hat{\mathbf{y}}) = \sigma^2\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$$

Again, σ is inherent to the system, but we choose the design, **X**.

The Model/Design Relationship – Aliasing

Suppose the best polynomial approximating model is:

$$\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\varepsilon}$$

But we estimate only β_1 using least-squares:

$$\hat{\boldsymbol{\beta}}_1 = (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{y}$$

Now the elements of the least-squares estimates of β_1 are biased by β_2, that is:

$$\mathrm{E}(\hat{\boldsymbol{\beta}}_1) = \boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2$$

where the alias matrix, A, is:

$$(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2$$

What makes a design good?

1. Low variance of the coefficients.
2. Low variance of predicted responses.
3. Minimal aliasing of terms in the model from likely effects that are not in the model (0.5 or less).
4. Correlations between likely effects that are not in the model are small (0.5 or less).

The first two deal with variance – the last two with bias.
Reducing variance and bias are fundamental goals.

Design Optimality Criteria

D-optimality $$\max_{d} |\mathbf{X_d}'\mathbf{X_d}|$$

I-optimality $$\min_{d} \frac{\int_{\chi} \mathbf{f}'(\mathbf{x})(\mathbf{X_d}'\mathbf{X_d})^{-1}\mathbf{f}(\mathbf{x})d\mathbf{x}}{\int_{\chi} d\mathbf{x}}$$

Alias optimality $$\min_{d} \mathrm{Tr}[\mathbf{A}(d)'\mathbf{A}(d)], \text{ subject to } D_e(d) \geq l_D$$

Important Points from the Fathers of DOE

DOE – Problem solving methodology for efficiently identifying cause-and-effect relationships.

Fisher's Four Fundamentals of DOE

1. Factorial principle
2. Randomization
3. Blocking
4. Replication

R.A. Fisher

"To discover what happens to a process when a factor is changed, you must actually change it!"

George Box

Module 1 – Conclusions

1. Remember Fisher's Four Principles
   1. Factorial Principle
   2. Randomization
   3. Blocking
   4. Replication
2. ANOVA models can be converted to regression models.
3. Variance and bias are fundamental criteria for evaluating designs.

Explorer Seminar – Module 2

Standard designs using an optimal design tool.

Goals

1. Give an examples of familiar designs created using an optimal design algorithm

Optimal <> Full Factorial

Full Factorial designs are D-optimal for the models they support.

Example:

2^k designs are optimal for main effects plus interactions of any order.

Photolithography Example

- Consider five factors in a photolithography process
  - A = aperture setting
  - B = exposure time
  - C = develop time
  - D = mask dimension
  - E = etch time

With each factor at two levels the resulting number of runs is:

$$2^5 = 32$$

Properties of this design

- Orthogonal
- Makes interpretation easy
- Minimizes the variance of the model coefficients
- Minimizes the average prediction variance
- Minimizes the maximum prediction variance
- You can’t do any better than this
  - (for five two-level factors and 32 runs)!

JMP Demo

Relative Variance of Coefficients

Significance Level	0.05
Signal to Noise Ratio	1

Effect	Variance	Power
Intercept	0.031	1
X1	0.031	1
X2	0.031	1
X3	0.031	1
X4	0.031	1
X5	0.031	1
X1*X2	0.031	1
X1*X3	0.031	1
X1*X4	0.031	1
X1*X5	0.031	1
X2*X3	0.031	1
X2*X4	0.031	1
X2*X5	0.031	1
X3*X4	0.031	1
X3*X5	0.031	1
X4*X5	0.031	1

Optimal <> Fractional Factorial

Fractional Factorial designs are D-optimal for the models they support.

Example:

2^{k-p} designs are optimal for main effects plus interactions up to an order dependent on the resolution of the design.

Resolution V

- Models for main effects + all two-factor interactions
- Recall the five factors from the photolithography process
  - A = aperture setting
  - B = exposure time
  - C = develop time
  - D = mask dimension
  - E = etch time
- The number of runs is half the number required for the full factorial design – 16.

The 2^{5-1}

- Aliases:
  - All main effects are clear of the two-factor interactions
  - All two-factor interactions are clear of each other
- Orthogonal
- Makes interpretation easy
- Minimizes the variance of the model coefficients
- Minimizes the average prediction variance
- Minimizes the maximum prediction variance
- Once again, you can’t do any better than this!

JMP Demo

Relative Variance of Coefficients

Significance Level	0.05
Signal to Noise Ratio	1

Effect	Variance
Intercept	0.063
X1	0.063
X2	0.063
X3	0.063
X4	0.063
X5	0.063
X1*X2	0.063
X1*X3	0.063
X1*X4	0.063
X1*X5	0.063
X2*X3	0.063
X2*X4	0.063
X2*X5	0.063
X3*X4	0.063
X3*X5	0.063
X4*X5	0.063

Module 2 - Summary

1. Main message is that standard designs are optimal designs.
2. Optimal design generators can reproduce standard designs for routine problems.

Module 3 – Modern Screening Methods

There is substantial new research in both design and analysis of screening experiments in the last 15 years.

