jmp™

Release 8

Design of Experiments

"The real voyage of discovery consists not in seeking new landscapes, but in having new eyes."

Marcel Proust

8.0.1

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Chapter **1**

Introduction to Designing Experiments

A Beginner's Tutorial

This tutorial chapter introduces you to the design of experiments (DOE) using JMP's custom designer. It gives a general understanding of how to design an experiment using JMP. Refer to subsequent chapters in this book for more examples and procedures on how to design an experiment for your specific project.

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About Designing Experiments

Increasing productivity and improving quality are important goals in any business. The methods for determining *how* to increase productivity and improve quality are evolving. They have changed from costly and time-consuming trial-and-error searches to the powerful, elegant, and cost-effective statistical methods that JMP provides.

Designing experiments in JMP is centered around factors, responses, a model, and runs. JMP helps you determine if and how a factor affects a response.

My First Experiment

If you have never used JMP to design an experiment, this section shows you how to design the experiment and how to understand JMP's output.

Tip: The recommended way to create an experiment is to use the custom designer. JMP also provides classical designs for use in textbook situations.

The Situation

Your goal is to find the best way to microwave a bag of popcorn. Because you have some experience with this, it is easy to decide on reasonable ranges for the important factors:

- how long to cook the popcorn (between 3 and 5 minutes)
- what level of power to use on the microwave oven (between settings 5 and 10)
- which brand of popcorn to use (Top Secret or Wilbur)

When a bag of popcorn is popped, most of the kernels pop, but some remain unpopped. You prefer to have all (or nearly all) of the kernels popped and no (or very few) unpopped kernels. Therefore, you define "the best popped bag" based on the ratio of popped kernels to the total number of kernels.

A good way to improve any procedure is to conduct an experiment. For each experimental run, JMP's custom designer determines which brand to use, how long to cook each bag in the microwave and what power setting to use. Each *run* involves popping one bag of corn. After popping a bag, enter the total number of kernels and the number of popped kernels into the appropriate row of a JMP data table. After doing all the experimental runs, use JMP's model fitting capabilities to do the data analysis. Then, you can use JMP's profiling tools to determine the optimal settings of popping time, power level, and brand.

Step 1: Design the Experiment

The first step is to select **DOE > Custom Design** (Figure 1.1). Then, define the responses and factors.

Figure 1.1 Select the Custom Designer
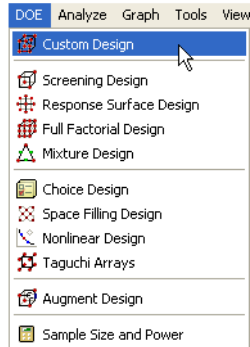
Define the Responses: Popped Kernels and Total Kernels

There are two responses in this experiment:

• the number of popped kernels
• the total number of kernels in the bag. After popping the bag add the number of unpopped kernels to the number of popped kernels to get the total number of kernels in the bag.

By default, the custom designer contains one response labeled Y (Figure 1.2).

Figure 1.2 Open and Close the Responses Panel by Clicking the Disclosure Icon
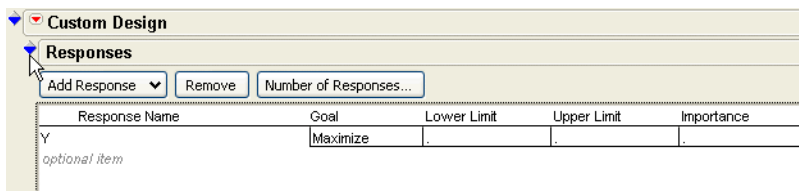
You want to add a second response to the Responses panel and change the names to be more descriptive:

1 To rename the Y response, double-click the name and type "Number Popped." Since you want to increase the number of popped kernels, leave the goal at **Maximize**.
2 To add the second response (total number of kernels), click **Add Response** and choose **None** from the menu that appears. JMP labels this response Y2 by default.
3 Double-click Y2 and type "Total Kernels" to rename it.

The completed Responses panel looks like Figure 1.3.

Figure 1.3 Renamed Responses with Specified Goals
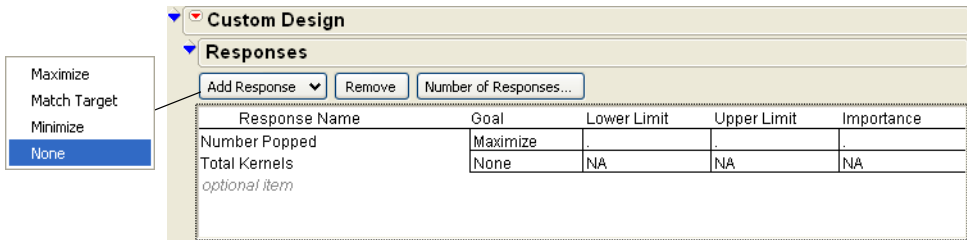
Define the Factors: Time, Power, and Brand

In this experiment, the factors are:

- brand of popcorn (Top Secret or Wilbur)
- cooking time for the popcorn (3 or 5 minutes)
- microwave oven power level (setting 5 or 10)

In the Factors panel, add Brand as a two-level categorical factor:

1 Click **Add Factor** and select **Categorical > 2 Level**.

2 To change the name of the factor (currently named X1), double-click on its name and type Brand.

3 To rename the default levels (L1 and L2), click the level names and type Top Secret and Wilbur.

Add Time as a two-level continuous factor:

4 Click **Add Factor** and select **Continuous**.

5 Change the default name of the factor (X2) by double-clicking it and typing Time.

6 Likewise, to rename the default levels (–1 and 1) as 3 and 5, click the current level name and type in the new value.

Add Power as a two-level continuous factor:

7 Click **Add Factor** and select **Continuous**.

8 Change the name of the factor (currently named X3) by double-clicking it and typing Power.

9 Rename the default levels (currently named **-1** and **1**) as 5 and 10 by clicking the current name and typing. The completed Factors panel looks like Figure 1.4.

Figure 1.4 Renamed Factors with Specified Values
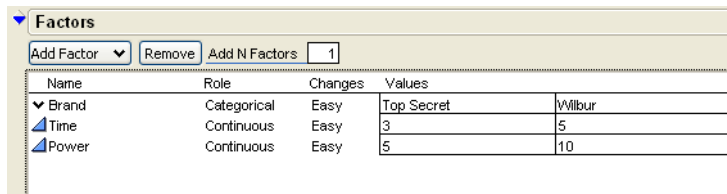
10 Click **Continue**.

Step 2: Define Factor Constraints

The popping time for this experiment is either 3 or 5 minutes, and the power settings on the micro-wave are 5 and 10. From experience, you know that

- popping corn for a long time on a high setting tends to scorch kernels.
- not many kernels pop when the popping time is brief and the power setting is low.

You want to constrain the combined popping time and power settings to be less than or equal to 13, but greater than or equal to 10. To define these limits:

1 Open the Constraints panel by clicking the disclosure button beside the **Define Factor Constraints** title bar (see Figure 1.5).

2 Click the **Add Constraint** button twice, once for each of the known constraints.

3 Complete the information, as shown to the right in Figure 1.5. These constraints tell the Custom Designer to avoid combinations of **Power** and **Time** that sum to less than 10 and more than 13. Be sure to change **<=** to **>=** in the second constraint.

The area inside the parallelogram, illustrated on the left in Figure 1.5, is the allowable region for the runs. You can see that popping for 5 minutes at a power of 10 is not allowed and neither is popping for 3 minutes at a power of 5.

Figure 1.5 Defining Factor Constraints
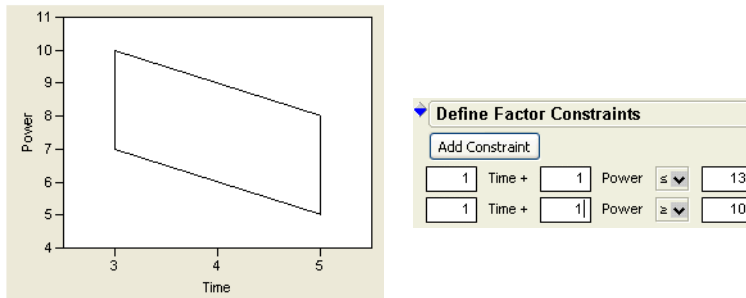
Step 3: Add Interaction Terms

You are interested in the possibility that the effect of any factor on the proportion of popped kernels may depend on the value of some other factor. For example, the effect of a change in popping time for the Wilbur popcorn brand could be larger than the same change in time for the Top Secret brand. This kind of synergistic effect of factors acting in concert is called a *two-factor interaction*. You can examine all possible two-factor interactions in your *a priori* model of the popcorn popping process.

1 Click **Interactions** in the Model panel and select **2nd**. JMP adds two-factor interactions to the model as shown to the left in Figure 1.6.

In addition, you suspect the graph of the relationship between any factor and any response might be curved. You can see whether this kind of curvature exists with a quadratic model formed by adding the second order powers of effects to the model, as follows.

2 Click **Powers** and select **2nd** to add quadratic effects of the continuous factors, **Power** and **Time**.

The completed Model should look like the one to the right in Figure 1.6.

Figure 1.6 Add Interaction and Power Terms to the Model
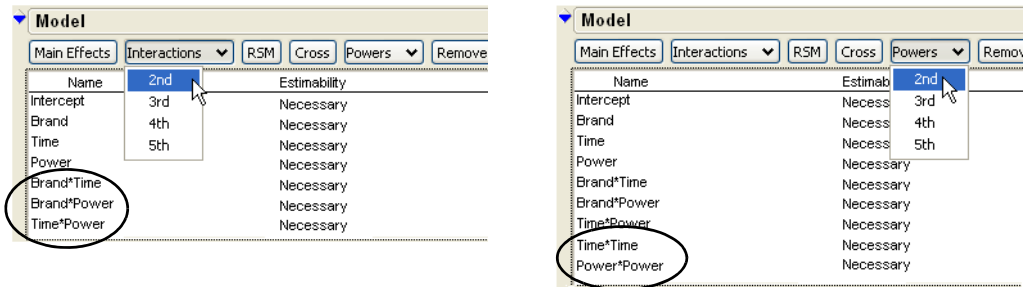
Step 4: Determine the Number of Runs

The Design Generation panel in Figure 1.7 shows the minimum number of runs needed to perform the experiment with the effects you've added to the model. You can use that minimum or the default number of runs, or you can specify your own number of runs as long as that number is more than the minimum. JMP has no restrictions on the number of runs you request. For this example, use the default number of runs, 16. Click **Make Design** to continue.

Figure 1.7 Model and Design Generation Panels
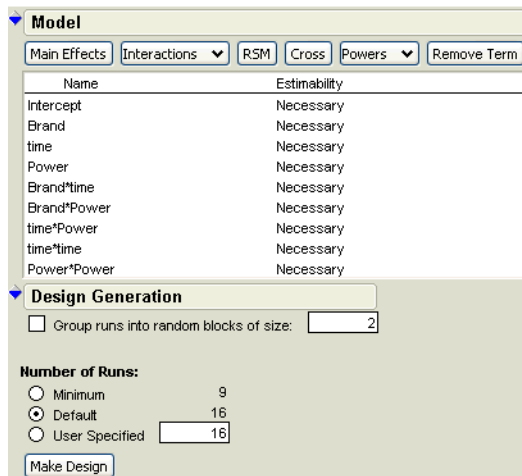
Step 5: Check the Design

When you click **Make Design**, JMP generates and displays a design, as shown on the left in Figure 1.8. Note that because JMP uses a random seed to generate custom designs and there is no unique optimal design for this problem, your table may be different than the one shown here. You can see in the table that the custom design requires 8 runs using each brand of popcorn.

Scroll to the bottom of the Custom Design window and look at the Output Options area (shown to the right in Figure 1.8. The Run Order option lets you designate the order you want the runs to appear in the data table when it is created. Keep the selection at Randomize so the rows (runs) in the output table appear in a random order.

Now click **Make Table** in the Output Options section.

Figure 1.8 Design and Output Options Section of Custom Designer
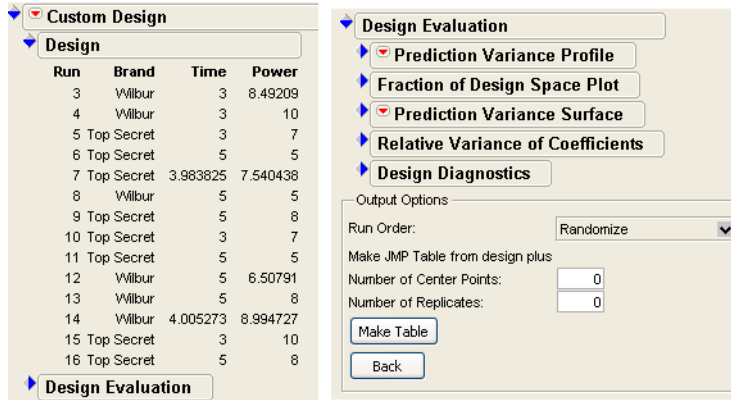
The resulting data table (Figure 1.9) shows the order in which you should do the experimental runs and provides columns for you to enter the number of popped and total kernels. According to the table, cook the first bag of Top Secret for five minutes using a power setting of eight (rounded value). Next, cook a bag of Wilbur for five minutes at a power of eight, then cook Top Secret for three minutes using a power setting of seven, and so forth.

You do not have fractional control over the power and time settings on a microwave oven, so you should round the power and time settings, as shown in the data table. Although this altered design is slightly less optimal than the one the custom designer suggested, the difference is negligible.

Tip: Note that optionally, before clicking **Make Table** in the Output Options, you could select **Sort Left to Right** in the Run Order menu to have JMP present the results in the data table according to the brand. We have conducted this experiment for you and placed the results, called Popcorn DOE Results.jmp, in the Sample Data folder installed with JMP. These results have the columns sorted from left to right

Figure 1.9 JMP Data Table of Design Runs Generated by Custom Designer

	Brand	Time	Power	Number Popped	Total Kernels
1	Top Secret	5	8	.	.
2	Wilbur	5	8	.	.
3	Top Secret	3	7	.	.
4	Top Secret	3	10	.	.
5	Wilbur	3	10	.	.
6	Wilbur	5	5	.	.
7	Wilbur	4	6	.	.
8	Top Secret	5	8	.	.
9	Top Secret	3	7	.	.
10	Top Secret	5	5	.	.
11	Wilbur	3	7	.	.
12	Wilbur	3	8	.	.
13	Wilbur	4	9	.	.
14	Wilbur	5	7	.	.
15	Top Secret	4	7	.	.
16	Top Secret	3	10	.	.

Step 6: Gather and Enter the Data

Pop the popcorn according to the design JMP provided. Then, count the number of popped and unpopped kernels left in each bag. Finally, enter the numbers shown below into the appropriate columns of the data table.

We have conducted this experiment for you and placed the results in the Sample Data folder installed with JMP. To see the results, open Popcorn DOE Results.jmp from the Design Experiment folder in the sample data. The data table is shown in Figure 1.10.

Figure 1.10 Results of the Popcorn DOE Experiment

	Brand	Time	Power	Number Popped	Total Kernels
1	Top Secret	3	7	30	420
2	Top Secret	3	7	120	420
3	Top Secret	3	10	120	400
4	Top Secret	4	8	250	430
5	Top Secret	5	5	370	420
6	Top Secret	5	5	400	420
7	Top Secret	5	8	350	420
8	Top Secret	5	8	370	380
9	Wilbur	3	7	374	400
10	Wilbur	3	8	340	440
11	Wilbur	3	10	20	410
12	Wilbur	4	6	440	460
13	Wilbur	4	9	340	400
14	Wilbur	5	5	170	370
15	Wilbur	5	7	370	380
16	Wilbur	5	8	420	450

scripts to analyze data

results from experiment

Step 7: Analyze the Results

After the experiment is finished and the number of popped kernels and total kernels have been entered into the data table, it is time to analyze the data. The design data table has a script, labeled **Model**, that shows in the top left panel of the table. When you created the design, a standard least squares analysis was stored in the **Model** script with the data table.

1   Click the red triangle for **Model** and select **Run Script**.

The default fitting personality in the model dialog is **Standard Least Squares**. One assumption of standard least squares is that your responses are normally distributed. But because you are modeling the proportion of popped kernels it is more appropriate to assume that your responses come from a binomial distribution. You can use this assumption by changing to a generalized linear model.

2   Change the Personality to **Generalized Linear Model**, Distribution to **Binomial**, and Link Function to **Logit**, as shown in Figure 1.11.

Figure 1.11 Fitting the Model
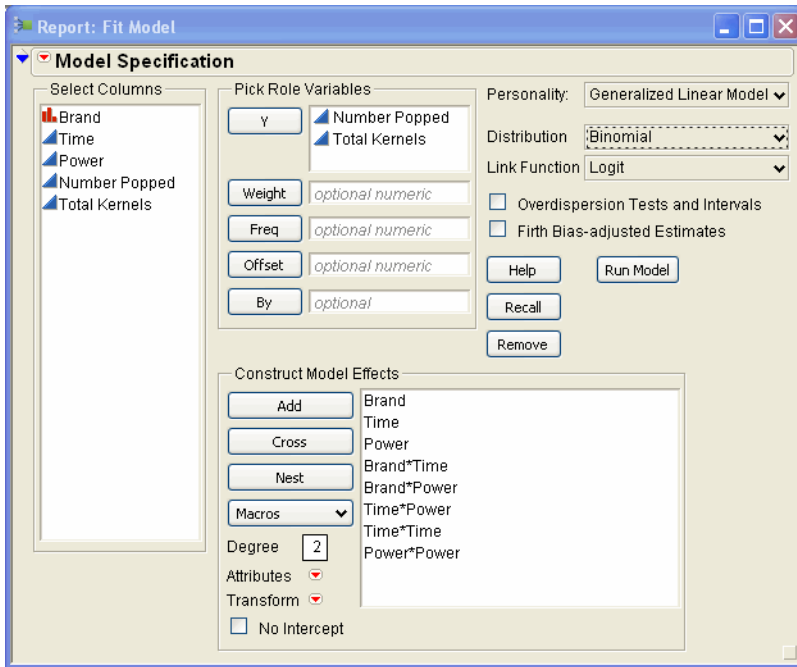
3   Click **Run Model**.
4   Scroll down to view the Effect Tests table (Figure 1.12) and look in the column labeled Prob>Chisq. This column lists *p*-values. A low *p*-value (a value less than 0.05) indicates that results are statistically significant. There are asterisks that identify the low *p*-values. You can therefore conclude that, in this experiment, all the model effects except for **Time*Time** are highly significant. You have confirmed that there is a strong relationship between popping time (**Time**), microwave setting (**Power**), popcorn brand (**Brand**), and the proportion of popped kernels.

Figure 1.12 Investigating *p*-Values

Effect Tests

		L-R	
Source	DF	ChiSquare	Prob>ChiSq
Brand	1	85.470408	<.0001*
Time(3,5)	1	717.99922	<.0001*
Power(5,10)	1	12.782254	0.0003*
Brand*Time	1	435.97692	<.0001*
Brand*Power	1	39.480267	<.0001*
Time*Power	1	7.8264948	0.0051*
Time*Time	1	3.3027281	0.0692
Power*Power	1	19.011628	<.0001*

p-values indicate significance.
Values with * beside them are
p-values that indicate the results
are statistically significant.

To further investigate, use the Prediction Profiler to see how changes in the factor settings affect the numbers of popped and unpopped kernels:

1   Choose **Profilers > Profiler** from the red triangle menu on the Generalized Linear Model Fit title bar. The Prediction Profiler is shown at the bottom of the report. Figure 1.13 shows the Prediction Profiler for the popcorn experiment. Prediction traces are displayed for each factor.

Figure 1.13 The Prediction Profiler

Disclosure icon to open or close the Prediction Profiler

Prediction trace for Brand

Prediction trace for Time

Prediction trace for Power

predicted value of the response

95% confidence interval on the mean response

Factor values (here, time = 4)
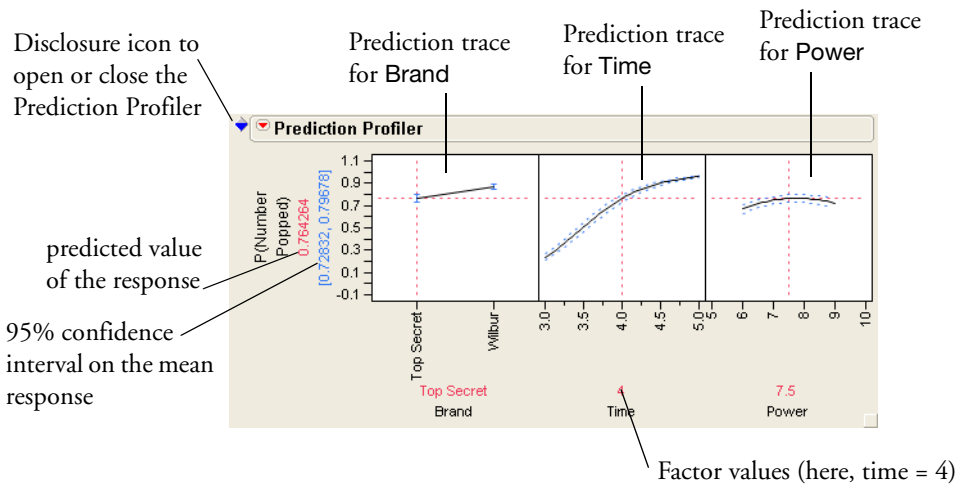
2   Move the vertical red dotted lines to see the effect that changing a factor value has on the response. For example, drag the red line in the Time graph right and left (Figure 1.14).

Figure 1.14 Moving the Time Value from 4 to Near 5
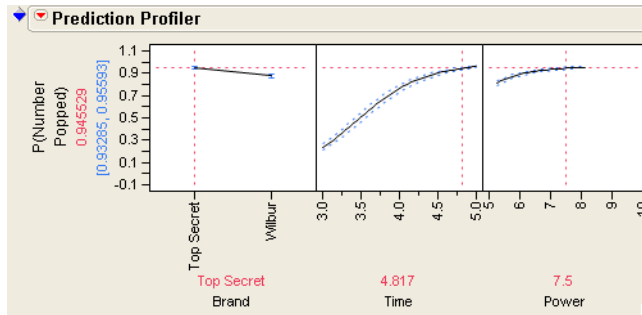
As Time increases and decreases, the curved Time and Power prediction traces shift their slope and maximum/minimum values. The substantial slope shift tells you there is an interaction (synergistic effect) involving Time and Power.

Furthermore, the steepness of a prediction trace reveals a factor's importance. Because the prediction trace for Time is steeper than that for Brand or Power (see Figure 1.14), you can see that cooking time is more important than the brand of popcorn or the microwave power setting.

Now for the final steps.

3   Click the red triangle icon in the Prediction Profiler title bar and select **Desirability Functions**.
4   Click the red triangle icon in the Prediction Profiler title bar and select **Maximize Desirability**. JMP automatically adjusts the graph to display the optimal settings at which the most kernels will be popped (Figure 1.15).

Our experiment found how to cook the bag of popcorn with the greatest proportion of popped kernels: use Top Secret, cook for five minutes, and use a power level of 8. The experiment predicts that cooking at these settings will yield greater than 96.5% popped kernels.

Figure 1.15 The Most Desirable Settings
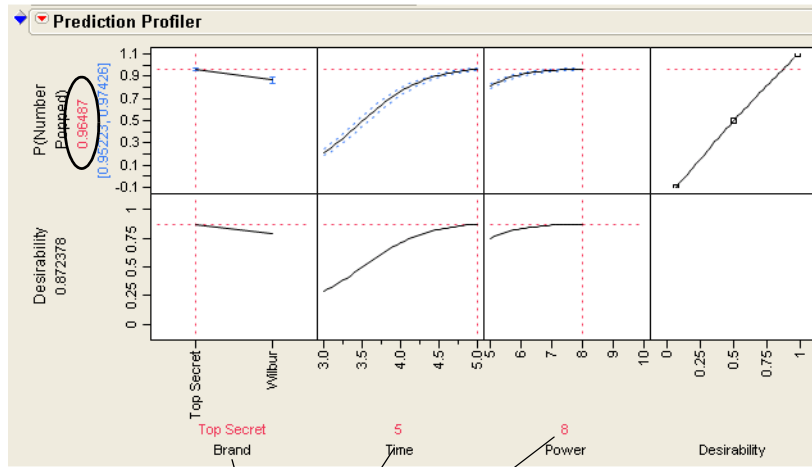
The best settings are:

- the Top Secret brand
- cooking time at 5
- power set at 8

Examples Using the Custom Designer

The use of statistical methods in industry is increasing. Arguably, the most cost-beneficial of these methods for quality and productivity improvement is statistical design of experiments. A trial-and -error search for the *vital few* factors that most affect quality is costly and time-consuming. The purpose of *experimental design* is to characterize, predict, and then improve the behavior of any system or process. Designed experiments are a cost-effective way to accomplish these goals.

JMP's custom designer is the recommended way to describe your process and create a design that works for your situation. To use the custom designer, you first enter the process variables and constraints, then JMP tailors a design to suit your unique case. This approach is more general and requires less experience and expertise than previous tools supporting the statistical design of experiments.

Custom designs accommodate any number of factors of any type. You can also control the number of experimental runs. This makes custom design more flexible and more cost effective than alternative approaches.

This chapter presents several examples showing the use of custom designs. It shows how to drive its interface to build a design using this easy step-by-step approach:

Key engineering steps: process knowledge and engineering judgement are important.

Describe	Design	Collect	Fit	Predict
Identify factors and responses.	Compute design for maximum information from runs.	Use design to set factors: measure response for each run.	Compute best fit of mathematical model to data from test runs.	Use model to find best factor settings for on-target responses and minimum variability.

Key mathematical steps: appropriate computer-based tools are empowering.

Contents

Creating Screening Experiments

You can use the screening designer in JMP to create screening designs, but the custom designer is more flexible and general. The straightforward screening examples described below show that 'custom' does not mean 'exotic.' The custom designer is a general purpose design environment that can create screening designs.

Creating a Main-Effects-Only Screening Design

To create a main-effects-only screening design using the custom designer:

1 Select **DOE > Custom Design**.

2 Enter six continuous factors into the Factors panel (see "Step 1: Design the Experiment," p. 3, for details). Figure 2.1 shows the six factors.

3 Click **Continue**. The default model contains only the main effects.

4 Using the default of eight runs, click **Make Design**.

Note to DOE experts: The result is a resolution-three screening design. All the main effects are estimable, but they are confounded with two factor interactions.

Figure 2.1 A Main-Effects-Only Screening Design

5 Click the disclosure button (◆ ◆ on Windows/Linux and ▶ ▼ on the Macintosh) to open the Alias Matrix. Figure 2.2 shows the Alias Matrix, which is a table of zeros, ones, and negative ones.

The Alias Matrix shows how the coefficients of the constant and main effect terms in the model are biased by any active two-factor interaction effects not already added to the model. The column labels identify interactions. For example, the columns labeled **2 6** and **3 4** in the table have a 1 in the row for X1. This means that the expected value of the main effect of X1 is actually the sum of the main effect of X1 and the two-factor interactions X2*X6 and X3*X4. You are assuming that these interactions are negligible in size compared to the effect of X1.

Figure 2.2 The Alias Matrix

Effect	1 2	1 3	1 4	1 5	1 6	2 3	2 4	2 5	2 6	3 4	3 5	3 6	4 5	4 6	5 6
Intercept	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X1	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0
X2	0	0	0	0	1	0	0	0	0	0	0	0	-1	0	0
X3	0	0	1	0	0	0	0	0	0	0	0	0	0	0	-1
X4	0	1	0	0	0	0	0	-1	0	0	0	0	0	0	0
X5	0	0	0	0	0	0	-1	0	0	0	0	-1	0	0	0
X6	1	0	0	0	0	0	0	0	0	0	-1	0	0	0	0

Note to DOE experts: The Alias matrix is a generalization of the confounding pattern in fractional factorial designs.

Creating a Screening Design to Fit All Two-Factor Interactions

There is risk involved in designs for main effects only. The risk is that two-factor interactions, if they are strong, can confuse the results of such experiments. To avoid this risk, you can create experiments resolving all the two-factor interactions.

Note to DOE experts: The result in this example is a resolution-five screening design. Two-factor interactions are estimable but are confounded with three-factor interactions.

1 Select **DOE > Custom Design**.
2 Enter five continuous factors into the Factors panel (see "Step 1: Design the Experiment" in Chapter 1, for details).
3 Click **Continue**.
4 In the Model panel, select **Interactions > 2nd**.
5 In the Design Generation Panel choose Minimum for **Number of Runs** and click **Make Design**.

Figure 2.3 shows the runs of the two-factor design with all interactions. The sample size, 16 (a power of two) is large enough to fit all the terms in the model. The values in your table may be different from those shown below.

Figure 2.3 All Two-Factor Interactions

6 Click the disclosure button to open the **Design Evaluation** outlines, then open **Alias Matrix**.
Figure 2.4 shows the alias matrix table of zeros and ones. The columns labels identify an interaction.
For example, the column labelled 1 2 refers to the interaction of the first and second effect, the column labelled 2 3 refers to the interaction between the second and third effect, and so forth.

Look at the column labelled 1 2. There is only one value of 1 in that column. All others are 0. The 1 occurs in the row labelled X1*X2. All the other rows and columns are similar. This means that the expected value of the two-factor interaction X1*X2 is not biased by any other terms. All the rows above the row labelled X1*X2 contain only zeros, which means that the Intercept and main effect terms are not biased by any two-factor interactions.

Figure 2.4 Alias Matrix Showing all Two-Factor Interactions Clear of all Main Effects

A Compromise Design Between Main Effects Only and All Interactions

In a screening situation, suppose there are six continuous factors and resources for n = 16 runs. The first example in this section showed an eight-run design that fit all the main effects. With six factors, there are 15 possible two-factor interactions. The minimum number of runs that could fit the constant, six main effects and 15 two-factor interactions is 22. This is more than the resource budget of 16 runs. It would be good to find a compromise between the main-effects only design and a design capable of fitting all the two-factor interactions.

This example shows how to obtain such a design compromise using the custom designer.

1 Select **DOE > Custom Design**.
2 Define six continuous factors (X1 - X6).
3 Click **Continue**. The model includes the main effect terms by default. The default estimability of these terms is **Necessary**.
4 Click the **Interactions** button and choose **2nd** to add all the two-factor interactions.
5 Select all the interaction terms and click the current estimability (**Necessary**) to reveal a menu. Change **Necessary** to **If Possible**, as shown in Figure 2.5.

Figure 2.5 Model for Six-Variable Design with Two-Factor Interactions Designated If Possible
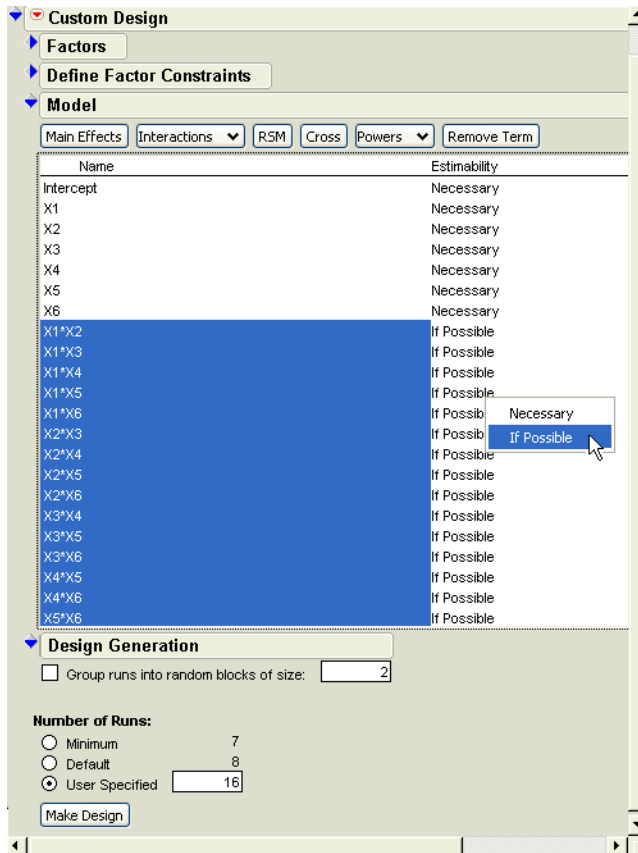
6 Type 16 in the **User Specified** edit box in the **Number of Runs** section, as shown. Although the

desired number of runs (16) is less than the total number of model terms, the custom designer builds a design to estimate as many two-factor interactions as possible.

7   Click **Make Design**.

After the custom designer creates the design, click the disclosure button beside Design Evaluation to open the Alias Matrix (Figure 2.6). The values in your table may be different from those shown below, but with a similar pattern.

Figure 2.6 Alias Matrix

Effect	12	13	14	15	16	23	24	25	26	34	35	36	45	46	56
Intercept	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X1*X2	0.333	0	0	0	0	0	0	0	0	0	0	0	0	0.333	0
X1*X3	0	0.333	0	0	0	0	0	0	0	0	0	0	0	0	0.333
X1*X4	0	0	0.333	0	0	0	0	0	0.333	0	0	0	0	0	0
X1*X5	0	0	0	0.333	0	0	0	0	0	0	0.333	0	0	0	0
X1*X6	0	0	0	0	0.25	0	0.25	0	0	0	0.25	0	0	0	0
X2*X3	0	0	0	0	0	0.333	0	0	0	0	0	0.333	0	0	0
X2*X4	0	0	0	0	0.25	0	0.25	0	0	0.25	0	0	0	0	0
X2*X5	0	0	0	0	0	0	0	0.333	0	0.333	0	0	0	0	0
X2*X6	0	0	0.333	0	0	0	0	0	0.333	0	0	0	0	0	0
X3*X4	0	0	0	0	0	0	0	0.333	0	0.333	0	0	0	0	0
X3*X5	0	0	0	0	0.25	0	0.25	0	0	0	0.25	0	0	0	0
X3*X6	0	0	0	0.333	0	0	0	0	0	0	0.333	0	0	0	0
X4*X5	0	0	0	0	0	0.333	0	0	0	0	0	0.333	0	0	0
X4*X6	0.333	0	0	0	0	0	0	0	0	0	0	0	0	0.333	0
X5*X6	0	0.333	0	0	0	0	0	0	0	0	0	0	0	0	0.333

All the rows above the row labelled X1*X2 contain only zeros, which means that the Intercept and main effect terms are not biased by any two-factor interactions. The row labelled X1*X2 has the value 0.333 in the 1 2 column and the same value in the 4 6 column. That means the expected value of the estimate for X1*X2 is actually the sum of X1*X2 and any real effect due to X4*X6.

Note to DOE experts: The result in this particular example is a resolution-four screening design. Two-factor interactions are estimable but are aliased with other two-factor interactions.

Creating 'Super' Screening Designs

This section shows how to use the technique shown in the previous example to create 'super' (supersaturated) screening designs. Supersaturated designs have fewer runs than factors, which makes them attractive for factor screening when there are many factors and experimental runs are expensive.

In a saturated design, the number of runs equals the number of model terms. In a supersaturated design, as the name suggests, the number of model terms exceeds the number of runs (Lin, 1993). A supersaturated design can examine dozens of factors using fewer than half as many runs as factors.

The Need for Supersaturated Designs

The 2^{7-4} and the 2^{15-11} fractional factorial designs available using the screening designer are both saturated with respect to a main effects model. In the analysis of a saturated design, you can (barely) fit the model, but there are no degrees of freedom for error or for lack of fit. Until recently, saturated designs represented the limit of efficiency in designs for screening.

Factor screening relies on the *sparsity* principle. The experimenter expects that only a few of the factors in a screening experiment are active. The problem is not knowing which are the vital few factors and which are the trivial many. It is common for brainstorming sessions to turn up dozens of factors. Yet, in practice, screening experiments rarely involve more than ten factors. What happens to winnow the list from dozens to ten or so?

If the experimenter is limited to designs that have more runs than factors, then dozens of factors translate into dozens of runs. Often, this is not economically feasible. The result is that the factor list is reduced without the benefit of data. In a supersaturated design, the number of model terms exceeds the number of runs, and you can examine dozens of factors using less than half as many runs.

There are drawbacks:

- If the number of *active* factors approaches the number of runs in the experiment, then it is likely that these factors will be impossible to identify. A rule of thumb is that the number of runs should be at least four times larger than the number of active factors. If you expect that there might be as many as five active factors, you should have at least 20 runs.

- Analysis of supersaturated designs cannot yet be reduced to an automatic procedure. However, using forward stepwise regression is reasonable and the new Screening platform (**Analyze** > **Modeling** > **Screening**) offers a more streamlined analysis.

Example: Twelve Factors in Eight Runs

As an example, consider a supersaturated design with twelve factors. Using model terms designated If Possible provides the software machinery for creating a supersaturated design.

In the last example, two-factor interaction terms were specified If Possible. In a supersaturated design, all terms—including main effects—are If Possible. Note in Figure 2.7, the only primary term is the intercept.

To see an example of a supersaturated design with twelve factors in eight runs:

1   Select **DOE > Custom Design**.
2   Add 12 continuous factors and click **Continue**.
3   Highlight all terms except the Intercept and click the current estimability (Necessary) to reveal the menu. Change Necessary to If Possible, as shown in Figure 2.7.

Figure 2.7 Changing the Estimability
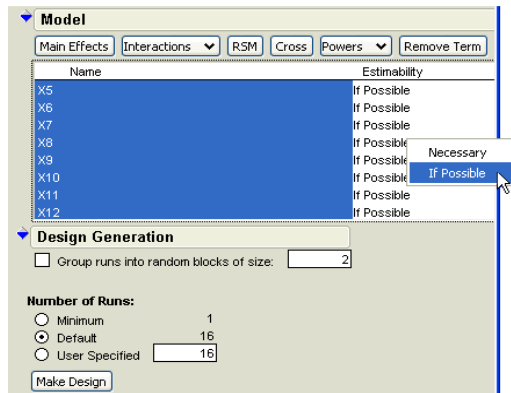
4   The desired number of runs is eight so type 8 in the User Specified edit box in the **Number of Runs** section.

5   Click the red triangle on the Custom Design title bar and select **Simulate Responses**, as shown in Figure 2.8.

Figure 2.8 Simulating Responses
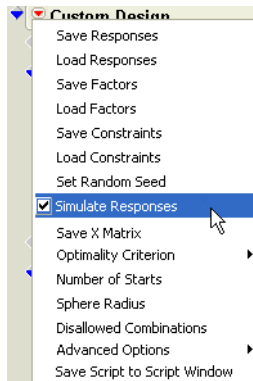
6   Click **Make Design**, then click **Make Table.** A window named Simulate Responses and a design table appear, similar to the one in Figure 2.9. The Y column values are controlled by the coefficients of the model in the Simulate Responses window. The values in your table may be different from those shown below.

Figure 2.9 Simulated Responses and Design Table

7 Change the default settings of the coefficients in the Simulate Responses dialog to match those in Figure 2.10 and click **Apply**. The numbers in the Y column change. Because you have set X2 and X10 as active factors in the simulation, the analysis should be able to identify the same two factors.

Note that random noise is added to the Y column formula, so the numbers you see might not necessarily match those in the figure. The values in your table may be different from those shown below.

Figure 2.10 Give Values to Two Main Effects and Specify the Standard Error as 0.5

To identify active factors using stepwise regression:

1 To run the Model script in the design table, click the red triangle beside **Model** and select **Run Script**.

2 Change the **Personality** in the Model Specification window from **Standard Least Squares** to **Stepwise**.

3 Click **Run Model** on the Fit Model dialog.

4 In the resulting display click the **Step** button two times. JMP enters the factors with the largest effects. From the report that appears, you should identify two active factors, X2 and X10, as shown in Figure 2.11. The step history appears in the bottom part of the report. Because random noise is added, your estimates will be slightly different from those shown below.

Figure 2.11 Stepwise Regression Identifies Active Factors

Note: This example defines two large main effects and sets the rest to zero. In real-world situations, it may be less likely to have such clearly differentiated effects.

Screening Designs with Flexible Block Sizes

When you create a design using the Screening designer (**DOE** > **Screening**), the available block sizes for the listed designs are a power of two. However, custom designs in JMP can have blocks of any size. The blocking example shown in this section is flexible because it is using three runs per block, instead of a power of two.

After you select **DOE > Custom Design** and enter factors, the blocking factor shows only one level in the Values section of the Factors panel because the sample size is unknown at this point. After you complete the design, JMP shows the appropriate number of blocks, which is calculated as the sample size divided by the number of runs per block.

For example, Figure 2.12 shows that when you enter three continuous factors and one blocking factor with three runs per block, only one block appears in the Factors panel.

Figure 2.12 One Block Appears in the Factors Panel
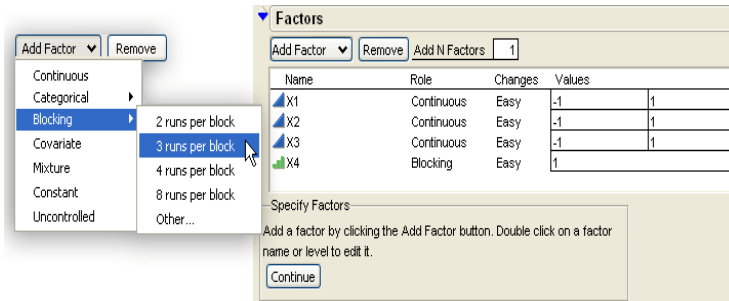
The default sample size of nine requires three blocks. After you click **Continue**, there are three blocks in the Factors panel (Figure 2.13). This is because the default sample size is nine, which requires three blocks with three runs each.

Figure 2.13 Three Blocks in the Factors Panel
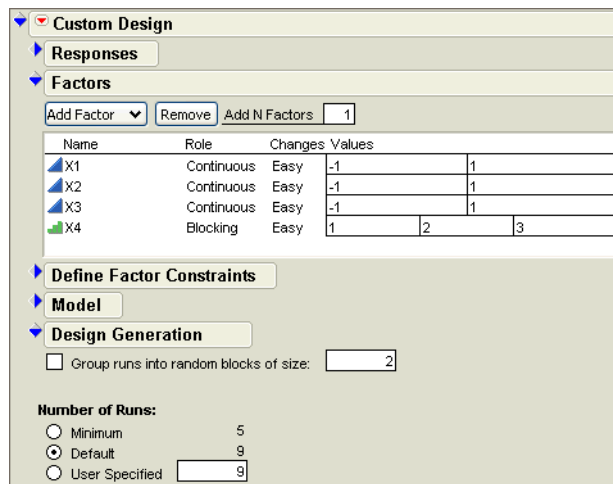
If you enter 24 runs in the User Specified box of the **Number of Runs** section, the Factors panel changes and now contains 8 blocks (Figure 2.14).

Figure 2.14 Number of Runs is 24 Gives Eight Blocks

If you add all the two-factor interactions and change the number of runs to 15, three runs per block produces five blocks (as shown in Figure 2.15), so the Factors panel displays five blocks in the Values section.

Figure 2.15 Changing the Runs to 15

Click **Make Design**, then click the disclosure button (◆ ◆ on Windows/Linux and ▶ ▼ on the Macintosh) to open the Relative Variance of Coefficients report. Figure 2.16 shows the variance of each coefficient in the model relative to the unknown error variance.

The values in your table may be slightly different from those shown below. Notice that the variance of each coefficient is about one-tenth the error variance and that all the variances are roughly the same size. The error variance is assumed to be 1.

Figure 2.16 Table of Relative Variance of the Model Coefficients

▼ Relative Variance of Coefficients		
Significance Level		0.050
Signal to Noise Ratio		1.000
Effect	**Variance**	**Power**
Intercept	0.070	0.802
X1	0.078	0.763
X2	0.106	0.638
X3	0.083	0.736
X4 1	0.099	0.668
X4 2	0.086	0.723
X4 3	0.085	0.731
X4 4	0.081	0.747
X1*X2	0.083	0.736
X1*X3	0.079	0.757
X2*X3	0.078	0.763

The main question here is whether the relative size of the coefficient variance is acceptably small. If not, adding more runs (18 or more) will lower the variance of each coefficient.

For more details, see "The Relative Variance of Coefficients and Power Table," p. 68.

Note to DOE experts: There are four rows associated with X4 (the block factor). That is because X4 has 5 blocks and, therefore, 4 degrees of freedom. Each degree of freedom is associated with one unknown coefficient in the model.

Checking for Curvature Using One Extra Run

In screening designs, experimenters often add center points and other check points to a design to help determine whether the assumed model is adequate. Although this is good practice, it is also *ad hoc*. The custom designer provides a way to improve on this *ad hoc* practice while supplying a theoretical foundation and an easy-to-use interface for choosing a design robust to the modeling assumptions.

The purpose of check points in a design is to provide a detection mechanism for higher-order effects that are contained in the assumed model. These higher-order terms are called *potential terms*. (Let q denote the potential terms, designated If Possible in JMP.) The assumed model consists of the *primary terms*. (Let p denote the primary terms designated Necessary in JMP.)

To take advantage of the benefits of the approach using If Possible model terms, the sample size should be larger than the number of Necessary (primary) terms but smaller than the sum of the Necessary and If Possible (potential) terms. That is, $p < n < p+q$. The formal name of the approach using If Possible model terms is *Bayesian D-Optimal design*. This type of design allows the precise estimation of all of the Necessary terms while providing omnibus detectability (and some estimability) for the If Possible terms.

For a two-factor design having a model with an intercept, two main effects, and an interaction, there are $p = 4$ primary terms. When you enter this model in the custom designer, the default minimum runs is a four-run design with the factor settings shown in Figure 2.17.

Figure 2.17 Two Continuous Factors with Interaction
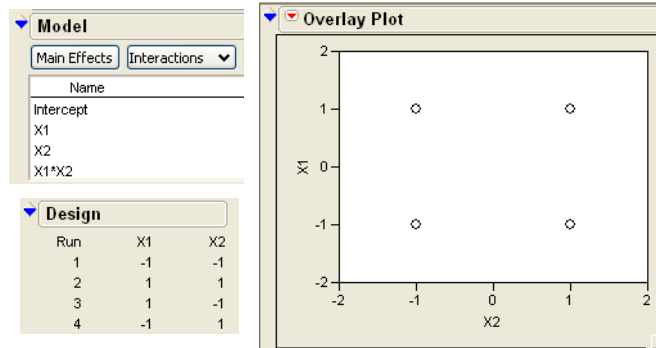
Now suppose you can afford an extra run ($n = 5$). You would like to use this point as a check point for curvature. If you leave the model the same and increase the sample size, the custom designer replicates one of the four vertices. Replicating any run is the optimal choice for improving the estimates of the terms in the model, but it provides no way to check for lack of fit.

Adding the two quadratic terms to the model makes a total of six terms. This is a way to model curvature directly. However, to do this the custom designer requires two additional runs (at a minimum), which exceeds your budget of five runs.

The Bayesian *D*-Optimal design provides a way to check for curvature while adding only one extra run. To create this design:

1 Select **DOE > Custom Design**.

2 Define two continuous factors (**X1** and **X2**).

3 Click **Continue**.

4 Choose **2nd** from the **Interactions** menu in the Model panel. The results appear as shown in Figure 2.18.

Figure 2.18 Second-Level Interactions
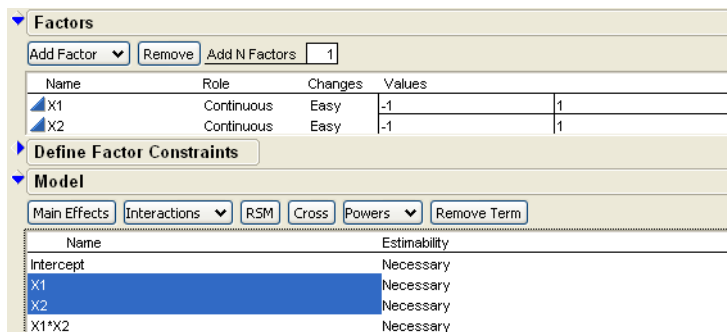
5 Choose **2nd** from the **Powers** button in the Model panel. This adds two quadratic terms.

6 Select the two quadratic terms (**X1*X1** and **X2*X2**) and click the current estimability (**Necessary**) to

see the menu and change Necessary to **If Possible**, as shown in Figure 2.19.

Figure 2.19 Changing the Estimability
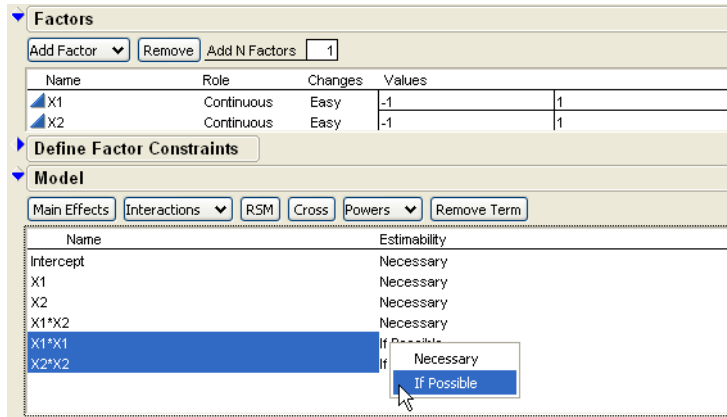
Now, the $p = 4$ primary terms (the intercept, two main effects, and the interaction) are designated as Necessary while the $q = 2$ potential terms (the two quadratic terms) are designated as If Possible. The desired number of runs, five, is between $p = 4$ and $p + q = 6$.

7 Enter 5 into the User Specified edit box in the Number of Runs section of the Design Generation panel.

8 Click **Make Design**. The resulting factor settings appear in Figure 2.20. The values in your design may be different from those shown below.

Figure 2.20 Five-Run Bayesian *D*-Optimal Design

9 Click **Make Table** to create a JMP data table of the runs.

10 Create the overlay plot in Figure 2.21 with **Graph > Overlay Plot**, and assign X1 as Y and X2 as X. The overlay plot illustrates how the design incorporates the single extra run. In this example the design places the factor settings at the center of the design instead of at one of the corners.

Figure 2.21 Overlay Plot of Five-run Bayesian *D*-Optimal Design
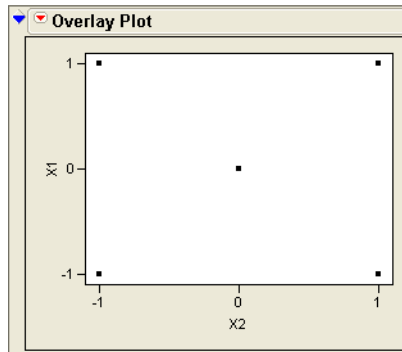
Creating Response Surface Experiments

Response surface experiments traditionally involve a small number (generally 2 to 8) of continuous factors. The *a priori* model for a response surface experiment is usually quadratic.

In contrast to screening experiments, researchers use response surface experiments when they already know which factors are important. The main goal of response surface experiments is to create a predictive model of the relationship between the factors and the response. Using this predictive model allows the experimenter to find better operating settings for the process.

In screening experiments one measure of the quality of the design is the size of the relative variance of the coefficients. In response surface experiments, the prediction variance over the range of the factors is more important than the variance of the coefficients. One way to visualize the prediction variance is JMP's prediction variance profile plot. This plot is a powerful diagnostic tool for evaluating and comparing response surface designs.

Exploring the Prediction Variance Surface

The purpose of the example below is to generate and interpret a simple Prediction Variance Profile Plot. Follow the steps below to create a design for a quadratic model with a single continuous factor.