Much of this new research calls into question the conventional strategy of the standard use of regular fractional factorial designs for screening.

We will introduce some of these new methods in this section.

Many of the new designs are orthogonal but have more desirable aliasing properties than the regular fractional factorial designs previously shown.

Standard Fractional Factorial Designs may not Always be the Best Choice for Screening

- In these designs the alias matrix consists of either 0, +1 or -1 entries
- That means that effects are completely confounded…

JMP Demo

Design

Run	A	B	C	D	E
1	1	-1	1	-1	1
2	1	1	-1	1	-1
3	-1	-1	-1	1	1
4	-1	1	1	1	1
5	-1	1	1	-1	-1
6	-1	-1	-1	-1	-1
7	1	1	-1	-1	1
8	1	-1	1	1	-1

Alias Matrix

Effect	A*B	A*C	A*D	A*E	B*C	B*D	B*E	C*D	C*E	D*E
Intercept	0	0	0	0	0	0	0	0	0	0
A	0	0	0	0	-1	0	0	0	0	-1
B	0	-1	0	0	0	0	0	0	0	0
C	-1	0	0	0	0	0	0	0	0	0
D	0	0	0	-1	0	0	0	0	0	0
E	0	0	-1	0	0	0	0	0	0	0

Plackett-Burman Designs

- These are an orthogonal design alternative
- The number of runs, N, is any multiple of four
- N = 4, 8, 12, 16, 20, 24, 28, 32, 36, 40, …
- The designs where N = 12, 20, 24, etc. are called **nongeometric** or **nonregular** PB designs
- These designs are D-optimal for the main-effects model.
- But…

The Alias Matrix for the 12-run Plackett-Burman Design

Alias Matrix

Effect	A*B	A*C	A*D	A*E	B*C	B*D	B*E	C*D	C*E	D*E
Intercept	0	0	0	0	0	0	0	0	0	0
A	0	0	0	0	-0.33	0.333	0.333	0.333	0.333	0.333
B	0	-0.33	0.333	0.333	0	0	0	-0.33	0.333	0.333
C	-0.33	0	0.333	0.333	0	-0.33	0.333	0	0	-0.33
D	0.333	0.333	0	0.333	-0.33	0	0.333	0	-0.33	0
E	0.333	0.333	0.333	0	0.333	0.333	0	-0.33	0	0

These designs are D-optimal for the main-effects model. But, the main-effects may suffer substantial bias from any active two-factor interactions. The literature refers to the above pattern as “complex” aliasing.

JMP Demo

Design

Run	A	B	C	D	E	Yield
1	-1	1	-1	1	-1	.
2	1	1	-1	1	1	.
3	1	-1	1	-1	1	.
4	-1	1	1	-1	1	.
5	1	-1	1	1	-1	.
6	-1	-1	-1	-1	1	.
7	-1	1	1	-1	-1	.
8	-1	-1	-1	1	1	.
9	-1	-1	1	1	-1	.
10	1	-1	-1	-1	-1	.
11	1	1	1	1	1	.
12	1	1	-1	-1	-1	.

Alias Matrix

Effect	A*B	A*C	A*D	A*E	B*C	B*D	B*E	C*D	C*E	D*E
Intercept	0	0	0	0	0	0	0	0	0	0
A	0	0	0	0	-0.33	0.333	0.333	0.333	0.333	0.333
B	0	-0.33	0.333	0.333	0	0	0	-0.33	0.333	0.333
C	-0.33	0	0.333	0.333	0	-0.33	0.333	0	0	-0.33
D	0.333	0.333	0	0.333	-0.33	0	0.333	0	-0.33	0
E	0.333	0.333	0.333	0	0.333	0.333	0	-0.33	0	0

Alias Optimal Design

Standard optimal designs (*D*, *I* and *G*) have a similar problem as fractional factorials. This is due to the fact that they focus all the effort on precise estimation of only one model.

In particular, there is no attention to possible aliasing of terms in this model by likely higher order terms.

Example:

> In screening designs we want to get good estimates of main effects but we do not want these estimates biased by two-factor interactions.

If only we could find a design with this alias matrix!

Alias Matrix

Effect	A*B	A*C	A*D	A*E	B*C	B*D	B*E	C*D	C*E	D*E
Intercept	0	0	0.333	0.333	-0.33	0	0	0	0	0.333
A	0	0	0	0	0	0	0	0	0	0
B	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0
D	0	0	0	0	0	0	0	0	0	0
E	0	0	0	0	0	0	0	0	0	0

Aliasing here not quite so "complex"
If only…!