1 Select **DOE > Custom Design**.
2 Add one continuous factor by selecting **Add Factor > Continuous** (Figure 2.22), and click **Continue**.
3 In the Model panel, select **Powers > 2nd** to create a quadratic term (Figure 2.22).

Figure 2.22 Adding a Factor and a Quadratic Term

4 In the Design Generation panel, use the default number of runs (six) and click **Make Design**
   (Figure 2.23). The number of runs is inversely proportional to the size of variance of the predicted
   response. As the number of runs increases, the prediction variances decrease.

Figure 2.23 Using the Default Number of Runs
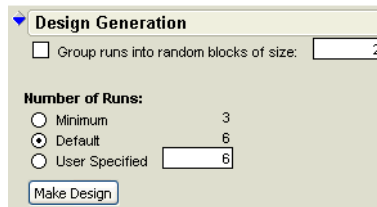
5 Click the disclosure button (◆ ◆ on Windows/Linux and ▶ ▼ on the Macintosh) to open the
   Design Evaluation outline node, and then the **Prediction Variance Profile**, as shown in
   Figure 2.24.

For continuous factors, the initial setting is at the mid-range of the factor values. For categorical factors,
the initial setting is the first level. If the design model is quadratic, then the prediction variance function is quartic. The y-axis is the relative variance of prediction of the expected value of the response.

In this design, the three design points are –1, 0, and 1. The prediction variance profile shows that the
variance is a maximum at each of these points on the interval –1 to 1.

Figure 2.24 Prediction Profile for Single Factor Quadratic Model
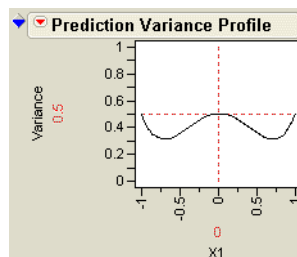
The prediction variance is relative to the error variance. When the relative prediction variance is one,
the absolute variance is equal to the error variance of the regression model. More detail on the Prediction Variance Profiler is in "Understanding Design Evaluation," p. 64.

6 To compare profile plots, click the **Back** button and choose **Minimum** in the Design Generation
   panel, which gives a sample size of three.
7 Click **Make Design** and then open the Prediction Variance Profile again.

Now you see a curve that has the same shape as the previous plot, but the maxima are at one instead of 0.5. Figure 2.25 compares plots for a sample size of six and sample size of three for this quadratic model. You can see the prediction variance increase as the sample size decreases. Since the prediction variance is inversely proportional to the sample size, doubling the number of runs halves the prediction variance. These profiles show settings for the maximum variance and minimum variance, for sample sizes six (top charts) and sample size three (bottom charts). The axes on the bottom plots are adjusted to match the axes on the top plot.

Figure 2.25 Comparison of Prediction Variance Profiles
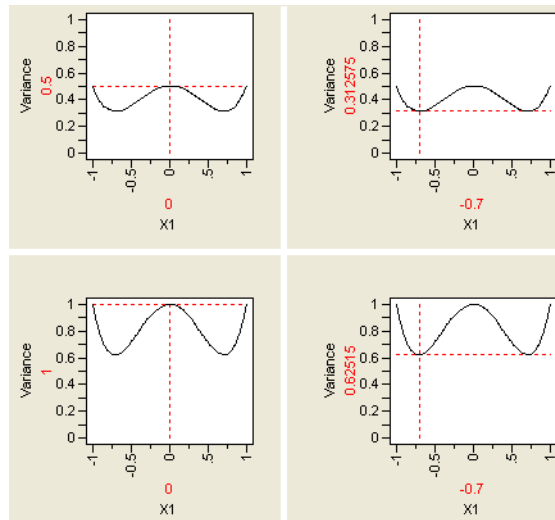
Tip: Control-click (Command-click on the Mac) on the factor to set a factor level precisely.

8 To create an unbalanced design, click the **Back** button and enter a sample size of 7 in the User Specified text edit box in the Design Generation panel, then click **Make Design**. The results are shown in Figure 2.26.

You can see that the variance of prediction at −1 is lower than the other sample points (its value is 0.33 instead of 0.5). The symmetry of the plot is related to the balance of the factor settings. When the design is balanced, the plot is symmetric, as shown in Figure 2.25. When the design is unbalanced, the prediction plot might not be symmetric, as shown in Figure 2.26.

Figure 2.26 Sample Size of Seven for the One-Factor Quadratic Model

Prediction variance at X1= 0   Prediction variance at X1= –1
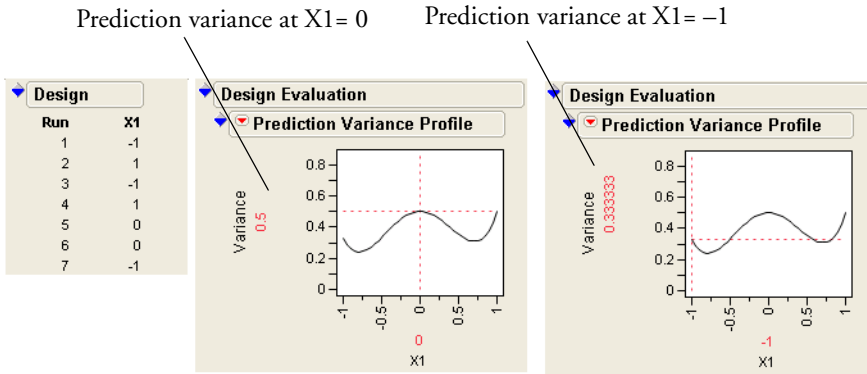
Introducing *I*-Optimal Designs for Response Surface Modeling

The custom designer generates designs using a mathematical optimality criterion. All the designs in this chapter so far have been *D*-Optimal designs. *D*-Optimal designs are most appropriate for screening experiments because the optimality criterion focuses on precise estimates of the coefficients. If an experimenter has precise estimates of the factor effects, then it is easy to tell which factors' effects are important and which are negligible. However, *D*-Optimal designs are not as appropriate for designing experiments where the primary goal is prediction.

I-Optimal designs minimize the average prediction variance inside the region of the factors. This makes *I*-Optimal designs more appropriate for prediction. As a result *I*-Optimality is the recommended criterion for JMP response surface designs.

An *I*-Optimal design tends to place fewer runs at the extremes of the design space than does a *D*-Optimal design. As an example, consider a one-factor design for a quadratic model using *n* = 12 experimental runs. The *D*-Optimal design for this model puts four runs at each end of the range of interest and four runs in the middle. The *I*-Optimal design puts three runs at each end point and six runs in the middle. In this case, the *D*-Optimal design places two-thirds of its runs at the extremes versus one-half for the *I*-Optimal design.

Figure 2.27 compares prediction variance profiles of the one-factor *I*- and *D*-Optimal designs for a quadratic model with (*n* = 12) runs. The variance function for the *I*-Optimal design is less than the corresponding function for the *D*-Optimal design in the center of the design space; the converse is true at the edges.

Figure 2.27 Prediction Variance Profiles for 12-Run *I*-Optimal (left) and *D*-Optimal (right) Designs
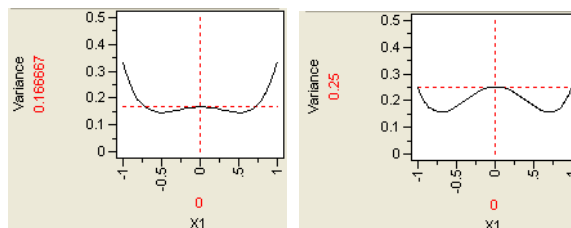
At the center of the design space, the average variance (relative to the error variance) for the *I*-Optimal design is 0.1667 compared to the *D*-Optimal design, which is 0.25. This means that confidence intervals for prediction will be nearly 10% shorter on average for the *I*-Optimal design.

To compare the two design criteria, create a one-factor design with a quadratic model that uses the *I*-Optimality criterion, and another one that uses *D*-Optimality:

1 Select **DOE > Custom Design**.
2 Add one continuous factor: X1.
3 Click **Continue**.
4 Click the **RSM** button in the Model panel to make the design *I*-Optimal.
5 Change the number of runs to 12.
6 Click **Make Design**.
7 Click the disclosure button (◆ ◆ on Windows/Linux and ▶ ▼ on the Macintosh) to open the **Prediction Variance Profile**, as shown on the left in Figure 2.27.
8 Repeat the same steps to create a *D*-Optimal design, but select **Optimality Criterion > Make D-Optimal Design** from the red triangle menu on the custom design title bar. The results in the Prediction Variance Profile should look the same as those on the right in Figure 2.27.

A Three-Factor Response Surface Design

In higher dimensions, the *I*-Optimal design continues to place more emphasis on the center of the region of the factors. The *D*-Optimal and *I*-Optimal designs for fitting a full quadratic model in three factors using 16 runs are shown in Figure 2.28.

To compare the two design criteria, create a three-factor design that uses the *I*-Optimality criterion, and another one that uses *D*-Optimality:

1 Select **DOE > Custom Design**.
2 Add three continuous factors: X1, X2, and X3.
3 Click **Continue**.
4 Click the **RSM** button in the Model panel to add interaction and quadratic terms to the model and to change the default optimality criterion to *I*-Optimal.
5 Use the default of 16 runs.
6 Click **Make Design**.
7 The design is shown in the Design panel (the left in Figure 2.28).
8 If you want to create a *D*-Optimal design for comparison, repeat the same steps but select **Optimality Criterion > Make D-Optimal Design** from the red triangle menu on the custom design title bar. The design should look similar to those on the right in Figure 2.28. The values in your design may be different from those shown below.

Figure 2.28 16-run *I*-Optimal and *D*-Optimal designs for RSM Model

I-Optimal Design					D-Optimal Design			
Run	X1	X2	X3		Run	X1	X2	X3
1	1	0	0		1	-1	1	1
2	-1	1	1		2	-1	-1	-1
3	-1	0	0		3	-1	1	-1
4	0	-1	0		4	0	1	1
5	1	-1	-1		5	-1	0	1
6	-1	-1	1		6	-1	-1	1
7	1	1	-1		7	1	1	1
8	0	0	-1		8	-1	-1	0
9	0	0	1		9	-1	1	0
10	-1	-1	-1		10	-1	0	-1
11	0	1	0		11	1	0	0
12	0	0	0		12	0	0	-1
13	1	-1	1		13	1	-1	-1
14	-1	1	-1		14	0	-1	0
15	1	1	1		15	1	-1	1
16	0	0	0		16	1	1	-1

Profile plots of the variance function are displayed in Figure 2.29. These plots show slices of the variance function as a function of each factor, with all other factors fixed at zero. The *I*-Optimal design has the lowest prediction variance at the center. Note that there are two center points in this design.

The *D*-Optimal design has no center points and its prediction variance at the center of the factor space is almost three times the variance of the *I*-Optimal design. The variance at the vertices of the *D*-Optimal design is not shown. However, note that the *D*-Optimal design predicts better than the *I*-Optimal design near the vertices.

Figure 2.29 Variance Profile Plots for 16 run *I*-Optimal and *D*-Optimal RSM Designs
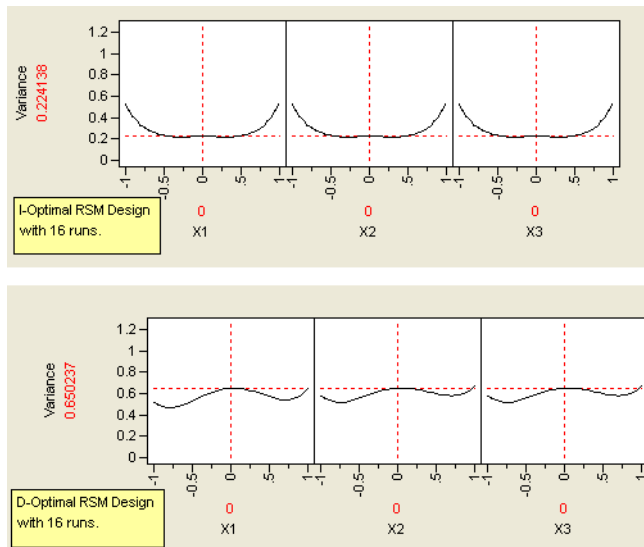
Response Surface with a Blocking Factor

It is not unusual for a process to depend on both qualitative and quantitative factors. For example, in the chemical industry, the yield of a process might depend not only on the quantitative factors temper-

ature and pressure, but also on such qualitative factors as the batch of raw material and the type of reactor. Likewise, an antibiotic might be given orally or by injection, a qualitative factor with two levels. The composition and dosage of the antibiotic could be quantitative factors (Atkinson and Donev, 1992).

The response surface designer (described in "Response Surface Designs," p. 115) only deals with quantitative factors. You could use the response surface designer to produce a Response Surface Model (RSM) design with a qualitative factor by replicating the design over each level of the factor. But, this is unnecessarily time-consuming and expensive. Using custom designer is simpler and more cost-effective because fewer runs are required. The following steps show how to accommodate a blocking factor in a response surface design using the custom designer:

1 First, define two continuous factors (X1 and X2).

2 Now, click **Add Factor** and select **Blocking > 4 runs per block** to create a blocking factor(X3). The blocking factor appears with one level, as shown in Figure 2.30, but the number of levels adjusts later to accommodate the number of runs specified for the design.

Figure 2.30 Add Two Continuous Factors and a Blocking Factor

3 Click **Continue,** and then click **RSM** in the Model panel to add the quadratic terms to the model (Figure 2.31). This automatically changes the recommended optimality criterion from *D*-Optimal to *I*-Optimal. Note that when you click RSM, a message reminds you that nominal factors (such as the blocking factor) cannot have quadratic effects.

Figure 2.31 Add Response Surface Terms

4 Enter 12 in the User Specified text edit box in the Design Generation panel, and note that the Factors panel now shows the Blocking factor, X3, with three levels (Figure 2.32). Twelve runs defines three blocks with four runs per block.

Figure 2.32 Blocking Factor Now Shows Three Levels

Factors						
Add Factor ▾	Remove	Add N Factors	1			
Name	Role	Changes	Values			
X1	Continuous	Easy	-1		1	
X2	Continuous	Easy	-1		1	
X3	Blocking	Easy	1	2		3

▶ Define Factor Constraints

Model	
Main Effects	Interactions ▾	RSM	Cross	Powers ▾	Remove Term
Name	Estimability
Intercept	Necessary
X1	Necessary
X2	Necessary
X3	Necessary
X1*X1	Necessary
X1*X2	Necessary
X2*X2	Necessary
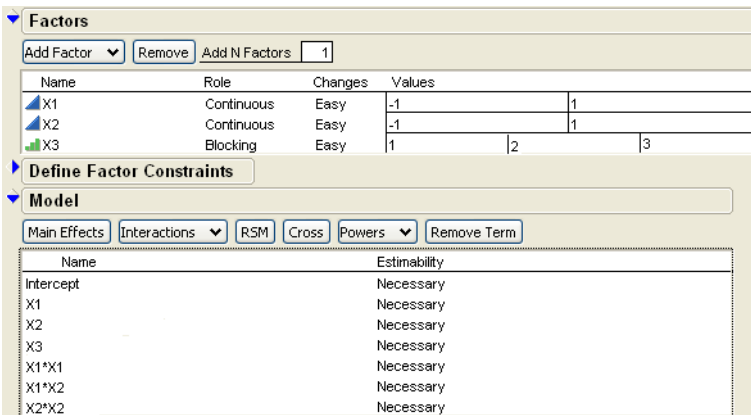
5 Click **Make Design**.

6 In the Output Options, select **Sort Right to Left** from the **Run Order** list.

7 Click **Make Table** to see an *I*-Optimal table similar to the one on the left in Figure 2.33.

Figure 2.33 compares the results of a 12-run *I*-Optimal design and a 12-run *D*-Optimal Design.

To see the *D*-Optimal design:

1 Click the **Back** button.

2 Click the red triangle icon on the Custom Design title bar and select **Optimality Criterion > Make D-Optimal Design**.

3 Click **Make Design**, then click **Make Table**.

Figure 2.33 JMP Design Tables for 12-Run *I*-Optimal and *D*-Optimal Designs

I-Optimal Design				D-Optimal Design			
Run	X1	X2	X3	Run	X1	X2	X3
1	1	-1	1	1	-1	-1	1
2	-1	0	1	2	0	-1	1
3	0	0	1	3	1	0	1
4	0	1	1	4	-1	1	1
5	0	-1	2	5	1	-1	2
6	0	0	2	6	0	0	2
7	-1	1	2	7	-1	1	2
8	1	1	2	8	1	1	2
9	-1	-1	3	9	-1	-1	3
10	0	0	3	10	1	-1	3
11	1	0	3	11	-1	0	3
12	0	1	3	12	0	1	3

Figure 2.34 gives a graphical view of the designs generated by this example. These plots were generated for the runs in each JMP table by choosing **Graph > Overlay Plot** from the main menu and using the blocking factor (X3) as the **Grouping** variable.

Note that there is a center point in each block of the *I*-Optimal design. The *D*-Optimal design has only one center point. The values in your graph may be different from those shown below.

Figure 2.34 Plots of *I*-Optimal (left) and *D*-Optimal (right) Design Points by Block.
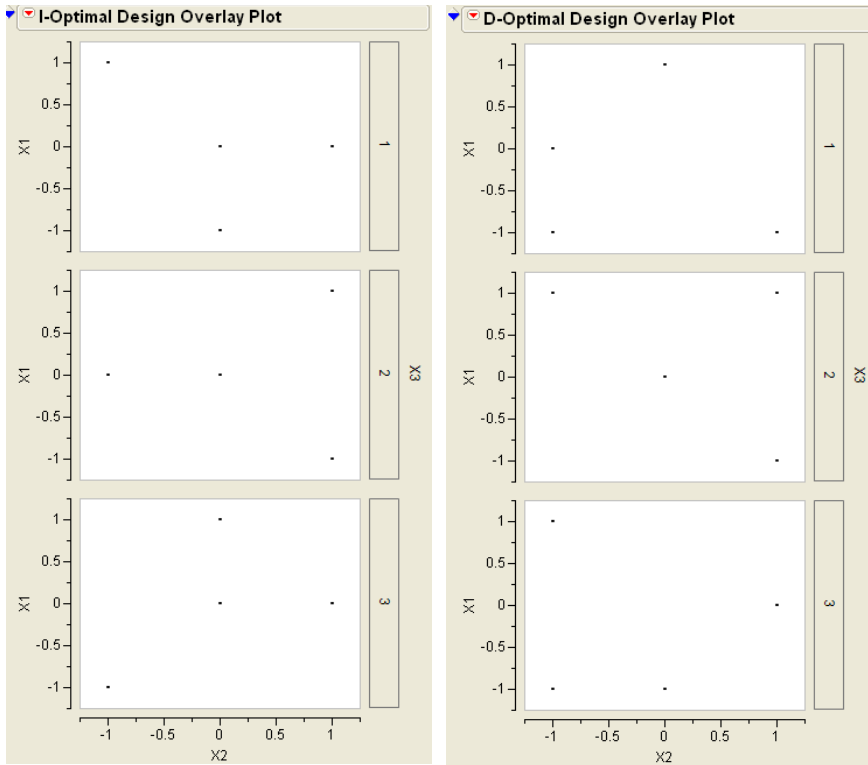
Either of the above designs supports fitting the specified model. The *D*-Optimal design does a slightly better job of estimating the model coefficients. The diagnostics (Figure 2.35) for the designs show beneath the design tables. In this example, the *D*-efficiency of the *I*-Optimal design is about 51%, and is 55% for the D-Optimal design.

The *I*-Optimal design is preferable for predicting the response inside the design region. Using the formulas given in "Technical Discussion," p. 53, you can compute the relative average variance for these designs. The average variance (relative to the error variance) for the *I*-Optimal design is 0.5 compared to 0.59 for the *D*-Optimal design (See Figure 2.35). This means confidence intervals for prediction will be almost 20% longer on average for *D*-Optimal designs.

Figure 2.35 Design Diagnostics for I-Optimal and D-Optimal Designs

Design Diagnostics	
I Optimal Design	
D Efficiency	50.85382
G Efficiency	76.47609
A Efficiency	37.51264
Average Variance of Prediction	0.49973
Design Creation Time (seconds)	0.083333

Design Diagnostics	
D Optimal Design	
D Efficiency	54.98822
G Efficiency	78.12922
A Efficiency	32.5789
Average Variance of Prediction	0.59188
Design Creation Time (seconds)	0.083333

Creating Mixture Experiments

If you have factors that are ingredients in a mixture, you can use either the custom designer or the specialized mixture designer. However, the mixture designer is limited because it requires all factors to be mixture components and you might want to vary the process settings along with the percentages of the mixture ingredients. The optimal formulation could change depending on the operating environment. The custom designer can handle mixture ingredients and process variables in the same study. You are not forced to modify your problem to conform to the restrictions of a special-purpose design approach.

Mixtures Having Nonmixture Factors

The following example from Atkinson and Donev (1992) shows how to create designs for experiments with mixtures where one or more factors are not ingredients in the mixture. In this example:

- The response is the electromagnetic damping of an acrylonitrile powder.
- The three mixture ingredients are copper sulphate, sodium thiosulphate, and glyoxal.
- The nonmixture environmental factor of interest is the wavelength of light.

Though wavelength is a continuous variable, the researchers were only interested in predictions at three discrete wavelengths. As a result, they treated it as a categorical factor with three levels. To create this custom design:

1 Select **DOE > Custom Design**.
2 Create Damping as the response. The authors do not mention how much damping is desirable, so right-click the goal and create Damping's response goal to be **None**.
3 In the Factors panel, add the three mixture ingredients and the categorical factor, Wavelength. The mixture ingredients have range constraints that arise from the mechanism of the chemical reaction. Rather than entering them by hand, load them from the Sample Data folder that was installed with JMP: click the red triangle icon on the Custom Design title bar and select **Load Factors**. Open Donev Mixture Factors.jmp, from the Design Experiment folder in the sample data. The custom design panels should now look like those shown in Figure 2.36.

Figure 2.36 Mixture Experiment Response Panel and Factors Panel
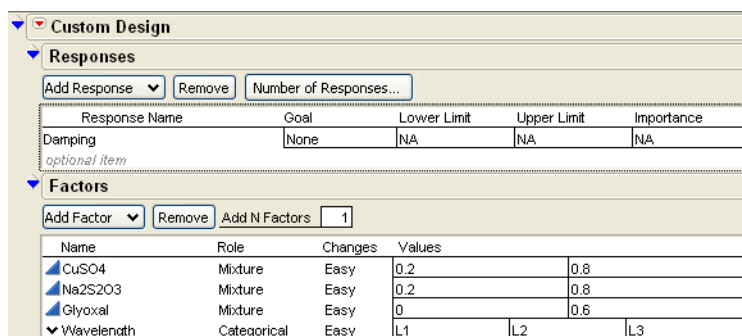
The model, shown in Figure 2.37 is a response surface model in the mixture ingredients along with the additive effect of the wavelength. To create this model:

1 Click **Interactions**, and choose **2nd**. A warning dialog appears telling you that JMP removes the

main effect terms for non-mixture factors that interact with all the mixture factors. Click **OK**.

2 In the Design Generation panel, type 18 in the User Specified text edit box (Figure 2.37), which results in six runs each for the three levels of the wavelength factor.

Figure 2.37 Mixture Experiment Design Generation Panel

3 Click **Make Design**, and then click **Make Table**.

The resulting data table is shown in Figure 2.38. The values in your table may be different from those shown below.

Figure 2.38 Mixture Experiment Design Table

Atkinson and Donev also discuss the design where the number of runs is limited to 10. In that case, it is not possible to run a complete mixture response surface design for every wavelength.

To view this:

1 Click the **Back** button.

2 Remove all the effects by highlighting them and clicking **Remove Term**.

3 Add the main effects by clicking the **Main Effects** button.

4 In the Design Generation panel, change the number of runs to **10** (Figure 2.39) and click **Make Design**. The Design table to the right in Figure 2.39 shows the factor settings for 10 runs.

Figure 2.39 Ten-Run Mixture Response Surface Design

Note that there are necessarily unequal numbers of runs for each wavelength. Because of this lack of balance it is a good idea to look at the prediction variance plot (top plot in Figure 2.40).

5 Open the **Design Evaluation** outline, then open the **Prediction Variance Profile**.

The prediction variance is almost constant across the three wavelengths, which is a good indication that the lack of balance is not a problem.

The values of the first three ingredients sum to one because they are mixture ingredients. If you vary one of the values, the others adjust to keep the sum constant.

6 Select **Maximize Desirability** from red triangle menu on the Prediction Variance Profile title bar, as

shown in the bottom profiler in Figure 2.40.

The most desirable wavelength is L2, with the CuSO4 percentage decreasing from about 0.4 to 0.2, Glyoxal percentage is zero, and Na2S2O3 is 0.8, which maintains the mixture.

Figure 2.40 Prediction Variance Plots for Ten-Run Design
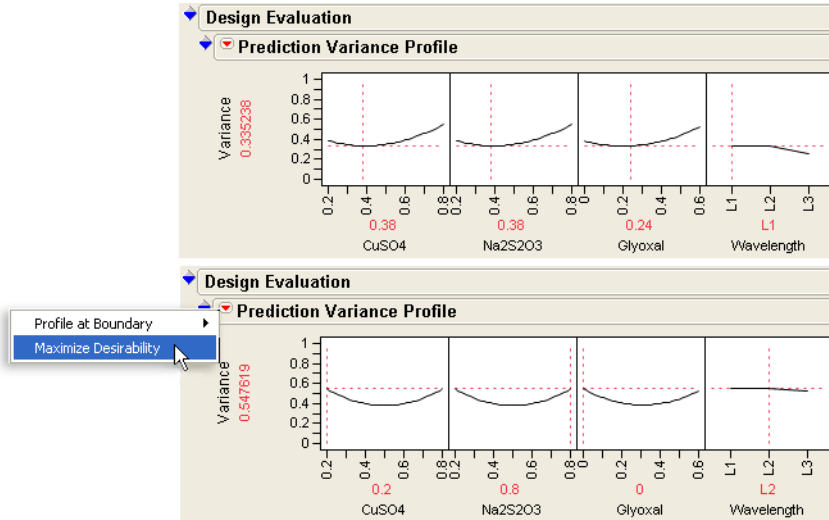
Experiments that are Mixtures of Mixtures

As a way to illustrate the idea of a 'mixture of mixtures' situation, imagine the ingredients that go into baking a cake and assume the following:

- dry ingredients composed of flour, sugar, and cocoa
- wet (or non-dry) ingredients consisting of milk, melted butter, and eggs.

These two components (wet and dry) of the cake are two mixtures that are first mixed separately and then blended together.

The dessert chef knows that the dry component (the mixture of flour, sugar, and cocoa) contributes 45% of the combined mixture and the wet component (butter, milk, and eggs) contributes 55%.

The objective of such an experiment might be to identify proportions within the two components that maximize some measure of taste or consistency.

This is a main effects model except that you must leave out one of the factors in order to avoid singularity. The choice of which factor to leave out of the model is arbitrary.

For now, consider these upper and lower levels of the various factors:

Within the dry mixture:

- cocoa must be greater than 10% but less than 20%
- sugar must be greater than 0% but less than 15%
- flour must be greater than 20% but less than 30%

Within the wet mixture:

- melted butter must be greater than 10% but less than 20%
- milk must be greater than 25% and less than 35%
- eggs constitute more than 5% but less than 20%

You want to bake cakes and measure taste on a scale from 1 to 10

Use the Custom Designer to set up this example, as follows:

1 In the Response Panel, enter one response and call it Taste.
2 Give Taste a Lower Limit of 1 and an Upper Limit of 10. (You are assuming a taste test where the respondents reply on a scale of 1 to 10.)
3 In the Factors Panel, enter the six cake factors described above.
4 Enter the given percentage values of the factors as proportions in the Values section of the Factors panel.

The completed Response and Factors panels should look like those shown in Figure 2.41.

Figure 2.41 Completed Responses and Factors Panel for the Cake Example

5 Next, click Continue.
6 Open the Constraints pane and click Add Constraint twice.
7 Enter the constraints as shown at the top in Figure 2.42.

By confining the dry factors to exactly 45% in this way, the mixture role of all the factors ensures that the wet factors constitute the remaining 55%.

8 Open the Model dialog and note that it lists all 6 effects. Because these are mixture factors, including all effects would render the model singular. Highlight any one of the terms in the model and click Remove Term, as shown.

Figure 2.42 Constraints to Define the Double Mixture Experiment
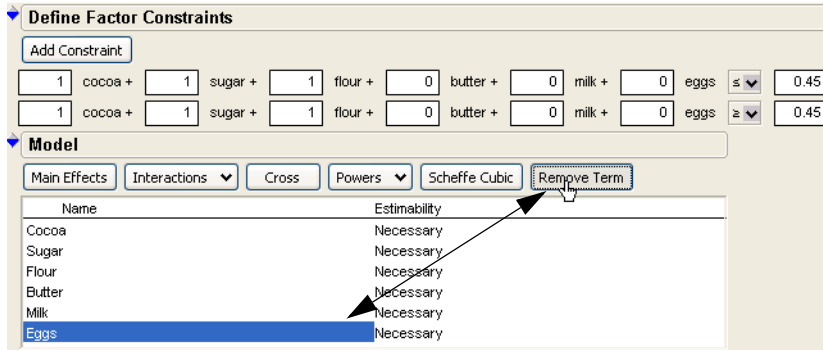
9 To see a completed example, choose **Simulate Responses** from the menu on the Custom Design title bar.

10 In the Design Generation panel, enter 10 as the number of runs for the example. That is, you would bake cakes with 10 different sets of ingredient proportions.

11 Click **Make Design** in the Design Generation panel, and then click **Make Table**.

The table inFigure 2.43 shows that the two sets of cake ingredients (dry and wet) adhere to the proportions 45% and 55% as defined by the entered constraints. In addition, the amount of each ingredient in each cake recipe (run) conforms to the upper and lower limits given in the factors dialog.

Figure 2.43 Cake Experiment Conforming to a Mixture of Mixture Design

	Cocoa	Sugar	Flour	Butter	Milk	Eggs	Taste
1	0.20	0.05	0.20	0.10	0.25	0.20	9.30
2	0.20	0.05	0.20	0.10	0.35	0.10	6.66
3	0.20	0.00	0.25	0.20	0.25	0.10	7.61
4	0.15	0.00	0.30	0.15	0.35	0.05	6.38
5	0.15	0.00	0.30	0.15	0.35	0.05	5.25
6	0.10	0.15	0.20	0.20	0.25	0.10	5.77
7	0.10	0.15	0.20	0.20	0.30	0.05	5.02
8	0.10	0.15	0.20	0.10	0.35	0.10	5.47
9	0.10	0.05	0.30	0.10	0.25	0.20	4.14
10	0.10	0.05	0.30	0.10	0.25	0.20	5.81

Each run sums to 0.45 (45%)   Each run sums to 0.55 (55%)

Note: As a word of caution, keep in mind that it is easy to define constraints in such a way that it is impossible to construct a design that fits the model. In such a case, you will get a message saying "Could not find a valid starting design. Please check your constraints for consistency."

Special-Purpose Uses of the Custom Designer

While some of the designs discussed in previous sections can be created using other designers in JMP or by looking them up in a textbook containing tables of designs, the designs presented in this section cannot be created without using the custom designer.

Designing Experiments with Fixed Covariate Factors

Pre-tabulated designs rely on the assumption that the experimenter controls all the factors. Sometimes you have quantitative measurements (a covariate) on the experimental units before the experiment begins. If this variable affects the experimental response, the covariate should be a design factor. The pre-defined design that allows only a few discrete values is too restrictive. The custom designer supplies a reasonable design option.

For this example, suppose there are a group of students participating in a study. A physical education researcher has proposed an experiment where you vary the number of hours of sleep and the calories for breakfast and ask each student to run 1/4 mile. The weight of the student is known and it seems important to include this information in the experimental design.

To follow along with this example that shows column properties, open Big Class.jmp from the Sample Data folder that was installed when you installed JMP.

Build the custom design as follows:

1 Select **DOE > Custom Design**.

2 Add two continuous variables to the models by clicking **Add Factors** and selecting **Continuous**, naming them calories and sleep.

3 Click **Add Factor** and select **Covariate**, as shown in Figure 2.44. The **Covariate** selection displays a list of the variables in the current data table.

Figure 2.44 Add a Covariate Factor
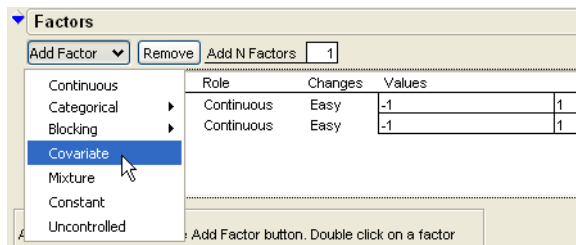
4 Select weight from the variable list (Figure 2.45) and click **OK**.

Figure 2.45 Design with Fixed Covariate
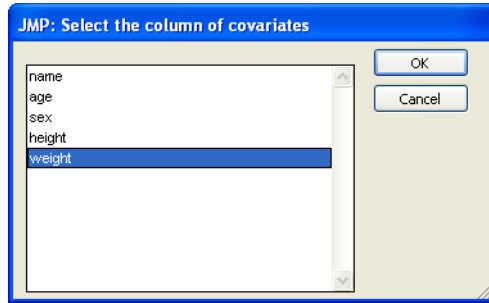
5 Click **Continue**.

6 Add the interaction to the model by selecting calories in the Factors panel, selecting sleep in the Model panel, and then clicking the **Cross** button (Figure 2.46).

Figure 2.46 Design With Fixed Covariate Factor
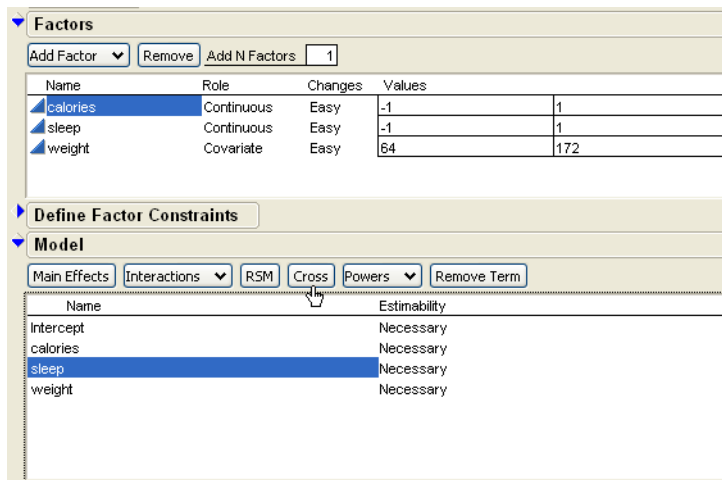
7 Click **Make Design**, then click **Make Table**. The data table in Figure 2.47 shows the design table. Your runs might not look the same because the order of the runs has been randomized.

Figure 2.47 Design Table for Covariate Example

	calories	sleep	weight	Y
1	-1	-1	95	.
2	1	1	123	.
3	1	-1	74	.
4	1	-1	145	.
5	-1	-1	64	.
6	1	1	84	.
7	1	1	128	.
8	1	-1	79	.
9	1	1	112	.
10	1	1	107	.
11	1	1	67	.
12	-1	1	98	.
13	-1	-1	105	.
14	-1	1	95	.

Note: Covariate factors cannot have missing values.

Remember that weight is the covariate factor, measured for each student, but it is not controlled. The custom designer has calculated settings for calories and sleep for each student. It would be desirable if the correlations between calories, sleep and weight were as small as possible. You can see how well the custom designer did by fitting a model of weight as a function of calories and sleep. If that fit has a small model sum of squares, that means the custom designer has successfully separated the effect of weight from the effects of calories and sleep.

8   Click the red triangle icon beside **Model** in the data table and select **Run Script**, as shown on the left in Figure 2.48.

Figure 2.48 Model Script

9   Rearrange the dialog so weight is Y and calories, sleep, and calories*sleep are the model effects, as shown to the right in Figure 2.48. Click **Run Model**.

The leverage plots are nearly horizontal, and the analysis of variance table shows that the model sum of squares is near zero compared to the residuals (Figure 2.49). Therefore, weight is independent of calories and sleep. The values in your analysis may be a little different from those shown below.

Figure 2.49 Analysis to Check That Weight is Independent of Calories and Sleep
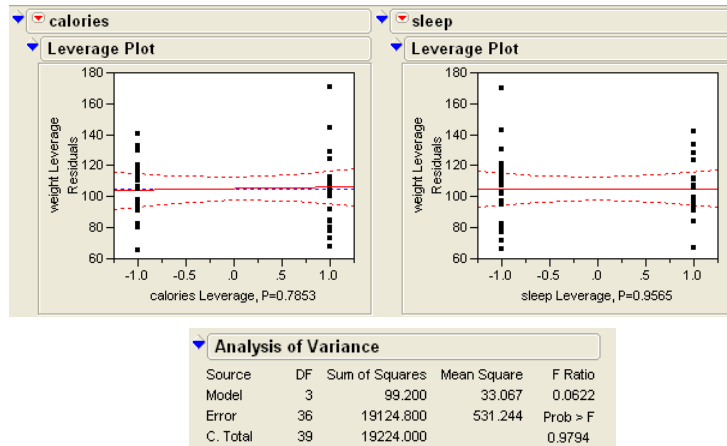
Creating a Design with Two Hard-to-Change Factors: Split Plot

While there is substantial research literature covering the analysis of split plot designs, it has only been possible in the last few years to create optimal split plot designs (Goos 2002). The split plot design capability accessible in the JMP custom designer is the first commercially available tool for generating optimal split plot designs.

The split plot design originated in agriculture, but is commonplace in manufacturing and engineering studies. In split plot experiments, hard-to-change factors only change between one whole plot and the next. The whole plot is divided into subplots, and the levels of the easy-to-change factors are randomly assigned to each subplot.

The example in this section is adapted from Kowalski, Cornell, and Vining (2002). The experiment studies the effect of five factors on the thickness of vinyl used to make automobile seat covers. The response and factors in the experiment are described below:

- Three of the factors are ingredients in a mixture. They are plasticizers whose proportions, m1, m2, and m3, sum to one. Additionally, the mixture components are the subplot factors of the experiment.

- Two of the factors are process variables. They are the rate of extrusion (extrusion rate) and the temperature (temperature) of drying. These process variables are the whole plot factors of the experiment. They are hard to change.

- The response in the experiment is the thickness of the vinyl used for automobile seat covers. The response of interest (thickness) depends both on the proportions of the mixtures and on the effects of the process variables.

To create this design in JMP:

1 Select **DOE > Custom Design**.
2 By default, there is one response, Y, showing. Double-click the name and change it to thickness. Use the default goal, **Maximize** (Figure 2.50).
3 Enter the lower limit of 10.

4 To add three mixture factors, type 3 in the box beside **Add N Factors,** and click **Add Factor > Mixture**.

5 Name the three mixture factors **m1**, **m2**, and **m3**. Use the default levels **0** and **1** for those three factors.

6 Add two continuous factors by typing 2 in the box beside **Add N Factors**, and click **Add Factor > Continuous**. Name these factors extrusion rate and temperature.

7 Ensure that you are using the default levels, –1 and 1, in the Values area corresponding to these two factors.

8 To make extrusion rate a whole plot factor, click **Easy** and select **Hard**.

9 To make temperature a whole plot factor, click **Easy** and select **Hard**. Your dialog should look like the one in Figure 2.50.

Figure 2.50 Entering Responses and Factors
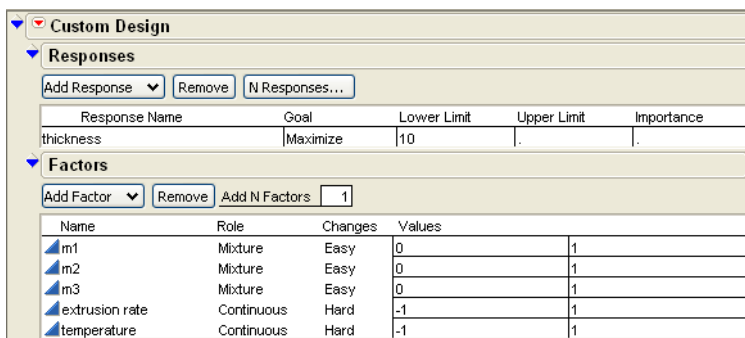
10 Click **Continue**.

11 Next, add interaction terms to the model by selecting **Interactions > 2nd** (Figure 2.51). This causes a warning that JMP removes the main effect terms for non-mixture factors that interact with all the mixture factors. Click **OK**.

Figure 2.51 Adding Interaction Terms
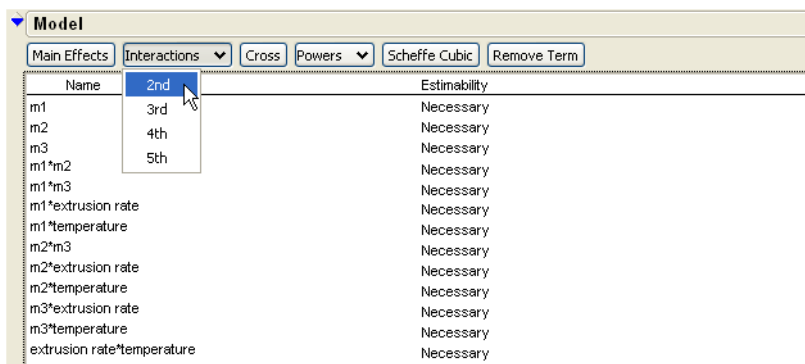
12 In the Design Generation panel, type 7 in the **Number of Whole Plots** text edit box.

13 For **Number of Runs**, type 28 in the User Specified text edit box (Figure 2.52).

Figure 2.52 Assigning the Number of Whole Plots and Number of Runs

Note: If you enter a missing value in the Number of Whole Plots edit box, then JMP considers many different numbers of whole plots and chooses the number that maximizes the information about the coefficients in the model. It maximizes the determinant of $\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}$ where $\mathbf{V}^{-1}$ is the inverse of the variance matrix of the responses. The matrix, $\mathbf{V}$, is a function of how many whole plots there are, so changing the number of whole plots changes $\mathbf{V}$, which can make a difference in the amount of information a design contains.

14 Click **Make Design**. The result is shown in Figure 2.53.

Figure 2.53 Partial Listing of the Final Design Structure

15 Click **Make Table**.

16 From the Sample Data folder that was installed with JMP, open Vinyl Data.jmp from the Design Experiment folder, which contains 28 runs as well as response values. The values in the table you generated with the custom designer may be different from those from the Sample Data folder, shown in Figure 2.54.

Figure 2.54 The Vinyl Data Design Table

17 Click the red triangle icon next to the Model script and select **Run Script**. The dialog in Figure 2.55 appears.

The models for split plots have a random effect associated with the whole plots' effect.

As shown in the dialog in Figure 2.55, JMP designates the error term by appending **&Random** to the name of the effect. REML will be used for the analysis, as indicated in the menu beside Method in Figure 2.55. For more information about REML models, see the *JMP Statistics and Graphics Guide*.

Figure 2.55 Define the Model in the Fit Model Dialog
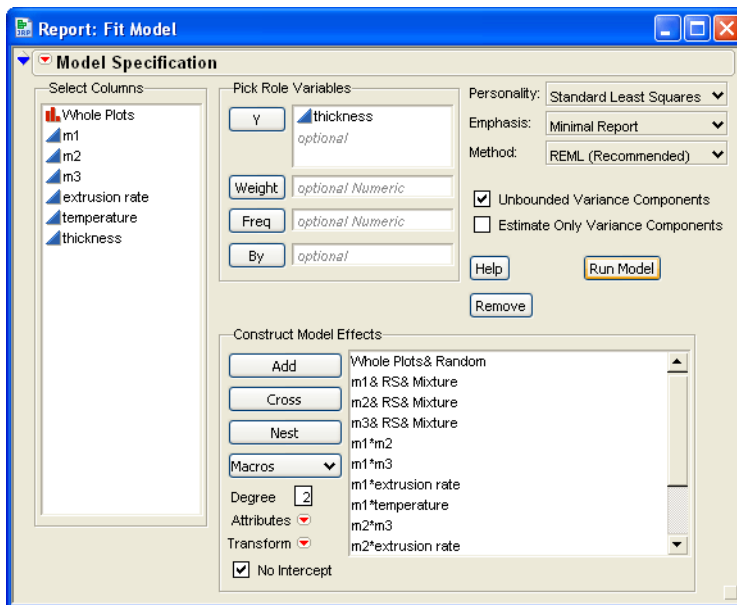
18 Click **Run Model** to run the analysis. The results are shown in Figure 2.56.

Figure 2.56 Split Plot Analysis Results

Technical Discussion

This section provides more technical information about *I*-, *D*-, and Bayesian *D*-Optimal designs in JMP.

D-**Optimality:**

- is the default design type produced by the custom designer except when the RSM button has been clicked to create a full quadratic model.

- minimizes the variance of the model coefficient estimates. This is appropriate for first-order models and in screening situations, because the experimental goal in such situations is often to identify the active factors; parameter estimation is key.

- is dependent on a pre-stated model. This is a limitation because in most real situations, the form of the pre-stated model is not known in advance.

- has runs whose purpose is to lower the variability of the coefficients of this pre-stated model. By focusing on minimizing the standard errors of coefficients, a *D*-Optimal design may not allow for checking that the model is correct. It will not include center points when investigating a first-order model. In the extreme, a *D*-Optimal design may have just *p* distinct runs with no degrees of freedom for lack of fit.

- maximizes *D* when

$$D = \det[\mathbf{X}'\mathbf{X}]$$

D-optimal split plot designs maximize *D* when

$$D = \det[\mathbf{X}' \mathbf{V}^{-1} \mathbf{X}]$$

where $\mathbf{V}^{-1}$ is the block diagonal variance matrix of the responses (Goos 2002).

Bayesian *D*-Optimality:

- is a modification of the *D*-Optimality criterion that effectively estimates the coefficients in a model, and at the same time has the ability to detect and estimate some higher-order terms. If there are interactions or curvature, the Bayesian *D*-Optimality criterion is advantageous.

- works best when the sample size is larger than the number of Necessary terms but smaller than the sum of the Necessary and If Possible terms. That is, $p + q > n > p$. The Bayesian *D*-Optimal design is an approach that allows the precise estimation of all of the Necessary terms while providing omnibus detectability (and some estimability) for the If Possible terms.

- uses the If Possible terms to force in runs that allow for detecting any inadequacy in the model containing only the Necessary terms. Let **K** be the $(p + q)$ by $(p + q)$ diagonal matrix whose first *p* diagonal elements are equal to 0 and whose last *q* diagonal elements are the constant, *k*. If there are 2-factor interactions then $k = 4$. Otherwise $k = 1$. The Bayesian *D*-Optimal design maximizes the determinant of $(\mathbf{X'X} + \mathbf{K})$. The difference between the criterion for *D*-Optimality and Bayesian *D*-Optimality is this constant added to the diagonal elements corresponding to the If Possible terms in the $\mathbf{X'X}$ matrix.

_I_-Optimality:

- minimizes the average variance of prediction over the region of the data.

- is more appropriate than *D*-Optimality if your goal is to predict the response rather than the coefficients, such as in response surface design problems. Using the *I*-Optimality criterion is more appropriate because you can predict the response anywhere inside the region of data and therefore find the factor settings that produce the most desirable response value. It is more appropriate when your objective is to determine optimum operating conditions, and also is appropriate to determine regions in the design space where the response falls within an acceptable range. Precise estimation of the response therefore takes precedence over precise estimation of the parameters.

- maximizes this criterion: If $f'(x)$ denotes a row of the **X** matrix corresponding to factor combinations *x*, then

$$I = \int_R f'(x)(\mathbf{X'X})^{-1} f(x) \, dx$$

$$= \text{Trace}[(\mathbf{X'X})^{-1} \mathbf{M}]$$

where

$$M = \int_R f(x) f(x)' \, dx$$

is a moment matrix that is independent of the design and can be computed in advance.

Bayesian *I*-Optimality:

Bayesian *I*-Optimality has a different objective function to optimize than the Bayesian D-optimal design, so the designs that result are different. The variance matrix of the coefficients for Bayesian

I-optimality is $\mathbf{X'X + K}$ where $\mathbf{K}$ is a matrix having zeros for the Necessary model terms and some constant value for the If Possible model terms.

The variance of the predicted value at a point x_0 is:

$$\text{var}\!\left(\hat{Y}\middle|x_0\right) = \left(\mathbf{x}_0'\!\left(\mathbf{X'X + K}\right)^{-1}\right)\mathbf{x}_0$$

The Bayesian *I*-Optimal design minimizes the average prediction variance over the design region:

$$= \text{Trace}[(\mathbf{X'X + K})^{-1}\mathbf{M}]$$

where $\mathbf{M}$ is defined as before.

Chapter **3**

Building Custom Designs

The Basic Steps

JMP can build a *custom* design that both matches the description of your engineering problem and remains within your budget for time and material. Custom designs are general, flexible, and good for routine factor screening or response optimization. To create these tailor-made designs, use the **Custom Design** command found on the **DOE** menu or the **Custom Design** button found on the **DOE** panel of the JMP Starter.

This chapter introduces you to the steps you need to complete to build a custom design.

Contents

Creating a Custom Design

To begin, select **DOE > Custom Design**, or click the **Custom Design** button on the JMP Starter **DOE** page. Then, follow the steps below.

- Enter responses and factors into the custom designer.
- Describe the model.
- Select the number of runs.
- Check the design diagnostics, if desired.
- Specify output options.
- Make the JMP design table.

The following sections describe each of these steps.

Enter Responses and Factors into the Custom Designer

How to Enter Responses

To enter responses, follow the steps in Figure 3.1.

Figure 3.1 Entering Responses

Click to enter lower and upper limits and importance weights.

To enter one response at a time, click then select a goal type: **Maximize**, **Match Target**, **Minimize**, or **None**.

Double-click to edit the response name, if desired.

Click to change the response goal, if desired.
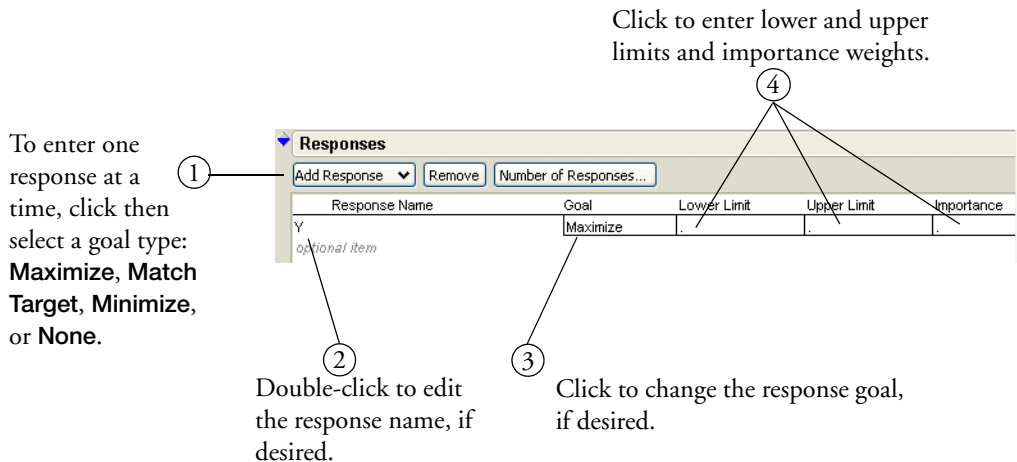
Tip: To quickly enter multiple responses, click **Number of Responses** and enter the number of responses you want.

Specifying Response Goal Types and Lower and Upper Limits

When entering responses, you can tell JMP that your goal is to obtain the maximum or minimum value possible, to match a specific value, or that there is no response goal.

The following description explains the relationship between the goal type (step 3 in Figure 3.1) and the lower and upper limits (step 4 in Figure 3.1):

- For responses such as strength or yield, the best value is usually the largest possible. A goal of **Maximize** supports this objective.

- The **Minimize** goal supports an objective of having the smallest value, such as when the response is impurity or defects.

- The **Match Target** goal supports the objective when the best value for a response is a specific target value, such as a dimension for a manufactured part. The default target value is assumed to be mid-way between the given lower and upper limits.

Note: If your target response is not equidistant from the lower and upper acceptable bounds, you can alter the default target after you make a table from the design. In the data table, open the Column Info dialog for the response column (**Cols** > **Column Info**) and enter the desired target value.

Understanding Response Importance Weights

To compute and maximize overall desirability, JMP uses the value you enter as the importance weight (step 4 in Figure 3.1) of each response. If there is only one response, then importance weight is unnecessary. With two responses you can give greater weight to one response by assigning it a higher importance value.

Adding Simulated Responses, If Desired

If you do not have values for specific responses, you might want to add simulated responses to see a prospective analysis in advance of real data collection:

1 Create the design.
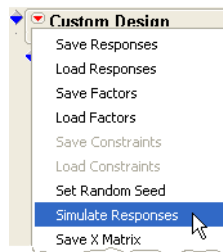
2 Before you click **Make Table**, click the red triangle icon in the title bar and select **Simulate Responses**.

3 Then, click **Make Table** to create the design table—the Y column contains values for simulated responses.

4 For custom and augment designs, a window (Figure 3.2) appears along with the design data table. In this window, enter values you want to apply to the Y column in the data table and click **Apply**. The numbers you enter represent the coefficients in an equation. An example of such an equation, as shown in Figure 3.2, would be, $y = 28 + 4X1 + 5X2 + random\ noise$, where the *random noise* is distributed with mean zero and standard deviation one.

Figure 3.2 In Custom and Augment Designs, Specify Values for Simulated Responses
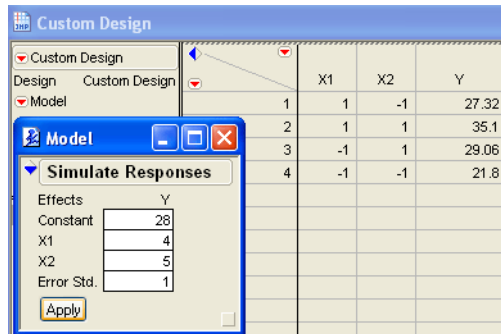
How to Enter Factors

To enter factors, follow the steps in Figure 3.3.

Figure 3.3 Entering Factors in a Custom Design

To add one factor, click **Add Factor** and select a factor type: **Continuous**, **Categorical**, **Blocking**, **Covariate**, **Mixture**, **Constant**, or **Uncontrolled** (see description below).

To add multiple factors, type the number of factors in the **Add N Factors** box, click the **Add Factor** button, and select the factor type.

Click and select **Add Level** to increase the number of levels.

Double-click to edit the factor name.

Click to indicate that changing a factor's setting from run to run is **Easy** or **Hard**. Changing to Hard will cause the resulting design to be a split plot design.

Click to enter or change factor values. To remove a level, click it, press the delete key on the keyboard, then press the Return or Enter key on the keyboard.

Types of Factors

When adding factors, click the **Add Factor** button and choose the type of factor.
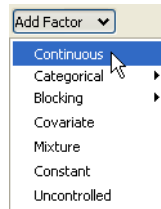
Continuous   Continuous factors are numeric data types only. In theory, you can set a continuous factor to any value between the lower and upper limits you supply.

Categorical   Either numeric or character data types. Categorical data types have no implied order. If the values are numbers, the order is the numeric magnitude. If the values are character, the order is the sorting sequence. The settings of a categorical factor are discrete and have no intrinsic order. Examples of categorical factors are machine, operator, and gender.

Blocking   Either numeric or character data types. Blocking factors are a special kind of categorical factor. Blocking factors differ from other categorical factors in that there is a limit to the number of runs that you can perform within one level of a blocking factor.

Covariate   Either numeric or character data types. Covariate factors are not controllable, but their values are known in advance of an experiment.

Mixture   Mixture factors are continuous factors that are ingredients in a mixture. Factor settings for a run are the proportion of that factor in a mixture and vary between zero and one.

Constant   Either numeric or character data types. Constant factors are factors whose values are fixed during an experiment.

Uncontrolled   Either numeric or character data types. Uncontrolled factors have values that cannot be controlled during an experiment, but they are factors you want to include in the model.

Factors that are Easy, Hard, or Very Hard, to Change - Creating Optimal Split-Plot and Split-Split-Plot Designs

Split plot experiments are performed in groups of runs where one or more factors are held constant within a group but vary between groups. In industrial experimentation this structure is desirable because certain factors may be difficult and expensive to change from one run to the next. It is convenient to make several runs while keeping such factors constant. Until now, commercial software has not supplied a general capability for the design and analysis of these experiments.

To indicate the difficulty level of changing a factor's setting, click in Changes column of the Factors panel for a given factor and select **Easy**, **Hard**, or **Very Hard** from the menu that appears. Changing to **Hard** results in a split-plot design and **Very Hard** results in a split-split-plot design.

See "Creating Random Block Designs," p. 71, for more details.

Defining Factor Constraints, If Necessary

Sometimes it is impossible to vary factors simultaneously over their entire experimental range. For example, if you are studying the affect of cooking time and microwave power level on the number of kernels popped in a microwave popcorn bag, the study cannot simultaneously set high power and long time without burning all the kernels. Therefore, you have factors whose levels are *constrained*.

To define the constraints:

1 After you add factors and click **Continue**, click the blue disclosure button (◆ ◆ on Windows/Linux and ▶ ▼ on the Macintosh) to open the Define Factor Constraints panel.

2 Click the **Add Constraint** button. Note that this feature is disabled if you have already controlled the design region by entering disallowed combinations or chosen a sphere radius.

3 Specify the coefficients and their limiting value in the boxes provided, as shown to the right. When you need to change the direction of the constraint, click on the default less than or equal button and select the greater than or equal to direction.

4 To add another constraint, click the **Add Constraint** button again and repeat the above steps.
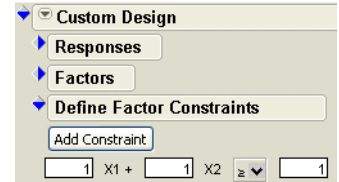
Describe the Model

Initially, the Model panel lists only the main effects corresponding to the factors you entered, as shown in Figure 3.4. However, you can add factor interactions or powers of continuous factors to the model. For example, to add all the two-factor interactions and quadratic effects at once, click the **RSM** button.

Figure 3.4 Add Terms
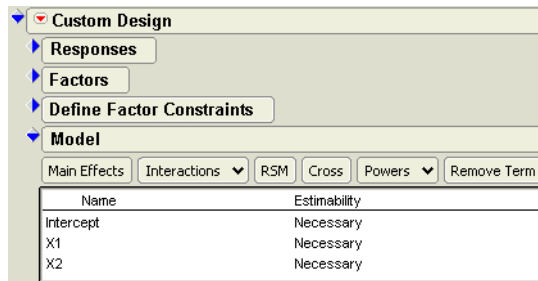
Table 3.1 summarizes the ways to add specific factor types to the model.

Table 3.1 How to Add Terms to a Model

Action	Instructions
Add interaction terms involving selected factors. If none are selected, JMP adds all of the interactions to the specified order.	Click the **Interactions** button and select **2nd**, **3rd**, **4th**, or **5th**. For example, if the factors are X1 and X2 and you click **Interactions > 2nd**, X1*X2 is added to the list of model terms.
Add all second-order effects, including two-factor interactions and quadratic effects	Click the **RSM** button. The design now uses *I*-Optimality criterion rather than *D*-Optimality criterion.
Add selected cross product terms	1 Highlight the factor names. 2 Highlight term(s) in the model list. 3 Click the **Cross** button.
Add powers of continuous factors to the model effects	Click the **Powers** button and select **2nd**, **3rd**, **4th**, or **5th**.

Select the Number of Runs

The Design Generation panel (Figure 3.5) shows the minimum number of runs needed to perform the experiment based on the effects you've added to the model (two main effects in the example above). It also shows alternate (default) numbers of runs, or lets you choose your own number of runs. Balancing the cost of each run with the information gained by extra runs you add is a judgment call that you control.

Figure 3.5 Options for Selecting the Number of Runs
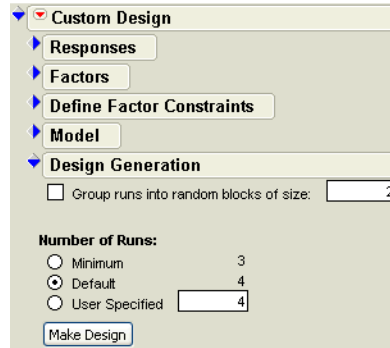
The Design Generation panel has these options for selecting the number of runs you want:

Minimum   is the smallest number of terms that can create a design. When you use Minimum, the resulting design is saturated (no degrees of freedom for error). This is an extreme and risky choice, and is appropriate only when the cost of extra runs is prohibitive.

Default   is a custom design suggestion for the number of runs. This value is based on heuristics for creating balanced designs with a few additional runs above the minimum.

User Specified   is a value that specifies the number of runs you want. Enter that value into the Number of Runs text box.

Note: In general, the custom design suggests a number of runs that is the smallest number that can be evenly divided by the number of levels of each of the factors and is larger than the minimum possible sample size. For designs with factors at two levels only, the default sample size is the smallest power of two larger than the minimum sample size.

When the Design Generation panel shows the number of runs you want, click **Make Design**.

Understanding Design Evaluation

After making the design, you can preview the design and investigate details by looking at various plots and tables that serve as design diagnostic tools.

Although different tools are available depending on the model you specify, most designs display

- the Prediction Variance Profile Plot
- the Fraction of Design Space Plot
- the Prediction Variance Surface Plot

- the Relative Variance of Coefficients and Power Table
- the Alias Matrix
- Design Diagnostic Table.

These diagnostic tools are outline nodes beneath the Design Evaluation panel, as shown in Figure 3.6. JMP always provides the Prediction Variance Profile, but the Prediction Surface Plot only appears if there are two or more variables.

Figure 3.6 Custom Design Diagnostic Tools
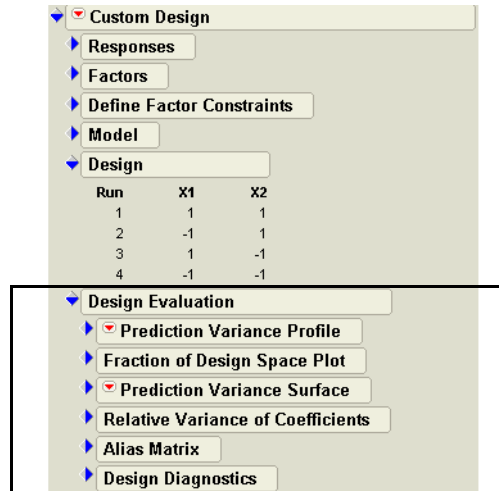
The Prediction Variance Profile

The example in Figure 3.7 shows the prediction variance profile for a response surface model (RSM) with 2 variables and 8 runs. To see a response surface design similar to this:

1 Chose **DOE** > **Custom Design**.
2 In the Factors panel, add 2 continuous factors.
3 Click **Continue**.
4 In the Model panel, click **RSM**.
5 Click **Make Design**.
6 Open the Prediction Variance Profile.

Figure 3.7 A Factor Design Layout For a Response Surface Design with 2 Variables
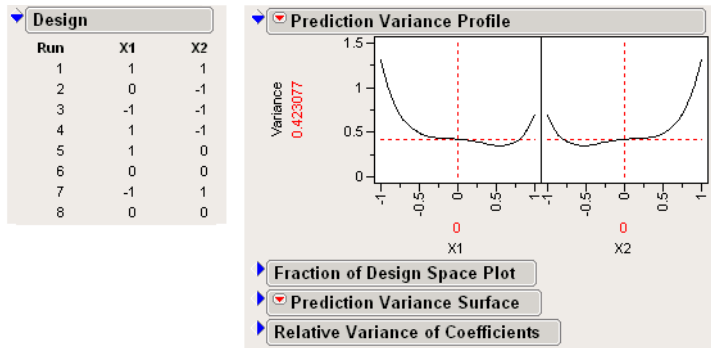
The prediction variance for any factor setting is the product of the error variance and a quantity that depends on the design and the factor setting. Before you collect the data the error variance is unknown, so the prediction variance is also unknown. However, the ratio of the prediction variance to the error variance is not a function of the error variance. This ratio, called the relative variance of prediction, depends only on the design and the factor setting and can be calculated before acquiring the data. The prediction variance profile plots the relative variance of prediction as a function of each factor at fixed values of the other factors.

After you run the experiment, collect the data, and fit the model, you can estimate the actual variance of prediction at any setting by multiplying the relative variance of prediction by the mean squared error (MSE) of the least squares fit.

It is ideal for the prediction variance to be small throughout the allowable regions of the factors. Generally, the error variance drops as the sample size increases. Comparing the prediction variance profilers for two designs side-by-side, is one way to compare two designs. A design that has lower prediction variance on the average is preferred.

In the profiler, drag the vertical lines in the plot to change the factor settings to different points. Dragging the lines reveals any points that have prediction variances that are larger than you would like.

Another way to evaluate a design, or to compare designs, is to try and minimize the maximum variance. You can use the **Maximize Desirability** command on the Prediction Variance Profile title bar to identify the maximum prediction variance for a model. Consider the Prediction Variance profile for the two-factor RSM model shown in Figure 3.8. The plots on the left are the default plots. The plots on the right identify the factor values where the maximum variance (or worst-case scenario) occur, which helps you evaluate the acceptability of the model.

Figure 3.8 Find Maximum Prediction Variance
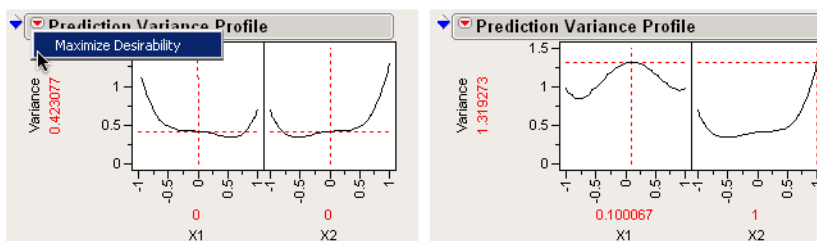
The Fraction of Design Space Plot

The Fraction of Design Space plot is a way to see how much of the model prediction variance lies above (or below) a given value. As a simple example, consider the Prediction Variance plot for a single factor quadratic model, shown on the left in Figure 3.9. The Prediction Variance plot shows that 100% of the values are smaller than 0.5. You can move the vertical trace and also see that all the values are above 0.332. The Fraction of Design Space plot displays the same information. The X axis is the proportion or percentage of prediction variance values, ranging from 0 to 100%, and the Y axis is the range of prediction variance values. In this simple example, the Fraction of Design plot verifies that 100% of the values are below 0.5 and 0% of the values are below approximately 0.3. You can use the crosshair tool and find the percentage of values for any value of the prediction variance. The example to the right in Figure 3.9 shows that 75% of the prediction variance values are below approximately 0.46.

The Fraction of Design space is most useful when there are multiple factors. It summarizes the prediction variance, showing the fractional design space for all the factors taken together.

Figure 3.9 Variance Profile and Fraction of Design Space
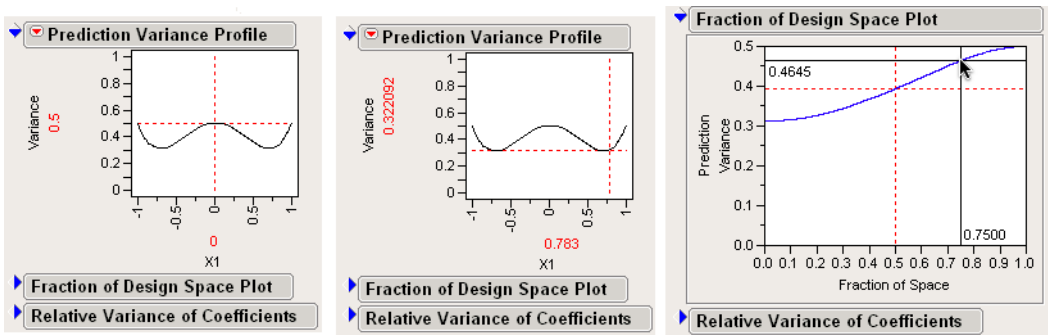
The Prediction Variance Surface

When there are two or more factors, the Prediction Variance Surface plots the surface of the prediction variance for any two variables. This feature uses the **Graph** > **Surface Plot** platform in JMP, and has all its functionality. Drag on the plot to rotate and change the perspective. Figure 3.10 shows the Prediction Variance Surface plot for a two-factor RSM model. The factors are on the x and y axes, and the prediction variance is on the z axis. You can clearly see the high and low variance areas for both factors. Compare this plot to the Prediction Variance Profile shown in Figure 3.8.

Figure 3.10 Prediction Variance Surface Plot for Two-Factor RSM Model
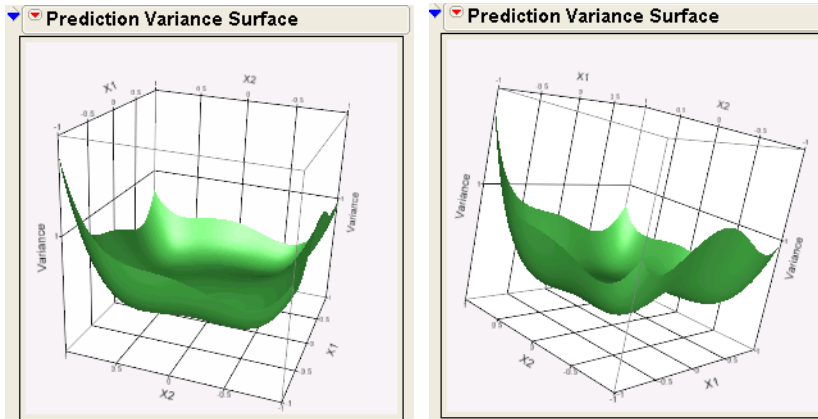
You can find complete documentation for the Surface Plot platform in *JMP Statistics and Graphics Guide*.

The Relative Variance of Coefficients and Power Table

Before clicking **Make Table** in the custom designer, click the disclosure button (◆ ◆ on Windows/ Linux and ▶ ▼ on the Macintosh) to open the Relative Variance of Coefficients table.

The Relative Variance of Coefficients table (Figure 3.11) shows the relative variance of all the coefficients for the example RSM custom design (see Figure 3.7). The variances are relative to the error variance, which is unknown before the experiment, and is assumed to be one. Once you complete the experiment and have an estimate for the error variance, you can multiply it by the relative variance to get the estimated variance of the coefficient. The square root of this value should match the standard error of prediction for the coefficient when you fit a model using **Analyze > Fit Model**.

The Power column shows the power of the design as specified to detect effects of a certain size. In the text edit boxes, you can change the alpha level of the test and the magnitude of the effects compared to the error standard deviation. The alpha level edit box is called **Significance Level**. The magnitude of the effects edit box is called **Signal to Noise Ratio**. This is the ratio of the absolute value of the regression parameter to sigma (the square root of the error variance).

If you enter a smaller alpha (requiring a more significant test), then the power falls. If you increase the magnitude of the effect you want to detect, the power rises.

The power reported is the probability of finding a significant model parameter if the true effect is Signal to Noise Ratio times sigma. The Relative Variance of Coefficients table on the left in Figure 3.11 shows the results for the two-factor RSM model.

As another example, suppose you have a 3-factor 8-run experiment with a linear model and you want to detect any regression coefficient that is twice as large as the error standard deviation, with an alpha level of 0.05. The Relative Variance of Coefficients table on the right in Figure 3.11 shows that the resulting power is 0.984 for all the parameters.

Figure 3.11 Table of Relative Variance of Coefficients
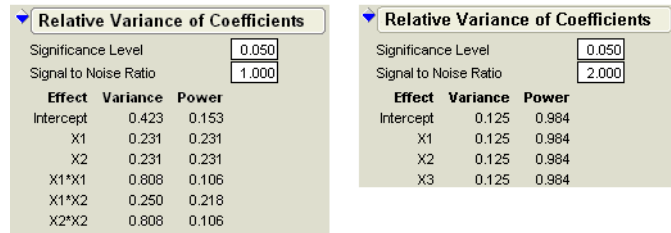
The Alias Matrix (Confounding Pattern)

Click the Alias Matrix disclosure button (◆ ◆ on Windows/Linux and ▶ ▼ on the Macintosh) to open the alias matrix (Figure 3.12).

The alias matrix only appears for custom designs if all factors are two-level factors. The table shows the aliasing (if any) between the model terms and all the two-factor interactions. It allows you to see the confounding pattern in *D*-Optimal and *I*-Optimal designs.

Figure 3.12 Alias Matrix
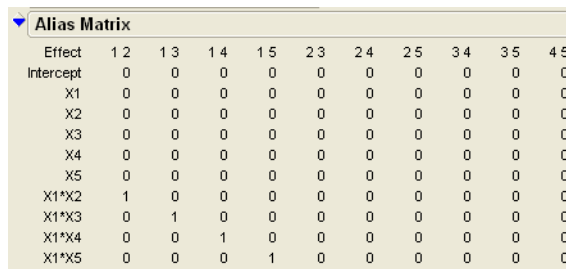
The Design Diagnostics Table

Open the Design Diagnostics outline node to display a table with relative *D*-, *G*-, and *A*-efficiencies, average variance of prediction, and length of time to create the design. The design efficiencies are computed as follows:

$$D\text{-efficiency} = 100\left(\frac{1}{N_D}|\mathbf{X}'\mathbf{X}|^{1/p}\right)$$

$$A\text{-efficiency} = 100\left(\frac{p}{\text{trace}(N_D(\mathbf{X}'\mathbf{X})^{-1})}\right)$$

$$G\text{-efficiency} = 100\left(\frac{\sqrt{\dfrac{p}{N_D}}}{\sigma_M}\right)$$

where

- N_D is the number of points in the design
- p is the number of effects in the model including the intercept
- σ_M is the maximum standard error for prediction over the design points.

These efficiency measures are single numbers attempting to quantify one mathematical design characteristic. While the maximum efficiency is 100 for any criterion, an efficiency of 100% is impossible for many design problems. It is best to use these design measures to compare two competitive designs with the same model and number of runs rather than as some absolute measure of design quality.

Figure 3.13 Custom Design Showing Diagnostics
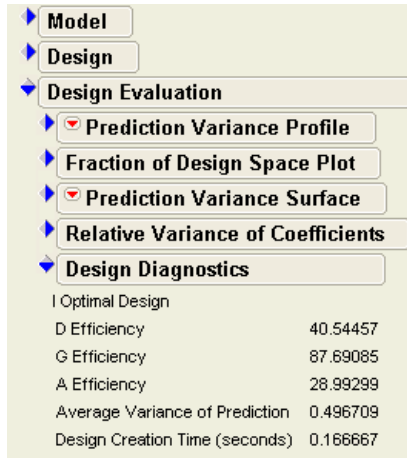
Specify Output Options

Use the Output Options panel to specify how you want the output data table to appear:

Run Order lets you designate the order you want the runs to appear in the data table when it is created. Choices are:

Keep the Same   the rows (runs) in the output table will appear as they do in the Design panel.

Sort Left to Right   the rows (runs) in the output table will appear sorted from left to right.

Randomize   the rows (runs) in the output table will appear in a random order.

Sort Right to Left   the rows (runs) in the output table will appear sorted from right to left.

Randomize within Blocks   the rows (runs) in the output table will appear in random order within the blocks you set up.

Add additional points using options from Make JMP Table from design plus

Number of Center Points: Specifies additional runs placed at the center of each continuous factor's range.

Number of Replicates: Specify the number of times to replicate the entire design, including centerpoints. Type the number of times you want to replicate the design in the associated text box. One replicate doubles the number of runs.

Make the JMP Design Table

When the Design panel shows the layout you want, click **Make Table**. Parts of the table contain information you might need to continue working with the table in JMP. The upper-left of the design table can have one or more of the following scripts:

- a Screening script runs the **Analyze** > **Modeling** > **Screening** platform when appropriate for the generated design.

- a Model script runs the **Analyze** > **Fit Model** platform with the model appropriate for the design.

- a constraint script that shows any model constraints you entered in the Define Factor Constraints panel of the Custom Design dialog.

- a DOE Dialog script that recreates the dialog used to generate the design table, and regenerates the design table.

Figure 3.14 Example Design Table

This area identifies the design type that generated the table. Click **Custom Design** to edit.

Model is a script. Click the red triangle icon and select **Run Script** to open the Fit Model dialog, which is used to generate the analysis appropriate to the design.

DOE Dialog is a script. Click the red trangle icon and select **Run Script** to recreate the DOE Custom Dialog and generate a new design table.

Creating Random Block Designs

It is often necessary to group the runs of an experiment into blocks. Runs within a block of runs are more homogeneous than runs in different blocks. For example, the experiment described in Goos (2002), describes a pastry dough mixing experiment that took several days to run. It is likely that random day-to-day differences in environmental variables have some effect on all the runs performed on a given day. Random block designs are useful in situations like this, where there is a non-reproducible shock to the system between each block of runs. In Goos (2002), the purpose of the experiment was to understand how certain properties of the dough depend on three factors: feed flow rate, initial moisture content, and rotational screw speed. It was only possible to conduct four runs a day. Because day-to-day

variation was likely, it was important to group the runs so that this variation would not compromise the information about the three factors. Thus, blocking the runs into groups of four was necessary. Each day's experimentation was one block. The factor, Day, is an example of a random block factor.

To create a random block, use the custom design and enter responses and factors, and define your model as usual. In the Design Generation panel, check the Group runs into random blocks of size check box and enter the number of runs you want in each block. When you select or enter the sample size, the number of runs specified are assigned to the blocks.

In this example, the Design Generation Panel shown here designates four runs per block, and the user-specified number of runs (28) indicates there will be seven days (blocks) of 4 runs. If the number of runs is not an even multiple of the random block size, some blocks will have a fewer runs than others.

Creating Split Plot Designs

Split plot experiments happen when it is convenient to run an experiment in groups of runs (called whole plots) where one or more factors stay constant within each group. Usually this is because these factors are difficult or expensive to change from run to run. JMP calls these factors **Hard** to change because this is usually how split plotting arises in industrial practice.

In a completely randomized design, any factor can change its setting from one run to the next. When certain factors are hard to change, the completely randomized design may require more changes in the settings of hard-to-change factors than desired.

If you know that a factor or two are difficult to change, then you can set the Changes setting of a factor from the default of **Easy** to **Hard**. Before making the design, you can set the number of whole plots you are willing to run.

For an example of creating a split plot design, see "Creating a Design with Two Hard-to-Change Factors: Split Plot," p. 49.

To create a split plot design using the custom designer:

1   In the factors table there is a column called Changes. By default, changes are **Easy** for all factors. If, however, you click in the changes area for a factor, you can choose to make the factor **Hard** to change.

2   Once you finish defining the factors and click continue, you see an edit box for supplying the number of whole plots. You can supply any value as long as it is above the minimum necessary to fit all the model parameters. You can also leave this field empty. In this case, JMP chooses a number of whole plots to minimize the omnibus uncertainty of the fixed parameters.

Note: If you enter a missing value in the Number of Whole Plots edit box, then JMP considers many different numbers of whole plots and chooses the number that maximizes the information about the coefficients in the model. It maximizes the determinant of $X'V^{-1}X$ where V^{-1} is the inverse of the variance matrix of the responses. The matrix, V, is a function of how many whole plots there are, so chang-

ing the number of whole plots changes **V**, which can make a difference in the amount of information a design contains.

To create a split plot design every time you use a certain factor, save steps by setting up that factor to be "hard" in all experiments. See "Identify Factor Changes Column Property," p. 87, for details.

Creating Split-Split Plot Designs

Split-split plot designs are a three stratum extension of split plot designs. Now there are factors that are Very-Hard-to-change, Hard-to-change, and Easy-to-change. Here, in the top stratum, the Very-Hard-to- change factors stay fixed within each whole plot. In the middle stratum the Hard-to-change factors stay fixed within each subplot. Finally, the Easy-to-change factors may vary (and should be reset) between runs within a subplot. This structure is natural when an experiment covers three processing steps. The factors in the first step are Very-Hard-to-change in the sense that once the material passes through the first processing stage, these factor settings are fixed. Now the material passes to the second stage where the factors are all Hard-to-change. In the third stage, the factors are Easy-to-change.

Schoen (1999) provides an example of three-stage processing involving the production of cheese that leads to a split-split plot design. The first processing step is milk storage. Typically milk from one storage facility provides the raw material for several curds processing units—the second processing stage. Then the curds are further processed to yield individual cheeses.

In a split-split plot design the material from one processing stage passes to the next stage in such a way that nests the subplots within a whole plot. In the example above, milk from a storage facility becomes divided into two curds processing units. Each milk storage tank provided milk to a different set of curds processors. So, the curds processors were nested within the milk storage unit.

Figure 3.15 shows an example of how factors might be defined for the cheese processing example.

Figure 3.15 Example of Split-Split Response and Factors in Custom Designer Dialog
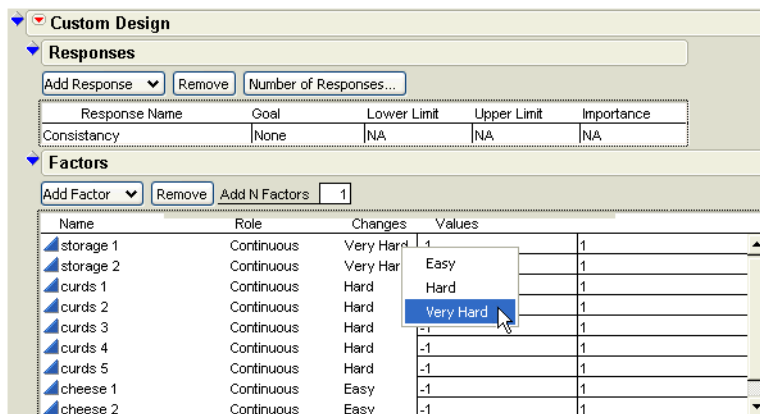
Creating Strip Plot Designs

In a strip plot design it is possible to reorder material between processing stages. Suppose units are labelled and go through the first stage in a particular order. If it is possible to collect all the units at the end of the first stage and reorder them for the second stage process, then the second stage variables are not nested within the blocks of the first stage variables. For example, in semiconductor manufacturing a boat of wafers may go through the first processing step together. However, after this step, the wafers in a given boat may be divided among many boats for the second stage.

To set up a strip plot design, enter responses and factors as usual, designating factors as Very Hard, Hard, or Easy to change. Then, in the Design Generation panel, check the box that says Hard to change factors can vary independently of Very Hard to change factors, as shown in Figure 3.16. Note that the Design Generation panel specified 6 whole plots, 12 subplots, and 24 runs.

When you click **Make Design**, the design table on the right in Figure 3.16 lists the run with subplots that are not nested in the whole plots.

Figure 3.16 Example of Strip Split Factors and Design Generation panel in Custom Designer Dialog

Special Custom Design Commands

After you select **DOE > Custom Design**, click the red triangle icon on the title bar to see the list of commands available to the Custom designer (Figure 3.17). The commands found on this menu vary, depending on which DOE command you select. However, the commands to save and load responses

and factors, the command to set the random seed, and the command to simulate responses are available to all designers. You should examine the red triangle menu for each designer you use to determine which commands are available. If a designer has additional commands, they are described in the appropriate chapter.

Figure 3.17 Click the Red Triangle Icon to Reveal Commands
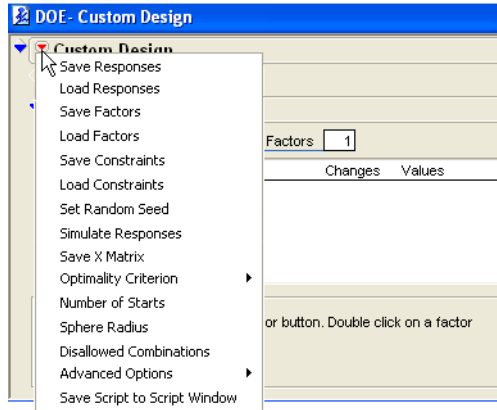
The following sections describe these menu commands and how to use them.

Save Responses and Save Factors

If you plan to do further experiments with factors and/or responses to which you have given meaningful names and values, you can save them for later use.

To save factors or responses:

1 Select a design type from the DOE menu.

2 Enter the factors and responses into the appropriate panels (see "Enter Responses and Factors into the Custom Designer," p. 59, for details).

3 Click the red triangle icon on the title bar and select **Save Responses** or **Save Factors.**

   Save Responses   creates a data table containing a row for each response with a column called Response Name that identifies the responses. Four additional columns identify more information about the responses: Lower Limit, Upper Limit, Response Goal, and Importance.

   Save Factors   creates a data table containing a column for each factor and a row for each factor level. The columns have a column property (noted with an asterisk icon in the column panel) called Design Role that identifies them as DOE factors and lists their type (continuous, categorical, blocking, and so on).

4 Save the data table.

Load Responses and Load Factors

If you have saved responses and factors, you can quickly apply them to your design and avoid retyping this information each time you run an experiment.

To design an experiment using responses or factors you have previously saved:

1 Open the data table that contains the factor names and levels.

2 Select a design type from the DOE menu.

3 Click the red triangle icon on the title bar (Figure 3.18) and select **Load Responses** or **Load
   Factors**.

Figure 3.18   Loading Factor Names and Values from a JMP Table
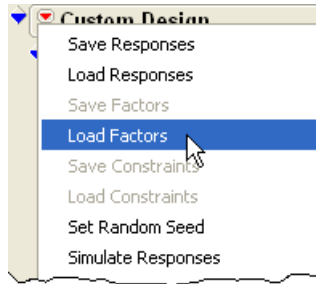
Tip: It is possible to create a factors table by keying data into an empty table, but remember to assign
each column a factor type. Do this by right-clicking the column name, selecting **Column Info**, and
then selecting **Column Properties > Design Role**. Lastly, click the button in the Design Role area and
select the appropriate role.

Save Constraints and Load Constraints

In custom, augment, and mixture designs, if you set up factor constraints and plan to do further exper-
iments with them, you can save them for later use. You can quickly apply these constraints to your
design and avoid retyping this information each time you run an experiment.

To save factor constraints:

1 Select a design type from the DOE menu.

2 Enter the factor constraints into the appropriate panels (see "Enter Responses and Factors into the
   Custom Designer," p. 59, for details).

3 Click the red triangle icon on the title bar (Figure 3.18) and select **Save Constraints. Save
   Constraints** creates a data table that contains the information you enter into a constraints panel.
   There is a column for each constraint. Each has a column property called Constraint State that iden-
   tifies it as a 'less than' or a 'greater than' constraint. There is a row for each variable and an additional
   row that has the inequality condition for each variable.

4 Save the data table.

To design an experiment using factor constraints you have previously saved:

1 Open the data table that contains the constraints.

2 Select a design type from the DOE menu.

3 Click the red triangle icon on the title bar (Figure 3.18) and select **Load Constraints**.

Set Random Seed: Setting the Number Generator

The design process begins with a random starting design. To set the random seed that the custom designer uses to create this starting design, click the red triangle icon in the design title bar (Figure 3.18) and select **Set Random Seed**.

The window that appears shows the *generating seed* for that design (Figure 3.19). From this window, you can set a new random number and then run the design again.

If you use the same seed as a previous design, you will get the same design again.

Figure 3.19 Setting the Random Seed
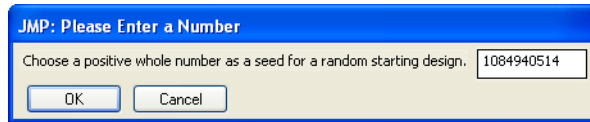
Note: The random seed is also used when you simulate responses to be used with a design, as described next.

Simulate Responses

Often, when you define a custom design (or any standard design), it may be useful to look at properties of the design with response data before you have collected data. The **Simulate Responses** command adds random response values to the JMP table that the custom designer creates. To use the command, select it before you click **Make Table**. When you click **Make Table** to create the design table, the Y column contains values for simulated responses.

For custom and augment designs, an additional window appears with the design data table that lists coefficients for the design you described in the designer panels. You can enter any coefficient values you want and click **Apply** to see new Y values in the data table. An example of an equation for a model with two factors and interaction (Figure 3.20) would be,

$$y = 19 + 2X1 + (-5)X2 + 6X1X2 + \textit{random noise},$$

where the *random noise* is distributed with mean zero and standard deviation one.

Figure 3.20 Example of a Custom Design with Simulated Responses
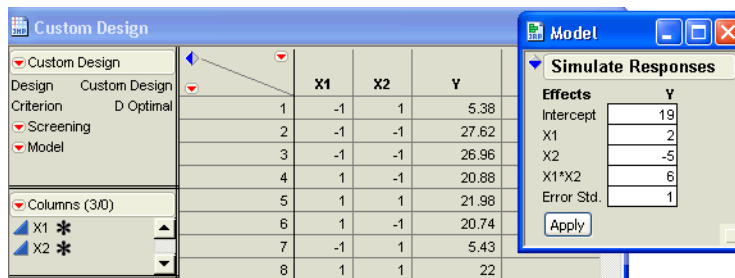
Save X Matrix: Viewing the Design (X) Matrix in the Log

To create a script and save the design matrix as a table property in a data table, click the red triangle icon in the Custom Design title bar (Figure 3.17) and select **Save X Matrix**. A script is saved as a table property called **Design Matrix**. When you run this script, JMP creates a global matrix called X and displays its number of rows in the log. If you do not have the log visible, select **View > Log (Window > Log** on the Macintosh).

Optimality Criterion: Changing the Design Criterion (*D*- or *I*- Optimality)

To change the design criterion, click the red triangle icon in the Custom Design title bar (Figure 3.21) and select **Optimality Criterion**, then choose **Make D-Optimal Design** or **Make I-Optimal Design**.

Figure 3.21 Changing the Design Criterion
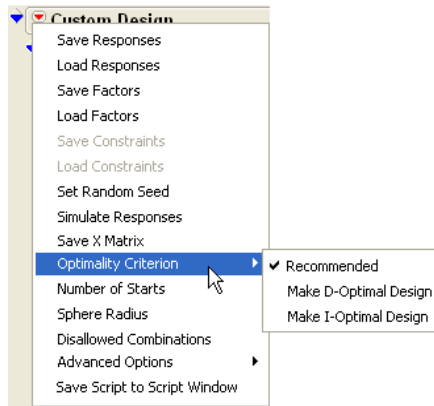
The default criterion for **Recommended** is *D*-optimal for all design types unless you have used the **RSM** button in the Model panel to add effects that make the model quadratic. For specific information about optimality criterion, see "Technical Discussion," p. 53.

Number of Starts: Changing the Number of Random Starts

To override the default number of random starts, click the red triangle icon in the Custom Design title bar (Figure 3.17) and select **Number of Starts**. When you select this command, the window shown here appears with an edit box for you to enter the number of random starts for the design you want to build. The number you enter overrides the default number of starts, which varies depending on the design.
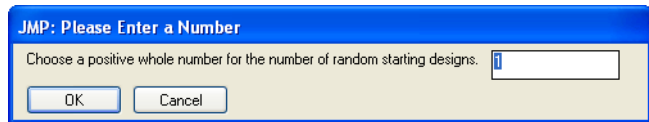
Note: If the design iterations are taking too long, click the **Cancel** button. The Custom Designer stops and gives the best design found at that point.

Why Change the Number of Starts?

One difficulty with the creation of optimal designs is that the methods used do not always find the globally optimal design in cases where the optimal design is known from theory. For example, orthogonal designs are *D*-optimal with respect to a linear additive model and a cubic design space.

As the number of factors and sample size increase, the optimization problem becomes harder. It is easy for an optimizer to converge to a local optimum instead of a global optimum.

It is useful to know that:

- If random starts are used for the optimization, the design produced at the end is not always the same. Increasing the number of random starts tends to improve the optimality of the resulting design.

- For designs with all two-level factors, there is a formula for the optimal determinant:
  If *D* is the determinant, *n* is the sample size, and *c* is the number of columns in the design matrix, the Log*D* = *c*Log*n*.

  If the determinants that result from the random starts match the formula above, the algorithm stops. The design is *D*-optimal and orthogonal.

Default Choice of Number of Random Starts: Technical Information

JMP does not start over with random designs until a jackpot is hit. The time it takes for one iteration of the algorithm (coordinate exchange) increases roughly as the product of the sample size and the number of terms in the model. By doing a large number of random starts for small sample sizes and reducing this number proportional to the square of the sample size as the designs get larger, the total time it takes to generate a design is kept roughly constant over the range of usual sample sizes.

The Custom Designer always attempts to find globally optimal designs when such designs are known from theory. For example,

- 2-level fractional factorial designs are globally D-optimal for all main effect and two-factor interaction models

- Latin-Square designs are D-optimal for main effect models assuming the right sample size and numbers of levels of the factors.

- Plackett-Burman designs are D-optimal for main effect models.

If the custom designer can identify one of these special cases, it does many more random starts. In general, however, the default number of random starts is controlled by the sample size, n, as follows:

Table 3.2 Sample Size and Random Starts

Sample Size	Number of Starts
9 or fewer	80
from 9 to 16	40
from 17 to 24	10
from 25 to 32	5
more than 32	2

Note the following exceptions:

- If each factor has only two levers, the number of terms in the model is one greater than the number of factors, and the sample size is a multiple of 4, then multiply the default number of starts shown in the table above by 40.
- If the design is I-optimal divide all the sample sizes in the table above by 2 and add 1.
- If the design could be a Latin Square, the Custom Designer does 1000 random starts.
- If the number of terms in the model is greater than 100, though, the number of random starts is 1.

After each random start, the design is checked to see if it is globally optimal, and if so, the iterations stop. Therefore, even if the default number of starts is large, it may only take a small fraction of the default number to find the globally optimal design. Again, if the process seems to be taking too long, use the **Cancel** button to see the best design found at that point.

Sphere Radius: Constraining a Design to a Hypersphere

You can constrain custom and augmented designs to a hypersphere by editing the sphere radius. Before making the design, click the red triangle icon in the Custom Design title bar (Figure 3.17) and select **Sphere Radius**. Enter the appropriate value and click **OK**.

Note that hypersphere constraints do not work with other constraints. Also, split plot designs cannot be generated with hypersphere constraints.

If you have designed any factor's changes as Hard (see "Factors that are Easy, Hard, or Very Hard, to Change - Creating Optimal Split-Plot and Split-Split-Plot Designs," p. 62, and "Creating Random Block Designs," p. 71), the sphere radius item becomes unavailable. Conversely, once you set the sphere radius, you cannot make a factor Hard to change.

Disallowed Combinations: Accounting for Factor Level Restrictions

JMP gives you the flexibility to disallow particular combinations of levels of factors. You can do this for custom and augmented designs except for experiments with mixture or blocking factors. This feature can also be used with continuous factors or mixed continuous and categorical factors.

For example, in a market research choice experiment, you might want to exclude a choice that allows all the best features of a product at the lowest price. In this case, the factor **Feature** has levels of worst (1), medium (2), and best (3), and the factor **Price** has levels of high (1), medium (2), and low (3). You want to exclude the third **Feature** level (best) and the third **Price** level (low).

To disallow a combination of factor levels:

1 Begin by adding the factors.
2 Click the red triangle icon in the title bar (Figure 3.17) of the designer window and select **Disallowed Combinations**. Note that this menu item is not available if you have already defined linear inequality constraints.
3 Enter a Boolean expression that identifies what you do not want allowed (Figure 3.22). JMP evaluates your expression, and when it sees it as true, it disallows the specified combination.

Note: When forming the expression, use the ordinal value of the level instead of the name of the level. If the level names of the factor called Price are high, medium, and low, their associated ordinal values are 1, 2, and 3.

For example, in Figure 3.22, `Feature==3 & Price==3` will not allow a run containing the best features at the lowest price. If there were two disallowed combinations in this example, you would use `Feature==3 & Price==3 | Quality==3 & Price==3`, which tells JMP to disallow a run with the best features at the lowest price or a run with the best quality and lowest price.

Figure 3.22 Enter a Boolean Expression
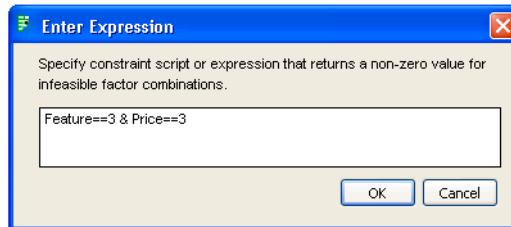
4 Make the design table. It excludes the combination of factors you specified, as shown in Figure 3.23.

Figure 3.23 No Row Contains L3 for Both Price and Feature

Advanced Options for the Custom Designer

The following options are for advanced design of experiment users.

Changing the Search Points Per Factor

For a main effects model, the coordinate exchange algorithm in the custom designer only considers the high and low values. However, you can change this so the algorithm considers more search points. For example, if you enter 5, then JMP considers five equally spaced settings for each factor. The 5 levels are considered, but all 5 levels may not appear in the output table. The Custom Designer finds a D- or I-Optimal design, which might not need to include all 5 levels.

To change the search points:

1 Select **DOE > Custom Design**.
2 Click the red triangle icon in the title bar (Figure 3.17) of the designer window and select **Advanced Options > Search Points Per Factor**.
3 Enter a positive integer and click **OK**.

4   Make the design.

Altering the Mixture Sum

If you want to keep a component of a mixture constant throughout an experiment, then the sum of the other mixture components must be between 0.001 and 1. You may have one or more fixed ingredients so that the sum of the remaining add to less than one but more than zero. To alter the mixture sum:

1   Select **DOE > Custom Design**.
2   Click the red triangle icon in the title bar (Figure 3.17) of the designer window and select **Advanced Options > Mixture Sum**.
3   Enter a positive number and click **OK**.
4   Make the design.

Split Plot Variance Ratio

The optimal split plot design depends on the ratio of the variance of the random whole plot variance to the error variance. By default, this variance is one. If you have some prior knowledge of this variance ratio, you can supply it by following these steps:

1   Select **DOE > Custom Design**.
2   Click the red triangle icon in the title bar (Figure 3.17) of the designer window and select **Advanced Options > Split Plot Variance Ratio**.
3   Enter a positive number and click **OK**.
4   Make the design.

Prior Parameter Variance

If you have specified **If Possible** as the Estimability for any factors in your model, then you can use this option to also specify the weight used for these terms. Default values are one. Larger values represent more prior information and a smaller variance. Variances are the reciprocals of the entered values.

1   Select **DOE > Custom Design**.
2   Click the red triangle icon in the title bar (Figure 3.17) of the designer window and select **Advanced Options > Prior Parameter Variance**.
3   Enter a positive number for each of the terms for which you want to specify a weight and click **OK**.
4   Make the design.

Save Script to Script Window

This command creates the script for the design you described in the Custom Designer and saves it in an open script window.

Assigning Column Properties

Columns in a data table can contain special column properties. Figure 3.24 shows that a column called Stretch has two special properties: **Role** and **Response Limits**, that were assigned by the Custom Designer when the table was created. To see the example in Figure 3.24, open Bounce Data.jmp from the Design Experiment folder found in the sample data installed with JMP. Then, right-click the column name in the data table and select **Column Info**. When the Column Info dialog appears, click on the property you want to see.

Figure 3.24 Column Properties Menu in the Column Info Dialog
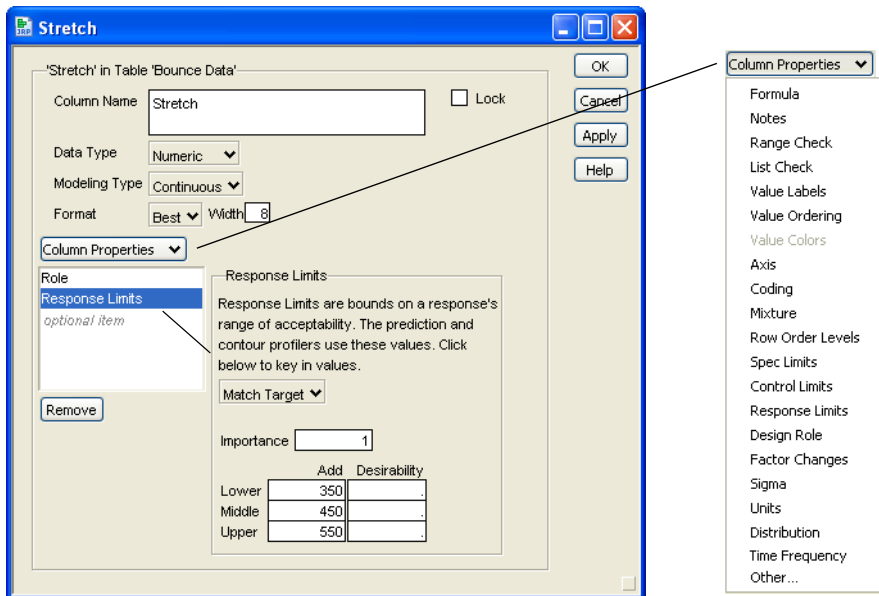
All special column properties are covered in the *JMP User Guide*. The following discussion gives details about properties specific to DOE and that are useful for analyzing DOE data.

Define Low and High Values (DOE Coding) for Columns

For continuous variables, the *Coding* column property transforms data in the range you specify from –1 to +1. When you analyze the coded variable, JMP uses those transformed data values to compute meaningful parameter estimates. You can specify the range in which the low and high values of the column are transformed.

By default, when JMP generates a design table from values entered in the Factors panel, it uses those values as the low and high values of the coding property. If a column has one or more limits missing, JMP substitutes the data's minimum and maximum for the high and low values.

You can use the Column Info dialog to manually add or delete a coding property, or change the range in which the low and high values are transformed. Figure 3.25 shows the coding values for the Temperature variable in the Reactor 8 Runs data table from the Design Experiment Sample Data.