Design we want is on the right

Plackett-Burman Design

Design

Run	A	B	C	D	E
1	-1	1	1	-1	-1
2	-1	-1	-1	1	1
3	1	1	-1	1	1
4	1	1	-1	-1	-1
5	-1	1	1	-1	1
6	1	-1	-1	-1	-1
7	1	-1	1	-1	1
8	-1	-1	1	1	-1
9	-1	1	-1	1	-1
10	1	1	1	1	1
11	1	-1	1	1	-1
12	-1	-1	-1	-1	1

Design Diagnostics

D Optimal

D Efficiency	100
G Efficiency	100
A Efficiency	100
Average Variance of Prediction	0.222222
Design Creation Time	0.283333

Alternative Design

Design

Run	A	B	C	D	E
1	-1	-1	1	-1	-1
2	-1	1	-1	1	-1
3	1	-1	1	-1	1
4	1	-1	1	1	-1
5	-1	-1	1	1	1
6	1	-1	-1	1	1
7	-1	-1	-1	-1	-1
8	1	1	-1	-1	-1
9	-1	1	-1	-1	1
10	-1	1	1	-1	-1
11	1	1	-1	1	1
12	1	1	1	1	1

Design Diagnostics

D Efficiency	93.27221
G Efficiency	92.70287
A Efficiency	87.59124
Average Variance of Prediction	0.245833
Design Creation Time	3.8

How do we get generate this design?

Constrained optimization:
Minimize the sum of squared elements of the alias matrix subject to a lower bound on d-efficiency.

Efficient Designs With Minimal Aliasing

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For some experimenters, a disadvantage of the standard optimal design approach is that it does not consider explicitly the aliasing of specified model terms with terms that are potentially important but are not included in the model. For example, when constructing an optimal design for a first-order model, aliasing of main effects and interactions is not considered. This can lead to designs that are optimal for estimation of the primary effects of interest, yet have undesirable aliasing structures. In this article, we construct exact designs that minimize the squared norm of the alias matrix subject to constraints on design efficiency. We demonstrate use of the method for the construction of screening and response surface designs.

KEY WORDS: Alias matrix; Bayesian design; Constrained design; D-optimality; Minimum bias design; Response surface design.

1. INTRODUCTION

In recent years, many statistical software packages with facilities for the design of experiments have incorporated capabilities for constructing optimal designs. A concern that many experimenters share when using optimal designs has to do with the potential over-reliance on a single model. Model robust designs (see, e.g., Läuter 1974; Cook and Nachtsheim 1982; Li and Nachtsheim 2000), model discriminating designs (see, e.g., Meyer, Steinberg, and Box 1996; Bingham and Chipman 2007; Jones et al. 2007), minimum bias designs (see, e.g., Draper and Lawrence 1965; Karson 1970; Karson and Spruill 1975; Evans and Manson 1978), and Bayesian D-optimal designs (DuMouchel and Jones 1994; Jones, Lin, and Nachtsheim 2008) represent alternative approaches to reducing the dependence on a single model.

One specific criticism of the basic optimal design approach is that standard criteria do not consider in any way the aliasing of specified model terms with terms that are potentially important but are not included in the model. Consider, for example, the following common design scenario. A researcher is considering two alternative designs for a 12-run screening experiment with six factors. The first design is a 12-run Plackett–Burman design. The Plackett–Burman design is orthogonal and optimal for the main-effects model. The experimenter has some concerns about using this design because she believes that the potential presence of active two-factor interactions could bias the results. Let $\mathbf{X}_1$ denote the (12×7) model matrix for the main-effects model (including the intercept) and let $\mathbf{X}_2$ denote the (12×15) model matrix corresponding to the 15 interaction columns. Suppose the true model is

$$\mathbf{Y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\varepsilon}, \tag{1}$$

where $\boldsymbol{\varepsilon}$ is the vector of residuals with $\mathrm{E}(\boldsymbol{\varepsilon}) = \mathbf{0}$; $\boldsymbol{\beta}_1$ is the (7×1) vector comprised of the intercept, β_0, and the six main effects coefficients, $\beta_1, \ldots, \beta_6$; and $\boldsymbol{\beta}_2$ is the (15×1) vector of interaction effects coefficients, $\beta_{12}, \beta_{13}, \ldots, \beta_{56}$. If the experimenter employs the main effects model for estimation:

$$\mathbf{Y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \boldsymbol{\varepsilon}^*, \tag{2}$$

it is well known that the expected value of the least squares estimator $\hat{\boldsymbol{\beta}}_1$ of $\boldsymbol{\beta}_1$ is

$$\mathrm{E}(\hat{\boldsymbol{\beta}}_1) = \boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2, \tag{3}$$

where the (7×15) *alias matrix*, $\mathbf{A}$, is given by $\mathbf{A} = (\mathbf{X}_1'\mathbf{X}_1)^{-1} \times \mathbf{X}_1'\mathbf{X}_2$. The alias matrix for the 12-run Plackett–Burman design is shown in Table 1. Clearly, in view of (3), the many nonzero entries in $\mathbf{A}$ are a concern. If any interaction effects are nonzero, the estimates of main effects will be biased. Following Bursztyn and Steinberg (2006), an omnibus measure of the potential for bias is given by the sum of squares of the entries in $\mathbf{A}$, which can be computed as $\mathrm{Trace}(\mathbf{A}'\mathbf{A})$. For the 12-run Plackett–Burman design, $\mathrm{Trace}(\mathbf{A}'\mathbf{A}) = 60/9 = 6.6667$.

A second design under consideration by the experimenter, produced using methods to be described in Sections 2 and 3, is shown in Table 2. The alias matrix for this design is displayed in Table 3. From Table 3, we see that all of the entries in the alias matrix corresponding to main effects β_1 through β_6 are zero. As a result, the experimenter's main effects estimates will be unbiased in the presence of any active two-factor interactions. The squared norm of the alias matrix is $\mathrm{Trace}(\mathbf{A}'\mathbf{A}) = 6/9 = 0.6667$, a 90% reduction compared to the Plackett–Burman design. These reductions in potential bias do come with a cost: relative to the Plackett–Burman design, the D-efficiency [defined below in (4)] of the alternative design is

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Photolithography Example Revisited

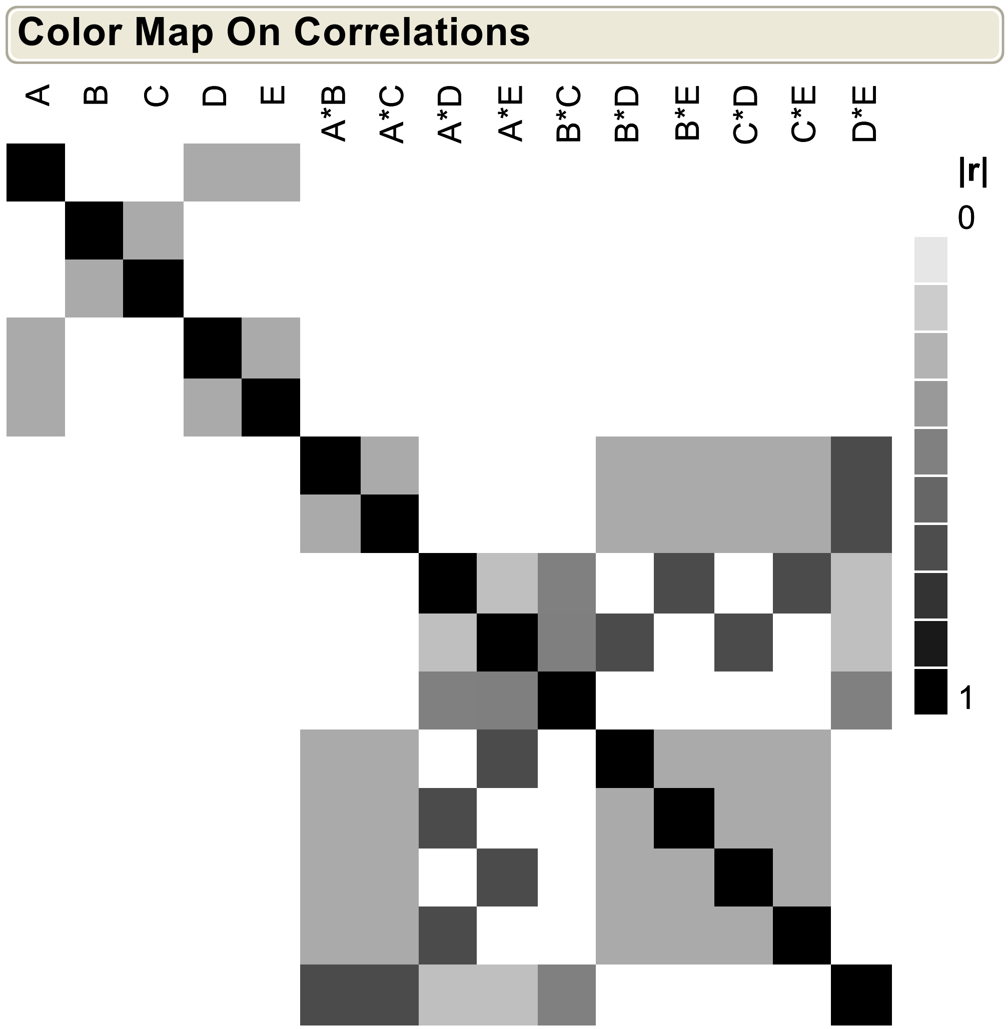
We showed the results of a photolithography study that was a full factorial design with 5 factors at 2 levels each.

Suppose that it was necessary to perform a 12 run screening experiment instead.

The D-optimal design is the orthogonal 12 run design that is isomorphic to the Plackett-Burman design.

We compare the performance of this design with the alias optimal design.

JMP Demo



Color Map On Correlations
A
B
C
D
E
A*B
A*C
A*D
A*E
B*C
B*D
B*E
C*D
C*E
D*E
|r|
0
1

Number of Orthogonal Designs versus Number of Factors

Number of Factors	Number of Different Orthogonal Designs
6	27
7	55
8	80
9	87
10	78
11	58
12	36
13	18
14	10
15	5

Alternatives to resolution IV screening designs in 16 runs

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Abstract: The resolution IV regular fractional factorial designs in 16 runs for six, seven, and eight factors are in standard use. They are economical and provide clear estimates of main effects when three-factor and higher-order interactions are negligible. However, because the two-factor interactions are completely confounded, experimenters are frequently required to augment the original fraction with new runs to resolve ambiguities in interpretation. We identify non-regular orthogonal fractions in 16 runs for these situations that have no complete confounding of two-factor interactions. These designs allow for the unambiguous estimation of models containing both main effects and a few two-factor interactions. We present the rationale behind the selection of these designs from the non-isomorphic 16-run fractions and illustrate how to use them with an example from the literature.