Figure 3.25 Coding Column Property in Column Info Dialog
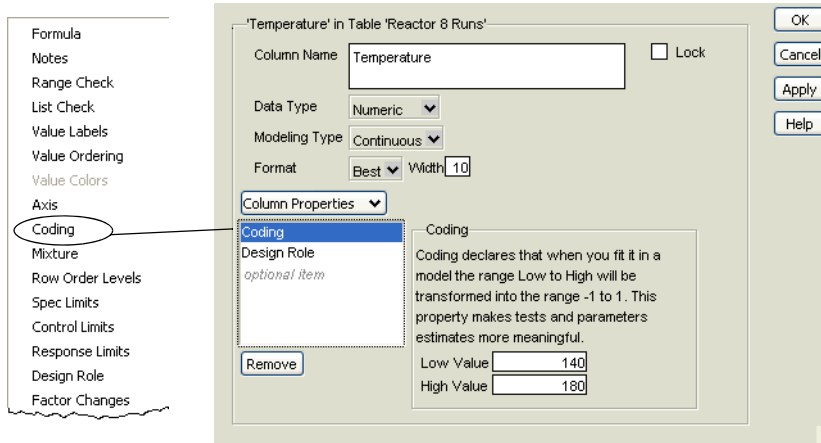
Set Columns as Factors for Mixture Experiments

You might have a column in a data table that is one of several factors that form 100% of a mixture. You can set up the column so JMP uses it to automatically generate a no-intercept model when you analyze the data with the Fit Model platform. The following example uses the Donev Mixture Data from the Design Experiment sample data

To set up the CuS04 column as a mixture factor, first select **Cols** > **Column Info** to see the Column Info dialog for CuS04. Then continue as follows:

1 Select **Mixture** from the **Column Properties** drop-down menu. Upper and Lower limits, and the sum of the limits appear in a panel on the dialog, as shown in Figure 3.26. You can use these limits, or enter your own values.

2 Optionally, check the boxes beside **L PseudoComponent Coding, U PseudoComponent Coding, or both L and U PseudoComponent Coding**. Using the example in Figure 3.26, where the mixture sum value is 1, the terms are coded as:

$$X_i L = (X_i - L_i)/(1 - L) \text{ for the } L \text{ pseudocomponent}$$

$$X_i U = (U_i - X_i)/(U - 1) \text{ for the } U \text{ pseudocomponent}$$

where L_i and U_i are the lower and upper bounds, L is the sum of L_i and U is the sum of U_i.

Note: If you check either **L PseudoComponent Coding** or **U PseudoComponent Coding** for the mixture coding of one mixture factor and you check the other alternative for one or more other mixture factors in the model, of if you check both boxes for one or more of the mixture factors, the Fit Model platform uses the L coding if $(1 - L) < (U - 1)$, and the U coding otherwise. If only one coding box is checked consistently for all mixture factors in the model, then only that one pseudocomponent coding is used.

In the Fit Model report, the main effects are labeled with the coding transformation. Crossed effects are not labeled, but coding values are used. All the features of fitting, such as the profilers and saved

formulas, respect the pseudocomponent coding but present the un-coded values in the tables and plots.

3   Select the **Design Role** Column Property, and choose **Mixture** from its drop down menu.

4   Click **OK**. The properties icon (✻) now appears next to the column name in the columns panel, indicating the column contains one or more column properties.

Figure 3.26 Column Info to Create Mixture Column For Analysis

5   Repeat the above steps for any other mixture factors that will be included in the model.

Define Response Column Values

You can save response limits in a column, which means you can run analyses without having to re-specify response limits each time. Saving these limits in a column facilitates consistency. For example, if you run an analysis that employs these limits, then come back later and change the data, you can run a new analysis using the same limits without having to reenter them. To see the example in Figure 3.27, open Bounce Data.jmp from the Design Experiment folder in the sample data installed with JMP.

Figure 3.27 shows the panel with values that specify lower, middle, and upper limits, and a desirability value. You can also select a possible goal for a DOE response variable: **Maximize**, **Match Target**, **Minimize**, or **None**. If you have more than one response, you can enter an importance value, which lets JMP know how to weigh the importance of one response against another.

To enter response limits:

1   Double-click the column name in the data grid. The Column Info dialog appears.

2   Select **Response Limits** from the **Column Properties** drop-down menu.

3 Complete the settings in the window, as described in Figure 3.27.

4 Click **OK**. The properties icon (✳) now appears next to the column name in the column panel of the data table to indicate that the column contains a property.

Figure 3.27 Define Response Column Values

Click to select a goal for the response variable. For example, if you are in the prediction profiler and want the desired value to be close to zero, select **Match Target**

When you have two responses, enter a number to indicate the amount of weight you want this response to have when JMP computes the over-all desirability

Enter the lower, middle and upper limits as well as the desirability values

Assign Columns a Design Role

The Custom designer in JMP assigns design roles to factors when you create the design. However, you can assign a property to a column that identifies a factor column as a continuous, categorical, blocking, covariate, mixture, constant, signal, or noise factor. The example in Figure 3.28 shows the Whole Plots factor in the Vinyl Data.jmp table from the Design Experiment sample data assigned the **Random Block** design role.

To give a column a design role:

1 Double-click the column name in the data grid. The Column Info window appears.

2 Select **Design Role** from the **Column Properties** drop-down menu, as shown in Figure 3.28. Design role information appears on the right.

3 Click the Design Role drop-down menu and select how you want JMP to use the factor column: **Continuous**, **Categorical**, **Blocking**, **Covariate**, **Mixture**, **Constant**, **Signal**, **Noise**, **Uncontrolled**, or **Random Block**.

4 Click **OK** to see the property icon (✳) next to the column name in the data table's column panel.

Figure 3.28 Assign a Design Role to a Factor Column
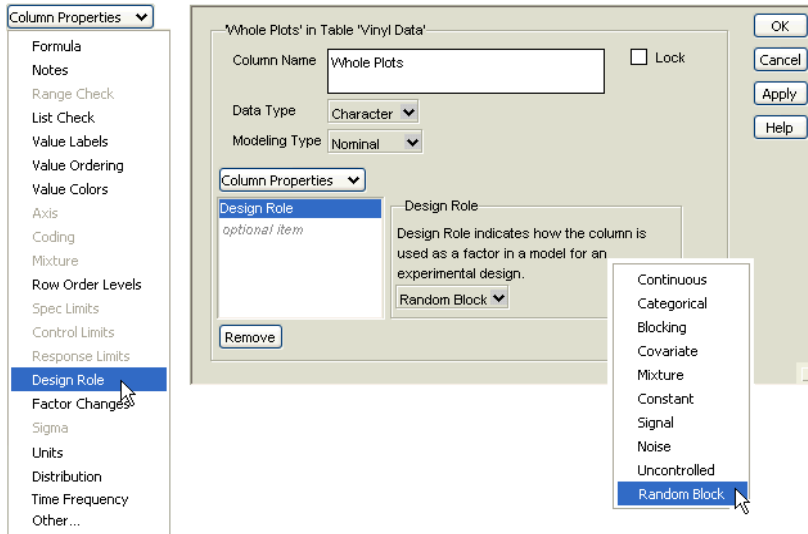
Identify Factor Changes Column Property

To create split plot or split-split plot designs, you must identify a factor as having values that are hard to change, or very hard to change. This is done in the DOE design panel (see "Creating Split Plot Designs," p. 72, for details) each time you design an experiment. However, if you know that every time you use that factor, you want it to be considered hard or very hard to change, you can save yourself steps by setting up a column property to be used in all experiments using that factor. To do this:

1 Double-click the column name in the data grid to see the Column Info dialog for that column.

2 Select **Factor Changes** from the **Column Properties** drop-down menu, as shown in Figure 3.29.

3 Click the Factor Changes button and select **Easy**, **Hard**, or **Very Hard** from the **Factor Changes** drop-down menu.

4 Click **OK**. The properties icon (✱) now appears next to the column name in the column panel of the data table.

Note: Although you can save design roles for factors, which are then automatically used each time those factors are loaded, you must always verify that the model for the design you create is correctly entered into the DOE custom designer.

Figure 3.29 Factor Changes Column Property
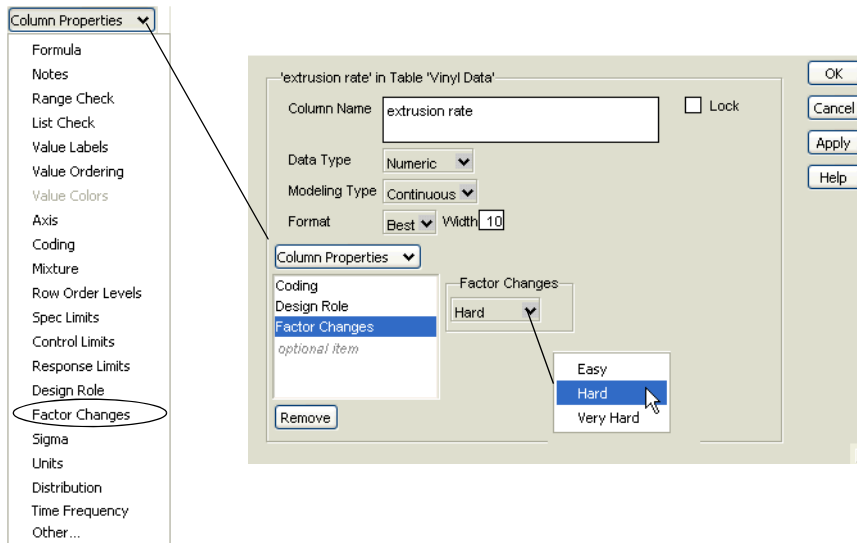
How Custom Designs Work: Behind the Scenes

The custom designer starts with a random set of points inside the range of each factor. The computational method is an iterative algorithm called *coordinate exchange* (Meyer and Nachtsheim, 1995). Each iteration of the algorithm involves testing every value of every factor in the design to determine if replacing that value increases the optimality criterion. If so, the new value replaces the old. This process continues until no replacement occurs for an entire iteration.

To avoid converging to a local optimum, the whole process is repeated several times using a different random start. The custom designer displays the best of these designs. For more details, see the section "Optimality Criterion: Changing the Design Criterion (D- or I- Optimality)," p. 78.

Sometimes a design problem can have several *equivalent* solutions. Equivalent solutions are designs with equal precision for estimating the model coefficients as a group. When this is true, the design algorithm may generate different (but equivalent) designs when you click the **Back** and **Make Design** buttons repeatedly.

Chapter **4**

Screening Designs

Screening designs are some of the most popular designs for industrial experimentation. They examine many factors to see which have the greatest effect on the results of a process.

Screening designs generally require fewer experimental runs, which is why they cost less. Thus, they are attractive because they are a relatively inexpensive and efficient way to begin improving a process.

Often screening designs are a prelude to further experiments. It is wise to spend only about a quarter of your resource budget on an initial screening experiment. You can then use the results to guide further study.

The efficiency of screening designs depends on the critical assumption of *effect sparsity*. Effect sparsity results because real-world processes usually have only a few driving factors; other factors are relatively unimportant. To understand the importance of effect sparsity, you can contrast screening designs to full factorial designs:

- Full factorial designs consist of all combinations of the levels of the factors. The number of runs is the product of the factor levels. For example, a factorial experiment with a two-level factor, a three-level factor, and a four-level factor has 2 x 3 x 4 = 24 runs.

- By contrast, screening designs reduce the number of runs by restricting the factors to two (or three) levels and by performing only a fraction of the full factorial design.

Each factor in a screening design is usually set at two levels to economize on the number of runs needed, and response measurements are taken for only a fraction of the possible combinations of levels. In the case described above, you can restrict the factors to two levels, which yield 2 x 2 x 2 = 8 runs. Further, by doing half of these eight combinations you can still assess the separate effects of the three factors. So the screening approach can reduce the original 24-run experiment to four runs.

Of course, there is a price for this reduction. This chapter discusses the screening approach in detail, showing both pros and cons. It also describes how to use JMP's screening designer, which supplies a list of popular screening designs for two or more factors. These factors can be continuous or categorical, with two or three levels. The list of screening designs you can use includes designs that group the experimental runs into blocks of equal sizes where the size is a power of two.

Contents

Screening Design Examples

This chapter is divided into two sections. The first section consists of two examples using screening designs. The second section outlines the procedures to follow to create a screening design to match your needs.

Using Two Continuous Factors and One Categorical Factor

Suppose an engineer wants to investigate a process that uses an electron beam welding machine to join two parts. The engineer fits the two parts into a welding fixture that holds them snugly together. A voltage applied to a beam generator creates a stream of electrons that heats the two parts, causing them to fuse. The ideal depth of the fused region is 0.17 inches. The engineer wants to study the welding process to determine the best settings for the beam generator to produce the desired depth in the fused region.

For this study, the engineer wants to explore the following three inputs, which are the *factors* for the study:

- Operator, who is the technician operating the welding machine
- Rotation Speed, which is the speed at which the part rotates under the beam
- Beam Current, which is a current that affects the intensity of the beam

After each processing run, the engineer cuts the part in half. This reveals an area where the two parts have fused. The Length of this fused area is the depth of penetration of the weld. This depth of penetration is the response for the study.

The goals of the study are to:

- find which factors affect the depth of the weld
- quantify those effects
- find specific factor settings that predict a weld depth of 0.17 inches

To begin this example, select **DOE > Screening Design** from the main menu. Note that in the Responses panel, there is a single default response called Y. Change the default response as follows:

1 Double-click the response name and change it to Depth (In.).
2 The default goal for the single default response is Maximize, but the goal of this process is to get a target value of 0.17 inches with a lower bound of 0.12 and an upper bound of 0.22. Click the **Goal** box and choose **Match Target** from the drop-down menu, as shown in Figure 4.1.

Figure 4.1 Screening Design Response With Match Target Goal

Click the **Goal** box
and choose **Match
Target**
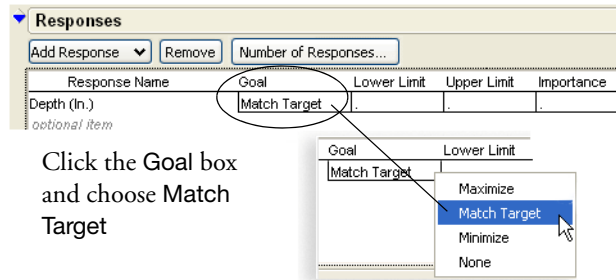
3 Click the **Lower Limit** text edit area and enter 0.12 as the lower limit (minimum acceptable value).
   Then click the **Upper Limit** text edit area and enter 0.22 as the upper limit (maximum acceptable
   value).

This example has one categorical factor (**Operator**) and two continuous factors (**Speed** and **Current**).

4 Add the categorical factor by clicking the **Add** button beside **2-Level Categorical**.

5 Add two continuous factors by typing **2** in the **Continuous** box and clicking the associated **Add**
   button.

6 Double-click the factor names and rename them **Operator**, **Speed**, and **Current**.

7 Set high and low values for **Speed** to 3 and 5 rpm. Set high and low values for **Current** to 150 and
   165 amps, and assign Mary and John as values for the categorical factor called Operator, as shown in
   Figure 4.2.

Figure 4.2 Screening Design with Two Continuous and One Categorical Factor
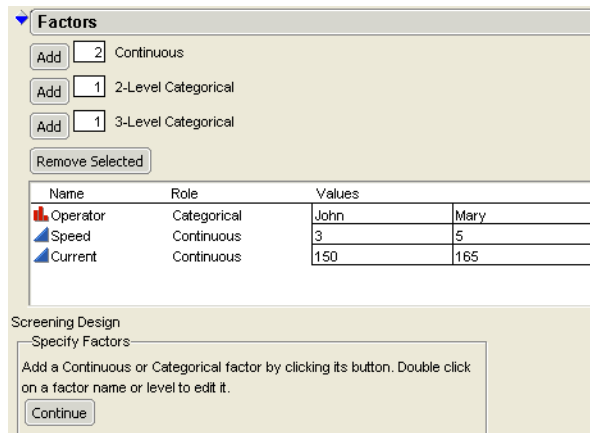
8 Click **Continue**.

9 Select **Full Factorial** in the list of designs, as shown in Figure 4.3, and then click **Continue**.

Figure 4.3 List of Screening Designs for Two Continuous and One Categorical Factors
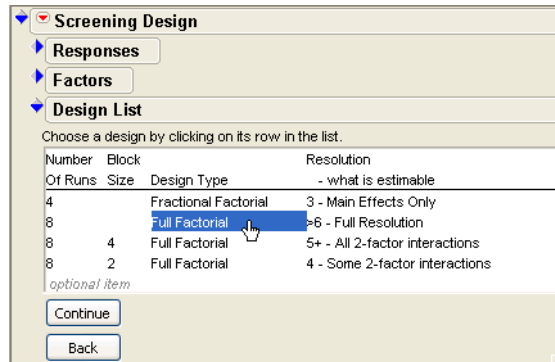
In the **Output Options** section of the Display and Modify Design panel that appears, click on the **Run Order** menu and select **Sort Left to Right**, which arranges the runs in the JMP design data table (see Figure 4.7). Then click **Make Table** to create the JMP table that contains the specified design.

The table in Figure 4.4 appears. The table uses the names for responses, factors, and levels you specified. The **Pattern** variable shows the coded design runs. You can also see the table produced in this example by selecting **Help > Sample Data > Design of Experiments >** DOE Example 1.jmp.

Figure 4.4 The Design Data Table

Using Five Continuous Factors

As illustrated in the previous section, experiments for screening the effects of many factors usually consider only two levels of each factor. This allows the examination of many factors with a minimum number of runs.

The following example, adapted from Meyer, *et al.* (1996), demonstrates how to use JMP's screening designer when you have many factors. In this study, a chemical engineer investigates the effects of five factors on the percent reaction of a chemical process. The factors are:

- feed rate, the amount of raw material added to the reaction chamber in liters per minute
- percentage of catalyst
- stir rate, the RPMs of a propeller in the chamber
- reaction temperature in degrees Celsius
- concentration of reactant

To start the example:

1 Select **DOE > Screening Design**.

2 You see one default response called Y. Change the default response name (Y) to Percent Reacted.

3 The Goal is to maximize the response, but change the minimum acceptable reaction percentage to 90 (**Lower Limit**), and upper limit to 99 (**Upper Limit**), as shown in Figure 4.5.

4 Add five continuous factors.

5 Change the default factor names (X1-X5) to Feed Rate, Catalyst, Stir Rate, Temperature, and Concentration.

6 Enter the high and low values, as shown in Figure 4.5.

Figure 4.5 Screening for Many Factors

7 Click **Continue**. Now, JMP lists the designs for the number of factors you specified, as shown to the left in Figure 4.6.

8 Select the first item in the list, which is an 8-run fractional factorial design with no blocks.

9 Click **Continue** to see the Display and Modify Design panel on the right in Figure 4.6.

Figure 4.6 Two-level Screening Design (left) and design output options (right)
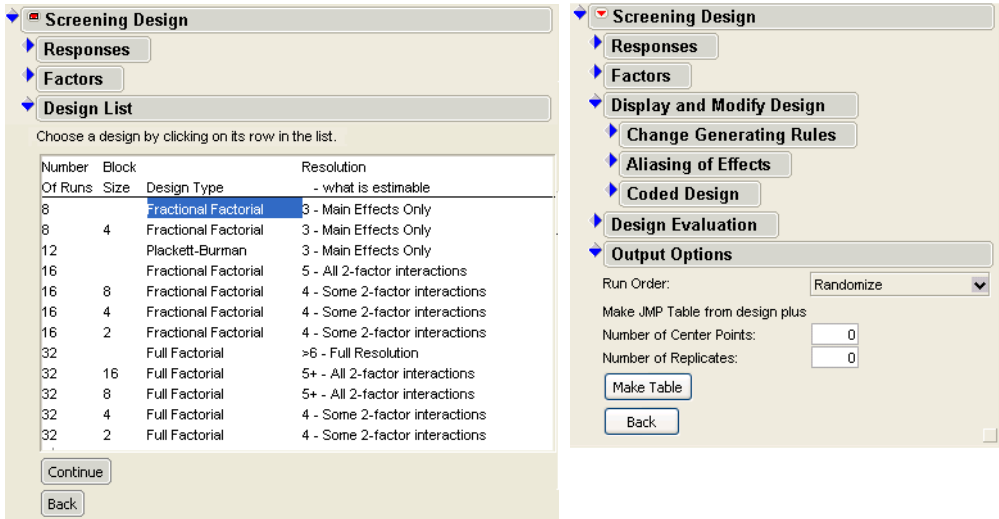
The design dialog has options shown in Figure 4.7 that can modify the final design table.

Figure 4.7 Output Options for Design Table
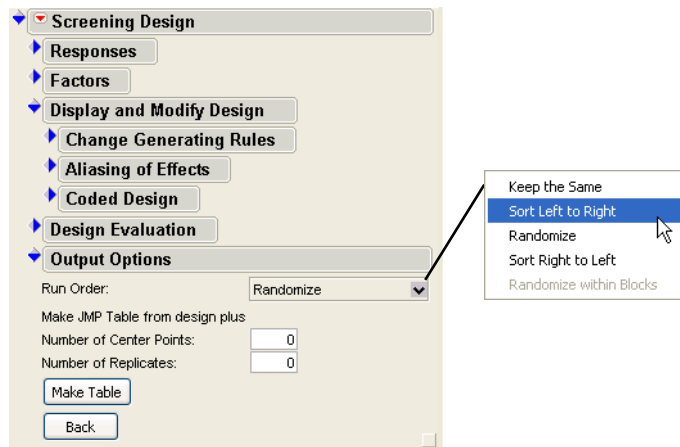
10 Click **Make Table** to create the data table shown in Figure 4.8 that lists the runs for the design you selected. Note that it also has a column called Percent Reacted for recording experimental results, showing as the rightmost column of the data table.

Figure 4.8 JMP Table of Runs for Screening Example

	Pattern	Feed Rate	Catalyst	Stir Rate	Temperature	Concentration	Percent Reacted
1	---++	10	1	100	180	6	.
2	--++-	10	1	120	180	3	.
3	-+--+	10	2	100	140	6	.
4	-++--	10	2	120	140	3	.
5	+----	15	1	100	140	3	.
6	+-+-+	15	1	120	140	6	.
7	++-+-	15	2	100	180	3	.
8	+++++	15	2	120	180	6	.

Columns (7/0):
Pattern
Feed Rate
Catalyst
Stir Rate
Temperature
Concentration
Percent Reacted

(Side panel: Fractional Factorial / Design Fractional Factorial / Screening / Model)

Of the five factors in the reaction percentage experiment, you expect a few to stand out in comparison to the others. Let's take an approach to the analysis that looks for active effects.

11 To run the model generated by the data shown in Figure 4.8, open Reactor 8 Runs.jmp from the Design Experiment folder found in the sample data that was installed with JMP. This table has the design runs and the results of the experiment.

12 In the design data table, click the Screening script that shows on the upper left of the data table, and select Run Script. Or, you can choose Analyze > Modeling > Screening to analyze the data. Select Percent Reacted as Y and all other continuous variables as X. Click OK. The report is shown in Figure 4.9.
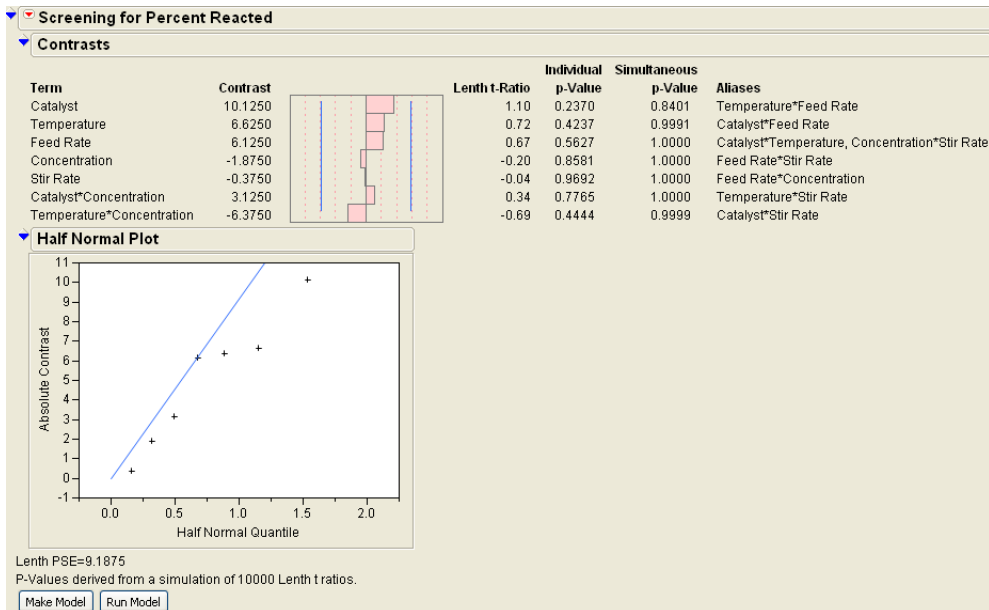
Figure 4.9 Report for Screening Example

Screening for Percent Reacted

Contrasts

Term	Contrast		Lenth t-Ratio	Individual p-Value	Simultaneous p-Value	Aliases
Catalyst	10.1250		1.10	0.2370	0.8401	Temperature*Feed Rate
Temperature	6.6250		0.72	0.4237	0.9991	Catalyst*Feed Rate
Feed Rate	6.1250		0.67	0.5627	1.0000	Catalyst*Temperature, Concentration*Stir Rate
Concentration	-1.8750		-0.20	0.8581	1.0000	Feed Rate*Stir Rate
Stir Rate	-0.3750		-0.04	0.9692	1.0000	Feed Rate*Concentration
Catalyst*Concentration	3.1250		0.34	0.7765	1.0000	Temperature*Stir Rate
Temperature*Concentration	-6.3750		-0.69	0.4444	0.9999	Catalyst*Stir Rate

Half Normal Plot

Lenth PSE=9.1875
P-Values derived from a simulation of 10000 Lenth t ratios.
Make Model   Run Model

Note: Analysis of the screening data is covered in the section "Create a Plackett-Burman design," at the end of this chapter.
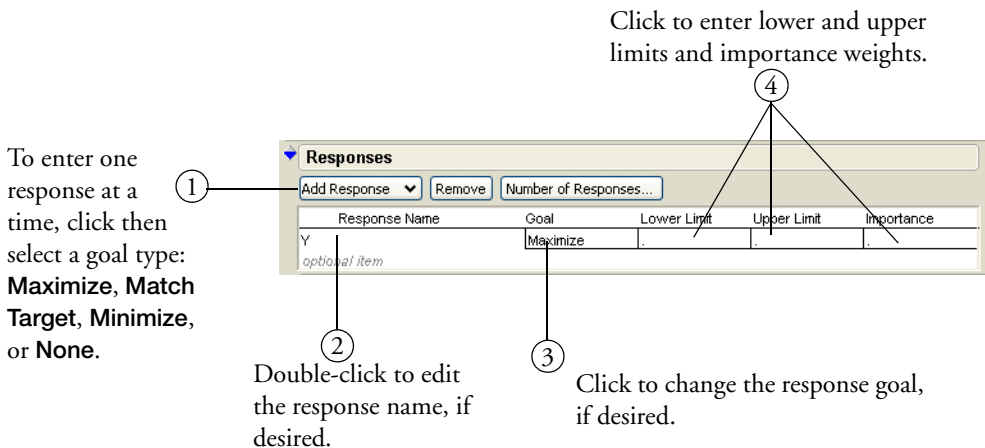
Create a Fractional Factorial Design

To begin, select **DOE > Screening Design**, or click the **Screening Design** button on the JMP Starter **DOE** page. Then, see the following sections for each step to create a screening design:

Enter Responses

To enter responses, follow the steps in Figure 4.10.

Figure 4.10 Entering Responses

Click to enter lower and upper limits and importance weights.

To enter one response at a time, click then select a goal type: **Maximize**, **Match Target**, **Minimize**, or **None**.

Double-click to edit the response name, if desired.

Click to change the response goal, if desired.

Tip: To quickly enter multiple responses, click the **Number of Responses** button and enter the number of responses you want.

Specifying Goal Types and Lower and Upper Limits

When entering responses, you can tell JMP that your goal is to obtain the maximum or minimum value possible, to match a specific value, or that there is no goal.

The following description explains the relationship between the goal type (step 3 in Figure 4.10) and the lower and upper limits (step 4 in Figure 4.10):

• For responses such as strength or yield, the best value is usually the largest possible. A goal of **Maximize** supports this objective.

- The **Minimize** goal supports an objective of having the smallest value be the most desirable, such as when the response is impurity or defects.

- The **Match Target** goal supports the objective when the best value for a response is a specific target value, such as dimensions of a manufactured part. The default target value is assumed to be midway between the lower and upper limits.

Note: If your target range is not symmetric around the target value, you can alter the default target after you make a table from the design. In the data table, open the response's Column Info dialog by double-clicking the column name, and enter an asymmetric target value.

Understanding Importance Weights

When computing overall desirability, JMP uses the value you enter as the importance weight (step 4 in Figure 4.10) as the weight of each response. If there is only one response, then specifying importance is unnecessary. With two responses you can give greater weight to one response by assigning it a higher importance value.

Enter Factors

Next, you enter factors. The Factors panel's appearance depends on the design you select. Entering factors is the same in **Screening Design**, **Space Filling Design**, **Mixture Design**, and **Response Surface Design**. This process is described below, in Figure 4.11.

Figure 4.11 Entering Factors

To enter factors, type the number of factors and click **Add**.

Highlight the factor and click the **Remove Selected** button to remove a factor in the list.

Double-click to edit the factor name.

Click to enter factor values. To remove a level, click it, press the delete key on your keyboard, then press the Return or Enter key on your keyboard.

Types of Factors

In general, when designing experiments, you can enter different types of factors in the model. Below is a description of factor types from which you can choose when creating screening designs:

Continuous   Continuous factors have numeric data types only. In theory, you can set a continuous factor to any value between the lower and upper limits you supply.

Categorical   Categorical factors (either numeric or categorical data types) have no implied order. If the values are numbers, the order is the numeric magnitude. If the values are character, the

order is the sorting sequence. The settings of a categorical factor are discrete and have no intrinsic order. Examples of categorical factors are machine, operator, and gender.

After you enter responses and factors, click **Continue**.

Choose a Design

The list of screening designs you can use includes designs that group the experimental runs into blocks of equal sizes where the size is a power of two. Highlight the type of screening design you want to use and click **Continue**.

Figure 4.12 Choosing a Type of Screening Design
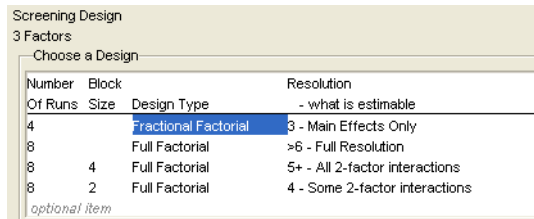
The screening designer provides the following types of designs:

Two-Level Full Factorial

A full factorial design has runs for all combinations of the levels of the factors. The samples size is the product of the levels of the factors. For two-level designs, this is 2^k where k is the number of factors. This can be expensive if the number of factors is greater than 3 or 4.

These designs are orthogonal. This means that the estimates of the effects are uncorrelated. If you remove an effect in the analysis, the values of the other estimates remain the same. Their p-values change slightly, because the estimate of the error variance and the degrees of freedom are different.

Full factorial designs allow the estimation of interactions of all orders up to the number of factors. Most empirical modeling involves first- or second-order approximations to the true functional relationship between the factors and the responses. The figure to the left in Figure 4.13 is a geometric representation of a two-level factorial.

Two-Level Fractional Factorial

A fractional factorial design also has a sample size that is a power of two. If k is the number of factors, the number of runs is 2^{k-p} where $p < k$. The fraction of the full factorial is 2^{-p}. Like the full factorial, fractional factorial designs are orthogonal.

The trade-off in screening designs is between the number of runs and the *resolution* of the design. If price is no object, you can run several replicates of all possible combinations of m factor levels. This provides a good estimate of everything, including interaction effects to the mth degree. But because running experiments costs time and money, you typically only run a fraction of all possible levels. This causes some of the higher-order effects in a model to become *nonestimable*. An effect is nonestimable when it is confounded with another effect. In fact, fractional factorials are designed by deciding in advance which interaction effects are confounded with the other interaction effects.

Resolution Number: The Degree of Confounding

In practice, few experimenters worry about interactions higher than two-way interactions. These higher-order interactions are assumed to be zero.

Experiments can therefore be classified by *resolution number* into three groups:

- Resolution = 3 means that main effects are confounded with one or more two-way interactions, which must be assumed to be zero for the main effects to be meaningful.
- Resolution = 4 means that main effects are not confounded with other main effects or two-factor interactions. However, two-factor interactions are confounded with other two-factor interactions.
- Resolution ≥ 5 means there is no confounding between main effects, between two-factor interactions, or between main effects and two-factor interactions.

All the fractional factorial designs are *minimum aberration* designs. A minimum aberration design is one in which there are a minimum number of confoundings for a given resolution. For DOE experts, the minimum aberration design of a given resolution minimizes the number of words in the defining relation that are of minimum length.

The figure on the right in Figure 4.13 is geometric representation of a two-level fractional factorial design.

Figure 4.13 Representation of Full Factorial (Left) and Two-Level Fractional Factorial (Right) Designs
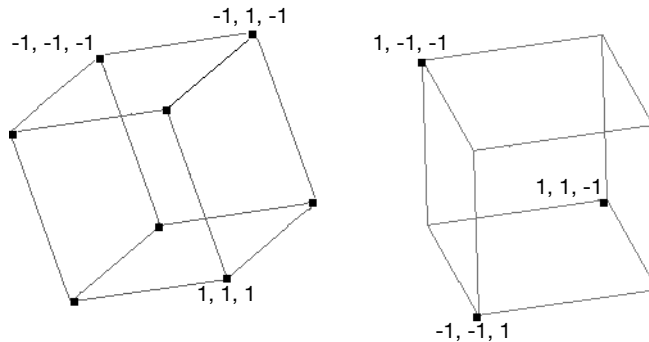
Plackett-Burman Designs

Plackett-Burman designs are an alternative to fractional factorials for screening. One useful characteristic is that the sample size is a multiple of four rather than a power of two. There are no two-level fractional factorial designs with sample sizes between 16 and 32 runs. However, there are 20-run, 24-run, and 28-run Plackett-Burman designs.

The main effects are orthogonal and two-factor interactions are only partially confounded with main effects. This is different from resolution-three fractional factorial where two-factor interactions are indistinguishable from main effects.

In cases of effect sparsity, a stepwise regression approach can allow for removing some insignificant main effects while adding highly significant and only somewhat correlated two-factor interactions. The new Screening platform in JMP, **Analyze** > **Modeling** > **Screening**, is a streamlined approach for looking at sparse data. This platform can accept multiple responses and multiple factors, then automatically fits a two-level design and shows significant effects with plots and statistics. See "Screening Designs," p. 89 of *JMP Statistics and Graphics Guide* for documentation of the Screening platform.

Mixed-Level Designs

If you have qualitative factors with three values, then none of the classical designs discussed previously are appropriate. For pure three-level factorials, JMP offers fractional factorials. For mixed two-level and three-level designs, JMP offers complete factorials and specialized orthogonal-array designs, listed in Table 4.1

If you have fewer than or equal to the number of factors for a design listed in the table, you can use that design by selecting an appropriate subset of columns from the original design. Some of these designs are not balanced, even though they are all orthogonal.

Table 4.1 Table of Mixed-Level Designs

Design	Two–Level Factors	Three–Level Factors
L18 John	1	7
L18 Chakravarty	3	6
L18 Hunter	8	4
L36	11	12

Cotter Designs

Cotter designs are used when you have very few resources and many factors, and you believe there may be interactions. Suppose you believe in effect sparsity— that very few effects are truly nonzero. You believe in this so strongly that you are willing to bet that if you add up a number of effects, the sum will show an effect if it contains an active effect. The danger is that several active effects with mixed signs will cancel and still sum to near zero and give a false negative.

Cotter designs are easy to set up. For k factors, there are $2k + 2$ runs. The design is similar to the "vary one factor at a time" approach many books call inefficient and naive.

A Cotter design begins with a run having all factors at their high level. Then follow k runs each with one factor in turn at its low level, and the others high. The next run sets all factors at their low level and sequences through k more runs with one factor high and the rest low. This completes the Cotter design, subject to randomizing the runs.

When you use JMP to generate a Cotter design, the design also includes a set of extra columns to use as regressors. These are of the form *factor*Odd and *factor*Even where *factor* is a factor name. They are constructed by adding up all the odd and even interaction terms for each factor. For example, if you have three factors, A, B, and C:

Table 4.2

|	
AOdd = A + ABC	AEven = AB + AC
BOdd = B + ABC	BEven = AB + BC
COdd = C + ABC	CEven = BC + AC

Because these columns in a Cotter design make an orthogonal transformation, testing the parameters on these combinations is equivalent to testing the combinations on the original effects. In the example of factors listed above, AOdd estimates the sum of odd terms involving A. AEven estimates the sum of the even terms involving A, and so forth.

Because Cotter designs have a false-negative risk, many statisticians discourage their use.

How to Run a Cotter Design

By default, JMP does not include a Cotter design in the list of available screening designs (Figure 4.12). However, if you want to make a Cotter design:

1 Immediately after entering responses and factors (and before clicking **Continue**), click the red triangle icon in the Screening Design title bar.
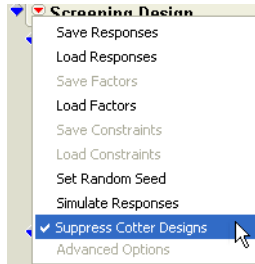
2 Select **Supress Cotter Designs** (to uncheck it), as shown to the right.

Changing the setting via the red triangle menu applies only to the *current* design. To alter the setting for *all* screening designs:

1 Select **File > Preferences**.
2 Click the **Platforms** icon.
3 Click **DOE** to highlight it.
4 Uncheck the box beside **Suppress Cotter Designs**.

Display and Modify a Design

After you select a design type, click the disclosure buttons (◆ ◆ on Windows/Linux and ▶ ▼ on the Macintosh) to display the design and show modification options using the Display and Modify Design panel to tailor the design (Figure 4.14).

Figure 4.14 Display and Modification Options
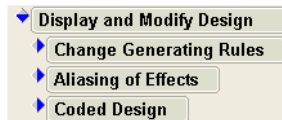
Change Generating Rules   Controls the choice of different fractional factorial designs for a given number of factors.

Aliasing of Effects   Shows the confounding pattern for fractional factorial designs.

Coded Design   Shows the pattern of high and low values for the factors in each run.

Aliasing of Effects

To see which effects are confounded with which other effects, click the disclosure button (◆ ◆ on Windows/Linux and ▶ ▼ on the Macintosh) to reveal the Aliasing of Effects panel. It shows effects and confounding up to two-factor interactions (Figure 4.15).

Figure 4.15 Generating Rules and Aliasing of Effects Panel
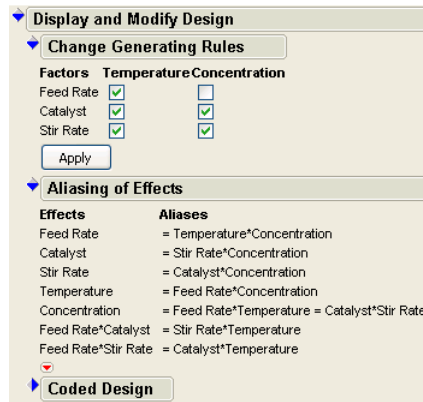
For example, a full factorial with five factors requires 2^5 = 32 runs. Eight runs can only accommodate a full factorial with three two-level factors. It is necessary to construct the two additional factors in terms of the first three factors.

The price of reducing the number of runs from 32 to eight is effect aliasing (confounding). Confounding is the direct result of the assignment of new factor values to products of the coded design columns.

In the example above, the values for Temperature are the product of the values for Feed Rate and Concentration. This means that you can't tell the difference of the effect of Temperature and the synergistic (interactive) effect of Feed Rate and Concentration.

In the example shown in Figure 4.15, all the main effects are confounded with two-factor interactions. This is characteristic of resolution-three designs.

Look at the Confounding Pattern

JMP can create a data table that shows the aliasing pattern for a specified level. To create this table:

1 Click the red triangle at the bottom of the Aliasing of Effects area.
2 Select **Show Confounding Pattern** (Figure 4.16).

Figure 4.16 Show Confounding Patterns
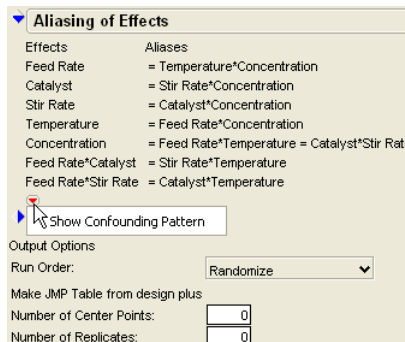
3 Enter the order of confounding you want to see (Figure 4.17).

Figure 4.17 Enter Order of Confounding in Text Edit Box

4 Click **OK**.

Figure 4.18 shows the third order aliasing for the five-factor reactor example. The effect names begin with C (Constant) and are shown by their order number in the design. Thus, **Temperature** appears as "4", with second order aliasing as "1 5" (**Feed Rate** and **Concentration**), and third order confounding as "1 2 3" (**Feed Rate**, **Catalyst**, and **Stir Rate**).

Figure 4.18 The Third Level Alias for the Five-Factor Reactor Example

Understanding Design Codes

In the Coded Design panel, each row represents a run. Plus signs designate high levels and minus signs represent low levels. As shown in Figure 4.19, rows for the first three columns of the coded design, which represent **Feed Rate**, **Catalyst**, and **Stir Rate** are all combinations of high and low values (a full factorial design). The fourth column (**Temperature**) of the coded design is the element-by-element product of the first three columns. Similarly, the last column (**Concentration**) is the product of the second and third columns.

Figure 4.19 Default Coded Designs

Changing the Coded Design

In the Change Generating Rules panel, changing the check marks and clicking **Apply** changes the coded design; it changes the choice of different fractional factorial designs for a given number of factors. The Coded Design table in Figure 4.19 shows how the last two columns are constructed in terms of the first three columns. The check marks in the Change Generating Rules table shown in Figure 4.20 for Temperature now show it is a function of Feed Rate, and Catalyst. The check marks for Concentration show it is a function of Feed Rate and Stir Rate.

If you check the options as shown in Figure 4.20 and click **Apply**, the Coded Design panel changes. The first three columns of the coded design remain a full factorial for the first three factors (Feed Rate, Catalyst, and Stir Rate). Temperature is now the product of Feed Rate and Catalyst, so the fourth column of the coded design is the element by element product of the first two columns. Concentration is a function of Feed Rate and Stir Rate.

Figure 4.20 Modified Coded Designs and Generating Rules
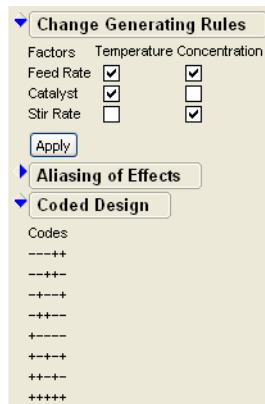
Specify Output Options

Use the Output Options panel (Figure 4.21) to specify how you want the output data table to appear. When the options are the way you want them, click **Make Table**.

Figure 4.21 Select the Output Options
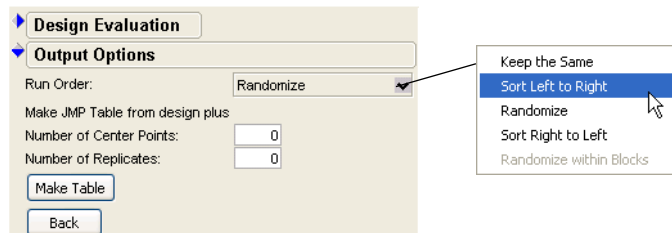
Run Order   Lets you designate the order you want the runs to appear in the data table when it is created. Choices are:

Keep the Same—the rows (runs) in the output table appear as they do in the Design panel.

Sort Left to Right—the rows (runs) in the output table appear sorted from left to right.

Randomize—the rows (runs) in the output table appear in a random order.

Sort Right to Left—the rows (runs) in the output table appear sorted from right to left.

Randomize within Blocks—the rows (runs) in the output table will appear in random order within the blocks you set up.

Number of Center Points   Specifies additional runs placed at the center points.

Number of Replicates   Specify the number of times to replicate the entire design, including centerpoints. Type the number of times you want to replicate the design in the associated text box. One replicate doubles the number of runs.

View the Design Table

Click **Make Table** to create a data table that contains the runs for your experiment. In the table, the high and low values you specified are displayed for each run.

Figure 4.22 The Design Data Table

The name of the table is the design type that generated it.

The column called **Pattern** shows the pattern of low values denoted "–" and high values denoted "+". **Pattern** is especially useful as a label variable in plots.

This script allows you to screen for active effects.

Create a Plackett-Burman design

The previous example shows an 8-run fractional factorial design for five continuous factors. But suppose you can afford 4 additional runs. First, repeat the steps shown in the previous sections. This time, use the Load Responses and Load Factors commands to define the design, as follows:

1 Select **DOE > Screening Design**.

2 Select **Load Responses** from the red triangle menu on the Screening Design title bar. Navigate to

the Design Experiment folder in the Sample Data installed with JMP and open the file called Reactor Response.jmp.

3 Next, select **Load Factors** from red triangle menu on the Screening Design title bar. Navigate to the Design Experiment folder in the Sample Data installed with JMP and open the file called Reactor Factors.jmp.

These two commands complete the DOE screening dialog for you, with the correct response and factor names, goal and limits for the response, and the values for the factors.

4 Click Continue on the completed Screening design dialog to see the list of designs in Figure 4.23, and chose the Plackett-Burman, as shown.

Figure 4.23 Design List for 5-factor Plackett-Burman Screening Design

5 Click Continue.

After you select the model from the Design list, the outlines for modifying and evaluating the model appear. In the Custom designer, you have the ability to form any model effects you want. The Screening designer creates the design effects based on the design you choose. In particular, the full factorial with all two-factor interactions has no aliasing of the included interactions, as shown in Figure 4.24.

Figure 4.24 No aliasing of the included interactions
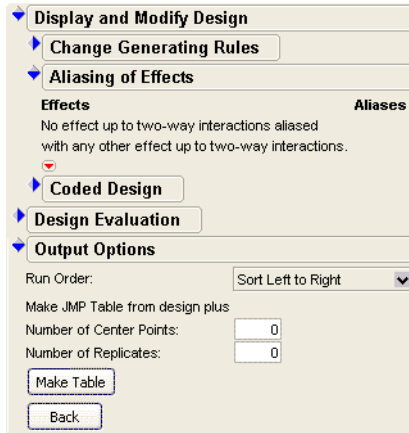
A complete discussion of the Design Evaluation options is found in Chapter 3, "Building Custom Designs."

To continue with this example, do the following:

6   Choose **Sort Left to Right** in the Output Options panel.

7   Click **Make Table** to see the design runs shown in Figure 4.25.

Examine the data table and note the Pattern variable to see the arrangement of plus and minus signs that define the runs. This table is used in the analysis sections that follow.

Figure 4.25 Listing of a 5-factor Placket-Burman Design Table with Results

Analysis of Screening Data

After creating and viewing the data table, you can now run analyses on the data. As an example, open the data table called Plackett-Burman.jmp, found in Design Experiment folder in the Sample Data installed with JMP. This table contains the design runs and the Percent Reacted experimental results for the 12-run Plackett-burman design created in the previous section.

Using the Screening Analysis Platform

The data table has two scripts called **Screening** and **Model**, showing in the upper-left corner of the table, that were created by the DOE Screening designer. You can use these scripts to analyze the data, however it is simple to run the analyses yourself.

1 Select **Analyze** > **Modeling > Screening** to see the completed launch dialog shown in Figure 4.26. When you create a DOE design table, the variable roles are saved with the data table and used by the launch platform to complete the dialog.

Figure 4.26 Launch Dialog for the Screening Platform
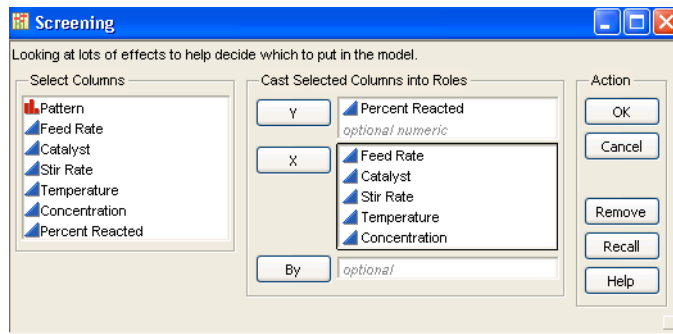
2 Click **OK** to see the Screening platform result shown in Figure 4.27.

The Contrasts section of the Screening platform results lists all possible model effects, a contrast value for each effect, Lenth *t*-ratios (calculated as the contrast value divided by the Lenth PSE (pseudo-standard error), individual and simultaneous *p*-values, and aliases if there are any. Significant and marginally significant effects are highlighted. See the chapter on analyzing Screening designs in the *Statistics and Graphics Guide* for complete documentation of the Screening analysis platform.

Figure 4.27 Results of the Screening Analysis
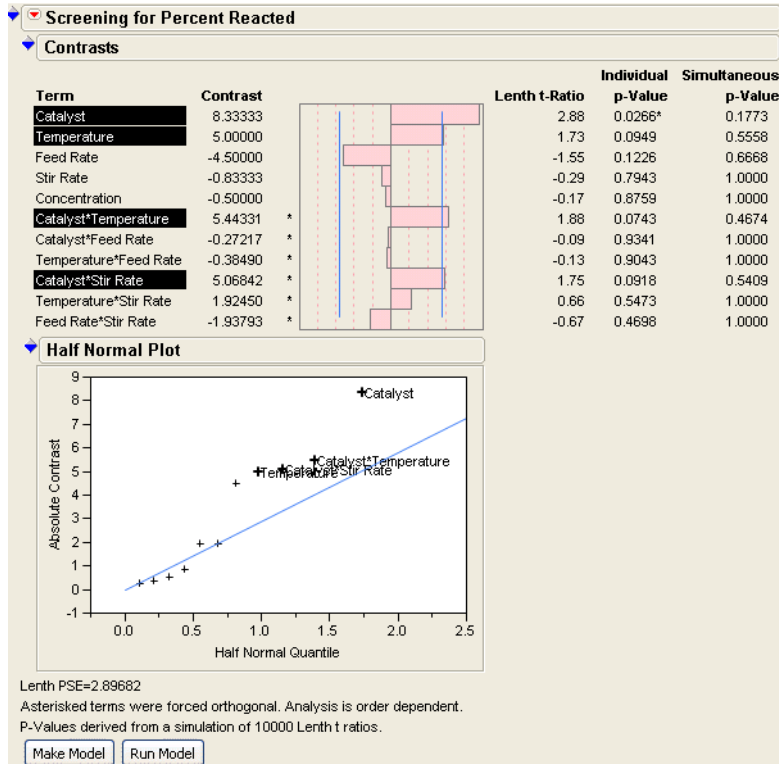
3 Examine the Half Normal plot in Figure 4.27.

Using the Fit Model Platform

The **Make Model** button beneath the Half Normal Plot creates a Fit Model dialog that includes all the highlighted effects. However, note that the Catalyst*Stir Rate interaction is highlighted, but the Stir Rate main effect is not. Therefore, that interaction shouldn't be in the model.