What if we are not willing to give up orthogonal main effects?

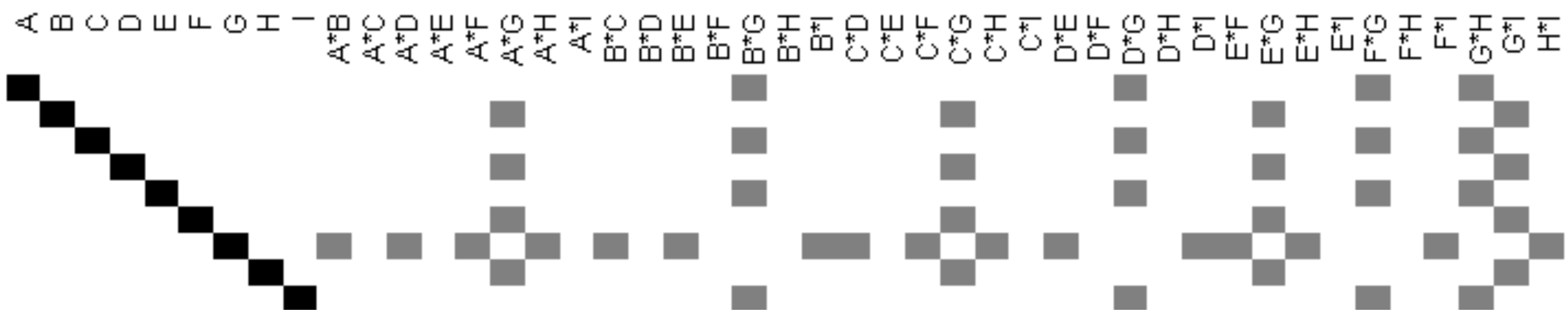
- For 9 to 14 factors and 16 runs the alias optimal criterion can generate orthogonal designs with
  - No complete confounding of main effects and two-factor interactions.
  - We call these designs “no confounding” designs

Recommended 9 Factor Design

Design

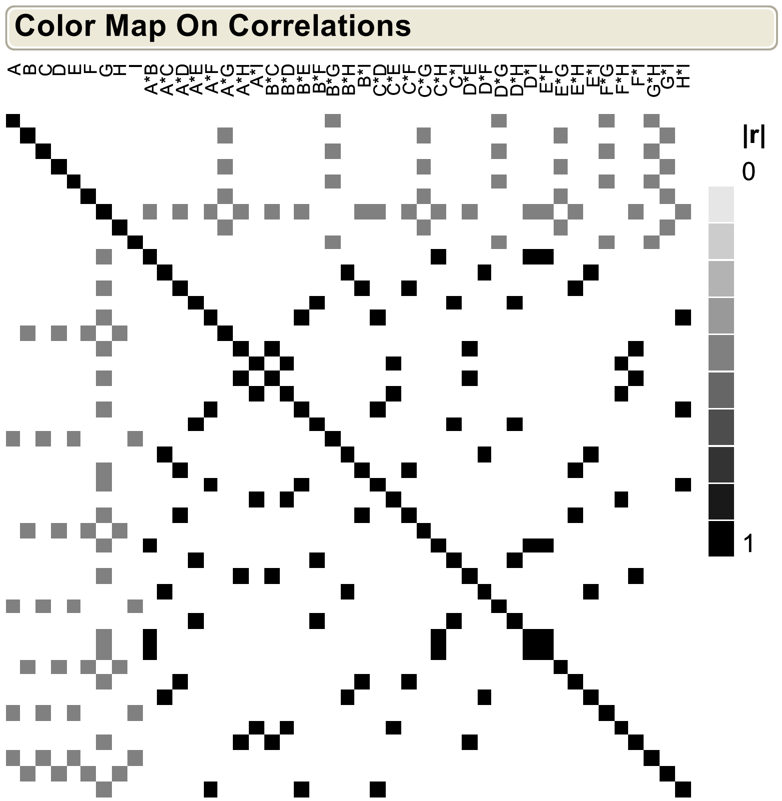
Run	A	B	C	D	E	F	G	H	I
1	-1	-1	-1	-1	1	1	-1	1	-1
2	1	-1	-1	-1	1	-1	1	-1	1
3	-1	-1	1	-1	-1	-1	-1	-1	-1
4	1	1	-1	-1	-1	-1	1	1	-1
5	1	-1	-1	1	-1	1	-1	-1	-1
6	1	-1	1	-1	-1	1	1	1	1
7	1	1	1	-1	1	1	-1	-1	-1
8	-1	1	-1	-1	-1	1	1	-1	1
9	-1	-1	-1	1	-1	-1	-1	1	1
10	-1	-1	1	1	1	1	1	-1	1
11	1	1	-1	1	1	1	-1	1	1
12	1	-1	1	1	1	-1	1	1	-1
13	1	1	1	1	-1	-1	-1	-1	1
14	-1	1	-1	1	1	-1	1	-1	-1
15	-1	1	1	1	-1	1	1	1	-1
16	-1	1	1	-1	1	-1	-1	1	1