4 Click the **Make Model** Button beneath the Half Normal Plot to see the completed Fit Model dialog in Figure 4.28.

5 Highlight the Catalyst*Stir Rate interaction and click **Remove** on the Fit Model dialog.

6 Then click **Run Model** to see the analysis results.

Figure 4.28 Create Fit Model Dialog and Remove Unwanted Effect
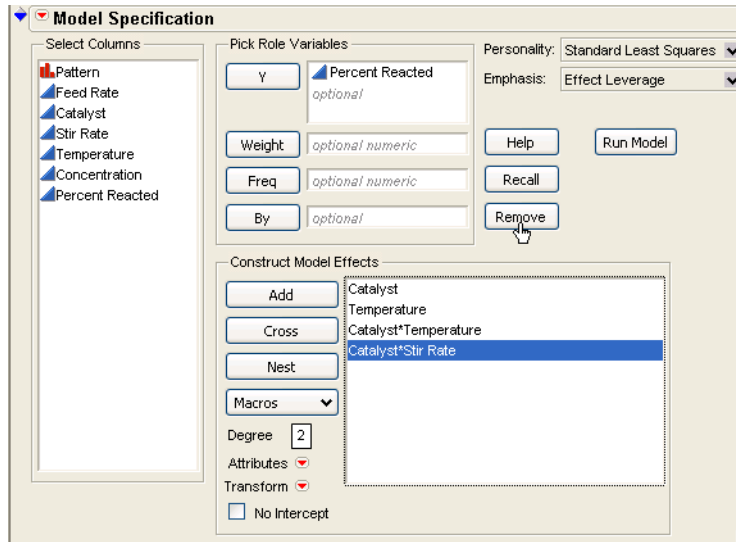
The Actual-by-Predicted Plot

The Whole Model actual-by-predicted plot, shown on the left in Figure 4.29, appears at the top of the Fit Model report. You see at a glance that this model fits well. The mean line falls outside the bounds of the 95% confidence curves (red-dotted lines), which tells you the model is significant. The model *p*-value (p = 0.0178), R^2, and RMSE appear below the plot. The RMSE is an estimate of the standard deviation of the process noise, assuming that the unestimated effects are negligible.

In this example, the Pattern variable is designated as a label column. To show labels in the plot (on the right in Figure 4.29), shift click to select points of interest, right-click the graph, and select **Row Label**. The pattern variable displayed in the data table serves as the label for each point. Also, you can hover over a point to see the label.

Figure 4.29 An Actual-by-Predicted Plot
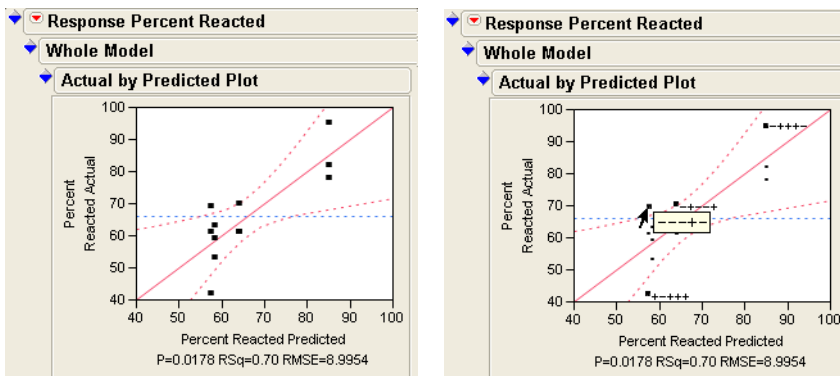
The Scaled Estimates Report
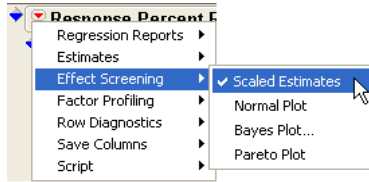
To see a scaled estimates report, use **Effect Screening** > **Scaled Estimates** found in the red triangle menu on the **Response Percent Reacted** title bar. When there are quadratic or polynomial effects, the coefficients and the tests for them are more meaningful if effects are scaled and coded. The Scaled Estimates report includes a bar chart of the individual effects embedded in a table of parameter estimates. The last column of the table has the *p*-values for each effect.

Figure 4.30 Example of a Scaled Estimates Report

Scaled Estimates					
Term	**Scaled Estimate**		**Std Error**	**t Ratio**	**Prob>|t|**
Intercept	66.166667		2.596739	25.48	<.0001*
Catalyst(1,2)	8.3333333		2.596739	3.21	0.0124*
Temperature(140,180)	5		2.596739	1.93	0.0903
Catalyst*Temperature	5.5		2.596739	2.12	0.0670
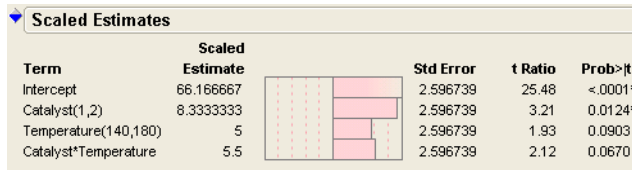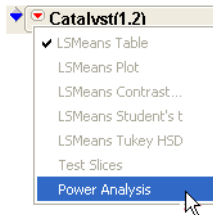
A Power Analysis

The Fit Model report has outline nodes for the Catalyst and Temperature effects. To run a power analysis for an effect, click the red triangle icon on its title bar and select **Power Analysis**.

This example shows a power analysis for the Catalyst variable, using default value for α (0.05), the root mean square error and parameter estimate for Catalyst, for a sample size of 12. The resulting power is 0.802, which means that in similar experiments, you can expect an 80% chance of detecting a significant effect for Catalyst.

Figure 4.31   Example of a Power Analysis

Refer to the *JMP Statistics and Graphics Guide* for details.

Response Surface Designs

Response surface designs are useful for modeling a curved quadratic surface to continuous factors. A response surface model can pinpoint a minimum or maximum response, if one exists inside the factor region. Three distinct values for each factor are necessary to fit a quadratic function, so the standard two-level designs cannot fit curved surfaces.
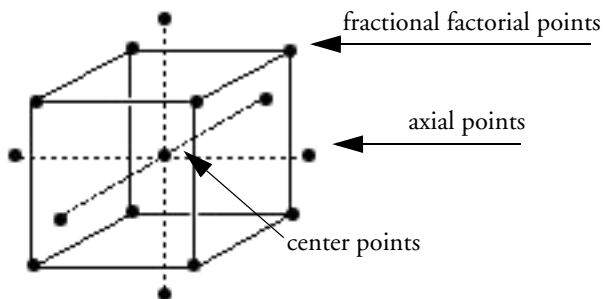
The most popular response surface design is the central composite design, illustrated in the figure to the left below. It combines a two-level fractional factorial and two other kinds of points:

• *Center points*, for which all the factor values are at the zero (or midrange) value.

• *Axial* (o*r star*) *points*, for which all but one factor are set at zero (midrange) and that one factor is set at outer (axial) values.

The Box-Behnken design, illustrated in the figure on the right below, is an alternative to central composite designs. One distinguishing feature of the Box-Behnken design is that there are only three levels per factor.

Another important difference between the two design types is that the Box-Behnken design has no points at the vertices of the cube defined by the ranges of the factors. This is sometimes useful when it is desirable to avoid these points due to engineering considerations. The price of this characteristic is the higher uncertainty of prediction near the vertices compared to the central composite design.

Central Composite Design

Box-Behnken Design

fractional factorial points

axial points

center points
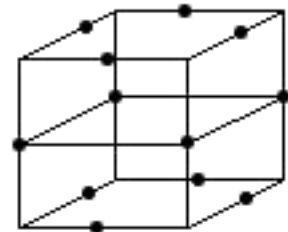
Contents

A Box-Behnken Design: The Tennis Ball Example

The Bounce Data.jmp sample data file has response surface data inspired by the tire tread data described in Derringer and Suich (1980). The objective of this experiment is to match a standardized target value (450) of tennis ball bounciness. The bounciness varies with amounts of Silica, Silane, and Sulfur used to manufacture the tennis balls. The experimenter wants to collect data over a wide range of values for these variables to see if a response surface can find a combination of factors that matches a specified bounce target. To follow this example:

1   Select **DOE > Response Surface Design**.

2   Load factors by clicking the red triangle icon on the Response Surface Design title bar and selecting **Load Factors**. Navigate to the Sample Data folder installed with JMP, and open Bounce Factors.jmp from the Design Experiment folder.

3   Load the responses by clicking the red triangle icon on the Response Surface Design title bar and selecting **Load Responses**. Navigate to the Sample Data folder, and open Bounce Response.jmp from the Design Experiment folder. Figure 5.1 shows the completed Response panel and Factors panel.

Figure 5.1 Response and Factors For Bounce Data
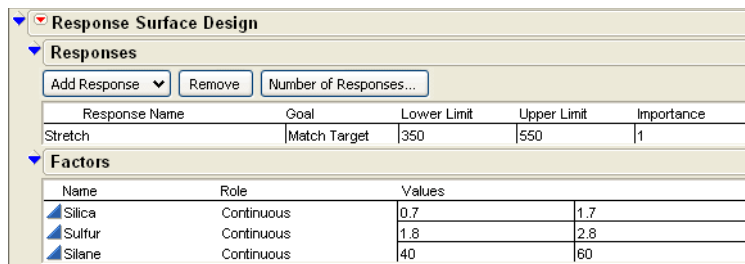
After the response data and factors data are loaded, the Response Surface Design Choice dialog lists the designs in Figure 5.2.

Figure 5.2 Response Surface Design Selection
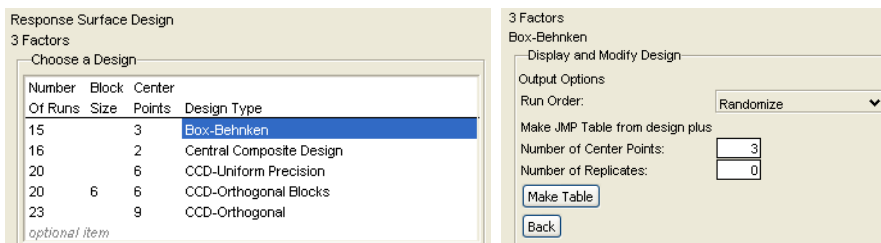
The Box-Behnken design selected for three effects generates the design table of 15 runs shown in Figure 5.3.

In real life, you would conduct the experiment and then enter the responses into the data table. Suppose you completed the experiment and the final data table is Bounce Data.jmp.

1   Open Bounce Data.jmp from the Design Experiment folder found in the sample data installed with JMP (Figure 5.3).

Figure 5.3 JMP Table for a Three-Factor Box-Behnken Design

	Pattern	Silica	Sulfur	Silane	Stretch
1	--0	0.7	1.8	50	570
2	-+0	0.7	2.8	50	285
3	+-0	1.7	1.8	50	260
4	++0	1.7	2.8	50	433
5	0--	1.2	1.8	40	422
6	0-+	1.2	1.8	60	351
7	0+-	1.2	2.8	40	278
8	0++	1.2	2.8	60	392
9	-0-	0.7	2.3	40	451
10	+0-	1.7	2.3	40	372
11	-0+	0.7	2.3	60	474
12	+0+	1.7	2.3	60	394
13	000	1.2	2.3	50	398
14	000	1.2	2.3	50	394
15	000	1.2	2.3	50	396

Bounce Data / Design Box-Behnken / Model
Columns (5/0): Pattern, Silica *, Sulfur *, Silane *, Stretch *
Rows: All rows 15, Selected 0, Excluded 0, Hidden 0, Labelled 0

After opening the Bounce Data.jmp data table, run a fit model analysis on the data. The data table contains a script labeled **Model**, showing in the upper left panel of the table.

2   Click the red triangle next to **Model** and select **Run Script** to start a fit model analysis.

3   When the Fit Model dialog appears, click **Run Model**.

The standard Fit Model analysis results appear in tables shown in Figure 5.4, with parameter estimates for all response surface and crossed effects in the model.

The prediction model is highly significant with no evidence of lack of fit. All main effect terms are significant as well as the two interaction effects involving Sulfur.

Figure 5.4 JMP Statistical Reports for a Response Surface Analysis of Bounce Data

Response Stretch

Summary of Fit

RSquare	0.999777
RSquare Adj	0.999375
Root Mean Square Error	1.987461
Mean of Response	391.3333
Observations (or Sum Wgts)	15

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	9	88453.583	9828.18	2488.146
Error	5	19.750	3.95	Prob > F
C. Total	14	88473.333		<.0001*

Lack Of Fit

Source	DF	Sum of Squares	Mean Square	F Ratio
Lack Of Fit	3	11.750000	3.91667	0.9792
Pure Error	2	8.000000	4.00000	Prob > F
Total Error	5	19.750000		0.5411
				Max RSq
				0.9999

Parameter Estimates

Effect Tests

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
Silica(0.7,1.7)	1	1	12880.125	3260.791	<.0001*
Silane(40,60)	1	1	968.000	245.0633	<.0001*
Sulfur(1.8,2.8)	1	1	5778.125	1462.816	<.0001*
Silane*Silica	1	1	0.250	0.0633	0.8114
Sulfur*Silica	1	1	52441.000	13276.20	<.0001*
Sulfur*Silane	1	1	8556.250	2166.139	<.0001*
Silica*Silica	1	1	2592.923	656.4362	<.0001*
Silane*Silane	1	1	0.231	0.0584	0.8186
Sulfur*Sulfur	1	1	4653.231	1178.033	<.0001*

See the chapter "Standard Least Squares: Introduction" of *JMP Statistics and Graphics Guide* for more information about interpretation of the tables in Figure 5.4.

The Response Surface report also has the tables shown in Figure 5.5.

Figure 5.5 Statistical Reports for a Response Surface Analysis

Summary of the parameter estimates

Lists the critical values of the surface factors and tells the kind of solution (maximum, minimum, or saddle point). The solution for this example is a saddle point. The table also warns that the critical values given by the solution are outside the range of data values.

Response Surface

Coef

	Silica(0.7,1.7)	Silane(40,60)	Sulfur(1.8,2.8)	Stretch
Silica(0.7,1.7)	26.5	-0.25	114.5	-40.125
Silane(40,60)	.	0.25	46.25	11
Sulfur(1.8,2.8)	.	.	-35.5	-26.875

Solution

Variable	Critical Value
Silica(0.7,1.7)	1.7912411
Silane(40,60)	23.424426
Sulfur(1.8,2.8)	2.1986422

Solution is a SaddlePoint
Critical values outside data range
Predicted Value at Solution 360.38388

Canonical Curvature

Eigenvalues and Eigenvectors

Eigenvalue	62.9095	3.2989	-74.9584
Silica(0.7,1.7)	0.82779	-0.29879	-0.47486
Silane(40,60)	0.19280	0.94634	-0.25937
Sulfur(1.8,2.8)	0.52687	0.12315	0.84097

Shows eigenvalues and eigenvectors of the effects. The eigenvector values show that the dominant negative curvature (yielding a maximum) is mostly in the Sulfur direction. The dominant positive curvature (yielding a minimum) is mostly in the Silica direction. This is confirmed by the prediction profiler in Figure 5.8.

See the chapter "Standard Least Squares: Exploring the Prediction Equation" of *JMP Statistics and Graphics Guide* for details about the response surface analysis tables in Figure 5.5.

The Prediction Profiler

Next, use the response Prediction Profiler to get a closer look at the response surface and help find the settings that produce the best response target. The Prediction Profiler is a way to interactively change variables and look at the effects on the predicted response.

1 If the Prediction Profiler is not already open, click the red triangle on the Response title bar and select **Factor Profiling > Profiler**, as shown in Figure 5.6.

Figure 5.6 The Profiler
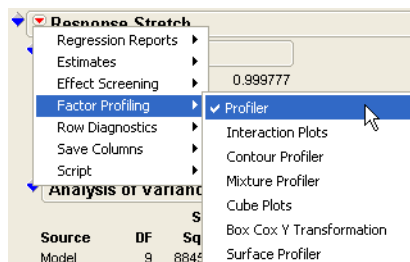
The first three plots in the top row of plots in the Prediction Profiler (Figure 5.7) display *prediction traces* for each *x* variable. A prediction trace is the predicted response as one variable is changed while the others are held constant at the current values (Jones 1991).

The current predicted value of Stretch, 396, is based on the default factor setting. It is represented by the horizontal dotted line that shows slightly below the desirability function target value (Figure 5.7). The profiler shows desirability settings for the factors Silica, Silane, and Sulfur that give a value for Stretch of 396, which is well away from the specified target of 450.

The bottom row has a plot for each factor, showing its *desirability trace*. The profiler also contains a Desirability column, which graphs desirability on a scale from 0 to 1 and has an adjustable desirability function for each *y* variable. The overall desirability measure is on the left of the desirability traces.

Figure 5.7 The Prediction Profiler
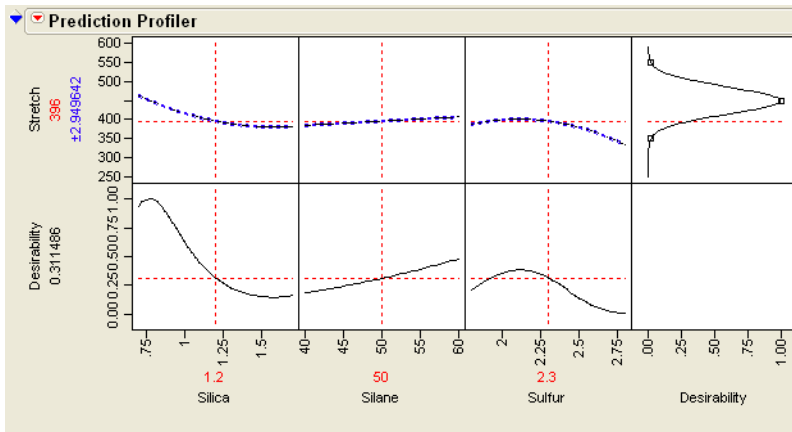
2   To adjust the prediction traces of the factors and find a Stretch value that is closer to the target, click the red triangle on the Prediction Profiler title bar and select **Maximize Desirability**. This command adjusts the profile traces to produce the response value closest to the specified target (the target given by the desirability function). The range of acceptable values is determined by the positions of the upper and lower handles.

Figure 5.8 shows the result of the most desirable settings. Changing the settings of Silica from 1.2 to 0.94, Silane from 50 to 46, and Sulfur from 2.3 to 2.1 raised the predicted response from 396 to the target value of 450. Finding maximum desirability is an iterative process so your results may differ slightly from those shown below.

Figure 5.8 Prediction Profiler with Maximum Desirability Set for a Response Surface Analysis
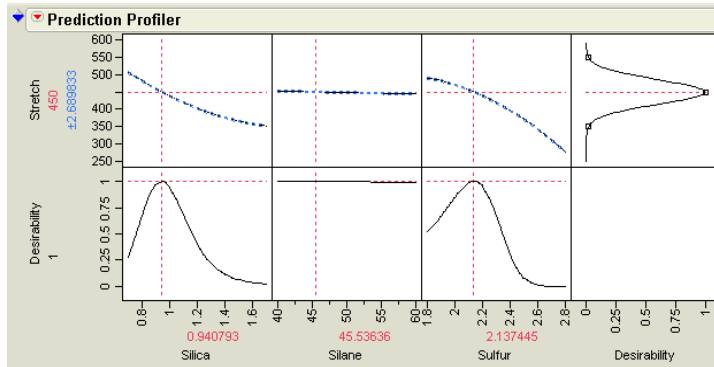
See the *JMP Statistics and Graphics Guide* for further discussion of the Prediction Profiler.

A Response Surface Plot (Contour Profiler)

Another way to look at the response surface is to use the Contour Profiler. Click the red triangle on the Response title bar and select **Factor Profiling > Contour Profiler** to display the interactive contour pro-filer, as shown in Figure 5.9.

The contour profiler is useful for viewing response surfaces graphically, especially when there are multi-ple responses. This example shows the profile to Silica and Sulfur for a fixed value of Silane.

Options on the Contour Profiler title bar can be used to set the grid density, request a surface plot (mesh plot), and add contours at specified intervals, like those shown in the contour plot in Figure 5.9. The sliders for each factor set values for Current X and Current Y.

Figure 5.9 Contour Profiler for a Response Surface Analysis
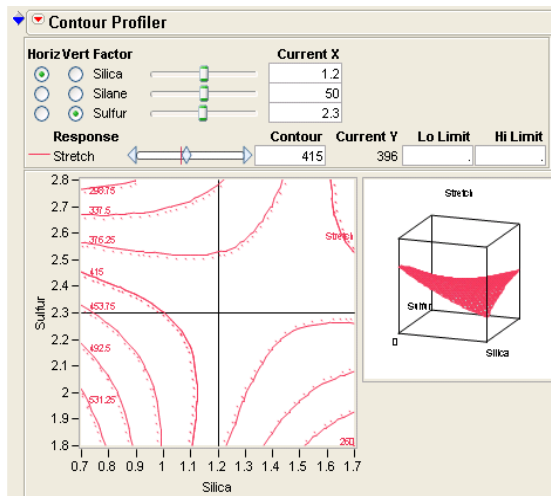
Figure 5.10 shows the Contour profile when the Current *x* values have Lo and Hi limits in effect, which cause shaded regions to show on the contour.

Figure 5.10 Contour Profiler with High and Low Limits

Enter Lo limit and Hi limit to see shaded unacceptable regions in contour plot.
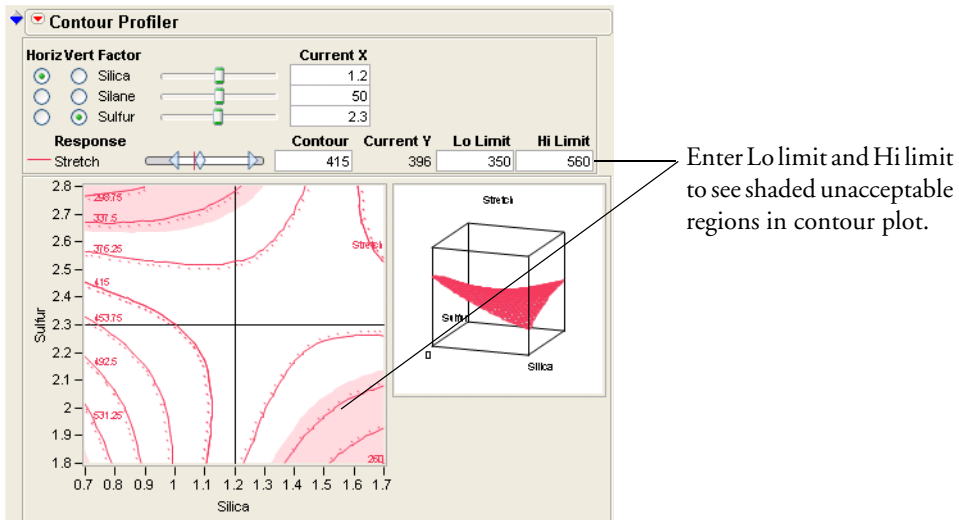
The Prediction Profiler and the Contour Profiler are discussed in more detail in the *JMP Statistics and Graphics Guide*.

Geometry of a Box-Behnken Design

The geometric structure of a design with three effects is seen by using the Scatterplot 3D platform. The plot shown in Figure 5.11 illustrates the three Box-Behnken design columns. You can clearly see the center points and the 12 points midway between the vertices. For details on how to use the Scatterplot 3D platform, see the *JMP Statistics and Graphics Guide*.

Figure 5.11 Scatterplot 3D Rendition of a Box-Behnken Design for Three Effects
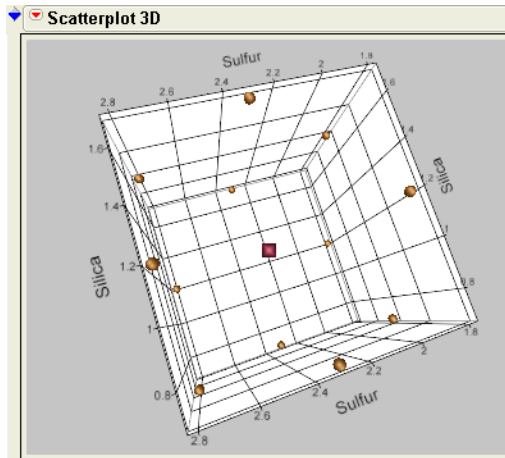
Creating a Response Surface Design

Response Surface Methodology (RSM) is an experimental technique invented to find the optimal response within specified ranges of the factors. These designs are capable of fitting a second-order prediction equation for the response. The quadratic terms in these equations model the curvature in the true response function. If a maximum or minimum exists inside the factor region, RSM can estimate it. In industrial applications, RSM designs usually involve a small number of factors. This is because the required number of runs increases dramatically with the number of factors. Using the response surface designer, you choose to use well-known RSM designs for two to eight continuous factors. Some of these designs also allow blocking.

Response surface designs are useful for modeling and analyzing curved surfaces.

To start a response surface design, select **DOE > Response Surface Design**, or click the **Response Surface Design** button on the JMP Starter **DOE** page. Then, follow the steps described in the following sections.

- "Enter Responses and Factors," p. 124
- "Choose a Design," p. 124
- "Specify Axial Value (Central Composite Designs Only)," p. 125
- "Specify Output Options," p. 126
- "View the Design Table," p. 126

Enter Responses and Factors

The steps for entering responses are the same in **Screening Design**, **Space Filling Design**, **Mixture Design**, **Response Surface Design**, **Custom Design**, and **Full Factorial Design**. These steps are outlined in "Enter Responses and Factors into the Custom Designer," p. 59

Factors in a response surface design can only be continuous. The Factors panel for a response surface design appears with two default continuous factors. To enter more factors, type the number you want in the Factors panel edit box and click **Add**, as shown in Figure 5.12.

Figure 5.12 Enter Factors into a Response Surface Design
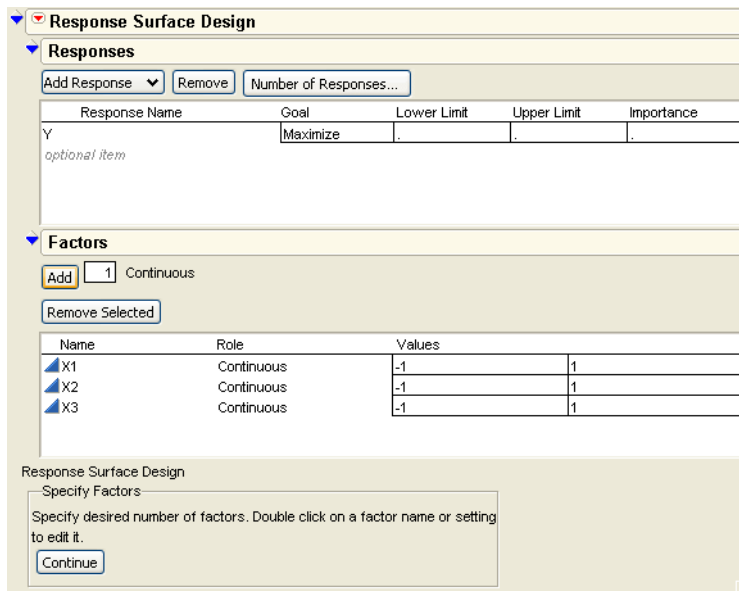
Click **Continue** to proceed to the next step.

Choose a Design

Highlight the type of response surface design you want and click **Continue**. The next sections describe the types of response surface designs shown in Figure 5.13.

Figure 5.13 Choose a Design Type
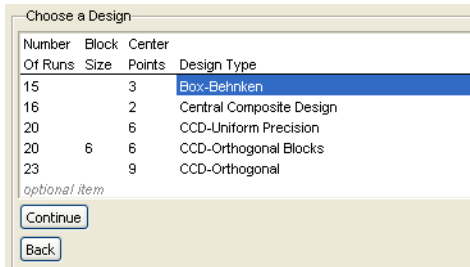
Box-Behnken Designs

The Box-Behnken design has only three levels per factor and has no points at the vertices of the cube defined by the ranges of the factors. This is sometimes useful when it is desirable to avoid extreme points due to engineering considerations. The price of this characteristic is the higher uncertainty of prediction near the vertices compared to the central composite design.

Central Composite Designs

The response surface design list contains two types of central composite designs: *uniform precision* and *orthogonal*. These properties of central composite designs relate to the number of center points in the design and to the axial values:

- Uniform precision means that the number of center points is chosen so that the prediction variance near the center of the design space is very flat.
- For orthogonal designs, the number of center points is chosen so that the second order parameter estimates are minimally correlated with the other parameter estimates.

Specify Axial Value (Central Composite Designs Only)

When you select a central composite (CCD-Uniform Precision) design and then click **Continue**, you see the panel in Figure 5.14. It supplies default axial scaling information. Entering 1.0 in the text box instructs JMP to place the axial value on the face of the cube defined by the factors, which controls how far out the axial points are. You have the flexibility to enter the values you want to use.

Figure 5.14 Display and Modify the Central Composite Design
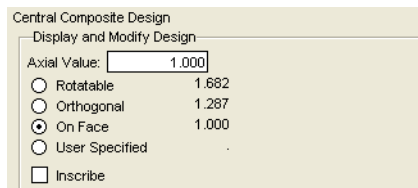
Rotatable   makes the variance of prediction depend only on the scaled distance from the center of the design. This causes the axial points to be more extreme than the range of the factor. If this factor range cannot be practically achieved, it is recommended that you choose **On Face** or specify your own value.

Orthogonal   makes the effects orthogonal in the analysis. This causes the axial points to be more extreme than the –1 or 1 representing the range of the factor. If this factor range cannot be practically achieved, it is recommended that you choose **On Face** or specify your own value.

On Face   leaves the axial points at the end of the -1 and 1 ranges.

User Specified   uses the value you enter in the Axial Value text box.

If you want to inscribe the design, click the box beside **Inscribe**. When checked, JMP rescales the whole design so that the axial points are at the low and high ends of the range (the axials are –1 and 1 and the factorials are shrunken based on that scaling).

Specify Output Options

Use the Output Options panel to specify how you want the output data table to appear. When the options are specified the way you want them, click **Make Table**. Note that the example shown in Figure 5.15 is for a Box-Behnken design. The Box-Behnken design from the design list and the Output Options request 3 center points for a single replicate.

Figure 5.15 Select the Output Options

```
Response Surface Design
3 Factors
Box-Behnken
   ┌Display and Modify Design─────────────┐
   Output Options
   Run Order:                    Randomize        ▼

   Make JMP Table from design plus
   Number of Center Points:           3
   Number of Replicates:              0
   Make Table
   Back
```
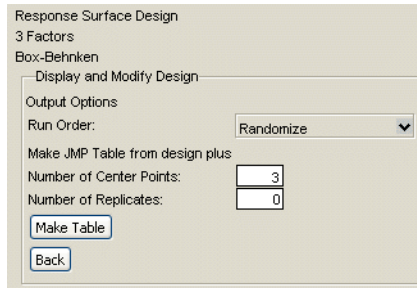
Run Order provides a menu with options for designating the order you want the runs to appear in the data table when it is created. Menu choices are:

  Keep the Same   the rows (runs) in the output table will appear as they do in the Design panel.

  Sort Left to Right   the rows (runs) in the output table will appear sorted from left to right.

  Randomize   the rows (runs) in the output table will appear in a random order.

  Sort Right to Left   the rows (runs) in the output table will appear sorted from right to left.

  Randomize within Blocks   the rows (runs) in the output table will appear in random order within the blocks you set up.

Add additional points with options given by Make JMP Table from design plus:

  Number of Center Points   Specifies additional runs placed at the center points.

  Number of Replicates   Specify the number of times to replicate the entire design, including centerpoints. Type the number of times you want to replicate the design in the associated text box. One replicate doubles the number of runs.

View the Design Table

Now you have a data table that outlines your experiment, as described in Figure 5.16.

Figure 5.16 The Design Data Table

The column called Pattern identifies the coding of the factors. It shows all the codings with "+" for high, "−" for low factor, "a" and "A" for low and high axial values, and "0" for midrange. Pattern is suitable to use as a label variable in plots because when you hover over a point in a plot of the factors, the pattern value shows the factor coding of the point.

The name of the table is the design type that generated it.

Runs are in a random order.

This script fits a model using the values in the design table.

The Y column is for recording experimental results.

There are three center points.

	Pattern	X1	X2	X3	Y
1	-0-	-1	0	-1	
2	000	0	0	0	
3	+-0	1	-1	0	
4	--0	-1	-1	0	
5	0-+	0	-1	1	
6	-+0	-1	1	0	
7	+0-	1	0	-1	
8	0+-	0	1	-1	
9	000	0	0	0	
10	0--	0	-1	-1	
11	++0	1	1	0	
12	0++	0	1	1	
13	+0+	1	0	1	
14	000	0	0	0	
15	-0+	-1	0	1	

Box-Behnken
Design   Box-Behnken
Model

Columns (5/0)
Pattern
X1 ✱
X2 ✱
X3 ✱
Y ✱

Rows
All rows   15
Selected   0
Excluded   0
Hidden   0
Labelled   0

Chapter **6**

Full Factorial Designs
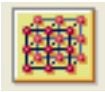
A full factorial design contains all possible combinations of a set of factors. This is the most fool proof design approach, but it is also the most costly in experimental resources. The full factorial designer supports both continuous factors and categorical factors with up to nine levels.

In full factorial designs, you perform an experimental run at every combination of the factor levels. The sample size is the product of the numbers of levels of the factors. For example, a factorial experiment with a two-level factor, a three-level factor, and a four-level factor has 2 x 3 x 4 = 24 runs.

Factorial designs with only two-level factors have a sample size that is a power of two (specifically 2^f where f is the number of factors). When there are three factors, the factorial design points are at the vertices of a cube as shown in the diagram below. For more factors, the design points are the vertices of a hypercube.

Full factorial designs are the most conservative of all design types. There is little scope for ambiguity when you are willing to try all combinations of the factor settings.

Unfortunately, the sample size grows exponentially in the number of factors, so full factorial designs are too expensive to run for most practical purposes.
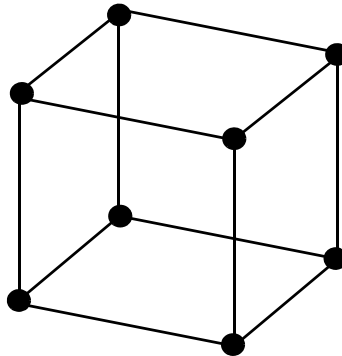
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The Five-Factor Reactor Example

The following example, adapted from Meyer *et al.* (1996) and Box, Hunter, and Hunter (1978), shows a five-factor reactor example.

Previously, the screening designer was used to investigate the effects of five factors on the percent reaction of a chemical process (see "Screening Designs," p. 89). The factors (Feed Rate, Catalyst, Stir Rate, Temperature, and Concentration) are all two-level continuous factors. The next example studies the same system using a full factorial design.

1 Select **DOE > Full Factorial Design**.

2 Click the red triangle icon on the Full Factorial Design title bar and select **Load Responses**.

3 In the sample data (installed with JMP), open Reactor Response.jmp found in the Design Experiment Sample Data folder.

4 Click the red triangle icon on the Full Factorial Design title bar and select **Load Factors**.

5 In the sample data (installed with JMP), open Reactor Factors.jmp found in the Design Experiment folder.

The completed dialog should look like the one shown in Figure 6.1.

Figure 6.1 Full Factorial Example Response and Factors Panels

6 Click **Continue** to see the Output Options panel. In the Output Options panel, select **Sort Left to Right** from the Run Order menu, as shown to the right. This command defines the order of runs as they will be in the final JMP design table.

7   Click **Make Table**.

The design data table (Figure 6.2) contains a run for every combination of high and low values for the five variables, which covers all combinations of five factors with two levels each. Since there are five variables, there are 2^5=32 runs. Initially, the table has an empty Y column named Percent Reacted for entering response values when the experiment is complete.

To see the completed experiment and continue this example, open Reactor 32 Runs.jmp found in the Design Experiment Sample Data folder.

Figure 6.2 Partial Listing of Reactor 32 Runs.jmp from the Sample Data Folder

	Pattern	Feed Rate	Catalyst	Stir Rate	Temperature	Concentration	Percent Reacted
1	-----	10	1	100	140	3	61
2	----+	10	1	100	140	6	56
3	---+-	10	1	100	180	3	69
4	---++	10	1	100	180	6	44
5	--+--	10	1	120	140	3	53
6	--+-+	10	1	120	140	6	59
7	--++-	10	1	120	180	3	66
8	--+++	10	1	120	180	6	49
9	-+---	10	2	100	140	3	63
10	-+--+	10	2	100	140	6	70
11	-+-+-	10	2	100	180	3	94
12	-+-++	10	2	100	180	6	78
13	-++--	10	2	120	140	3	54
14	-++-+	10	2	120	140	6	67
15	-+++-	10	2	120	180	3	95

Panel at left:
- Reactor 32 Runs
- Design   2x2x2x2 Factorial
- Fit Model
- Columns (7/0)
  - Pattern
  - Feed Rate ✱
  - Catalyst ✱
  - Stir Rate ✱
  - Temperature ✱
  - Concentration ✱
  - Percent Reacted ✱
- Rows
  - All rows   32
  - Selected   0
  - Excluded   0
  - Hidden   0

Analyze the Reactor Data

Begin the analysis with a quick look at the response data before fitting the factorial model.

1   Select **Analyze > Distribution**.
2   Highlight Percent Reacted and click **Y, Columns**. Then click **OK**.
3   Click the red triangle icon on the Percent Reacted title bar and select **Normal Quantile Plot**. The results are shown in Figure 6.3.

Figure 6.3 Distribution of Response Variable for Reactor Data

Note that this initial analysis shows some experimental runs with a very high percent reacted response.
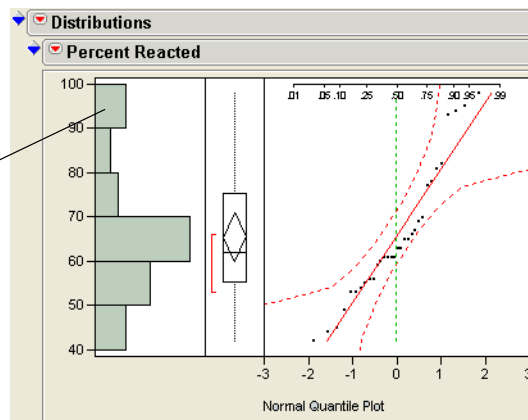
Start the formal analysis with a stepwise regression. The data table has a script stored with it that automatically defines an analysis of the model with main effects and all two-factor interactions.

4   Click the red triangle icon next to the Fit Model script and select **Run Script**. The stepwise analysis begins with the Stepwise Regression Control panel shown in Figure 6.4.

5   The probability to enter a factor (**Prob to Enter**) in the model should be 0.05.

6   The probability to remove a factor (**Prob to Leave**) should be 0.1.

Figure 6.4 Stepwise Control Panel

7   A useful way to use the Stepwise platform is to check all the main effects in the Current Estimates table. However, make sure that the menu beside **Direction** in the Stepwise Regression Control panel specifies **Mixed** (see Figure 6.4).

8   Check the boxes for the main effects of the factors as shown in Figure 6.5.

9   Click **Go**.

Figure 6.5 Starting Model For Stepwise Process

		SSE	DFE	MSE	RSquare	RSquare Adj	Cp	AIC
		2642.75	26	101.64423	0.6192	0.5460	210.64	153.2429

Lock	Entered	Parameter	Estimate	nDF	SS	"F Ratio"	"Prob>F"
✓	✓	Intercept	65.5	1	0	0.000	1.0000
☐	✔	Feed Rate(10,15)	-0.6875	1	15.125	0.149	0.7028
☐	✔	Catalyst(1,2)	9.75	1	3042	29.928	0.0000
☐	✔	Stir Rate(100,120)	-0.3125	1	3.125	0.031	0.8622
☐	✔	Temperature(140,180)	5.375	1	924.5	9.095	0.0057
☐	✔	Concentration(3,6)	-3.125	1	312.5	3.074	0.0913
☐	☐	Catalyst*Feed Rate	0	1	15.125	0.144	0.7076
☐	☐	Stir Rate*Feed Rate	0	1	4.5	0.043	0.8381
☐	☐	Temperature*Feed Rate	0	1	6.125	0.058	0.8115
☐	☐	Concentration*Feed Rate	0	1	0.125	0.001	0.9728
☐	☐	Stir Rate*Catalyst	0	1	6.125	0.058	0.8115
☐	☐	Temperature*Catalyst	0	1	1404.5	28.357	0.0000
☐	☐	Concentration*Catalyst	0	1	32	0.306	0.5848
☐	☐	Concentration*Temperature	0	1	968	14.450	0.0008

The mixed stepwise procedure removes insignificant main effects and adds important interactions. The end result is shown in Figure 6.6. Note that the Feed Rate and Stir Rate factors are no longer in the model.

Figure 6.6 Model After Mixed Stepwise Regression

10 Click the **Make Model** button in the Stepwise Regression Control panel. The Model Specification window that appears is automatically set up with the appropriate effects (Figure 6.7).

Figure 6.7 Fitting a Prediction Model

11 Click **Run Model** to see the analysis for a candidate prediction model (Figure 6.8).

The figure on the left in Figure 6.8 shows the actual by predicted plot for the model. The predicted model covers a range of predictions from 40% to 95% reacted. The size of the random noise as measured by the RMSE is only 3.3311%, which is more than an order of magnitude smaller than the range of predictions. This is strong evidence that the model has good predictive capability.

The figure on the right in Figure 6.8 shows a table of model coefficients and their standard errors (labeled Parameter Estimates). All effects selected by the stepwise process are highly significant.

Figure 6.8 Actual by Predicted Plot and Prediction Parameter Estimates Table
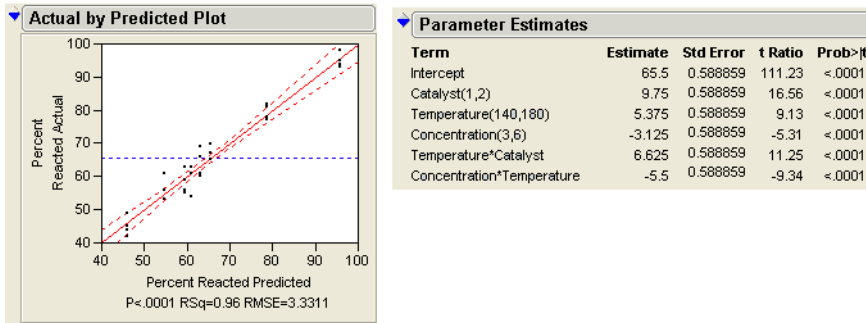
The factor Prediction Profiler also gives you a way to compare the factors and find optimal settings.

1   To open the Prediction Profiler, click the red triangle on the Response Percent Reacted title bar and select **Factor Profiling > Profiler**, as shown in Figure 6.9.

Figure 6.9 Selecting the Profiler
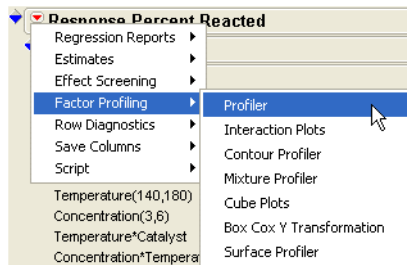
Figure 6.10 shows the profiler's initial display. The Prediction Profiler is discussed in more detail in the chapter "Response Surface Designs," p. 115, and in the chapter "Standard Least Squares: Exploring the Prediction Equation" of *JMP Statistics and Graphics Guide*.

Figure 6.10 Viewing the Profiler
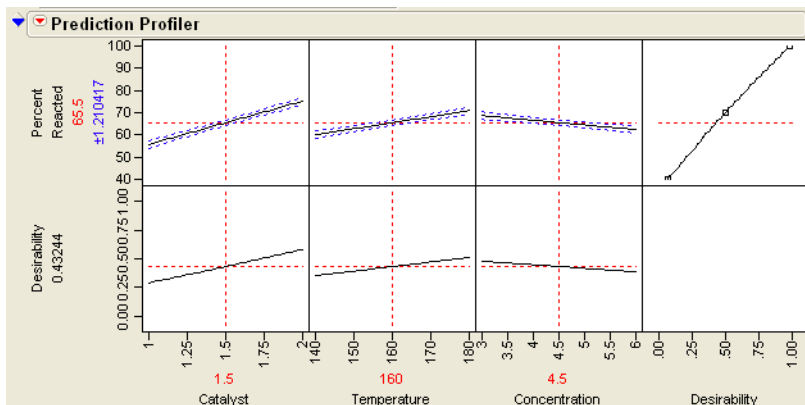
2   Click the red triangle on the Prediction Profiler title bar and select **Maximize Desirability** to see the profiler in Figure 6.11.

Figure 6.11 Viewing the Prediction Profiles at the Optimum Settings
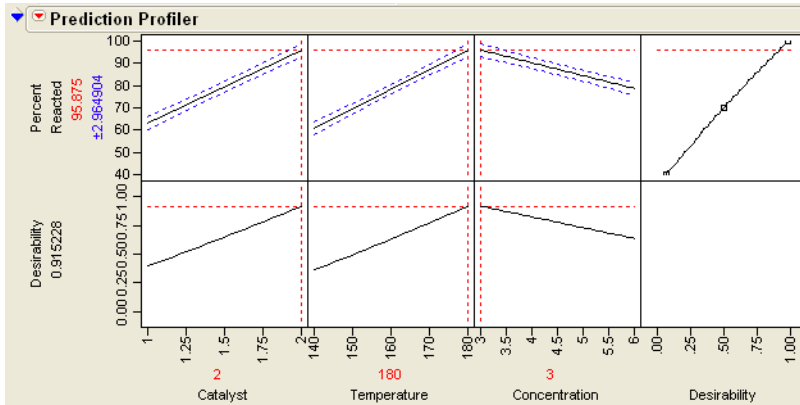
The goal is to maximize Percent Reacted. The reaction is unfeasible economically unless the Percent Reacted is above 90%. Percent Reacted increases from 65.5 at the center of the factor ranges to 95.875 ± 2.96 at the most desirable settings. The best settings of all three factors are at the ends of their ranges. Future experiments could investigate what happens as you continue moving further in this direction.

Creating a Factorial Design

To start a full factorial design, select **DOE > Full Factorial Design**, or click the **Full Factorial Design** button on the JMP Starter **DOE** page. Then, follow the steps below:

- "Enter Responses and Factors," p. 136
- "Select Output Options," p. 137
- "Make the Table," p. 138

Enter Responses and Factors

The steps for entering responses are outlined in "Enter Responses and Factors into the Custom Designer," p. 59

The steps for entering factors in a full factorial design are unique to this design. To add factors, see Figure 6.12.

Figure 6.12 Entering Factors in a Full Factorial Design

To enter factors, click either the **Continuous**
button or the **Categorical** button and select a
factor type, level 2 - 9.
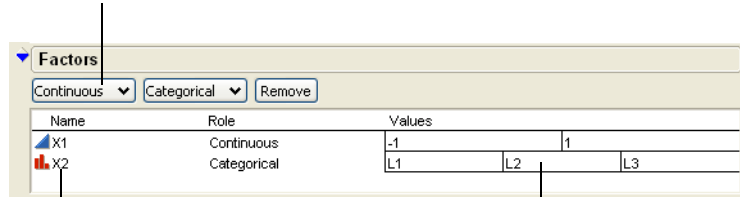
Double-click to edit
the factor name.

Click to enter values or change the level names. To remove
a level, click it, press the delete key on the keyboard, then
press the Return or Enter key on the keyboard.

When you finish adding factors, click **Continue**.

Select Output Options

Use the Output Options panel to specify how you want the output data table to appear, as illustrated in
Figure 6.13:

Figure 6.13 Output Options Panel
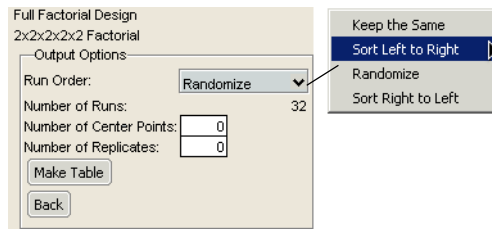
Run Order gives options to designate the order you want the runs to appear in the data table when it is
created. Choices are:

Keep the Same   the rows (runs) in the output table will appear as they do in the Design panel.

Sort Left to Right   the rows (runs) in the output table will appear sorted from left to right.

Randomize   the rows (runs) in the output table will appear in a random order.

Sort Right to Left   the rows (runs) in the output table will appear sorted from right to left.

Add additional points to the data table with these options:

Number of Center Points   Specifies additional runs placed at the center of each continuous factor's
range.

Number of Replicates   Specify the number of times to replicate the entire design, including cen-
terpoints. Type the number of times you want to replicate the design in the associated text box.
One replicate doubles the number of runs.
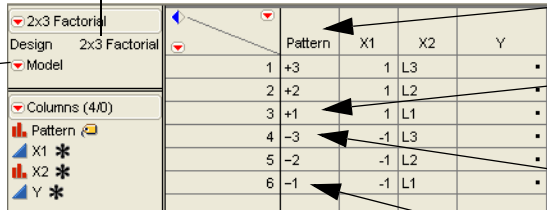
Make the Table

When you click **Make Table**, the table shown in Figure 6.14 appears.

Figure 6.14 Factorial Design Table

The name of the table is the design type that generated it.

values in the Pattern column describe the run each row represents

This script automates fitting a model using values in the design table.

for continuous factors, a plus sign represents high levels

for continuous factors, a minus sign represents low levels

level numbers represent values of categorical factors

	Pattern	X1	X2	Y
1	+3	1	L3	.
2	+2	1	L2	.
3	+1	1	L1	.
4	-3	-1	L3	.
5	-2	-1	L2	.
6	-1	-1	L1	.

▼2x3 Factorial
Design   2x3 Factorial
▼Model

▼Columns (4/0)
Pattern
X1 ✳
X2 ✳
Y ✳

Chapter **7**

Mixture Designs

The mixture designer supports experiments with factors that are ingredients in a mixture. You can choose among several classical mixture design approaches, such as simplex, extreme vertices, and lattice. For the extreme vertices approach you can supply a set of linear inequality constraints limiting the geometry of the mixture factor space.

The properties of a mixture are almost always a function of the relative proportions of the ingredients rather than their absolute amounts. In experiments with mixtures, a factor's value is its proportion in the mixture, which falls between zero and one. The sum of the proportions in any mixture recipe is one (100%).

Designs for mixture experiments are fundamentally different from those for screening. Screening experiments are orthogonal. That is, over the course of an experiment, the setting of one factor varies independently of any other factor. Thus, the interpretation of screening experiments is relatively simple, because the effects of the factors on the response are separable.

With mixtures, it is impossible to vary one factor independently of all the others. When you change the proportion of one ingredient, the proportion of one or more other ingredients must also change to compensate. This simple fact has a profound effect on every aspect of experimentation with mixtures: the factor space, the design properties, and the interpretation of the results.

Because the proportions sum to one, mixture designs have an interesting geometry. The feasible region for the response in a mixture design takes the form of a simplex. For example, consider three factors in a 3-D graph. The plane where the sum of the three factors sum to one is a triangle-shaped slice. You can rotate the plane to see the triangle face-on and see the points in the form of a ternary plot.
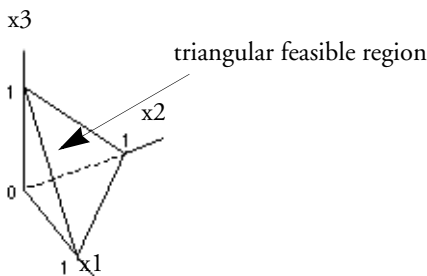
Contents

Mixture Design Types

To create a mixture design, choose **DOE > Mixture Design**, enter the responses and factors into the initial mixture designer panel, and click **Continue**. You then see the Choose Mixture Design Type panel shown in Figure 7.1. Select one of the designs from the panel:

Optimal   invokes the custom designer with all the mixture variables already defined.

Simplex Centroid   lets you specify the degree to which the factor combinations are made.

Simplex Lattice   lets you specify how many levels you want on each edge of the grid.

Extreme Vertices   lets you specify linear constraints or restrict the upper and lower bounds to be within the 0 to 1 range.

ABCD Design   generates a screening design for mixtures devised by Snee (1975).