Absolute Column Correlations: White = 0 Grey = 0.5

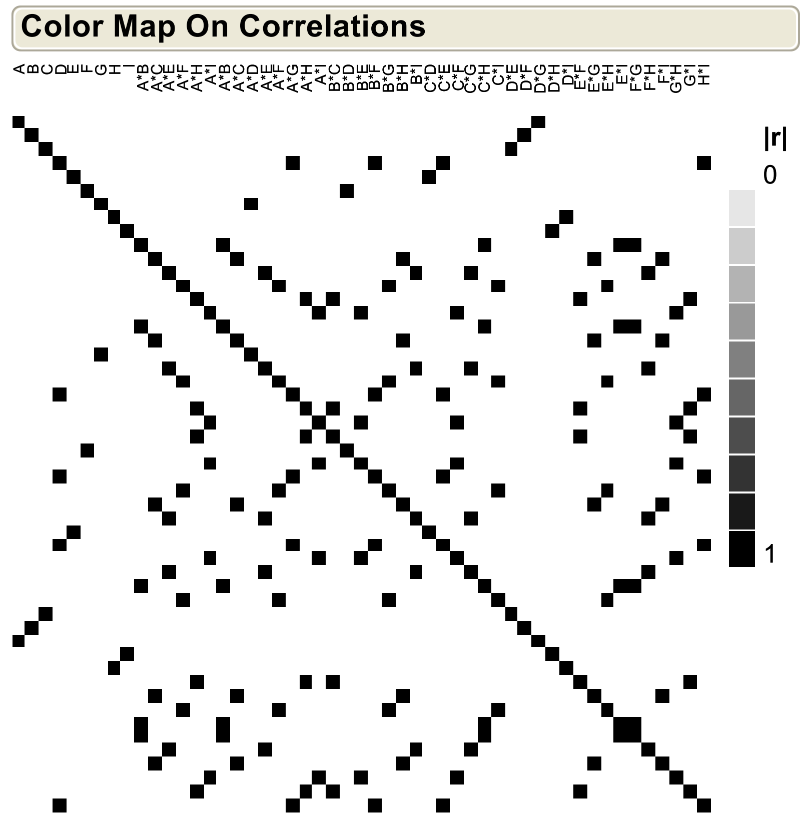


JMP Demo

Alias Optimal



Standard Fractional Factorial



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

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Screening designs are attractive for assessing the relative impact of a large number of factors on a response of interest. Experimenters often prefer quantitative factors with three levels over two-level factors because having three levels allows for some assessment of curvature in the factor–response relationship. Yet, the most familiar screening designs limit each factor to only two levels. We propose a new class of designs that have three levels, provide estimates of main effects that are unbiased by any second-order effect, require only one more than twice as many runs as there are factors, and avoid confounding of any pair of second-order effects. Moreover, for designs having six factors or more, our designs allow for the efficient estimation of the full quadratic model in any three factors. In this respect, our designs may render follow-up experiments unnecessary in many situations, thereby increasing the efficiency of the entire experimentation process. We also provide an algorithm for design construction.

Key Words: Alias; Confounding; Coordinate Exchange Algorithm; D-Efficiency; Response Surface Designs; Robust Designs; Screening Designs.

Definitive Screening Designs

Engineers often prefer designs for quantitative factors to have three levels. Yet the most familiar screening designs are two-level designs.

Definitive screening designs are three-level designs for quantitative factors with some very nice properties.

Robust Screening Design Properties

1. The number of required runs is only one more than twice the number of factors.
2. Unlike resolution III designs, main effects are completely independent of two-factor interactions. As a result, estimates of main effects are not biased by the presence of active two-factor interactions, regardless of whether the interactions are included in the model.
3. Unlike resolution IV designs, two-factor interactions are not completely confounded with other two-factor interactions, although they may be correlated.
4. Unlike resolution III, IV and V designs with added center points, all quadratic effects are estimable in models comprised of any number of linear and quadratic main effects terms.
5. Quadratic effects are orthogonal to main effects and not completely confounded (though correlated) with interaction effects.
6. With six or more factors, the designs are capable of estimating all possible full quadratic models involving three or fewer factors.