Figure 7.1 Mixture Design Selection Dialog

After you select the design type, choose the number of runs in the Design Generation panel and click **Make Design**.

The following sections describe each mixture design type and show examples.

The Optimal Mixture Design

The **Optimal** mixture design choice invokes the custom designer with the mixture variables entered into the response and factors panels. To create an optimal mixture design:

1 Select **DOE > Mixture Design**.

2 Enter factors and responses. The steps for entering responses are outlined in "Enter Responses and Factors into the Custom Designer," p. 59.

3 After you enter responses and factors, click **Continue**.

4 Click **Optimal** on the Choose Mixture Design Type panel.

5 Add effects to the model using the instructions below.

Adding Effects to the Model

Initially, the Model panel lists only the main effects corresponding to the factors you entered, as shown in Figure 7.2.

Figure 7.2 The Model Panel
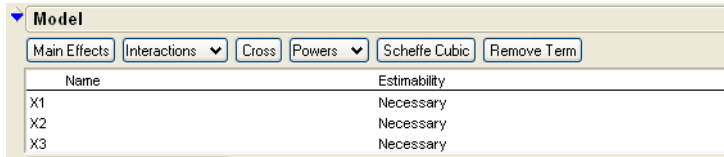
However, you can add factor interactions, specific crossed factor terms, powers, or Scheffe Cubic terms to the model.

- To add interaction terms to a model, click the **Interactions** button and select **2nd**, **3rd**, **4th**, or **5th**. For example, if you have factors X1 and X2, click **Interactions > 2nd** and X1*X2 is added to the list of model effects.

- To add crossed effects to a model, highlight the factors and effects you want to cross and click the **Cross** button.

- To add powers of continuous factors to the model, click the **Powers** button and select **2nd**, **3rd**, **4th**, or **5th**.

- When you want a mixture model with third-degree polynomial terms, the **Scheffe Cubic** button provides a polynomial specification of the surface by adding terms of the form X1*X2*(X1-X2).

The Simplex Centroid Design

A simplex centroid design of degree k with n factors is composed of mixture runs with

- all one factor
- all combinations of two factors at equal levels
- all combinations of three factors at equal levels
- and so on up to k factors at a time combined at k equal levels.

A center point run with equal amounts of all the ingredients is always included.

Creating the Design

To create a simplex centroid design:

1 Select **DOE > Mixture Design**.

2 Enter factors and responses. The steps for entering responses are outlined in "Enter Responses and Factors into the Custom Designer," p. 59.

3 After you enter responses and factors, click **Continue**.

4 Enter the number of ingredients in the box labeled **K**. JMP will create runs for each ingredient with-

out mixing, then create runs that mix equal proportions of K ingredients at a time to the specified limit.

5   Click the **Simplex Centroid** button.

6   View factor settings and Output Options, as illustrated in Figure 7.3.

Figure 7.3 Example of Factor Settings and Output Options
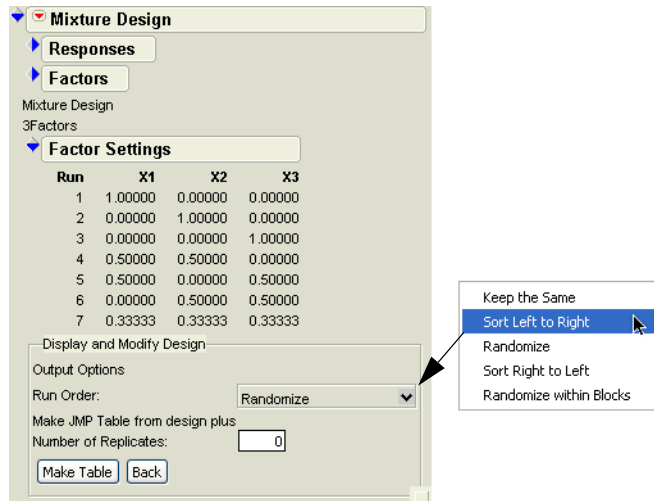
7   Specify Run Order, which is the order you want the runs to appear in the data table when it is created. Run order choices are:

Keep the Same   the rows (runs) in the output table will appear as they do in the Design panel.

Sort Left to Right   the rows (runs) in the output table will appear sorted from left to right.

Randomize   the rows (runs) in the output table will appear in a random order.

Sort Right to Left   the rows (runs) in the output table will appear sorted from right to left.

Randomize within Blocks   the rows (runs) in the output table will appear in random order within the blocks you set up.

8   Specify Number of Replicates. The number of replicates is the number of times to replicate the entire design, including centerpoints. Type the number of times you want to replicate the design in the associated text box. One replicate doubles the number of runs.

9   Click **Make Table**.

Simplex Centroid Design Examples

The table of runs for a design of degree 1 with three factors (left in Figure 7.4) shows runs for each single ingredient followed by the center point. The table of runs to the right is for three factors of degree 2. The first three runs are for each single ingredient, the second set shows each combination of two ingredients in equal parts, and the last run is the center point.

Figure 7.4 Three-Factor Simplex Centroid Designs of Degrees 1 and 2
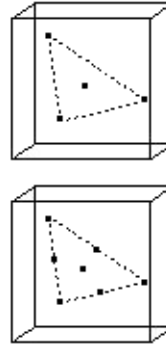
To generate the two sets of runs in Figure 7.4:

1 Choose **DOE > Mixture Design**.
2 Enter three mixture factors.
3 Click **Continue**.
4 Enter **1** in the **K** box, and click **Simplex Centroid** to see the design on the left in Figure 7.5.
5 Click the **Back** button, then click **Continue**, and enter **2** in the **K** box. Then click **Simplex Centroid** to see the design on the right in Figure 7.5.

Figure 7.5 Create Simplex Centroid Designs of Degrees 1 and 2

As another example:

1 Choose **DOE > Mixture Design**.
2 Enter five factors and click **Continue**.
3 Use the default value, **4**, in the **K** box.
4 Click **Simplex Centroid**.
5 Click **Make Table** to see the 31-run JMP data table shown in Figure 7.6.

Figure 7.6 Partial Listing of Factor Settings for Five-Factor Simplex Centroid Design

The Simplex Lattice Design

The simplex lattice design is a space filling design that creates a triangular grid of runs. The design is the set of all combinations where the factors' values are i / m, where i is an integer from 0 to m such that the sum of the factors is 1.

To create simplex lattice designs:

1 Select **DOE > Mixture Design**.
2 Enter factors and responses. The steps for entering responses are outlined in "Enter Responses and Factors into the Custom Designer," p. 59.
3 Click **Continue**.
4 Specify the number of levels you want in the Mixture Design Type dialog (Figure 7.1) and click **Simplex Lattice**.

Figure 7.7 shows the runs for three-factor simplex lattice designs of degrees 3, 4, and 5, with their corresponding geometric representations. In contrast to the simplex centroid design, the simplex lattice design does not necessarily include the centroid.

Figure 7.7 Three-Factor Simplex Lattice Designs for Factor Levels 3, 4, and 5

Factor Settings

Run	X1	X2	X3
1	0.00000	0.00000	1.00000
2	0.00000	0.33333	0.66667
3	0.00000	0.66667	0.33333
4	0.00000	1.00000	0.00000
5	0.33333	0.00000	0.66667
6	0.33333	0.33333	0.33333
7	0.33333	0.66667	0.00000
8	0.66667	0.00000	0.33333
9	0.66667	0.33333	0.00000
10	1.00000	0.00000	0.00000

Factor Settings

Run	X1	X2	X3
1	0.00000	0.00000	1.00000
2	0.00000	0.25000	0.75000
3	0.00000	0.50000	0.50000
4	0.00000	0.75000	0.25000
5	0.00000	1.00000	0.00000
6	0.25000	0.00000	0.75000
7	0.25000	0.25000	0.50000
8	0.25000	0.50000	0.25000
9	0.25000	0.75000	0.00000
10	0.50000	0.00000	0.50000
11	0.50000	0.25000	0.25000
12	0.50000	0.50000	0.00000
13	0.75000	0.00000	0.25000
14	0.75000	0.25000	0.00000
15	1.00000	0.00000	0.00000

Factor Settings

Run	X1	X2	X3
1	0.00000	0.00000	1.00000
2	0.00000	0.20000	0.80000
3	0.00000	0.40000	0.60000
4	0.00000	0.60000	0.40000
5	0.00000	0.80000	0.20000
6	0.00000	1.00000	0.00000
7	0.20000	0.00000	0.80000
8	0.20000	0.20000	0.60000
9	0.20000	0.40000	0.40000
10	0.20000	0.60000	0.20000
11	0.20000	0.80000	0.00000
12	0.40000	0.00000	0.60000
13	0.40000	0.20000	0.40000
14	0.40000	0.40000	0.20000
15	0.40000	0.60000	0.00000
16	0.60000	0.00000	0.40000
17	0.60000	0.20000	0.20000
18	0.60000	0.40000	0.00000
19	0.80000	0.00000	0.20000
20	0.80000	0.20000	0.00000
21	1.00000	0.00000	0.00000

Figure 7.8 lists the runs for a simplex lattice of degree 3 for five effects. In the five-level example, the runs creep across the hyper-triangular region and fill the space in a grid-like manner.

Figure 7.8 JMP Design Table for Simplex Lattice with Five Variables, Order (Degree) 3

5Factors

Factor Settings

Run	X1	X2	X3	X4	X5
1	0.00000	0.00000	0.00000	0.00000	1.00000
2	0.00000	0.00000	0.00000	0.33333	0.66667
3	0.00000	0.00000	0.00000	0.66667	0.33333
4	0.00000	0.00000	0.00000	1.00000	0.00000
5	0.00000	0.00000	0.33333	0.00000	0.66667
6	0.00000	0.00000	0.33333	0.33333	0.33333
7	0.00000	0.00000	0.33333	0.66667	0.00000
8	0.00000	0.00000	0.66667	0.00000	0.33333
9	0.00000	0.00000	0.66667	0.33333	0.00000
10	0.00000	0.00000	1.00000	0.00000	0.00000
11	0.00000	0.33333	0.00000	0.00000	0.66667
12	0.00000	0.33333	0.00000	0.33333	0.33333
13	0.00000	0.33333	0.00000	0.66667	0.00000
14	0.00000	0.33333	0.33333	0.00000	0.33333
15	0.00000	0.33333	0.33333	0.33333	0.00000
16	0.00000	0.33333	0.66667	0.00000	0.00000
17	0.00000	0.66667	0.00000	0.00000	0.33333
18	0.00000	0.66667	0.00000	0.33333	0.00000
19	0.00000	0.66667	0.33333	0.00000	0.00000
20	0.00000	1.00000	0.00000	0.00000	0.00000
21	0.33333	0.00000	0.00000	0.00000	0.66667
22	0.33333	0.00000	0.00000	0.33333	0.33333
23	0.33333	0.00000	0.00000	0.66667	0.00000
24	0.33333	0.00000	0.33333	0.00000	0.33333
25	0.33333	0.00000	0.33333	0.33333	0.00000
26	0.33333	0.00000	0.66667	0.00000	0.00000
27	0.33333	0.33333	0.00000	0.00000	0.33333
28	0.33333	0.33333	0.00000	0.33333	0.00000
29	0.33333	0.33333	0.33333	0.00000	0.00000
30	0.33333	0.66667	0.00000	0.00000	0.00000
31	0.66667	0.00000	0.00000	0.00000	0.33333
32	0.66667	0.00000	0.00000	0.33333	0.00000
33	0.66667	0.00000	0.33333	0.00000	0.00000
34	0.66667	0.33333	0.00000	0.00000	0.00000
35	1.00000	0.00000	0.00000	0.00000	0.00000

The Extreme Vertices Design

The extreme vertices design accounts for factor limits and selects vertices and their averages (formed by factor limits) as design points. Additional limits are usually in the form of range constraints, upper bounds, and lower bounds on the factor values.

The extreme vertices design finds the corners (vertices) of a factor space constrained by limits specified for one or more of the factors. The property that the factors must be non-negative and must add up to one is the basic mixture constraint that makes a triangular-shaped region.

Sometimes other ingredients need range constraints that confine their values to be greater than a lower bound or less than an upper bound. Range constraints chop off parts of the triangular-shaped (simplex) region to make additional vertices. It is also possible to have a linear constraint, which defines a linear combination of factors to be greater or smaller than some constant.

The geometric shape of a region bound by linear constraints is called a simplex, and because the vertices represent extreme conditions of the operating environment, they are often the best places to use as design points in an experiment.

You usually want to add points between the vertices. The average of points that share a constraint boundary is called a *centroid* point, and centroid points of various degrees can be added. The centroid point for two neighboring vertices joined by a line is a second degree centroid because a line is two dimensional. The centroid point for vertices sharing a plane is a third degree centroid because a plane is three dimensional, and so on.

If you specify an extreme vertices design but give no constraints, a simplex centroid design results.

Creating the Design

Follow these steps to create an extreme vertices design. The next sections show examples with specific constraints.

1 Select **DOE > Mixture Design**.
2 Enter factors and responses. These steps are outlined in "Enter Responses and Factors into the Custom Designer," p. 59. Remember to enter the upper and lower limits in the factors panel (see Figure 7.9).
3 Click **Continue**.
4 In the **Degree** text box, enter the degree of the centroid point you want to add. The centroid point is the average of points that share a constraint boundary.
5 If you have linear constraints, click the **Linear Constraints** button for each constraint you want to add. Use the text boxes that appear to define a linear combination of factors to be greater or smaller than some constant.
6 Click **Extreme Vertices** to see the factor settings.

7 (Optional) Change the order of the runs in the data table when it is created. Run order choices are:

   Keep the Same—the rows (runs) in the output table will appear as they do in the Design panel.

   Sort Left to Right—the rows (runs) in the output table will appear sorted from left to right.

   Randomize—the rows (runs) in the output table will appear in a random order.

   Sort Right to Left—the rows (runs) in the output table will appear sorted from right to left.

   Randomize within Blocks—the rows (runs) in the output table will appear in random order
   within the blocks you set up.

8 (Optional) Type the sample size you want in the **Choose desired sample size** text box.

9 (Optional) Click **Find Subset** to generate the optimal subset having the number of runs specified in
   sample size box described in Step 8. The **Find Subset** option uses the row exchange method (not
   coordinate exchange) to find the optimal subset of rows.

10 Click **Make Table**.

An Extreme Vertices Example with Range Constraints

The following example design table is for five factors with the range constraints shown in Figure 7.9,
where the ranges are smaller than the default 0 to 1 range.

1 Select **DOE > Mixture Design**.

2 Add two additional factors (for a total of 5 factors) and give them the values shown in Figure 7.9.

3 Click **Continue**.

4 Enter '4' in the **Degree** text box (Figure 7.9).

Figure 7.9 Example of Five-factor Extreme Vertices

5 Click **Exreme Vertices**.

6 Select **Sort Left to Right** from the Run Order menu.

7 Click **Make Table.** Figure 7.10 shows a partial listing of the resulting table. Note that the Rows panel in the data table shows that the table has the default 116 runs.

Figure 7.10 JMP Design Table for Extreme Vertices with Range Constraints

	X1	X2	X3	X4	X5	Y
1	0.05	0.1	0.2	0.4	0.25	.
2	0.05	0.1	0.25	0.4	0.2	.
3	0.05	0.1	0.26666667	0.36666667	0.21666667	.
4	0.05	0.1	0.3	0.4	0.15	.
5	0.05	0.15	0.15	0.4	0.25	.
6	0.05	0.15	0.3	0.4	0.1	.
7	0.05	0.2	0.1	0.4	0.25	.
8	0.05	0.2	0.2	0.4	0.15	.
9	0.05	0.2	0.3	0.4	0.05	.
10	0.05	0.25	0.1	0.4	0.2	.
11	0.05	0.25	0.25	0.4	0.05	.
12	0.05	0.26666667	0.1	0.36666667	0.21666667	.
13	0.05	0.26666667	0.26666667	0.36666667	0.05	.
14	0.05	0.3	0.1	0.4	0.15	.
15	0.05	0.3	0.15	0.4	0.1	.
16	0.05	0.3	0.2	0.4	0.05	.
17	0.05	0.1	0.25	0.35	0.25	

Extreme Vertices / Design Extreme Vertices / Model / Columns (6/0): X1 ✳, X2 ✳, X3 ✳, X4 ✳, X5 ✳, Y ✳ / Rows — All rows 116, Selected 0, Excluded 0, Hidden 0, Labelled 0

Suppose you want fewer runs. You can go back and enter a different sample size (number of runs).

8 Click **Back**, then click **Continue**.

9 Enter '4' in the **Degree** text box and click **Exreme Vertices**.

10 In the sample size text box, enter '10' as the sample size.

11 Click **Find Subset** to generate the optimal subset having the number of runs specified. The resulting design (Figure 7.11) is the optimal 10-run subset of the 116 current runs. This is useful when the extreme vertices design generates a large number of vertices.

Figure 7.11 JMP Design Table for 10-Run Subset of the 116 Current Runs

	X1	X2	X3	X4	X5	Y
1	0.05	0.1	0.3	0.4	0.15	.
2	0.05	0.3	0.2	0.4	0.05	.
3	0.05	0.3	0.3	0.1	0.25	.
4	0.05	0.3	0.1	0.3	0.25	.
5	0.15	0.1	0.1	0.4	0.25	.
6	0.25	0.1	0.3	0.1	0.25	.
7	0.25	0.1	0.3	0.3	0.05	.
8	0.25	0.2	0.1	0.4	0.05	.
9	0.25	0.3	0.1	0.1	0.25	.
10	0.25	0.3	0.3	0.1	0.05	.

Extreme Vertices / Design Extreme Vertices / Model / Columns (6/0): X1 ✳, X2 ✳, X3 ✳, X4 ✳, X5 ✳, Y ✳ / Rows — All rows 10, Selected 0

Note: The **Find Subset** option uses the row exchange method (not coordinate exchange) to find the optimal subset of rows.

An Extreme Vertices Example with Linear Constraints

Consider the classic example presented by Snee (1979) and Peipel (1988). This example has three factors, X1, X2, and X3, with five individual factor bound constraints and three additional linear constraints:

Table 7.1 Linear Constraints for the Snee and Peipel Example

X1 ≥ 0.1	90 ≤ 85*X1 + 90*X2 + 100*X3
X1 ≤ 0.5	85*X1 + 90*X2 + 100*X3 ≤ 95
X2 ≥ 0.1	.4 ≤ 0.7*X1 + X3
X2 ≤ 0.7	
X3 ≤ 0.7	

To enter these constraints:

1 Enter the upper and lower limits in the factors panel.

2 Click **Continue**.

3 Click the **Linear Constraint** button three times. Enter the constraints as shown in Figure 7.12.

4 Click the **Extreme Vertices** button.

5 Change the run order to **Sort Right to Left,** and keep the sample size at 13 to see the 13-run factor settings like those shown on the right in Figure 7.12.

6 Click **Make Table**.

Figure 7.12 Constraints

This example is best understood by viewing the design as a ternary plot, as shown at the end of this chapter, in Figure 7.14. The ternary plot shows how close to one a given component is by how close it is to the vertex of that variable in the triangle. See "Creating Ternary Plots," p. 152, for details.

Extreme Vertices Method: How It Works

If there are linear constraints, JMP uses the CONSIM algorithm developed by R.E. Wheeler, described in Snee (1979) and presented by Peipel (1988) as CONVRT. The method is also described in Cornell (1990, Appendix 10a). The method combines constraints and checks to see if vertices violate them. If so, it drops the vertices and calculates new ones. The method named CONAEV for doing centroid points is by Peipel (1988).

If there are no linear constraints (only range constraints), the extreme vertices design is constructed using the XVERT method developed by Snee and Marquardt (1974) and Snee (1975). After the vertices are found, a simplex centroid method generates combinations of vertices up to a specified order.

The XVERT method first creates a full 2^{nf-1} design using the given low and high values of the $nf-1$ factors with smallest range. Then, it computes the value of the one factor left out based on the restriction that the factors' values must sum to one. It keeps the point if it is in that factor's range. If not, it increments or decrements it to bring it within range, and decrements or increments each of the other factors in turn by the same amount, keeping the points that still satisfy the initial restrictions.

The above algorithm creates the vertices of the feasible region in the simplex defined by the factor constraints. However, Snee (1975) has shown that it can also be useful to have the centroids of the edges and faces of the feasible region. A generalized n-dimensional face of the feasible region is defined by $nf-n$ of the boundaries and the centroid of a face defined to be the average of the vertices lying on it. The algorithm generates all possible combinations of the boundary conditions and then averages over the vertices generated on the first step.

The ABCD Design

This approach by Snee (1975) generates a screening design for mixtures. To create an ABCD design:

1 Select **DOE > Mixture Design**.
2 Enter factors and responses. The steps for entering responses are outlined in "Enter Responses and Factors into the Custom Designer," p. 59.
3 After you enter responses and factors, click **Continue**.
4 Click the **ABCD** button.
5 View factor settings and Output Options.
6 Specify **Run Order**, which is the order you want the runs to appear in the data table when it is created. Run order choices are:

   Keep the Same—the rows (runs) in the output table will appear as they do in the Design panel.

   Sort Left to Right—the rows (runs) in the output table will appear sorted from left to right.

   Randomize—the rows (runs) in the output table will appear in a random order.

   Sort Right to Left—the rows (runs) in the output table will appear sorted from right to left.

   Randomize within Blocks—the rows (runs) in the output table will appear in random order within the blocks you set up.

7 Specify **Number of Replicates**. The number of replicates is the number of times to replicate the entire design, including centerpoints. Type the number of times you want to replicate the design in

the associated text box. One replicate doubles the number of runs.

8   Click **Make Table**.

Creating Ternary Plots

A mixture problem in three components can be represented in two dimensions because the third component is a linear function of the others. The *ternary plot* in Figure 7.14 shows how close to one (1) a given component is by how close it is to the vertex of that variable in the triangle. The plot to the left in Figure 7.13 illustrates a ternary plot.

Figure 7.13 Ternary Plot (left) and Tetrary Plot (right) for Mixture Design
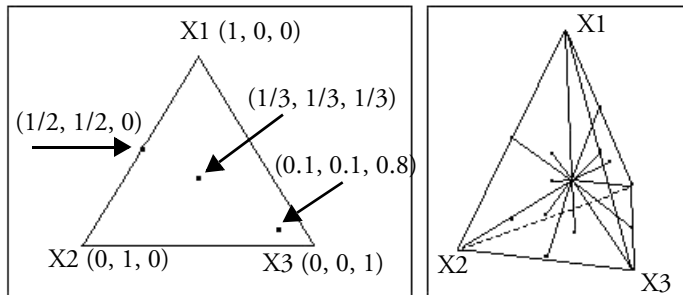
The Peipel (1979) example referenced in "An Extreme Vertices Example with Linear Constraints," p. 150 is best understood by the ternary plot shown in Figure 7.14.

To view a mixture design as a ternary plot:

1   Create the Peipel mixture data as shown previously, or open the table called Peipel.jmp, found in the Design Experiments folder of the Sample Data Library.

2   Choose **Graph > Ternary Plot**.

3   In the ternary plot launch dialog, specify the three mixture components and click **OK**.

The JMP Ternary plot platform recognizes the three factors as mixture factors, and also considers the upper and lower constraints entered into the Factors panel when the design was created. The Ternary plot uses shading to exclude the unfeasible areas excluded by those constraints.

The Peipel data had additional constraints, entered as linear constraints for the extreme vertices design. Each constraint is a line, drawn by the line graphics tool on the ternary plot. There are six active constraints, six vertices, and six centroid points shown on the plot, as well as two inactive (redundant) constraints. The feasible area is the inner white polygon delimited by the design points and constraint lines.

Figure 7.14 Diagram of Ternary Plot Showing Peipel Example Constraints
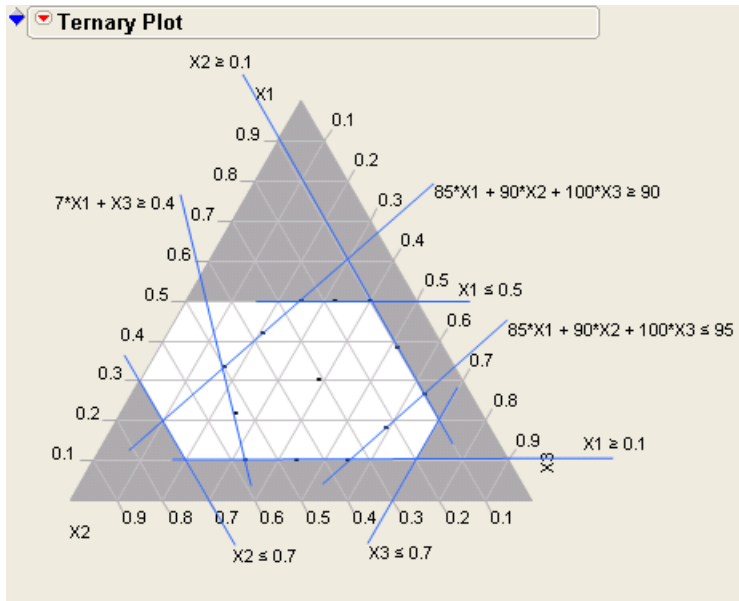
Fitting Mixture Designs

When fitting a model for mixture designs, you must take into account that all the factors add up to a constant, and thus a traditional full linear model will not be fully estimable.

The recommended response surface model, called the Scheffé polynomial (Scheffé 1958), does the following:

- suppresses the intercept
- includes all the linear main-effect terms
- excludes all the square terms (such as X1*X1)
- includes all the cross terms (such as X1*X2)

To fit a model:

1 Choose **DOE > Mixture Design** and make the design data table. Remember that to fit a model, the Y column in the data table must contain values, so either assign responses or click the red triangle menu and select **Simulate Responses** before you click **Make Table**.
2 The design data table stores the model in the data table as a table property. This table property is a JSL script called **Model**, located in the left panel of the table.
3 Right-click the model and select **Run Script** to launch the Fit Model dialog, which is automatically filled with the saved model.
4 Click **Run Model** on the Fit Model dialog.

In this model, the parameters are easy to interpret (Cornell 1990). The coefficients on the linear terms are the fitted response at the extreme points where the mixture consists of a single factor. The coefficients on the cross terms indicate the curvature across each edge of the factor space. Your values may be different from those shown below.

Figure 7.15   Fitting a Mixture Design
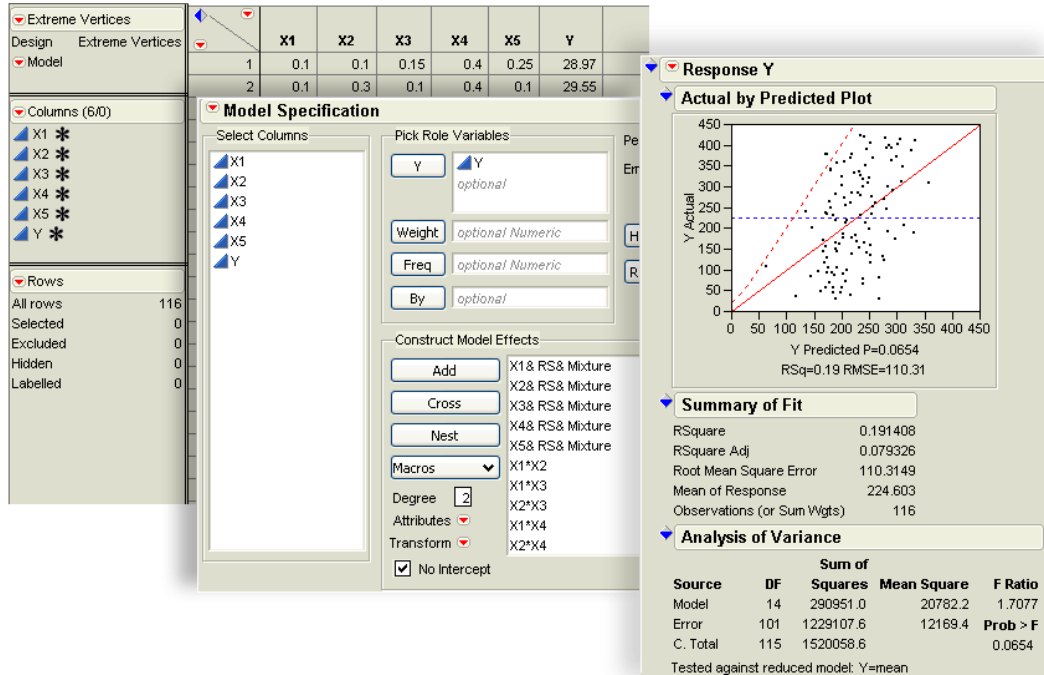
The model report usually has several sections of interest, including the whole model tests, Analysis of Variance reports, and response surface reports, which are described below.

Whole Model Tests and Analysis of Variance Reports

In a whole-model Analysis of Variance table, JMP traditionally tests that all the parameters are zero except for the intercept. In a mixture model without an intercept, JMP looks for a hidden intercept, in the sense that a linear combination of effects is a constant. If it finds a hidden intercept, it does the whole model test with respect to the intercept model rather than a zero-intercept model. This test is equivalent to testing that all the parameters are zero except the linear parameters, and testing that they are equal.

The hidden-intercept property also causes the R^2 to be reported with respect to the intercept model rather than reported as missing.

Understanding Response Surface Reports

When there are effects marked as response surface effects "&RS," JMP creates additional reports that analyze the fitted response surface. These reports were originally designed for full response surfaces, not mixture models. However, if JMP encounters a no-intercept model and finds a hidden intercept with linear response surface terms, but no square terms, then it *folds* its calculations, collapsing on the last response surface term to calculate critical values for the optimum. This can be done for any combination that yields a constant and involves the last response surface term.

The contour plot feature of these reports does not fold to handle mixtures. If you want a contour plot of the surface, you can do any of the following:

- Save the model prediction formula and then create a ternary plot with **Graph > Ternary Plot**.
- Refit the model using a full response surface that omits the last factor.
- Create a separate contour plot with **Graph > Contour Plot**, and add points to make the plot less granular.

A Chemical Mixture Example

Three plasticizers (p1, p2, and p3) comprise 79.5% of the vinyl used for automobile seat covers (Cornell, 1990). Within this 79.5%, the individual plasticizers are restricted by the following constraints: $0.409 \leq x1 \leq 0.849$, $0 \leq x2 \leq 0.252$, and $0.151 \leq x3 \leq 0.274$.

Create the Design

To create Cornell's mixture design in JMP:

1 Select **DOE > Mixture Design**.
2 In the Factors panel, use the three default factors but name them p1, p2, and p3, and enter the high and low constraints as shown in Figure 7.16. Or, load the factors with the **Load Factors** command in the red triangle on the Mixture Design title bar. To import the factors, open Plastifactors.jmp, found in the Design Experiment Sample Data folder that was installed with JMP.

Figure 7.16 Factors and Factor Constraints for the Plasticizer Experiment

3 Click **Continue**.
4 Enter **3** in the **Degree** text box.
5 Click **Exreme Vertices**.

6   Click **Make Table**. JMP uses the 9 factor settings to generate a JMP table (Figure 7.17).

Figure 7.17 Extreme Vertices Mixture Design

7   Add an extra five design runs by duplicating the vertex points and center point, to give a total of 14 rows in the table.

Note: To identify the vertex points and the center (or interior) point, use the sample data script called LabelMixturePoints.jsl in the Sample Scripts folder installed with JMP.

---

8   Run the LabelMixturePoints.jsl to see the results inFigure 7.18, and highlight the vertex points and the interior point as shown.

Figure 7.18 Identify Vertices and Center Point with Sample Data Script

9   Select **Edit > Copy**, to copy the selected rows to the clipboard.

10 Select **Rows > Add Rows** and enter **5** as the number of rows to add

11 Click the **At End** radio button on the dialog, then click **OK**.

12 Highlight the new rows and select **Edit > Paste** to add the duplicate rows to the table.

The Plasticizer data with the results (*Y* values) that Cornell obtained are available in the Sample data. Open Plasticizer.jmp in the Sample Data folder installed with JMP to see this table (Figure 7.19).

Figure 7.19 Plasticizer.jmp Data Table from the Sample Data Library

Analyze the Mixture Model

Use the Cornell plasticizer data from the Sample Data library (Figure 7.19) to run the mixture model:

1 Right-click the table property named Model on the upper-left of the data table and select **Run Script**, which runs a script that displays a completed Fit Model dialog. Click Run Model to see the response surface analysis.

2 Plasticizer.jmp contains a column called **Pred Formula Y**. This column was added after the analysis by selecting **Save Columns > Prediction Formula** from the red triangle menu in the Response Y title bar of the analysis report. To see the prediction formula, right-click (Ctrl+click on the Mac) the column name and select **Formula**:

```
0–50.1465*p1 – 282.1982*p2 – 911.6484*p3 + p2*p1*317.363 +
    p3*p1*1464.3298 + p3*p2*1846.2177
```

Your values may be different from those shown here.

Note: These results correct the coefficients reported in Cornell (1990).

The Response Surface Solution report (Figure 7.20) shows that a maximum predicted value of 19.570299 occurs at point (0.63505, 0.15568, 0.20927).

Figure 7.20 Mixture Response Surface Analysis
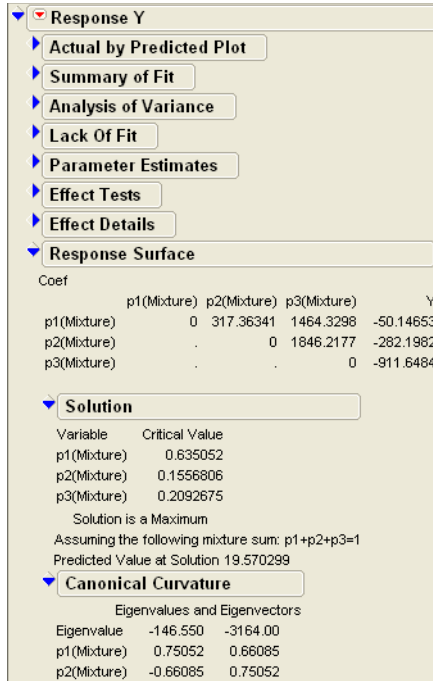
The Prediction Profiler

The report contains a prediction profiler.

3 If the profiler is not visible, click the red triangle in the Response Y title bar and select **Factor Profiling > Profiler**. You should see the initial profiler shown in Figure 7.21.

The crossed effects show as curvature in the prediction traces. Drag one of the vertical reference lines, and the other two move in the opposite direction maintaining their ratio.

Note: The axes of prediction profiler traces range from the upper and lower bounds of the factors, p1, p2, and p3, entered to create the design and the design table. When you experiment moving a variable trace, you see the other traces move such that their ratio is preserved. As a result, when the limit of a variable is reached, it cannot move further and only the third variable changes.
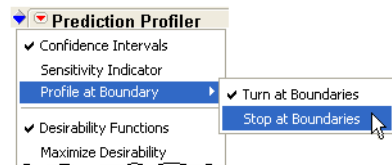
4 To limit the visible profile curves to bounds that use all three variables, use the **Stop at Boundaries** command from the menu on the Prediction Profiler title bar.

5 If needed, select the **Desirability Functions** command to display the desirability function showing to the right of the prediction profile plots in Figure 7.22.

6 Then select **Maximize Desirabilty** from the Prediction Profiler menu to see the best factor settings.

The profiler in Figure 7.22, displays optimal settings (rounded) of 0.6350 for p1, 0.1557 for p2, and 0.2093 for p3, which give an estimated response of 19.5703.

Figure 7.21 Initial Prediction Profiler
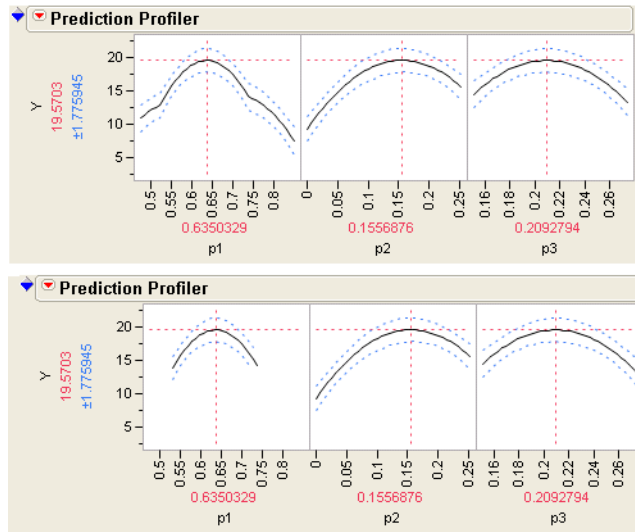
Figure 7.22 Maximum Desirability in Profiler for Mixture Analysis Example
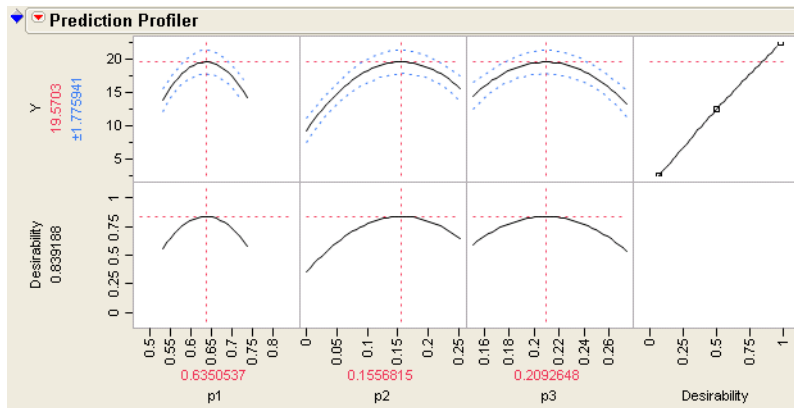
The Mixture Profiler

The Fit Model report also has a **Mixture Profiler** that is useful for visualizing and optimizing response surfaces from mixture experiments.

Many of the features are the same as those of the Contour Profiler however some are unique to the Mixture Profiler:

- A ternary plot is used instead of a Cartesian plot, which enables you to view three mixture factors at a time.

- If you have more than three factors, radio buttons let you choose which factors to plot.

- If the factors have constraints, you can enter their low and high limits in the Lo Limit and Hi Limit columns. This shades non-feasible regions in the profiler.

7   Select **Factor Profiling** > **Mixture Profiler** from the menu on the Response Y title bar to see the mixture profiler for the plasticizer data, shown in Figure 7.23.
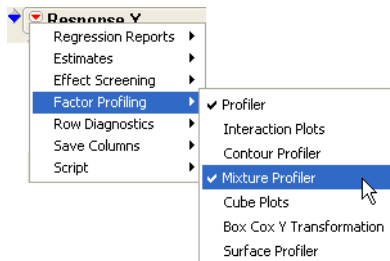
Figure 7.23 Mixture Profiler for Plasticizer Example
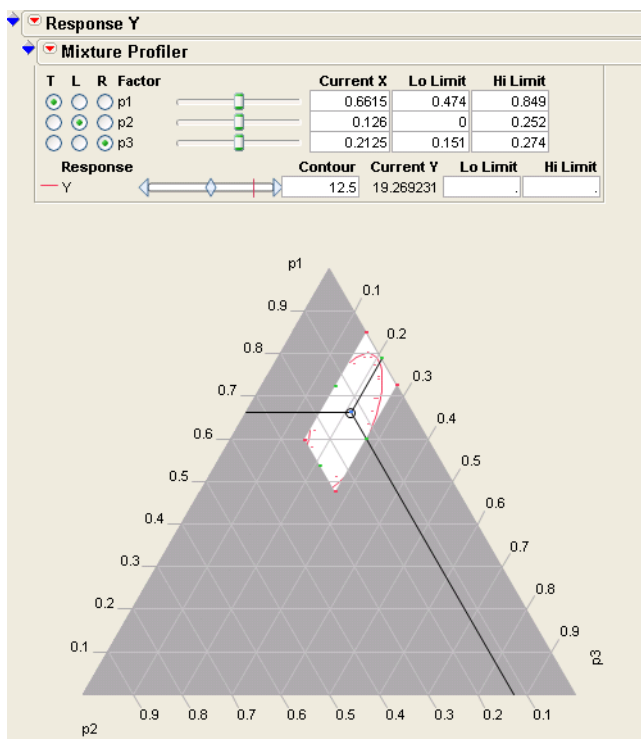
A Ternary Plot of the Mixture Response Surface

You can also plot the response surface of the plasticizer data as a ternary plot using the Ternary graph platform and contour the plot with information from an additional variable:

1 Choose **Graph > Ternary Plot**.

2 Specify plot variables (p1, p2, and p3) and click **X, Plottting**, as shown in Figure 7.24. To identify the contour variable (the prediction equation), select **Pred Formula Y** and click the **Contour Formula** button. The contour variable must have a prediction formula to form the contour lines, as shown by the ternary plots at the bottom in Figure 7.25. If there is no prediction formula, the ternary plot only shows points.

Figure 7.24 Launch Dialog for the Ternary Plot Platform
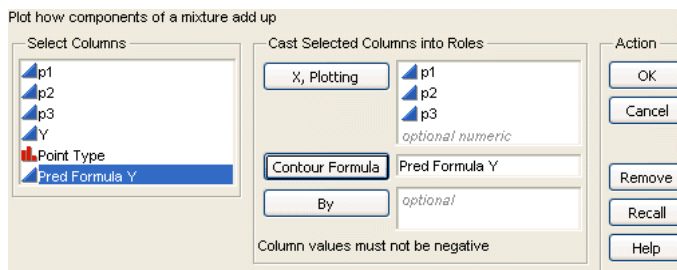
3 Click **OK** and view the results, as shown in Figure 7.25. By default, the ternary plot displays contour lines only, but you can request a fill, as shown, with the **Contour Fill** command found in the red triangle menu on the Ternary Plot title bar.

Figure 7.25 Ternary Plot of a Mixture Response Surface
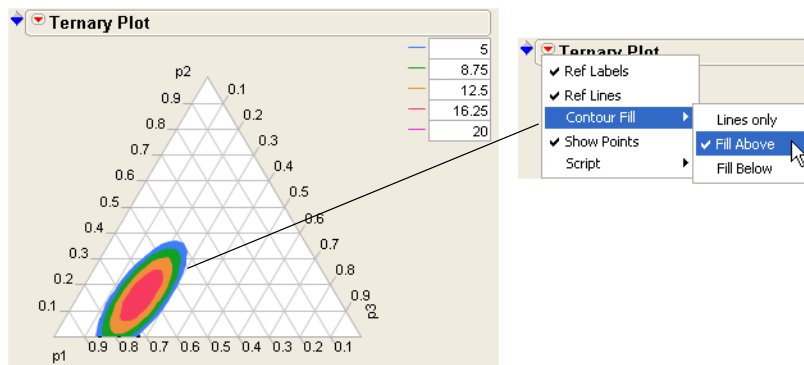
Chapter **8**

Discrete Choice Designs

The Discrete Choice designer creates experiments with factors that are product attributes. A collection of attributes is called a product profile. Respondents choose one in each set of product profiles.

Industrial experimentation deals with the question of how to improve processes to deliver better products. Choice experiments help a company prioritize product features for their market. The purpose of a choice experiment is to define a product that people want to buy.

Choice experiments always involve people comparing prospective products and picking the one they prefer. For example, suppose a computer company wants to update its high-end laptop. Laptops have many features that are important to customers such as processor speed, hard disk size, screen size, battery life, and price. To build a laptop that customers want, the computer company needs to know the relative importance of each feature. Most people prefer a faster computer with more storage, longer battery life, and a low price. What the company does not know is how much more an extra hour of battery life is worth to a customer or whether doubling the hard disk size is as important as doubling the processor speed. A choice experiment can answer these questions and indicate the optimal set of trade-offs among product features.

Contents

Introduction

Most choice experiments involve conducting a market research survey. The survey consists of a series of questions about attributes of interest about a potential new product or product modification. For example, a computer manufacturer might be interested in manufacturing a new laptop and wants information about customer preference before beginning an expensive development process. Computer characteristics change so rapidly that it is crucial to quickly identify the attributes that help the manufacturers to design and build a new machine most likely to capture enough market share to be profitable.

Often, the attributes are obvious. For example, the consumer wants a laptop that has a large screen, weighs almost nothing, costs almost nothing, and lasts forever on a single battery charge. The question, then, is how much is the customer willing to compromise these desires? How important is each of these attributes, and which kinds of trade off is the customer most likely to accept and still purchase a new machine?

Assume a simple situation where a computer manufacturer wants to examine preferences for four possible laptop configurations. Notice that there are no 'right' or 'wrong' selections. Instead there are just preferences. A well designed questionnaire and proper analysis of results can tell a manufacturer how to proceed. The manufacturer wants information about the following four laptop attributes.

- size of hard drive disk (40 GB or 80 GB)
- speed of processor (1.5 GHz or 2.0 GHz)
- battery life (4 Hrs or 6 Hrs)
- cost of computer ($1000, $1200 or $1500)

If a survey were constructed that offered the possibility of choosing any combination of these attributes, a respondent would be forced to evaluate 24 possible combinations and make a single response. Instead each respondent usually evaluates several choice sets and for each choice set, chooses the preferred profile. In the simplest situation, each respondent chooses between sets of two profiles.

Then, you analyze the choices of multiple respondents. A well designed choice experiment, correctly analyzed is a efficient way to give the researcher the most information for the least time and expense.

Table 1 shows hypothetical results from a single *survey* designed to collect information about consumer preferences about laptop computers.

- Each column in the survey identifies a laptop *attribute.*
- Each line in the survey defines a laptop *profile*, which is a collection of attribute values.
- Each *choice set* consists of two attribute profiles.
- All of the attribute values are allowed to change across the two profiles in a choice set.

Table 8.1 Hypothetical Choice Survey Results from a single Respondent, Subject ID 2

		Disk Size	Speed	Battery Life	Price	Preference
1	1	40 GB	1.5 GHz	6 hours	$1,000	_X_
	2	80 GB	1.5 GHz	4 hours	$1,200	____
2	1	40 GB	1.5 GHz	4 hours	$1,500	____
	2	80 GB	2.0 GHz	4 hours	$1,200	_X_
3	1	40 GB	2.0 GHz	4 hours	$1,200	_X_
	2	80 GB	2.0 GHz	6 hours	$1,500	____
4	1	40 GB	2.0 GHz	4 hours	$1,000	_X_
	2	80 GB	1.5 GHz	6 hours	$1,200	____
5	1	40 GB	1.5 GHz	6 hours	$1,000	_X_
	2	40 GB	2.0 GHz	4 hours	$1,500	____
6	1	40 GB	2.0 GHz	6 hours	$1,200	_X_
	2	80 GB	1.5 GHz	4 hours	$1,500	____
7	1	40 GB	2.0 GHz	6 hours	$1,500	____
	2	80 GB	1.5 GHz	4 hours	$1,000	_X_
8	1	40 GB	1.5 GHz	4 hours	$1,200	____
	2	80 GB	2.0 GHz	4 hours	$1,000	_X_

For each pair, please check the combination of attributes you find most appealing.

The DOE Choice designer can create a survey like that shown in Table 8.1. However, to create an effective design, the Choice designer needs information about the attributes. For example, most laptop attributes have values that are intrinsic preferences. That is, a bigger disk size is better, longer battery life is better, and so forth. The purpose of conducting a choice survey is to find out how the potential laptop purchasers feels about the advantages of a collection of tractates.

One way to gain prior information about attributes in a survey is to conduct a single example survey, analyze the results, and use those results as prior information to create the final survey instrument.

This chapter shows how to create a sample survey and use its results as prior information for a final survey design

Create an Example Choice Experiment

The Choice design can create a survey like the one in Table 1. As an example,

1 Choose **Doe** > **Choice Design**, and complete the initial dialog as shown in Figure 8.1.

Figure 8.1 Choice Design Dialog with Attributes Defined

2 Click **Continue**. For this example, use the default values in the Model Control panel and in the Design Generation panel, as shown in Figure 8.2.

Optionally, you can use the DOE Model Controls panel to add interactions to the choice model in situations where you expect there are interactions and want to generate profile sets that will help detect them.

Figure 8.2 Design Generation Panel for the Laptop Experiment

The values in the Design Generation panel describe the laptop survey.

Number of attributes that can change within a choice set   There are four laptop attributes. Entering 4 as the number of attributes that can change within a choice set means that the Choice designer can change 4 or fewer attribute values within a single choice set. You can enter fewer than the total number of attributes to constrain the total number that can be changed within a choice set. This might be a reasonable thing to do if you had a large number of attributes and you want to make it easier for the respondents to make a choice. For example, a survey might be

interested in 20 or more attributes of a cell phone, but show and change only 5 or fewer attributes in a choice set.

Number of profiles per choice set   This example has two profiles per choice set. You can design choice experiments with more than two profiles in a choice set.

Number of choice sets per survey   There are eight choice sets in the example survey but often there are many more.

Number of surveys   The example only shows a single survey. Normally you expect multiple respondents and would request more than one survey.

Expected number of respondents per survey   You might want to give surveys to 10 people, but use two different surveys. So you enter 2 as the Number of surveys and 5 as the Expected number of respondents per survey.

Note: Recall that this first example is used to generate prior information, then used to create a more realistic survey. This example is a single survey given to a single respondent.

3   Click **Make Design** to see the example survey results in Figure 8.3.

Figure 8.3 Survey Results based on a Simple Model and Default Prior Information

The Radio buttons beneath the design settings let you choose between having the survey settings in one JMP table and gathering survey results in a second table, or generating a single table that shows the settings and has an additional column for the choice response.

You can see that there are eight choice sets, each consisting of two laptop profiles. At this point you can press **Back** and modify the design, or click **Make Table** and generate the JMP table shown in Figure 8.4.

This default design was created with no given prior information. Without prior information, the Choice designer has no way of knowing which attribute levels are better. That is, the Choice designer

cannot know that a lower price might be more desirable than a higher price, a faster machine is better than a slower machine, and so forth. As a result, you can see that some choice sets might not convey useful information. The analysis results are used as prior information in a new Choice design dialog.

Figure 8.4 JMP Data Table for Preliminary Laptop Choice Survey

	Choice Set	Response Indicator	Disk Size	Speed	Battery Life	Price
1	1	·	40 GB	1.5 GHz	6 Hrs	$1,000
2	1	·	80 GB	1.5 GHz	4 Hrs	$1,200
3	2	·	40 GB	1.5 GHz	4 Hrs	$1,500
4	2	·	80 GB	2.0 GHz	4 Hrs	$1,200
5	3	·	40 GB	2.0 GHz	4 Hrs	$1,200
6	3	·	80 GB	2.0 GHz	6 Hrs	$1,500
7	4	·	40 GB	2.0 GHz	4 Hrs	$1,000
8	4	·	80 GB	1.5 GHz	6 Hrs	$1,200
9	5	·	40 GB	1.5 GHz	6 Hrs	$1,000
10	5	·	40 GB	2.0 GHz	4 Hrs	$1,500
11	6	·	40 GB	2.0 GHz	6 Hrs	$1,200
12	6	·	80 GB	1.5 GHz	4 Hrs	$1,500
13	7	·	40 GB	2.0 GHz	6 Hrs	$1,500
14	7	·	80 GB	1.5 GHz	4 Hrs	$1,000
15	8	·	40 GB	1.5 GHz	4 Hrs	$1,200
16	8	·	80 GB	2.0 GHz	4 Hrs	$1,000

Choice Profiles
Design   Discrete Choice
Choice

Columns (6/0)
Choice Set
Response Indicator
Disk Size
Speed
Battery Life
Price

Rows
All rows   16
Selected   0
Excluded   0

Analyze the Example Choice Experiment

Once a survey deign is complete, a respondent chooses one profile from each set, entering '1' for the chosen profile and '0' for the rejected profile. Suppose a respondent completed the example survey as shown in Figure 8.5. You can now analyze these results using the Choice platform in the **Analyze** menu (**Analyze** > **Modeling** > **Choice**).