Robust Screening Design Structure

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

Definitive Screening Designs for 4 to 12 Factors

m = 4

```
1   0+--
2   0-++
3   -0-+
4   +0+-
5   --0-
6   ++0+
7   -++0
8   +--0
9   0000
```

m = 5

```
1   0++--
2   0--++
3   +0--+
4   -0++-
5   +-0+-
6   -+0-+
7   +-+0+
8   -+-0-
9   ++++0
10  ----0
11  00000
```

m = 6

```
1   0+----
2   0-++++
3   +0-++-
4   -0+--+
5   --0+--
6   ++0-++
7   -++0+-
8   +--0-+
9   +-+-0-
10  -+-+0+
11  ++++-0
12  ----+0
13  000000
```

m = 7

```
1   0+-+-+-
2   0-+-+-+
3   -0+-++-
4   +0-+--+
5   +-0++++
6   -+0----
7   +--0+--
8   -++0-++
9   --++0--
10  ++--0++
11  -+-++0+
12  +-+--0-
13  +++++-0
14  -----+0
15  0000000
```

m = 8

```
1   0-++-+++
2   0+--+---
3   -0-++++-
4   +0+----+
5   --0++--+
6   ++0--++-
7   +-+0++--
8   -+-0--++
9   --+-0-+-
10  ++-+0+-+
11  +---+0++
12  -+++-0--
13  -++-++0+
14  +--+--0-
15  +++++-+0
16  -----+-0
17  00000000
```

m = 9

```
1   0++++++++
2   0--------
3   +0+-+--+-
4   -0-+-++-+
5   -+0-+-+--
6   +-0+-+-++
7   --+0+---+
8   ++-0-+++-
9   +-+-0++--
10  -+-+0--++
11  ----+0+++
12  ++++-0---
13  ++--++0-+
14  --++--0+-
15  ---+++-0-
16  +++---+0+
17  -++--+-+0
18  +--++-+-0
19  000000000
```

m = 10

```
1   0++-++++-+
2   0--+----+-
3   +0-++-++--
4   -0+--+--++
5   -+0---+---
6   +-0+++-+++
7   -++0+--++-
8   +--0-++--+
9   ----0++++-
10  ++++0----+
11  -+-++0+-++
12  +-+--0-+--
13  ++----0+++
14  --++++0---
15  ++++-++0+-
16  ----+--0-+
17  ++--++--0-
18  --++--++0+
19  +-+-+-+-+0
20  -+-+-+-+-0
21  0000000000
```

m = 11

```
1   0-+-----+-+
2   0+-+++++-+-
3   -0--+----++
4   +0++-++++--
5   --0++++---+
6   ++0----+++-
7   ---0-++-++-
8   +++0+--+--+
9   +--+0+-++++
10  -++-0-+----
11  --++-0-+-+-
12  ++--+0+-+-+
13  ---++-0++--
14  +++--+0--++
15  -+++--+0+++
16  +---++-0---
17  -+---+-+0-+
18  +-+++-+-0+-
19  +-----++-0+
20  -+++++--+0-
21  ++-+------0
22  --+-++++++0
23  00000000000
```

m = 12

```
1   0--+-+-+++-+
2   0++-+-+---+-
3   -0+++++++---
4   +0-------+++
5   ++0-++-++-++
6   --0+--+--+--
7   +--0+-+-+--+
8   -++0-+-+-++-
9   ++++0-++++++
10  ----0+------
11  +-+-+0++-+-+
12  -+-+-0--+-+-
13  ++++-+0----+
14  ----+-0++++-
15  --+++--0--++
16  ++---++0++--
17  +-++++--0++-
18  -+----++0--+
19  ++-++--+-0--
20  --+--++-+0++
21  -+-++++--+0+
22  +-+----++-0-
23  +--+-+++--+0
24  -++-+---++-0
25  000000000000
```

Definitive Screening Data Using Five Columns from the Six Factor Design

Design

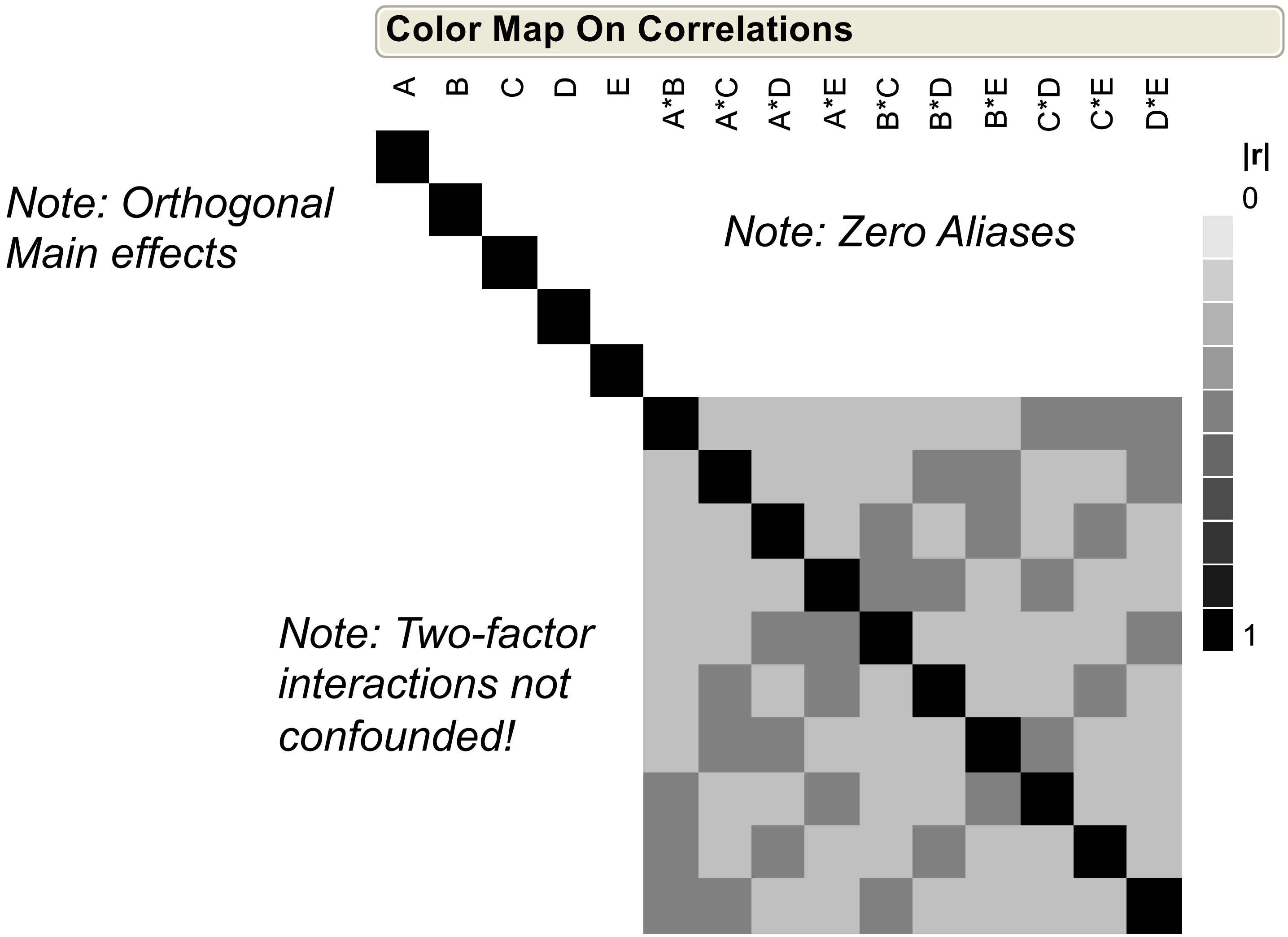
Run	A	B	C	D	E	Yield
1	0	-1	-1	-1	-1	8
2	0	1	1	1	1	50
3	-1	0	-1	1	-1	21
4	1	0	1	-1	1	39
5	1	1	0	-1	-1	60
6	-1	-1	0	1	1	14
7	-1	1	1	0	-1	42
8	1	-1	-1	0	1	12
9	-1	-1	1	-1	0	14
10	1	1	-1	1	0	54
11	1	-1	1	1	-1	20
12	-1	1	-1	-1	1	34
13	0	0	0	0	0	28

Alias Matrix

Alias Matrix

Effect	A*B	A*C	A*D	A*E	B*C	B*D	B*E	C*D	C*E	D*E
Intercept	0	0	0	0	0	0	0	0	0	0
A	0	0	0	0	0	0	0	0	0	0
B	0	0	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0	0	0
D	0	0	0	0	0	0	0	0	0	0
E	0	0	0	0	0	0	0	0	0	0

Definitive Screening Correlation Map



Definitive Screening Coefficient Variances

Relative Variance of Coefficients

Significance Level	0.05
Signal to Noise Ratio	2

Effect	Variance	Power
Intercept	0.077	1
A	0.1	1
B	0.1	1
C	0.1	1
D	0.1	1
E	0.1	1

Definitive Screening Main-Effects Model

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	30.461538	1.3637	22.34	<.0001 *
A	6	1.554858	3.86	0.0062 *
B	17.2	1.554858	11.06	<.0001 *
C	3.6	1.554858	2.32	0.0538
D	0.4	1.554858	0.26	0.8044
E	-0.2	1.554858	-0.13	0.9013

Definitive Screening Stepwise Result

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	30.461538	0.506978	60.08	<.0001 *
A	6	0.578044	10.38	<.0001 *
B	17.2	0.578044	29.76	<.0001 *
C	3.6	0.578044	6.23	0.0003 *
B*A	4.25	0.646273	6.58	0.0002 *

Module 3 - Conclusions

- The traditional approach to screening is to use regular fractional factorial designs.
- Recent research in design has found alternative designs that are strong competitors to these designs.
- In any case where two-factor interactions are likely and you cannot afford to run a resolution V design, these new designs are preferred.

Explorers 2011 – Final Thoughts

1. Optimal design framework is general and powerful for handling all kinds of DOX problems.
2. Modern software makes it easy to generate optimal designs for virtually any problem incorporating constraints on
    1. Factor combinations
    2. Model requirements
    3. Restrictions on sample size
    4. Restrictions on randomization
3. It is time to break away from traditional methods
4. Make the design fit the problem don't force your problem into the constraints of a classical design.

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