Note: When you create a survey data table, the default name of the table is Choice Profiles. A Choice analysis is saved with the table as a script that references the default data table name. This example table is saved as Laptop Design.jmp in the Design of Experiment folder of the Sample data. Note in Figure 8.5 that the script was modified to reference the table named Laptop Design.

Figure 8.5 JMP Table with Survey Choice Sets and Responses

Use the Choice
script to analyze
the data.

	Choice Set	Response Indicator	Disk Size	Speed	Battery Life	Price
1	1	1	40 GB	1.5 GHz	6 Hrs	$1,000
2	1	0	80 GB	1.5 GHz	4 Hrs	$1,200
3	2	0	40 GB	1.5 GHz	4 Hrs	$1,500
4	2	1	80 GB	2.0 GHz	4 Hrs	$1,200
5	3	1	40 GB	2.0 GHz	4 Hrs	$1,200
6	3	0	80 GB	2.0 GHz	6 Hrs	$1,500
7	4	1	40 GB	2.0 GHz	4 Hrs	$1,000
8	4	0	80 GB	1.5 GHz	6 Hrs	$1,200
9	5	1	40 GB	1.5 GHz	6 Hrs	$1,000
10	5	0	40 GB	2.0 GHz	4 Hrs	$1,500
11	6	1	40 GB	2.0 GHz	6 Hrs	$1,200
12	6	0	80 GB	1.5 GHz	4 Hrs	$1,500
13	7	0	40 GB	2.0 GHz	6 Hrs	$1,500
14	7	1	80 GB	1.5 GHz	4 Hrs	$1,000
15	8	0	40 GB	1.5 GHz	4 Hrs	$1,200
16	8	1	80 GB	2.0 GHz	4 Hrs	$1,000

Columns (6/0)
- Choice Set
- Response Indicator
- Disk Size
- Speed
- Battery Life
- Price

Rows
All rows   16
Selected   0
Excluded   0

```
Choice(
    Profile DataTable( "Laptop Design" ),
    Profile Grouping( :Choice Set ),
    Profile ID( :Response Indicator ),
    Profile Effects( :Disk Size, :Speed, :Battery Life, :Price ),
    Launch Dialog
)
```

4   Click the Choice script in the Laptop Design data table and select **Run** to analyze that data with the
Choice modelling platform from the **Analyze** menu.

When you run the Choice model script, the Choice launch dialog shown in Figure 8.6 appears, The
Choice dialog is designed to cover a variety of choice survey results, which can include data saved in
multiple data tables. This example has all data contained in a single table. For details about using the
Choice analysis dialog, see Chapter 30, "Choice Modeling," in the JMP Statistics and Graphics User
Guide.

Figure 8.6 Choice Model Fitting Dialog

Choice Dialog

Profile Data

Select Data Table   Laptop Design

Run Model

Help

Remove

☑ Firth Bias-adjusted Estimates

Select Columns
- Choice Set
- Response Indicator
- Disk Size
- Speed
- Battery Life
- Price

Pick Role Variables
- Profile ID | Response Indicator
- Grouping | Choice Set
- optional

Construct Model Effects
- Add | Disk Size
- Speed
- Cross | Battery Life
- Price
- Nest
- Macros ⌄
- Degree   2
- Transform ⌄

5 Click **Run Model** on the Choice model fitting dialog.

6 An additional dialog then appears asking if this is a one-table analysis with all the data in the Profile Table, which is the case in this sample survey. Click **Yes** in this dialog to continue.

The analysis shows as in Figure 8.7.

To design the final choice survey using prior information, you will need to enter estimates of the mean and variance of the attribute parameter estimates. The analysis on the left in Figure 8.7 has estimates of the attribute means, called **Estimate**, and estimates of the standard deviation of the attributes, called **Std Error**. An easy way to see the variance of the attributes is to capture the analysis in a JMP table and compute the variance:

7 Right click on the Parameter Estimates report and choose **Make into Data Table** from the menu, as shown.

8 In the new **Untitled** data table, create a new column and call it **Var**.

9 Select **Formula** from the **Cols** menu (**Cols** > **Formula**), or right-click at the top of the **Var** column and select **Formula** for the menu that shows.

10 In the Formula Editor, click the **Std Error** column in the column list and click the exponent button (x^y) on the formula editor panel to compute the variance shown on the right in Figure 8.7.

Figure 8.7 Analysis of the sample Laptop Survey
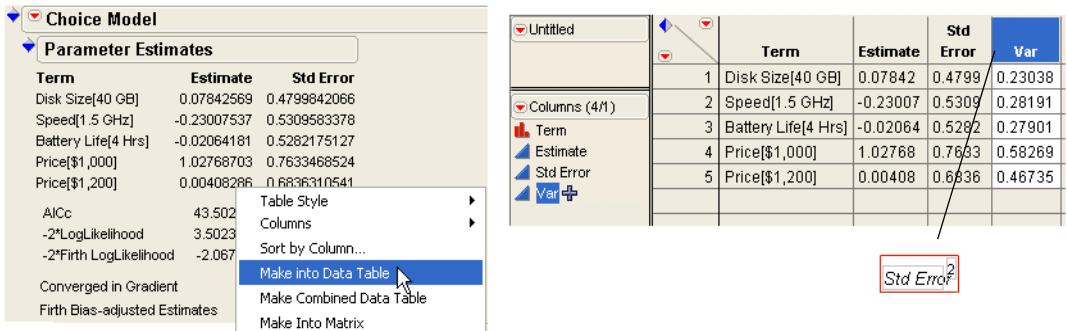
This preliminary survey with its analysis gives you the information needed to design a final survey appropriate for gathering information from multiple respondents. Keep in mind that in a real situation, you might have prior information about factor attributes and not need to do a sample design.

Note: Leave the **Untitled** data table with the mean and variance information open to be used in the next example.

Design a Choice Experiment Using Prior Information

In some situations, you will know from previous surveys or experience how to give prior information to the Choice designer about product attributes. This example continues by designing the laptop experiment again, using the analysis information gained from the sample design.

1 Choose **DOE** > **Choice Design** and enter the attributes and values as before.

2   Click **Continue** to see the Choice design panels in Figure 8.8.

3   Now enter the values from the JMP table created by the previous analysis into the Prior Mean and
    Prior Variance Matrix panels of the Choice Design dialog, as shown in Figure 8.8. You can
    copy-and-paste to transfer the values from the data table to the Choice dialog panels.

Figure 8.8 Enter Prior Mean and Variance Information from Preliminary Survey

4   Enter the values into the Design Generation panel, as shown in Figure 8.9.

•   Four or fewer attribute levels can change within a choice set.

•   There are two profiles per choice set.

•   Each survey has eight choice sets.

•   The design generates two separate surveys.

•   Five respondents are expected to complete each survey (for a total of 10 respondents).

Figure 8.9 Design Specifications for final Laptop Survey

5 Click Make Design to see a design similar to the one shown in Figure 8.10.

Figure 8.10 Design Runs for Two Choice Surveys

6 Click **Make Table**. The final data table will have runs for ten survey respondents, giving a total of 160 observations (2 profiles * 8 choice sets * 2 surveys * 5 respondents = 160 observations).

Administer the Survey and Analyze Results

The survey data table with is results is stored in the Sample Data Design Experiment folder installed with JMP. Figure 8.11 is a partial listing of the survey data table with results. The Choice script created by the Choice designer and saved with the survey data table can be used to analyze the data. As shown previously, the default script accesses the default data table created by the Choice designer named Choice Profiles. If necessary, change the data table name in the script to the name you used for the final design table. Note in Figure 8.11, the data table name is changed to Laptop Results.

1 To continue with this example, open the table called Laptop Results, saved in the Design Experi-

ment folder of the Sample Data.

Figure 8.11 Partial Listing of Final Survey with Results

	Respondent	Survey	Choice Set	Response Indicator	Disk Size	Speed	Battery Life	Price
22	2	2	11	0	80 GB	1.5 GHz	4 Hrs	$1,000
23	2	2	12	0	40 GB	1.5 GHz	4 Hrs	$1,200
24	2	2	12	1	80 GB	2.0 GHz	6 Hrs	$1,000
25	2	2	13	1	40 GB	2.0 GHz	6 Hrs	$1,200
26	2	2	13	0	80 GB	1.5 GHz	4 Hrs	$1,500
27	2	2	14	0	40 GB	1.5 GHz	6 Hrs	$1,200
28	2	2	14	1	80 GB	2.0 GHz	4 Hrs	$1,500
29	2	2	15	1	40 GB	2.0 GHz	4 Hrs	$1,200
30	2	2	15	0	80 GB	1.5 GHz	6 Hrs	$1,500
31	2	2	16	1	40 GB	2.0 GHz	4 Hrs	$1,000
32	2	2	16	0	80 GB	1.5 GHz	6 Hrs	$1,200
33	3	1	1	1	80 GB	1.5 GHz	4 Hrs	$1,200
34	3	1	1	0	40 GB	2.0 GHz	6 Hrs	$1,000
35	3	1	2	0	40 GB	2.0 GHz	4 Hrs	$1,200
36	3	1	2	1	80 GB	1.5 GHz	6 Hrs	$1,000

Laptop Results
Design Discrete Choic
Choice
  Run Script
  Edit
  Delete

Columns (8/0)
  Respondent
  Survey
  Choice Set
  Response Indicator
  Disk Size
  Speed
  Battery Life
  Price

```
Choice(
    Profile DataTable( "Laptop Results" ),
    Profile Grouping( :Respondent, :Survey, :Choice Set ),
    Profile ID( :Response Indicator ),
    Profile Effects( :Disk Size, :Speed, :Battery Life, :Price )
    Launch Dialog
)
```

Initial Choice Platform Analysis

2   To analyze the data, click the Choice script saved with the data and select **Run Script** from the menu to see the completed dialog shown in Figure 8.12.

Note that this dialog has three grouping variables (Respondent, Survey, and Choice Set, whereas the dialog shown Figure 8.6 had only the Choice Set grouping variable because there was a single survey and a single respondent. This example included multiple surveys and respondents, which must be included in the analysis.

Figure 8.12 Choice Model Fitting Dialog to Analyze the Laptop Survey

Choice Dialog
Profile Data

Select Data Table | Laptop Results

Run Model
Help
Remove
☑ Firth Bias-adjusted Estimates

Select Columns
  Respondent
  Survey
  Choice Set
  Response Indicator
  Disk Size
  Speed
  Battery Life
  Price

Pick Role Variables
  Profile ID | Response Indicator
  Grouping | Respondent
           Survey
           Choice Set

Construct Model Effects
  Add | Disk Size
        Speed
  Cross | Battery Life
          Price
  Nest
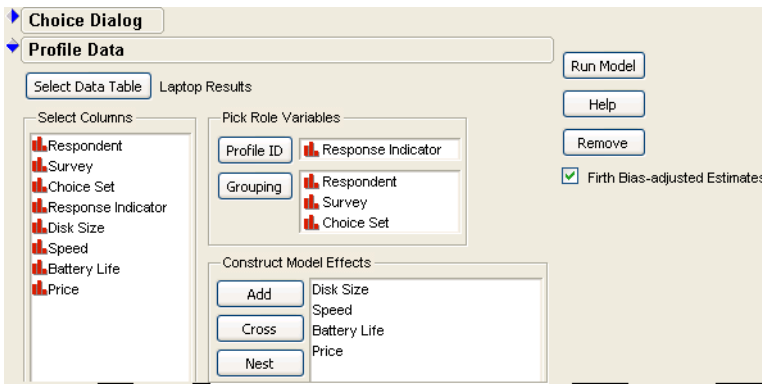
3   Click **Run Model** on the Fit Model dialog. The query again appears asking if the analysis is a

one-table analysis with all the data in the profile table. Click **Yes** to see the initial analysis result shown in Figure 8.13.

The results are clear. The most significant attribute is Speed (Prob < .0001). Disk Size and Price are also significant, but Battery Life is not.

Figure 8.13 Initial Analysis of the Final Laptop Survey
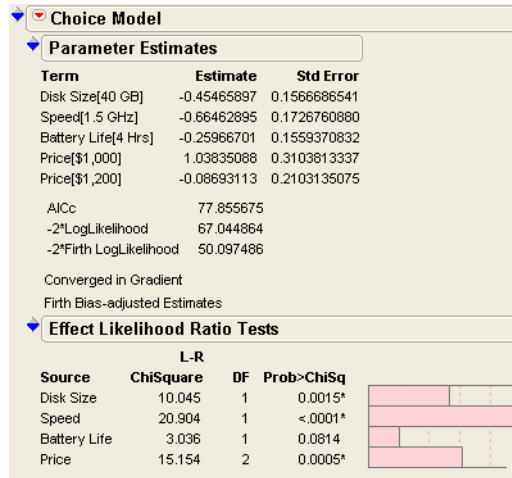
Find Unit Cost and Trade Off Costs with the Profiler

You would like to know how changing the price, or other characteristics, of a laptop affects the desirability as perceived by potential buyers. This desirability is called the *utility value* of the laptop attributes. The profiler shows the utility value and how it changes as the laptop attributes change.

4 Select **Profiler** from the menu on the Choice Model title bar to see the Prediction Profiler in Figure 8.14.

Figure 8.14 Default Prediction Profiler for Laptop Choice Analysis
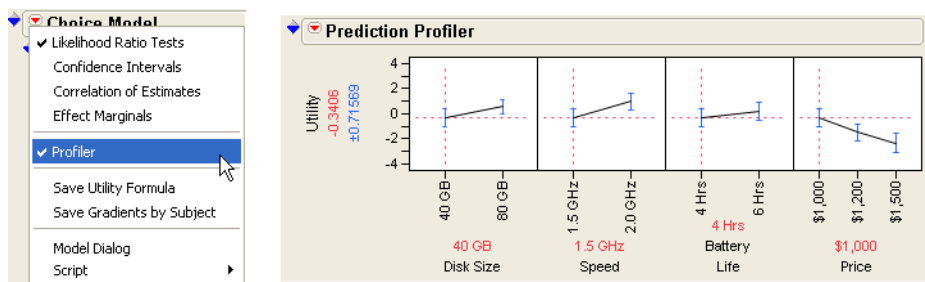
When each attribute value is set to its lowest value, the Utility value is –0.3406. The first thing you want to know is the unit utility cost.

5 To find the unit utility cost, move the trace for price to and note how the Utility value changes.

Compare the Utility values in Figure 8.14 and Figure 8.15. The value of Utility changes from –0.3406 to –2.3303 when cost is raised from $1,000 to $1,500. That is, raising the price of a laptop $500.00 lowers the utility (or desirability) approximately 2 units. Thus, you can say that the unit utility cost is roughly $250.00.

Figure 8.15 Compare Change in Utility Over Price
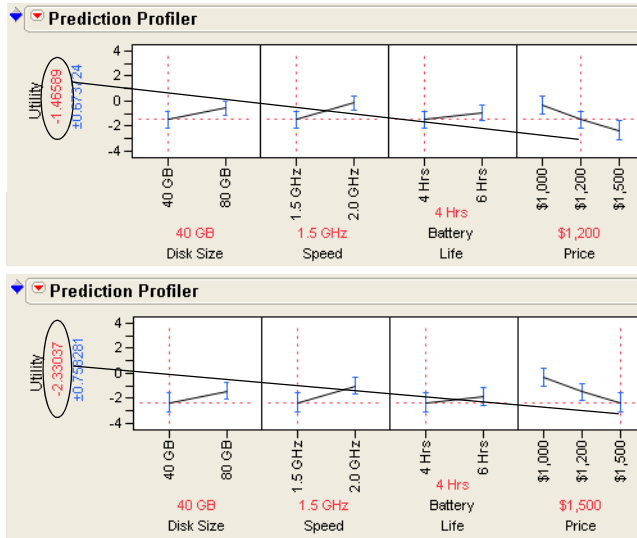
With this unit utility cost estimate you can now vary the other attributes, note the change in utility, and find an approximate dollar value associated with that attribute change. For example, the most significant attribute is speed (see Figure 8.13).

6 In the Prediction Profiler, set Price to its lowest value and change Speed to its higher value.

You can see in Figure 8.16 that the Utility value changes from the original value shown in Figure 8.14 of –0.3406 to 0.9886, for a total change of 1.3292 units. If the unit utility cost is estimated to be $250.00, as shown above, then the increase in price for a 2.0 GHz laptop over a 1.5 GHz laptop can be computed to be 1.3292*$250.00 = $332.30. This is the dollar value the Choice survey provides the manufacturer as a basis for pricing different laptop products. You can make similar calculations for the other attributes.

Figure 8.16 Change Speed in Profiler and Note Utility Value
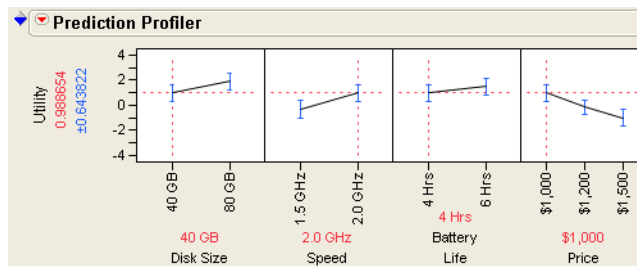
This simple Choice survey and its analysis shows how this kind if information can be used to help manufacturers and retailers identify important product attributes and assign values to them.

The Choice designer allows more complex designs, such as designs with interactions and other terms. The Choice analysis platform can be used to analyze complex designs, and it can be used to incorporate data from multiple data sets that include demographic information about the respondents.

Chapter **9**

Space-Filling Designs

Space-filling designs are useful in situations where run-to-run variability is of far less concern than the form of the model. Sensitivity studies of computer simulations is one such situation. For this case, and any mechanistic or deterministic modeling problem, any variability is small enough to be ignored.

For systems with no variability, randomization and blocking are irrelevant. Replication is undesirable because repeating the same run yields the same result. In space-filling designs, there are two objectives:

- The first objective is to prevent replicate points by spreading the design points out to the maximum distance possible between any two points.
- The second objective is to space the points uniformly.

The following methods are implemented for these types of designs:

- The Sphere-Packing method emphasizes spread of points.
- The Latin Hypercube method is a compromise between spread of points and uniform spacing.
- The Uniform method mimics the uniform probability distribution.
- The Minimum Potential method minimizes energy designs in a hypersphere.
- The Maximum Entropy method measures the amount of information contained in the distribution of a set of data.
- The Gaussian Process IMSE Optimal method creates a design that minimizes the integrated mean squared error of the gaussian process over the experimental region.
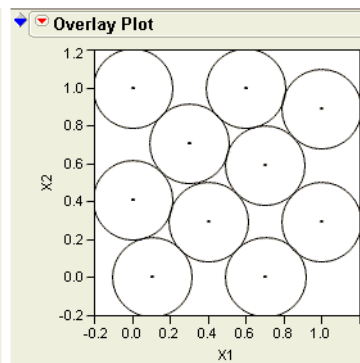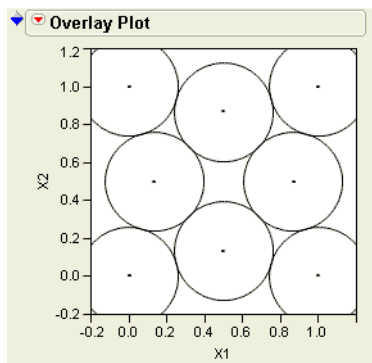
Contents

Introduction to Space-Filling Designs

Space-filling designs are useful for modeling systems that are deterministic or near-deterministic. One example of a deterministic system is a computer simulation. Such simulations can be very complex involving many variables with complicated interrelationships. A goal of designed experiments on these systems is to find a simpler empirical model that adequately predicts the behavior of the system over limited ranges of the factors.

In experiments on systems where there is substantial random noise, the goal is to minimize the variance of prediction. In experiments on deterministic systems, there is no variance but there is *bias*. Bias is the difference between the approximation model and the true mathematical function. The goal of space-filling designs is to bound the bias.

There are two schools of thought on how to bound the bias. One approach is to spread the design points out as far from each other as possible consistent with staying inside the experimental boundaries. The other approach is to space the points out evenly over the region of interest.

The **Space Filling** designer supports the following design methods:

Sphere Packing   maximizes the minimum distance between pairs of design points.

Latin Hypercube   maximizes the minimum distance between design points but requires even spacing of the levels of each factor. This method produces designs that mimic the uniform distribution. The Latin Hypercube method is a compromise between the Sphere-Packing method and the Uniform design method.

Uniform   minimizes the discrepancy between the design points (which have an empirical uniform distribution) and a theoretical uniform distribution.

Minimum Potential   spreads points out inside a sphere around the center.

Maximum Entropy   measures the amount of information contained in the distribution of a set of data.

Gaussian Process IMSE Optimal   creates a design that minimizes the integrated mean squared error of the Gaussian process over the experimental region.

Sphere-Packing Designs

The Sphere-Packing design method maximizes the minimum distance between pairs of design points. The effect of this maximization is to spread the points out as much as possible inside the design region.

Creating a Sphere-Packing Design

To use the Sphere-Packing method:

1 Select **DOE > Space Filling Design**.
2 Enter responses and factors. (See "Enter Responses and Factors into the Custom Designer," p. 59.)
3 Alter the factor level values, if necessary. For example, Figure 9.1 shows the two existing factors, X1 and X2, with values that range from 0 to 1 (instead of the default –1 to 1).

4 Click **Continue** in the dialog.

Figure 9.1 Space-Filling Dialog for Two Factors
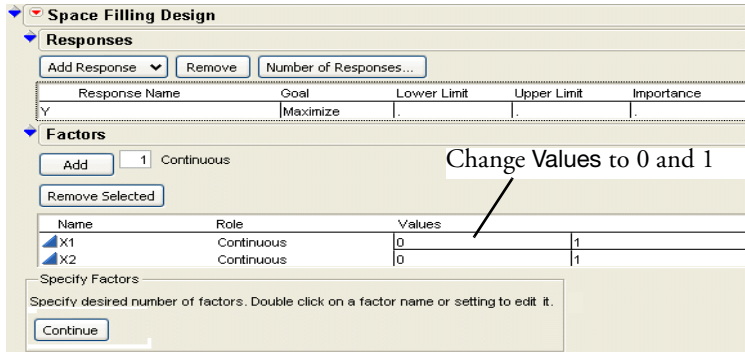
5 In the design specification dialog, specify a sample size (**Number of Runs**). Figure 9.2 shows a sample size of eight.

Figure 9.2 Space-Filling Design Dialog
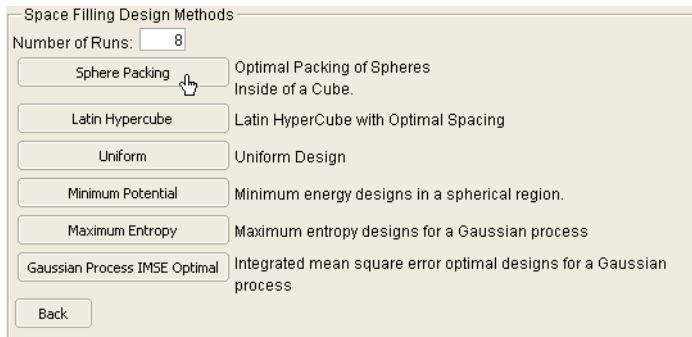
6 Click **Sphere Packing.**

JMP creates the design and displays the design runs and the design diagnostics. Figure 9.3 shows the Design Diagnostics panel open with 0.518 as the **Minimum Distance**. Your results might differ slightly from the ones below, but the minimum distance will be the same.

Figure 9.3 Sphere-Packing Design Settings and Design Diagnostics
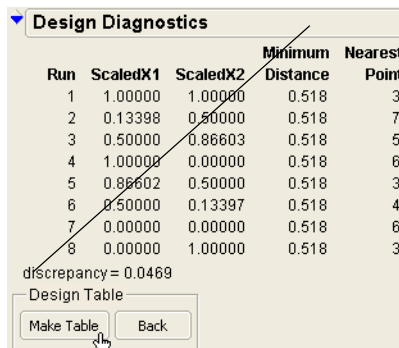
7 Click **Make Table**. Use this table to complete the visualization example, described next.

Visualizing the Sphere-Packing Design

To visualize the nature of the Sphere-Packing technique, create an overlay plot, adjust the plot's frame size, and add circles using the minimum distance from the diagnostic report shown in Figure 9.3 as the radius for the circles. Using the table you just created:

1 Select **Graph > Overlay Plot**.
2 Specify X1 as X and X2 as Y, then click **OK**.
3 Adjust the frame size so that the frame is square by right-clicking the plot and selecting
   Size/Scale > Size to Isometric.
4 Right-click the plot and select **Customize**. When the Customize panel appears, click the plus sign
   to see a text edit area and enter the following script:
   `For Each Row(Circle({:X1, :X2}, 0.518/2))`
   where `0.518` is the minimum distance number you noted in the Design Diagnostics panel. This
   script draws a circle centered at each design point with radius 0.259 (half the diameter, 0.518), as
   shown on the left in Figure 9.4. This plot shows the efficient way JMP packs the design points.
5 Now repeat the procedure exactly as described in the previous section, but with a sample size of 10
   instead of eight.

   Remember to change `0.518` in the graphics script to the minimum distance produced by 10 runs.
   When the plot appears, again set the frame size and create a graphics script using the minimum dis-
   tance from the diagnostic report as the diameter for the circle. You should see a graph similar to the
   one on the right in Figure 9.4. Note the irregular nature of the sphere packing. In fact, you can
   repeat the process a third time to get a slightly different picture because the arrangement is depen-
   dent on the random starting point.

Figure 9.4 Sphere-Packing Example with Eight Runs (left) and 10 Runs (right)
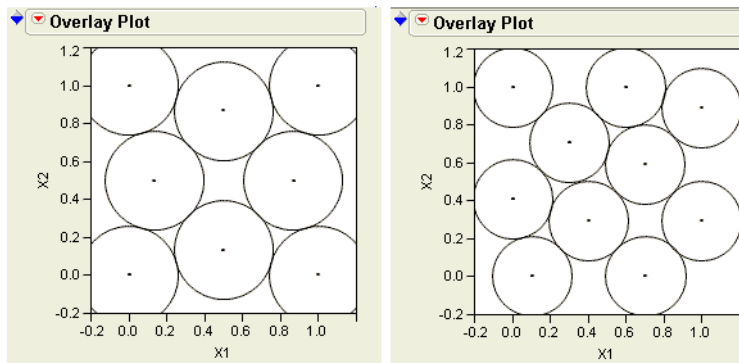
Latin Hypercube Designs

In a Latin Hypercube, each factor has as many levels as there are runs in the design. The levels are spaced evenly from the lower bound to the upper bound of the factor. Like the sphere-packing method, the Latin Hypercube method chooses points to maximize the minimum distance between design points, but with a constraint. The constraint maintains the even spacing between factor levels.

Creating a Latin Hypercube Design

To use the Latin Hypercube method:

1   Select **DOE > Space Filling Design**.

2   Enter responses, if necessary, and factors. (See "Enter Responses and Factors into the Custom Designer," p. 59.)

3   Alter the factor level values, if necessary. For example, Figure 9.5 shows adding two factors to the two existing factors and changing their values to 1 and 8 instead of the default –1 and 1.

Figure 9.5 Space-Filling Dialog for Four Factors
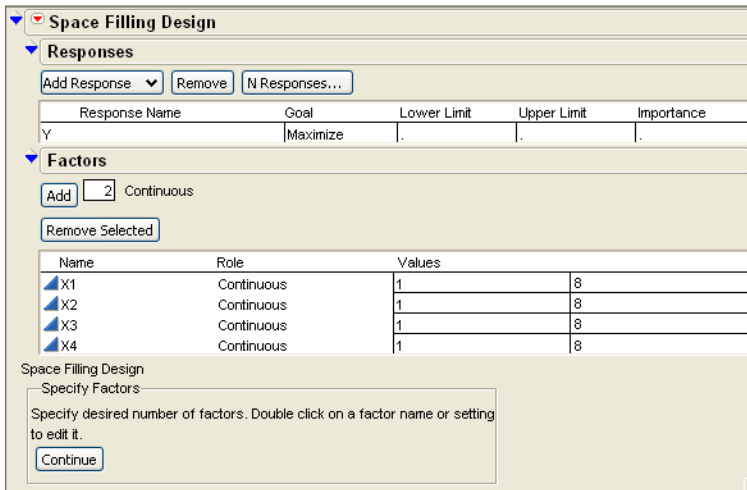
4   Click **Continue.**

5   In the design specification dialog, specify a sample size (**Number of Runs**). This example uses a sample size of eight.

6   Click **Latin Hypercube** (see Figure 9.2). Factor settings and design diagnostics results appear similar to those in Figure 9.6, which shows the Latin Hypercube design with four factors and eight runs.

Note: The purpose of this example is to show that each column (factor) is assigned each level only once, and each column is a different permutation of the levels.

Figure 9.6 Latin Hypercube Design for Four Factors and Eight Runs with Eight Levels

Visualizing the Latin Hypercube Design

To visualize the nature of the Latin Hypercube technique, create an overlay plot, adjust the plot's frame size, and add circles using the minimum distance from the diagnostic report as the radius for the circle.

1 First, create another Latin Hypercube design using the default X1 and X2 factors.
2 Be sure to change the factor values so they are 0 and 1 instead of the default −1 and 1.
3 Click **Continue**.
4 Specify a sample size of eight (**Number of Runs**).
5 Click **Latin Hypercube**. Factor settings and design diagnostics are shown in Figure 9.7.

Figure 9.7 Latin Hypercube Design with two Factors and Eight Runs

6 Click **Make Table**.
7 Select **Graph > Overlay Plot**.
8 Specify X1 as X and X2 as Y, then click **OK**.
9 Right-click the plot and select **Size/Scale > Size to Isometric** to adjust the frame size so that the frame is square.

10 Right-click the plot, select **Customize** from the menu. In the Customize panel, click the large plus sign to see a text edit area, and enter the following script:

```
For Each Row(Circle({:X1, :X2}, 0.404/2)),
```

where `0.404` is the minimum distance number you noted in the Design Diagnostics panel (Figure 9.7). This script draws a circle centered at each design point with radius 0.202 (half the diameter, 0.404), as shown on the left in Figure 9.8. This plot shows the efficient way JMP packs the design points.

11 Repeat the above procedure exactly, but with 10 runs instead of eight (step 5). Remember to change `0.404` in the graphics script to the minimum distance produced by 10 runs.

You should see a graph similar to the one on the right in Figure 9.8. Note the irregular nature of the sphere packing. In fact, you can repeat the process to get a slightly different picture because the arrangement is dependent on the random starting point.

Figure 9.8 Comparison of Latin Hypercube Designs with Eight Runs (left) and 10 Runs (right)
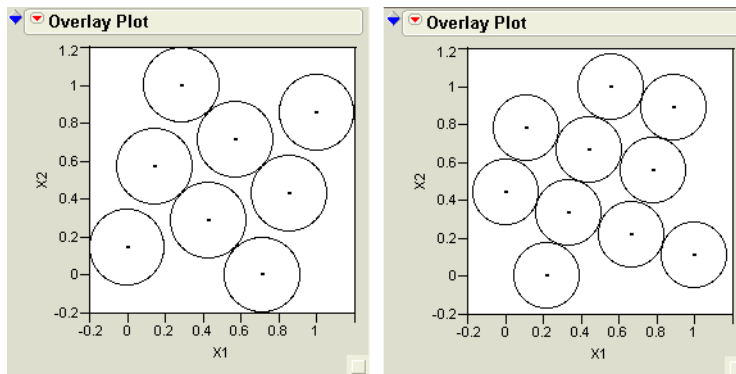
Note that the minimum distance between each pair of points in the Latin Hypercube design is smaller than that for the Sphere-Packing design. This is because the Latin Hypercube design constrains the levels of each factor to be evenly spaced. The Sphere-Packing design maximizes the minimum distance without any constraints.

Uniform Designs

The Uniform design minimizes the discrepancy between the design points (empirical uniform distribution) and a theoretical uniform distribution.

Note: These designs are most useful for getting a simple and precise estimate of the integral of an unknown function. The estimate is the average of the observed responses from the experiment.

1 Select **DOE > Space Filling Design**.
2 Enter responses, if necessary, and factors. (See "Enter Responses and Factors into the Custom Designer," p. 59.)
3 Alter the factor level values to 0 and 1.

4 Click **Continue.**

5 In the design specification dialog, specify a sample size. This example uses a sample size of eight (**Number of Runs**).

6 Click the **Uniform** button. JMP creates this design and displays the design runs and the design diagnostics as shown in Figure 9.9.

Note: The emphasis of the Uniform design method is not to spread out the points. The minimum distances in Figure 9.9 vary substantially.

Figure 9.9 Factor Settings and Diagnostics for Uniform Space-Filling Designs with Eight Runs

Run	X1	X2		Run	ScaledX1	ScaledX2	Minimum Distance	Nearest Point
1	0.43532	0.93541		1	0.43532	0.93541	0.284	3
2	0.56091	0.31491		2	0.56091	0.31491	0.352	6
3	0.69276	0.81486		3	0.69276	0.81486	0.277	7
4	0.18514	0.69286		4	0.18514	0.69286	0.285	5
5	0.06460	0.43504		5	0.06460	0.43504	0.285	4
6	0.30959	0.06908		6	0.30959	0.06908	0.352	2
7	0.81410	0.56557		7	0.81410	0.56557	0.277	3
8	0.92607	0.19080		8	0.92607	0.19080	0.386	2

Factor Settings | Design Diagnostics

discrepancy = 0.0046

7 Click **Make Table**.

A Uniform design does not guarantee even spacing of the factor levels. However, increasing the number of runs and running a distribution on each factor (use **Analyze** > **Distribution**) shows flat histograms.

Figure 9.10 Histograms are Flat for each Factor when Number of Runs is Increased to 20
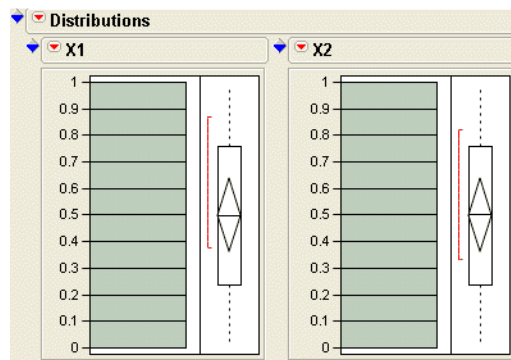
Comparing Sphere-Packing, Latin Hypercube, and Uniform Methods

To compare space-filling design methods, create the **Sphere Packing**, **Latin Hypercube**, and **Uniform** designs, as shown in the previous examples. The Design Diagnostics tables show the values for the factors scaled from zero to one. The minimum distance is based on these scaled values and is the mini-

mum distance from each point to its closest neighbor. The discrepancy value is the integrated difference between the design points and the uniform distribution.

Figure 9.11 shows a comparison of the design diagnostics for three eight-run space-filling designs. Note that the discrepancy for the Uniform design is the smallest (best). The discrepancy for the Sphere-Packing design is the largest (worst). The discrepancy for the Latin Hypercube takes an intermediate value that is closer to the optimal value.

Also note that the minimum distance between pairs of points is largest (best) for the Sphere-Packing method. The Uniform design has pairs of points that are only about half as far apart. The Latin Hypercube design behaves more like the Sphere-Packing design in spreading the points out.

For both spread and discrepancy, the Latin Hypercube design represents a healthy compromise solution.

Figure 9.11 Comparison of Diagnostics for Three Eight-Run Space-Filling Methods

Design Diagnostics - Sphere Packing

Run	ScaledX1	ScaledX2	Minimum Distance	Nearest Point
1	0.00000	1.00000	0.518	2
2	0.50000	0.86603	0.518	1
3	0.86603	0.50000	0.518	4
4	1.00000	1.00000	0.518	3
5	1.00000	0.00000	0.518	6
6	0.50000	0.13397	0.518	5
7	0.00000	0.00000	0.518	8
8	0.13397	0.50000	0.518	7

discrepancy = 0.0469

Sphere-Packing

Design Diagnostics - Latin Hypercube

Run	ScaledX1	ScaledX2	Minimum Distance	Nearest Point
1	0.57143	0.71429	0.404	6
2	0.85714	0.42857	0.404	1
3	1.00000	0.85714	0.452	1
4	0.00000	0.14286	0.452	5
5	0.42857	0.28571	0.404	7
6	0.28571	1.00000	0.404	1
7	0.14286	0.57143	0.404	5
8	0.71429	0.00000	0.404	5

discrepancy = 0.0092

Latin Hypercube

Design Diagnostics - Uniform

Run	ScaledX1	ScaledX2	Minimum Distance	Nearest Point
1	0.43909	0.68509	0.276	6
2	0.69031	0.93093	0.351	1
3	0.07393	0.19080	0.346	6
4	0.81410	0.56585	0.282	7
5	0.56496	0.06460	0.44	7
6	0.31491	0.43909	0.276	1
7	0.93092	0.30959	0.282	4
8	0.18696	0.81304	0.283	1

discrepancy = 0.0046

Uniform

Another point of comparison is the time it takes to compute a design. The Uniform design method requires the most time to compute. Also, the time to compute the design increases rapidly with the number of runs. For comparable problems, all the space-filling design methods take longer to compute than the *D*-optimal designs in the Custom Designer.

Minimum Potential Designs

The Minimum Potential design spreads points out inside a sphere. To understand how this design is created, imagine the points as electrons with springs attached to every other point, as illustrated to the right. The coulomb force pushes the points apart, but the springs pull them together. The design is the spacing of points that minimizes the potential energy of the system.
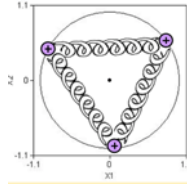
Minimum Potential designs:

- have spherical symmetry
- are nearly orthogonal
- have uniform spacing

To see a Minimum Potential example:

1 Select **DOE > Space Filling Design**.
2 Enter responses and factors. (See "Enter Responses and Factors into the Custom Designer," p. 59.)
3 Alter the factor level values to 0 and 1, if necessary.
4 Click **Continue.**
5 In the design specification dialog (shown on the left in Figure 9.12), enter a sample size (**Number of Runs**). This example uses a sample size of 12.
6 Click the **Minimum Potential** button. JMP creates this design and displays the design runs (shown on the right in Figure 9.12) and the design diagnostics.

Figure 9.12 Space-Filling Methods and Design Diagnostics for Minimum Potential Design

7 Click **Make Table**.

You can see the spherical symmetry of the Minimum Potential design using the Scatterplot 3D graphics platform.

1 After you make the JMP design table, choose the **Graph** > **Scatterplot 3D** command.

2 In the Scatterplot 3D launch dialog, select X1, X2, and X3 as **Y, Columns** and click **OK** to see the initial three dimensional scatterplot of the design points.

3 To see the results similar to those in Figure 9.13, double-click on the axes to scale them, and use the **Normal Contour Ellipsoids** option from the menu in the Scatterplot 3D title bar.

Now it is easy to see the points spread evenly on the surface of the ellipsoid.

Figure 9.13 Minimum Potential Design Points on Sphere
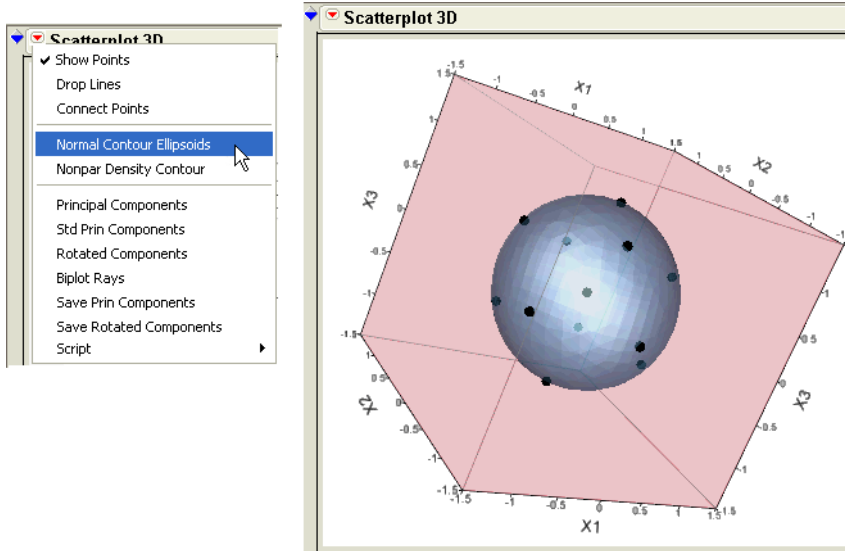
Maximum Entropy Designs

The Latin Hypercube design is currently the most popular design assuming you are going to analyze the data using a Gaussian-Process model. Computer simulation experts like to use the Latin Hypercube design because all its projections onto the coordinate axes are uniform.

However, as the example at the top in Figure 9.14 shows, the Latin Hypercube design does not necessarily do a great job of space filling. This is a two-factor Latin Hypercube with 16 runs. Note that this design appears to leave a hole in the bottom right of the overlay plot.

Figure 9.14 Two-factor Latin Hypercube Design

	X1	X2
1	-1	-0.8666667
2	0.06666667	-0.6
3	-0.2	0.33333333
4	-0.3333333	-0.2
5	0.33333333	0.46666667
6	0.2	-0.0666667
7	-0.0666667	0.86666667
8	-0.6	0.73333333
9	-0.7333333	0.2
10	0.6	-1
11	0.46666667	1
12	0.73333333	0.06666667
13	0.86666667	0.6
14	-0.4666667	-0.7333333
15	-0.8666667	-0.3333333
16	1	-0.4666667

Space Filling Latin Hypercub
Design Space Filling Latin Hype
Model
Overlay Plot

Columns (3/0)
X1 *
X2 *
Y *

Rows
All rows   16
Selected   0
Excluded   0

Overlay Plot

Note empty area in
Latin Hypercube design

The Maximum Entropy design is a competitor to the Latin Hypercube design for computer experiments because it optimizes a measure of the amount of information contained in an experiment. See the technical note below. The two-factor Maximum Entropy design shown in Figure 9.15 covers the region better than the Latin hypercube design in Figure 9.14. The space-filling property improves as the number of runs increases without bound.

Figure 9.15 Two-Factor Maximum Entropy Design

	X1	X2
1	0.75	1
2	-0.375	-1
3	1	-0.25
4	0.5	-0.5
5	0.5	0.125
6	-0.125	-0.375
7	-1	-0.875
8	1	-1
9	1	0.5
10	-0.25	1
11	0.25	0.625
12	0.25	-1
13	-1	1
14	-0.25	0.25
15	-1	0.375
16	-0.75	-0.25

Maximum Entropy
Design   Maximum Entropy
Model
Overlay Plot

Columns (3/0)
X1 *
X2 *
Y *

Rows
All rows   16
Selected   0
Excluded   0
Hidden   0
Labelled   0

Overlay Plot
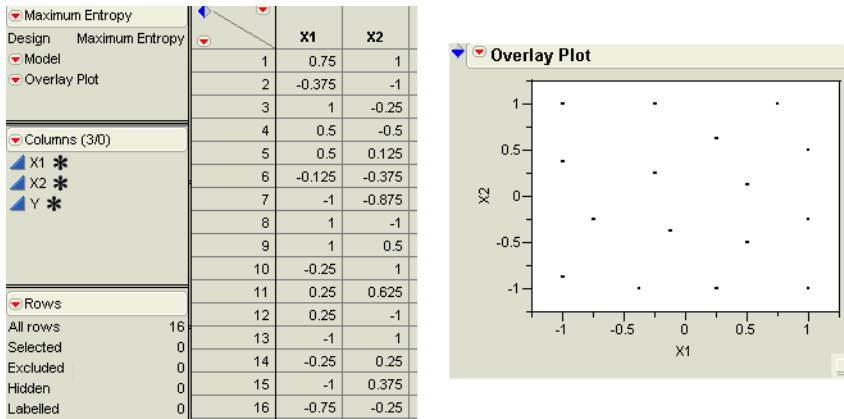
Technical Note: Maximum Entropy designs maximize the Shannon information (Shewry and Wynn (1987)) of an experiment, assuming that the data come from a normal $(m, s^2 R)$ distribution, where

$$R_{ij} = \exp\left(-\sum_k \theta_k (x_{ik} - x_{jk})^2\right)$$

is the correlation of response values at two different design points, x_i and x_j. Computationally, these designs maximize $|R|$, the determinant of the correlation matrix of the sample. When x_i and x_j are far apart, then R_{ij} approaches zero. When x_i and x_j are close together, then R_{ij} is near one.

Gaussian Process IMSE Optimal Designs

The Gaussian process IMSE optimal design is also a competitor to the Latin Hypercube design because it minimizes the integrated mean squared error of the Gaussian process model over the experimental region.

You can compare the IMSE optimal design to the Latin Hypercube (shown previously in Figure 9.14). The table and overlay plot in Figure 9.16 show a Gaussian IMSE optimal design. You can see that the design provides uniform coverage of the factor region.

Figure 9.16 Comparison of Two-factor Latin Hypercube and Gaussian IMSE Optimal Designs
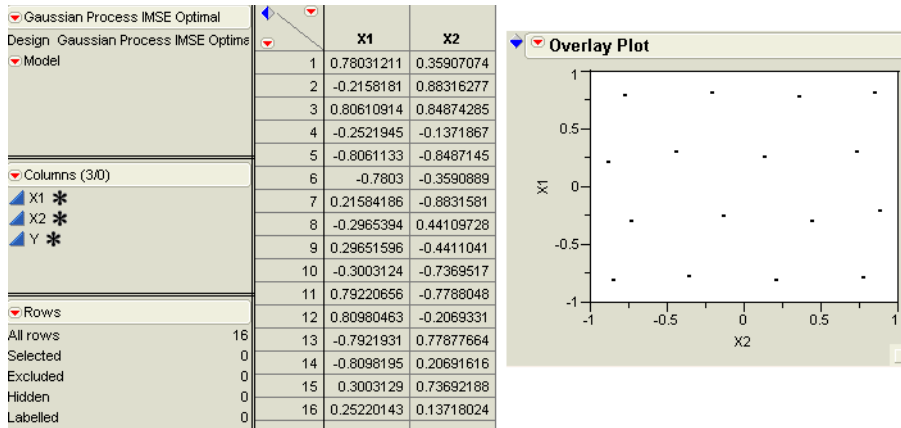
Note: Both the Maximum Entropy design and the Gaussian Process IMSE Optimal design were created using 100 random starts.

Borehole Model: A Sphere-Packing Example

Worley (1987) presented a model of the flow of water through a borehole that is drilled from the ground surface through two aquifers. The response variable y is the flow rate through the borehole in m^3/year and is determined by the equation

$$y = \frac{2\pi T_u (H_u - H_l)}{\ln(r/r_w)\left[1 + \dfrac{2LT_u}{\ln(r/r_w)r_w^2 K_w} + \dfrac{T_u}{T_l}\right]}$$

There are eight inputs to this model.

r_w = radius of borehole, 0.05 to 0.15 m

r = radius of influence, 100 to 50,000 m

T_u = transmissivity of upper aquifer, 63,070 to 115,600 m^2/year

H_u = potentiometric head of upper aquifer, 990 to 1100 m

T_l = transmissivity of lower aquifer, 63.1 to 116 m^2/year

H_l = potentiometric head of lower aquifer, 700 to 820 m

L = length of borehole, 1120 to 1680 m

K_w = hydraulic conductivity of borehole, 9855 to 12,045 m/year
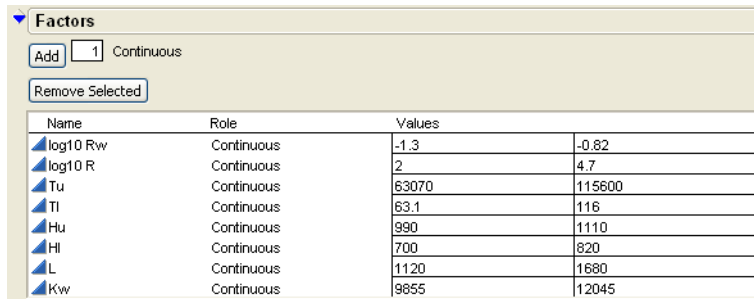
This example is atypical of most computer experiments because the response can be expressed as a simple, explicit function of the input variables. However, this simplicity is useful for explaining the design methods.

Create the Sphere-Packing Design for the Borehole Data

To create a Sphere-Packing design for the borehole problem:

1 Select **DOE > Space Filling Design**.
2 Click the red triangle icon on the Space Filling Design title bar and select **Load Factors**.
3 Open the Sample Data folder installed with JMP. In the DOE folder, open Borehole Factors.jmp from the Design Experiment folder to load the factors (Figure 9.17).

Figure 9.17 Factors Panel with Factor Values Loaded for Borehole Example

Name	Role	Values	
log10 Rw	Continuous	-1.3	-0.82
log10 R	Continuous	2	4.7
Tu	Continuous	63070	115600
Tl	Continuous	63.1	116
Hu	Continuous	990	1110
Hl	Continuous	700	820
L	Continuous	1120	1680
Kw	Continuous	9855	12045

Note: The logarithm of r and r_w are used in the following discussion.

4 Click **Continue**.
5 Specify a sample size of 32 runs, as shown in Figure 9.18.

Figure 9.18 Space-Filling Design Method Panel Showing 32 Runs
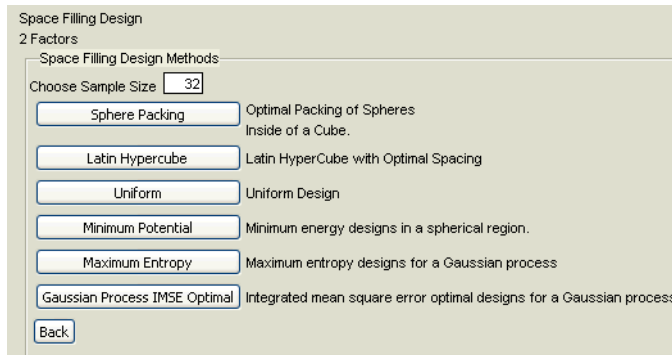
6 Click the **Sphere Packing** button to produce the design.

7 Click **Make Table** to make a table showing the design settings for the experiment. The factor set-
   tings in the example table might not have the same ones you see when generating the design because
   the designs are generated from a random seed.

8 To see a completed data table for this example, open Borehole Sphere Packing.jmp (Figure 9.19)
   from the Design Experiment Sample Data folder installed with JMP. This table also has a table vari-
   able that contains a script to analyze the data. The results of the analysis are saved as columns in the
   table.

Figure 9.19 Borehole Sample Data

Guidelines for the Analysis of Deterministic Data

It is important to remember that deterministic data has no random component. As a result, p-values
from fitted statistical models do not have their usual meanings. A large F statistic (low p-value) is an
indication of an effect due to a model term. However, you cannot make valid confidence intervals
about the size of the effects or about predictions made using the model.

Residuals from any model fit to deterministic data are not a measure of noise. Instead, a residual shows the model bias for the current model at the current point. Distinct patterns in the residuals indicate new terms to add to the model to reduce model bias.

Results of the Borehole Experiment

The example described in the previous sections produced the following results:

- A stepwise regression of the response, log y, versus the full quadratic model in the eight factors, led to the prediction formula column.
- The prediction bias column is the difference between the true model column and the prediction formula column.
- The prediction bias is relatively small for each of the experimental points. This indicates that the model fits the data well.

In real world examples, the true model is generally not available in a simple analytical form. As a result, it is impossible to know the prediction bias at points other than the observed data without doing additional runs.

In this case, the true model column contains a formula that allows profiling the prediction bias to find its value anywhere in the region of the data. To understand the prediction bias in this example:

1 Select **Graph > Profiler**.
2 Highlight the prediction bias column and click the **Y, Prediction Formula** button.
3 Check the **Expand Intermediate Formulas** box, as shown at the bottom on the Profiler dialog in Figure 9.20, because the prediction bias formula is a function of columns that are also created by formulas.
4 Click **OK**.

The profile plots at the bottom in Figure 9.20 show the prediction bias at the center of the design region. If there were no bias, the profile traces would be constant between the value ranges of each factor. In this example, the variables Hu and Hl show nonlinear effects.

Figure 9.20 Profiler Dialog and Profile of the Prediction Bias in the Borehole Sphere-Packing Data
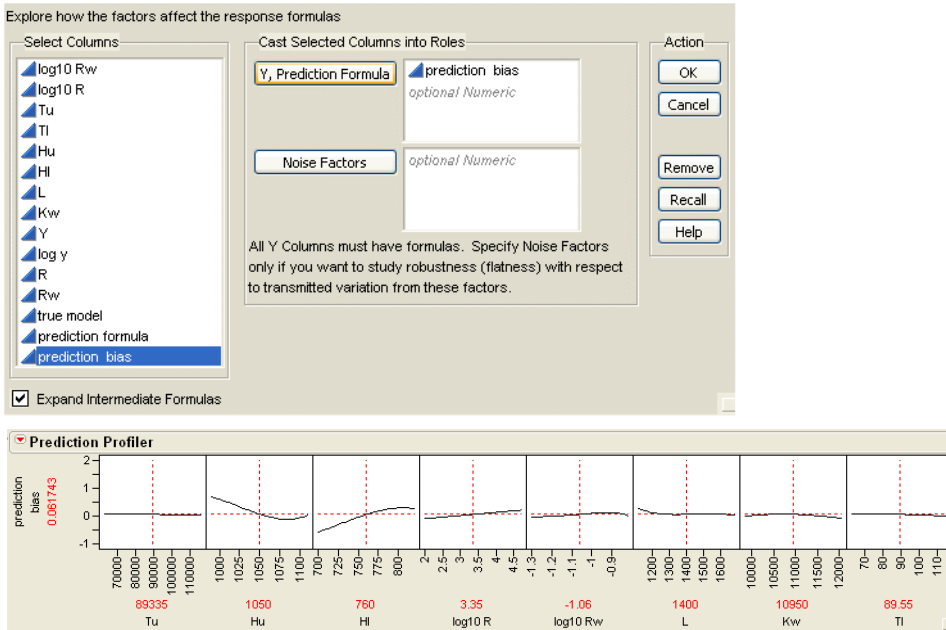
The range of the prediction bias on the data is smaller than the range of the prediction bias over the entire domain of interest. To see this, look at the distribution analysis (**Analyze > Distribution**) of the prediction bias in Figure 9.21. Note that the maximum bias is 1.826 and the minimum is –0.684 (the range is 2.51).

Figure 9.21 Distribution of the Prediction Bias
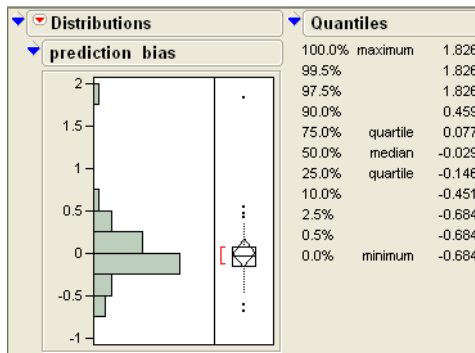
The top plot in Figure 9.22 shows the maximum bias (2.91) over the entire domain of the factors. The plot at the bottom shows the comparable minimum bias (–4.84). This gives a range of 7.75. This is more than three times the size of the range over the observed data.

Figure 9.22 Prediction Plots showing Maximum and Minimum Bias Over Factor Domains
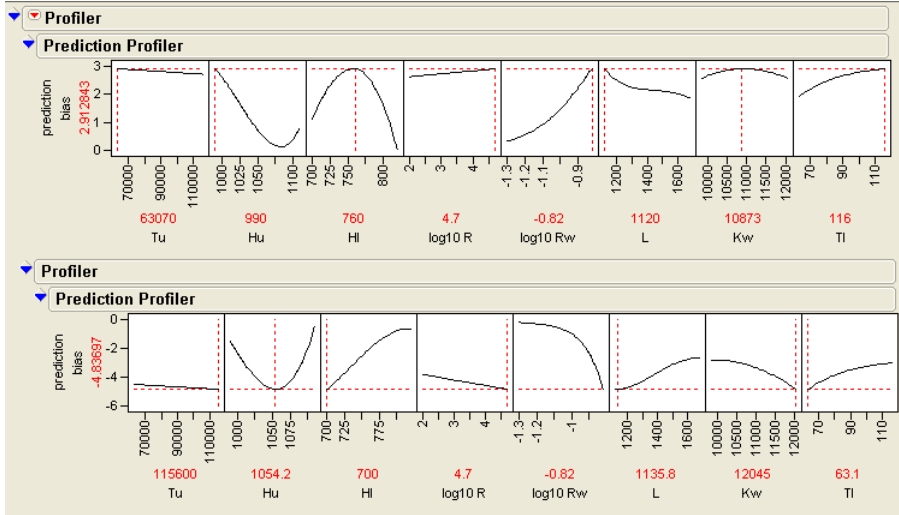
Keep in mind that, in this example, the true model is known. In any meaningful application, the response at any factor setting is unknown. The prediction bias over the experimental data underestimates the bias throughout the design domain.

There are two ways to assess the extent of this underestimation:

- Cross-validation refits the data to the model while holding back a subset of the points and looks at the error in estimating those points.
- Verification runs (new runs performed) at different settings to assess the lack of fit of the empirical model.

Chapter **10**

Nonlinear Designs
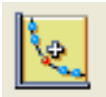
Design of experiments with models that are nonlinear in their parameters is available using either the DOE menu or the JMP Starter DOE category, as shown below.

Nonlinear designs offer both advantages and disadvantages compared to designs for linear models.

On the positive side, predictions using a well chosen model are likely to be good over a wider range of factor settings. It is also possible to model response surfaces with more curvature and with asymptotic behavior.

On the negative side, the researcher needs a greater understanding of both the system and of the nonlinear design tool.
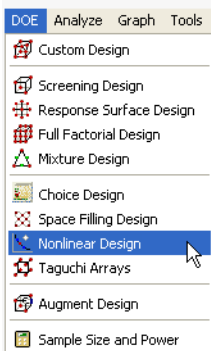
DOE Menu   **JMP Starter**
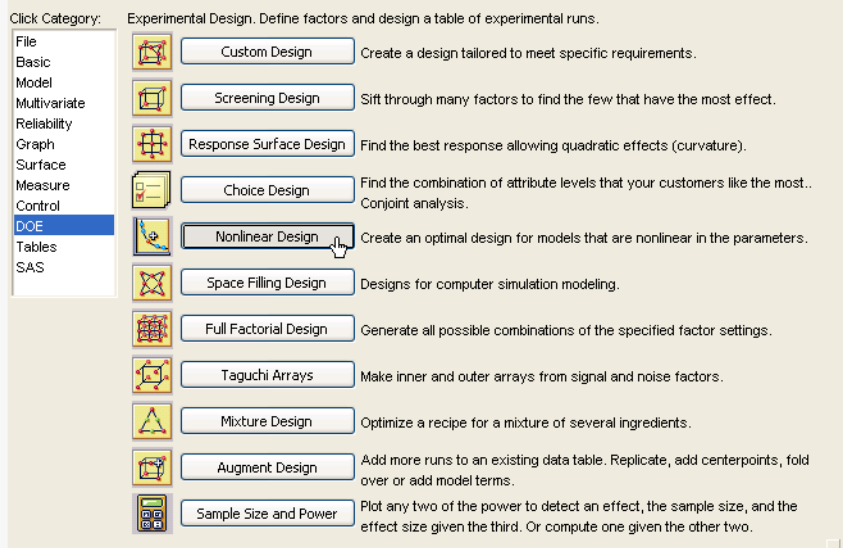
Contents

Examples of Nonlinear Designs

The Nonlinear Designer allows scientists to generate optimal designs and optimally augment data for fitting models that are nonlinear in their parameters. Such models, when they are descriptive of the underlying process, can yield more accurate prediction of process behavior than is possible with the standard polynomial models.

To use the Nonlinear Designer, you first need a data table that has

- one column for each factor
- one column for the response
- a column that contains a formula showing the functional relationship between the factor(s) and the response.

This is the same format for a table you would supply to the nonlinear platform for modeling.

The first example in this section describes how to approach creating a nonlinear design when there is prior data. The second example describes how to approach creating the design without data, but with reasonable starting values for the parameter estimates.

Using Nonlinear Fit to Find Prior Parameter Estimates

Suppose you have already collected experimental data and placed it in a JMP data table. That table can be used to create a nonlinear design for improving the estimates of the model's parameters.

To follow along with this example, open Chemical Kinetics.jmp from the Nonlinear Examples folder found in the sample data installed with JMP.

Chemical Kinetics.jmp (Figure 10.1) contains a column (Model (x))whose values are formed by a formula with a poor guess of the parameter values.

Figure 10.1 Chemical Kinetics.jmp

First, fit the data to the model using nonlinear least squares to get better parameter values.

1. Select **Analyze > Modeling > Nonlinear**.
2. Select Velocity (y) and click **Y, Response** on the nonlinear launch dialog.
3. Select Model (x) and click **X, Predictor Formula** (see Figure 10.2). Note that the formula given by Model (X) shows in the launch dialog.

Figure 10.2 Initial Nonlinear Analysis Launch Dialog
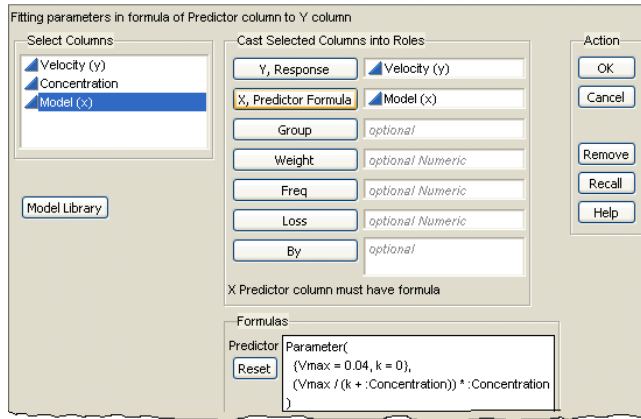
4 Click **OK** on the launch dialog to see the Nonlinear control panel.

5 Click the **Go** button on the Nonlinear control panel to see the results (Figure 10.3).

Figure 10.3 Nonlinear Fit Results
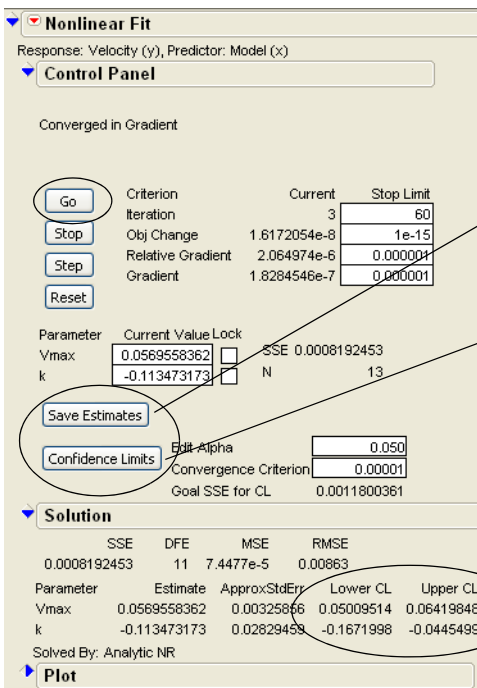
The **Save Estimates** button adds the new fitted parameter values in the Model (x) column in the Chemical Kinetics.jmp data table.

The **Confidence Limits** button computes confidence intervals used to create a nonlinear design.

These ranges are the intervals for **Vmax** and **k**. They are asymptotically normal. Use these limits to create a nonlinear design in JMP.

6 Click the **Confidence Limits** button to produce confidence intervals.

7 Click **Save Estimates** to add the new fitted parameter values in the Model (x) column in the Chemical Kinetics.jmp data table, which contains the formula:

$$\frac{Vmax}{\left(k + Concentration \right)} * Concentration$$

Note: Leave the nonlinear analysis report open because these results are needed in the DOE nonlinear design dialog described next.

Now create a design for fitting the model's nonlinear parameters.

1 With the Chemical Kinetics.jmp data table open, select **DOE > Nonlinear Design**.

2 Complete the launch dialog the same way as the Nonlinear Analysis launch dialog shown previously. That is, Select Velocity (y) and click **Y, Response**. Select Model (x) and click the **X, Predictor Formula**. Figure 10.4 shows the completed dialog.

Figure 10.4 Initial Nonlinear Design Launch Dialog
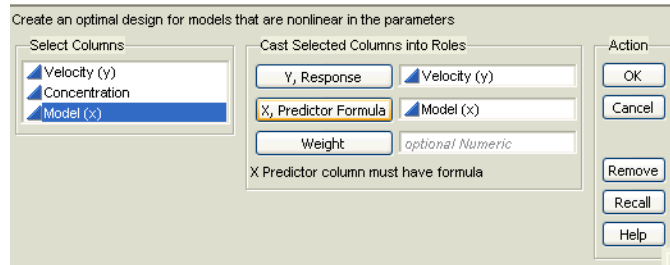
3 Click **OK** to see the completed Design panels for factors and parameters, as shown in Figure 10.5.

Figure 10.5 Nonlinear Design Panels for Factors and Parameters
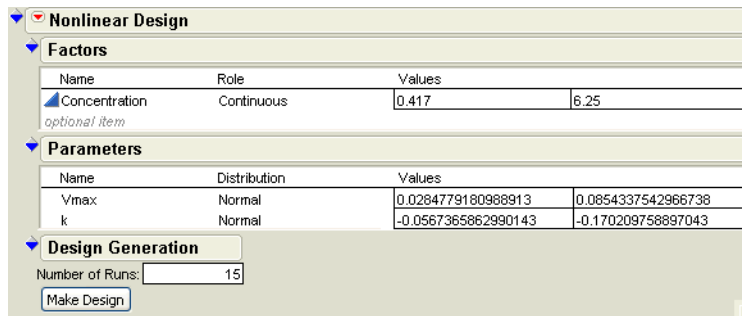
Note that in Chemical Kinetics.jmp (Figure 10.1), the range of data for Concentration goes from 0.417 to 6.25. Therefore, these values initially appear as the high and low values in the Factors control panel as follows:

4 Change the factor range for Concentration to a broader interval—from 0.1 to 7 (Figure 10.6).

Note that the *a priori* distribution of the parameters Vmax and k is Normal, which is correct for this example. Change the current level of uncertainty in the two parameters using the analysis results.

5 Look back at the analysis report inFigure 10.3 and locate the upper and lower confidence limits for Vmax and k in the Solution table. Change the values for Vmax and k to correspond to those limits, as shown in Figure 10.6.

Now you have described the current level of uncertainty of the two parameters.

Figure 10.6 Change Values for Factor and Parameters

6   If necessary, type the desired number of runs (15) into the text box.

Use commands from the menu on the Nonlinear Design title bar to get the best possible design:

7   Select **Number of Starts** from the menu on the title bar and enter 100 in the text box.

8   Select **Advanced Options** > **Number of Monte Carlo Samples** and enter 2 in the text box.

9   Click **Make Design** to preview the design (Figure 10.7). Your results may differ slightly than those shown for the additional runs.

Figure 10.7 Selecting the Number of Runs

10 Click **Make Table**.

This creates a new JMP design table (Figure 10.8) whose rows are the runs defined by the nonlinear design.

Note: This example creates a new table to avoid altering the sample data table Chemical Kinetics.jmp. In most cases, however, you can augment the original table using the **Augment Table** option in the Nonlinear Designer instead of making a new table. This option adds the new runs shown in the Design to the existing data table.

Figure 10.8 Making a Table with the Nonlinear Designer

The new runs use the wider interval of allowed concentration, which leads to more precise estimates of k and Vmax.

Creating a Nonlinear Design with No Prior Data

This next example describes how to create a design when you have not yet collected data, but have a guess for the unknown parameters.

To follow along with this example, open Reaction Kinetics Start.jmp, found in the Design Experiment folder in the sample data installed with JMP. Notice that the table is a template. That is, the table has columns with properties and formulas, but there are no observations in the table. The design has not yet been created and data has not been collected.

This table is used to supply the formula in the yield model column to the Nonlinear DOE platform. The formula is used to create a nonlinear design for fitting the model's nonlinear parameters. The formula looks like this:

$$100 * \frac{\mathrm{Exp}\left[t1 - \dfrac{1.9279 * 10^4}{Reaction\ Temperature}\right] * \left[\mathrm{Exp}\left[-\mathrm{Exp}\left[t1 - \dfrac{1.9279 * 10^4}{Reaction\ Temperature}\right] * Reaction\ Time\right] - \mathrm{Exp}\left[-\mathrm{Exp}\left[t3 - \dfrac{1.6819 * 10^4}{Reaction\ Temperature}\right] * Reaction\ Time\right]\right]}{\left[\mathrm{Exp}\left[t3 - \dfrac{1.6819 * 10^4}{Reaction\ Temperature}\right] - \mathrm{Exp}\left[t1 - \dfrac{1.9279 * 10^4}{Reaction\ Temperature}\right]\right]}$$

This model is from Box and Draper (1987). The formula arises from the fractional yield of the intermediate product in a consecutive chemical reaction. It is written as a function of time and temperature.

1 With the Reaction Kinetics Start.jmp data table open, select **DOE > Nonlinear Design** to see the initial launch dialog.

2 Select observed yield and click **Y, Response**.

3 Select yield model (the column with the formula) and click **X, Predictor Formula**.

The completed dialog should look like the one in Figure 10.9.

Figure 10.9 Nonlinear Design launch Dialog
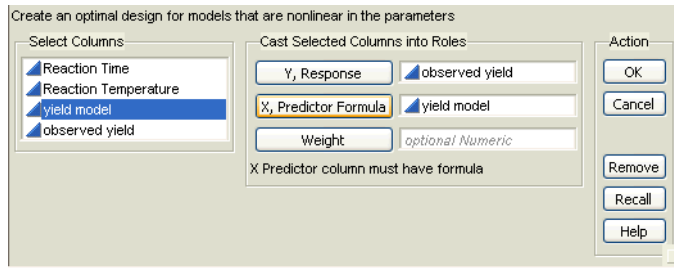
4 Click **OK** to see the nonlinear design Factors and Parameters panels in Figure 10.10.

5 Change the two factors' values to be a reasonable range of values. (In your experiment, these values might have to be an educated guess.) For this example, use the values 510 and 540 for Reaction Temperature. Use the values 0.1 and 0.3 for Reaction Time.

6 Change the values of the parameter t1 to 25 and 50, and t3 to 30 and 35.

7 Click on the Distribution of each parameter and select **Uniform** from the menu to change the distribution from the default **Normal** (see Figure 10.10).

8 Change the number of runs to 12 in the Design Generation panel.

Figure 10.10 Change Factor Values, Parameter Distributions, and Number of Runs
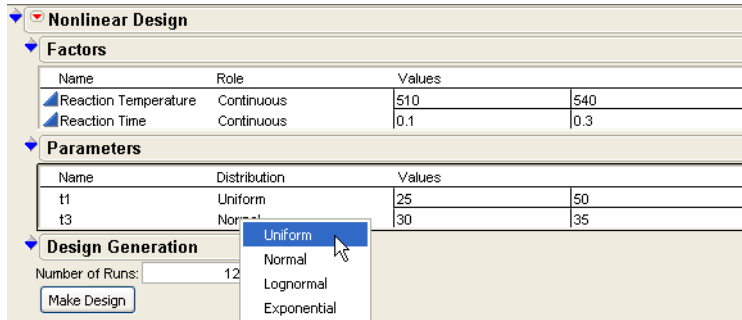
9 Click **Make Design**, then **Make Table**. Your results should look similar to those in Figure 10.11.

Figure 10.11 Design Table

10 To analyze data that contains values for the response, observed yield, open Reaction Kinetics.jmp

from the Design Experiment folder in the sample data installed with JMP (Figure 10.12).

11 To analyze data that contains values for the response, observed yield, open Reaction Kinetics.jmp from the Design Experiment folder in the sample data installed with JMP (Figure 10.12).

Figure 10.12 Reaction Kinetics.jmp

First, examine the design region with an overlay plot.

12 Selecting **Graph > Overlay Plot**.

13 Select Reaction Temperature and click **Y**

14 Select Reaction Time and click **X** as shown in the Overlay Plot launch dialog in Figure 10.13.

15 Click **OK** to see the overlay plot in Figure 10.13.

Figure 10.13 Create an Overlay Plot
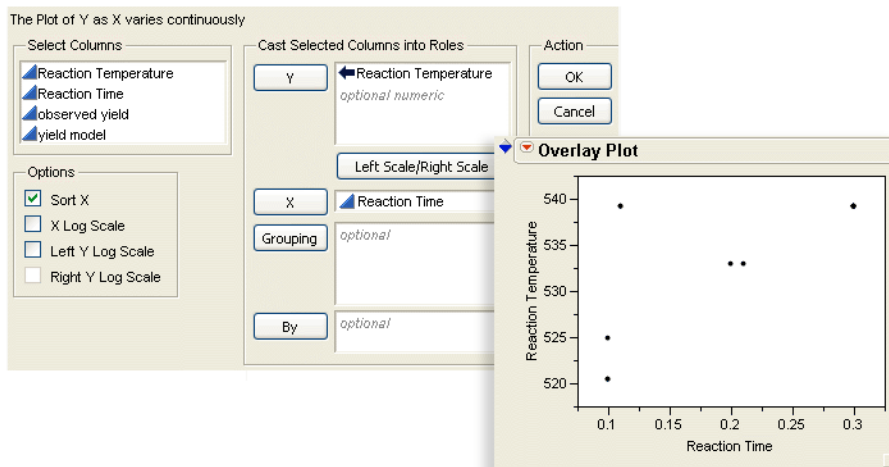
Notice that the points are not at the corners of the design region. In particular, there are no points at low temperature and high time—the lower right corner of the graph.

16 Select **Analyze > Modeling > Nonlinear**.

17 Select observed yield and click **Y, Response**.

18 Select yield model and click the **X, Predictor Formula**, then click **OK**.

19 Click **Go** on the Nonlinear control panel.

20 Now, choose **Profilers > Profiler** from the red triangle menu on the Nonlinear Fit title bar.

21 To maximize the yield, choose **Maximize Desirability** from the red triangle menu on the Prediction Profiler title bar.

The maximum yield is approximately 63.5% at a reaction temperature of 540 degrees Kelvin and a reaction time of 0.1945 minutes.

Figure 10.14 Time and Temperature Settings for Maximum Yield
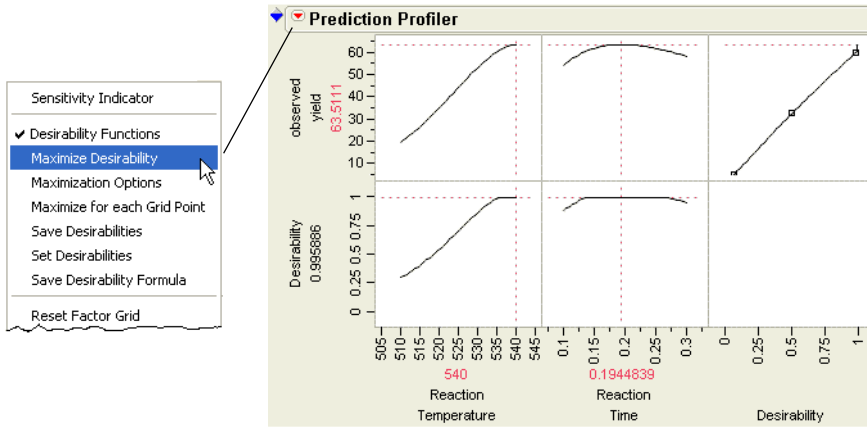
Creating a Nonlinear Design

To begin, open a data table that has a column whose values are formed by a formula (for details about formulas, see the *JMP User Guide*). This formula must have parameters.

Select **DOE >Nonlinear Design**, or click the **Nonlinear Design** button on the JMP Starter **DOE** page. Then, follow the steps below:

- "Identify the Response and Factor Column with Formula," p. 208
- "Set Up Factors and Parameters in the Nonlinear Design Dialog," p. 209
- "Enter the Number of Runs and Preview the Design," p. 210
- "Make Table or Augment the Table," p. 211

Identify the Response and Factor Column with Formula

1 Open a data table that contains a column whose values are formed by a formula that has parameters. This example uses **Corn.jmp** from the **Nonlinear Examples** folder in the sample data installed with JMP.

2 Select **DOE > Nonlinear Design** to see the initial launch dialog.

3 Select yield and click **Y, Response**. The response column cannot have missing values.

4 Select quad and click **X, Predictor Formula**. The quad variable has a formula that includes **nitrate** and three parameters (Figure 10.15).

5 Click **OK** on the launch dialog to see the Nonlinear Design DOE panels.

Figure 10.15 Identify Response (Y) and the Column with the Nonlinear Formula (X)
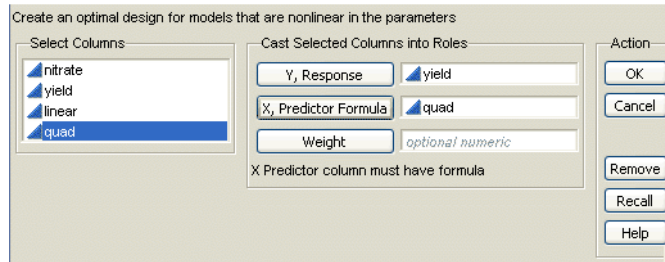
Set Up Factors and Parameters in the Nonlinear Design Dialog

First, look at the formula for quad, shown in Figure 10.16, and notice there are three parameters. These parameters show in the Parameters panel of the Nonlinear design dialog, with initial parameter values.

Figure 10.16 Formula for quad has Parameters a, b, and c

Use Figure 10.17 to understand how to set up factor and parameter names and values.

- The initial values for the factor and the parameters are reasonable and do not need to be changed.
- If necessary, change the Distribution of the parameters to Uniform, as shown in Figure 10.17.

Figure 10.17 Example of Setting Up Factors and Parameters

Double-click to edit the factor
or parameter name.

Click to enter or change factor values.

Click to edit the distribution: Uniform,
Normal, Lognormal, or Exponential.
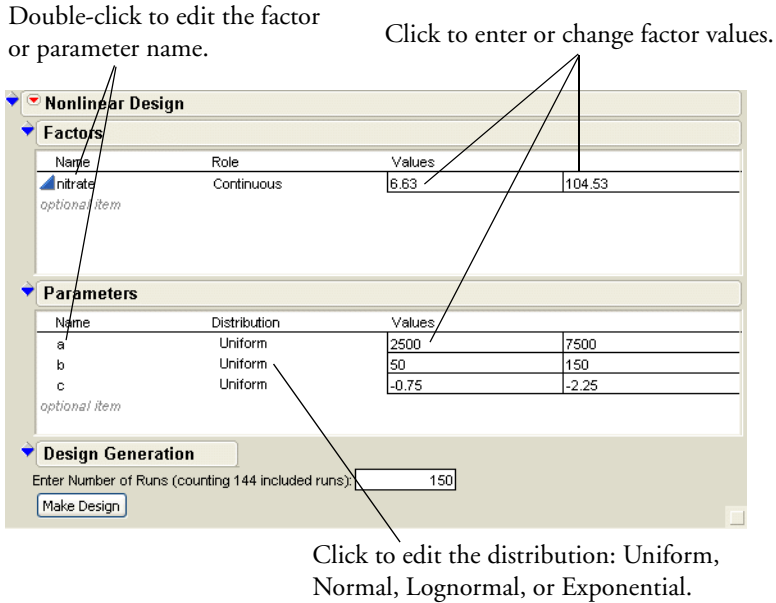
Enter the Number of Runs and Preview the Design

1 The Design Generation panel shows a default number of runs needed to perform the experiment. This example needs one run for each observation (144) plus three additional runs for the three parameters giving 147 as a total minimum number of runs. Enter 147 in the Number of Runs edit box.

2 Click **Make Design** before creating the data table to preview the design. Figure 10.18 shows a partial listing of the design.

Figure 10.18 Example Preview Design

Make Table or Augment the Table

3 The last step is to click either **Make Table** or **Augment Table**. The **Make Table** command creates a new table (Figure 10.19) with all runs included. The **Augment Table** command adds the new runs to the existing table.

Figure 10.19 Partial Listing of an Example Nonlinear Design Table

Advanced Options for the Nonlinear Designer

For advanced users, the Nonlinear Designer has the two additional options, as shown in Figure 10.20. These advanced options are included because finding nonlinear DOE solutions involves minimizing the integral of the log of the determinant of the Fisher information matrix with respect to the prior distribution of the parameters. These integrals are complicated and have to be calculated numerically.

The way the integration is done for Normal distribution priors uses a numerical integration technique where the integral is reparameterized into a radial direction, and the number of parameters minus one

angular directions. The radial part of the integral is handled using Radau-Gauss-Laguerre quadrature with an evaluation at radius=0. A randomized Mysovskikh quadrature is used to calculate the integral over the spherical part, which is equivalent to integrating over the surface of a hypersphere.

Note: If some of the prior distributions are not Normal, then the integral is reparameterized so that the new parameters have normal distribution, and then the radial-spherical integration method is applied. However, if the prior distribution set for the parameters does not lend itself to a solution, sometimes the process fails and gives the message that the Fisher information is singular in a region of the parameter space, and advises changing the prior distribution or the ranges of the parameters.

Figure 10.20 Advanced Options for the Nonlinear Designer
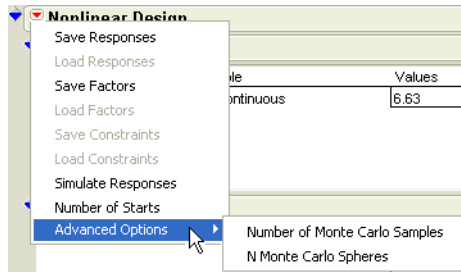
The following is a technical description for these two advanced options:

> **Number of Monte Carlo Samples**   sets the number of octahedra per sphere. Because each octahedron is a fixed unit, this option can be thought of as setting the number of octahedra per sphere.

> **N Monte Carlo Spheres**   are the number of nonzero radius values used. The default is two spheres and one center point. Each radial value requires integration over the angular dimensions. This is done by constructing a certain number of hyperoctahedra (the generalization of an octagon in arbitrary dimensions), and randomly rotating each of them.

Technical Note: The reason for the approach given by these advanced options is to get good integral approximations much faster than using standard methods. For instance, with six parameters, using two radii and one sample per sphere, these methods give a generalized five-point rule that needs only 113 observations to get a good approximation. Using the most common approach (Simpson's rule) would need $5^6 = 15,625$ evaluations. The straight Monte Carlo approach also requires thousands of function evaluations to get the same level of quality in the answer.

Keep in mind that if the number of radii is set to zero, then just the center point is used, which gives a local design that is optimal for a particular value of the parameters. For some people this is good enough for their purposes. These designs are created much faster than if the integration is performed.

Chapter 11

Taguchi Designs

Quality was the watchword of 1980s, and Genichi Taguchi was a leader in the growth of quality consciousness. One of Taguchi's technical contributions to the field of quality control was a new approach to industrial experimentation. The purpose of the *Taguchi method* was to develop products that worked well in spite of natural variation in materials, operators, suppliers, and environmental change. This is *robust* engineering.

Much of the Taguchi method is traditional. His *orthogonal arrays* are two-level, three-level, and mixed-level fractional factorial designs. The unique aspects of his approach are the use of *signal* and *noise* factors, *inner* and *outer arrays*, and *signal-to-noise ratios*.

The goal of the Taguchi method is to find control factor settings that generate acceptable responses despite natural environmental and process variability. In each experiment, Taguchi's design approach employs two designs called the *inner* and *outer* array. The Taguchi experiment is the cross product of these two arrays. The *control* factors, used to tweak the process, form the inner array. The *noise* factors, associated with process or environmental variability, form the outer array. Taguchi's *signal-to-noise ratios* are functions of the observed responses over an outer array. The Taguchi designer supports all these features of the Taguchi method. You choose from inner and outer array designs, which use the traditional Taguchi orthogonal arrays, such as L4, L8, and L16.

Dividing system variables according to their signal and noise factors is a key ingredient in robust engineering. Signal factors are system control inputs. Noise factors are variables that are typically difficult or expensive to control.

The inner array is a design in the signal factors and the outer array is a design in the noise factors. A signal-to-noise ratio is a statistic calculated over an entire outer array. Its formula depends on whether the experimental goal is to maximize, minimize or match a target value of the quality characteristic of interest.

A Taguchi experiment repeats the outer array design for each run of the inner array. The response variable in the data analysis is not the raw response or quality characteristic; it is the signal-to-noise ratio.

The **Taguchi** designer in JMP supports signal and noise factors, inner and outer arrays, and signal-to-noise ratios as Taguchi specifies.

Contents

The Taguchi Design Approach

The Taguchi method defines two types of factors: control factors and noise factors. An *inner* design constructed over the control factors finds optimum settings. An *outer* design over the noise factors looks at how the response behaves for a wide range of noise conditions. The experiment is performed on all combinations of the inner and outer design runs. A performance statistic is calculated across the outer runs for each inner run. This becomes the response for a fit across the inner design runs. The table below lists the recommended performance statistics.

Table 11.1

Goal	S/N Ratio Formula
nominal is best	$\dfrac{S}{N} = 10\log\!\left(\dfrac{\bar{Y}^2}{s^2}\right)$
larger-is-better (maximize)	$\dfrac{S}{N} = -10\log\!\left(\dfrac{1}{n}\sum_i \dfrac{1}{Y_i^2}\right)$
smaller-is-better (minimize)	$\dfrac{S}{N} = -10\log\!\left(\dfrac{1}{n}\sum_i Y_i^2\right)$

Taguchi Design Example

The following example is an experiment done at Baylock Manufacturing Corporation and described by Byrne and Taguchi (1986). The objective of the experiment is to find settings of predetermined control factors that simultaneously maximize the adhesiveness (pull-off force) and minimize the assembly costs of nylon tubing.

To follow along with this example, open the Byrne Taguchi Data.jmp table found in the Design Experiment folder of the Sample Data installed with JMP. Or, generate the original design table on your own using **DOE > Taguchi Arrays**.

The signal and noise factors in the Byrne Taguchi Data for this example appear in the table below.

Table 11.2

Factor Name	Type	Levels	Comment
Interfer	control	3	tubing and connector interference
Wall	control	3	the wall thickness of the connector
Depth	control	3	insertion depth of the tubing into the connector
Adhesive	control	3	percent adhesive
Time	noise	2	the conditioning time
Temperature	noise	2	temperature
Humidity	noise	2	the relative humidity

To start this example:

1 Select **DOE > Taguchi**.

2 Click the red triangle icon on the Taguchi Design title bar and select **Load Factors**.

3 When the Open File dialog appears, open the factors table, Byrne Taguchi Factors.jmp found in the Design Experiment Sample Data folder installed with JMP.

The factors panel then shows the four three-level control (signal) factors and three noise factors, as shown in Figure 11.1.

Figure 11.1 Response, and Signal and Noise Factors for the Byrne-Taguchi Example
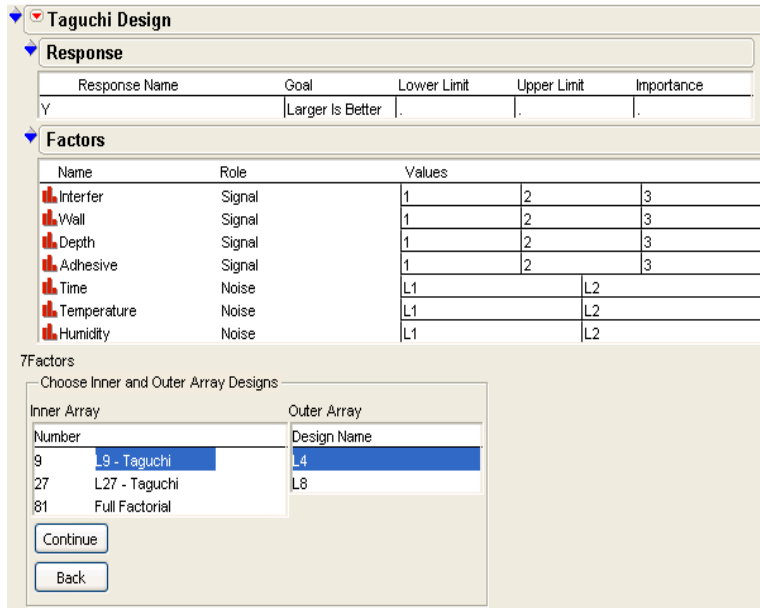
4 Highlight **L9-Taguchi** to give the L9 orthogonal array for the inner design.

5 Highlight **L8** to give an eight-run outer array design.

6 Click **Continue**.

The outer design has three two-level factors. A full factorial in eight runs is generated. However, it is only used as a guide to identify a new set of eight columns in the final JMP data table—one for each combination of levels in the outer design.

7 Click **Make Table** to create the design table shown in Figure 11.2.

Figure 11.2 Taguchi Design Before Data Entry

	Interfer	Wall	Depth	Adhesive	Pattern	---	--+	-+-	-++	+--	+-+	++-	+++	Mean	SN Ratio
1	1	1	1	1	----	.	.	.	.	.	.	.	.	.	.
2	1	2	2	2	-000	.	.	.	.	.	.	.	.	.	.
3	1	3	3	3	-+++	.	.	.	.	.	.	.	.	.	.
4	2	1	2	3	0-0+	.	.	.	.	.	.	.	.	.	.
5	2	2	3	1	00+-	.	.	.	.	.	.	.	.	.	.
6	2	3	1	2	0+-0	.	.	.	.	.	.	.	.	.	.
7	3	1	3	2	+-+0	.	.	.	.	.	.	.	.	.	.
8	3	2	1	3	+0-+	.	.	.	.	.	.	.	.	.	.
9	3	3	2	1	++0-	.	.	.	.	.	.	.	.	.	.

Now suppose the pull-off adhesive force measures are collected and entered into the columns containing missing data, as shown in Figure 11.3. The missing data column names are appended with the letter **Y** before the levels (+ or –) of the noise factors for that run. For example, **Y---** is the column of measurements taken with the three noise factors set at their low levels.

8   To see the completed experiment, open the data table, Byrne Taguchi Data.jmp found in the Design Experiment Sample Data folder installed with JMP. Figure 11.3 shows the completed design.

Figure 11.3 Complete Taguchi Design Table (Byrne Taguchi Data.jmp)

	Interfer	Wall	Depth	Adhesive	Pattern	Y---	Y--+	Y-+-	Y-++	Y+--	Y+-+	Y++-	Y+++	Mean Y	SN Ratio Y
1	1	1	1	1	----	15.6	9.5	16.9	19.9	19.6	19.6	20	19.1	17.525	24.02534
2	1	2	2	2	-000	15	16.2	19.4	19.6	19.7	19.8	24.2	21.9	19.475	25.52164
3	1	3	3	3	-+++	16.3	16.7	19.1	15.6	22.6	18.2	23.3	20.4	19.025	25.33476
4	2	1	2	3	0-0+	18.3	17.4	18.9	18.6	21	18.9	23.2	24.7	20.125	25.90425
5	2	2	3	1	00+-	19.7	18.6	19.4	25.1	25.6	21.4	27.5	25.3	22.825	26.90753
6	2	3	1	2	0+-0	16.2	16.3	20	19.8	14.7	19.6	22.5	24.7	19.225	25.32574
7	3	1	3	2	+-+0	16.4	19.1	18.4	23.6	16.8	18.6	24.3	21.6	19.85	25.71081
8	3	2	1	3	+0-+	14.2	15.6	15.1	16.8	17.8	19.6	23.2	24.4	18.3375	24.83231
9	3	3	2	1	++0-	16.1	19.9	19.3	17.3	23.1	22.7	22.6	28.6	21.2	26.15198

The column named **SN Ratio Y** is the performance statistic computed with the formula shown below. In this case, it is the "larger-the-better" (LTB) formula, which is –10 times the common logarithm of the average squared reciprocal:

$$-10 Log10 \left[Mean \left[\frac{1}{(Y---)^2}, \frac{1}{(Y--+)^2}, \frac{1}{(Y-+-)^2}, \frac{1}{(Y-++}^2}, \frac{1}{(Y+--)^2}, \right. \right.$$

$$\left. \left. \frac{1}{(Y+-+)^2}, \frac{1}{(Y++-)^2}, \frac{1}{(Y+++)^2} \right] \right]$$

This expression is large when all of the individual *y* values are small.

Analyze the Data

The data in Byrne Taguchi Data.jmp are now ready to analyze. The goal of the analysis is to find factor settings that maximize both the mean and the signal-to-noise ratio.

1 Click the red triangle icon next to Model on the upper left of the data table and select **Run Script**.

The Model script produces the Fit Model dialog shown in Figure 11.4.

The Fit Model dialog that appears automatically has the appropriate effects. It includes the main effects of the four signal factors. The two responses are the mean (Mean Y) and signal-to-noise ratio (SN Ratio Y) over the outer array.

Figure 11.4 Fit Model Dialog for Taguchi Data
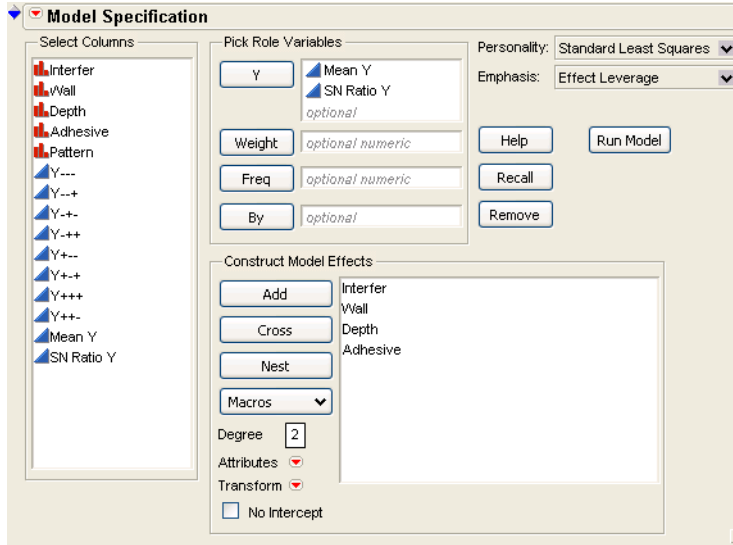
2 Click **Run Model** on the Fit Model dialog.

The prediction profiler is a quick way to find settings that give the highest signal-to-noise ratio for this experiment.

3 To open the Prediction Profiler, click the red triangle on the Response Mean Y title bar and select **Factor Profiling > Profiler**.

The profile traces (Figure 11.5) indicate that different settings of the first three factors would increase SN Ratio Y.

Figure 11.5 The Prediction Profiler
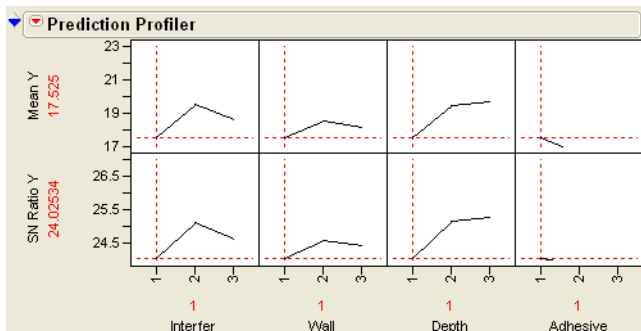
4 To find optimal settings, click the red triangle on the Prediction Profiler title bar and select **Desirability Functions**. This adds the row of traces and a column of function settings to the pro-

filer, as shown in Figure 11.6. The default desirability functions are set to larger-is-better, which is what you want in this experiment. See the chapter "Standard Least Squares: Perspectives on the Estimates" of *JMP Statistics and Graphics Guide* for more details about the prediction profiler.

5 Again click the red triangle on the Prediction Profiler title bar and select **Maximize Desirability** to automatically set the prediction traces that give the best results according to the desirability functions.

In this example, the settings for Interfer and Wall changed from L1 to L2 (see Figure 11.5 and Figure 11.6). The Depth setting changed from L1 to L3. The settings for Adhesive did not change. These new settings increased the signal-to-noise ratio from 24.0253 to 26.9075.

Figure 11.6 Best Factor Settings for Byrne Taguchi Data
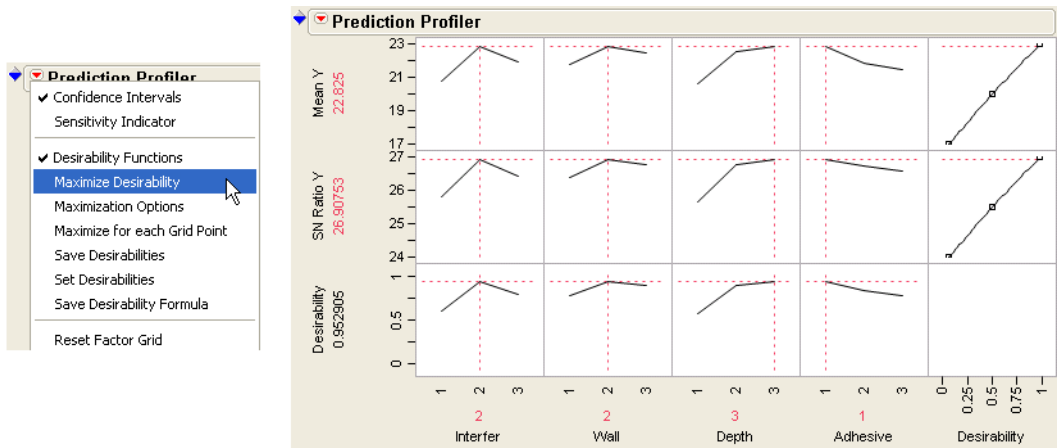
Creating a Taguchi Design

To start a Taguchi design, select **DOE** >**Taguchi Arrays**, or click the **Taguchi Arrays** button on the JMP Starter **DOE** page. Then, follow the steps below:

- "Detail the Response and Add Factors," p. 219
- "Choose Inner and Outer Array Designs," p. 220
- "Display Coded Design," p. 221
- "Make the Design Table," p. 221

Detail the Response and Add Factors

The Responses panel has a single default response. The steps for setting up the details of this response are outlined in Figure 11.7. For information on importance weights and lower and upper limits, see "Understanding Response Importance Weights," p. 60.

Figure 11.7 Setting Up the Response

Click to enter lower and upper
limits and importance weights.

③ Double-click to edit
the response name.

② Click to change the response goal:
Larger Is Better, Nominal is Best,
Smaller is Better, or None.
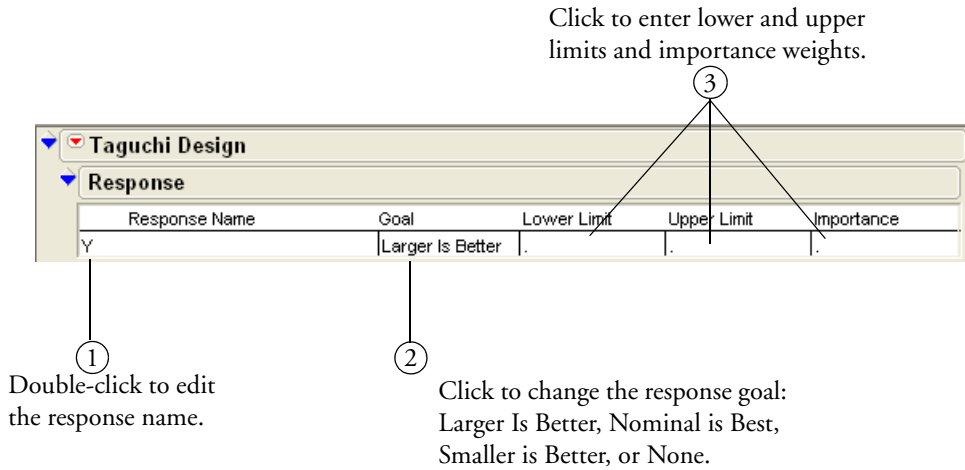
The steps for setting up the factors are outlined in Figure 11.8.

Figure 11.8 Entering Factors

Click to add a signal, then select a
signal type: **2 Level**, or **3 Level**.

or

Click to add a noise.

To change the value of a signal or noise,
click and then type the new value.

② Double-click to edit
the factor name.
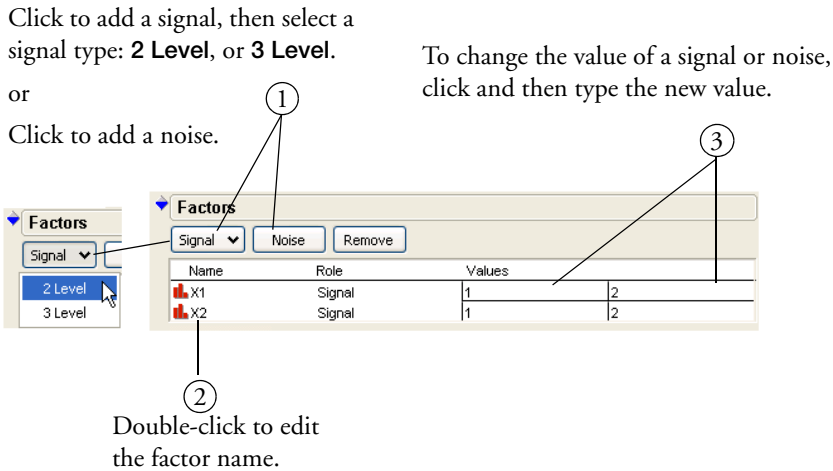
When you finish adding factors, click **Continue**.

Choose Inner and Outer Array Designs

Your choice for inner and outer arrays depends on the number and type of factors you have.
Figure 11.9 shows the available inner array choices when you have eight signal factors. If you also have
noise factors, choices include designs for the outer array. To follow along, enter eight two-level **Signal**
factors and click **Continue**. Then highlight the design you want and again click **Continue**. This exam-
ple uses the L12 design.

Figure 11.9 Selecting a Design for Eight Signal Factors
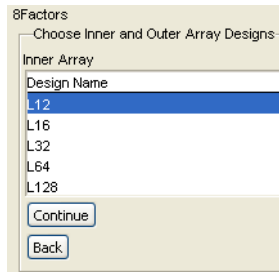
After you click **Continue**, a dialog appears that asks to you specify how many times you want to perform each inner array run. Specify one (1) for this example.

Display Coded Design

After you select a design type, click the disclosure buttons (◆ ◆ on Windows/Linux and ▶ ▼ on the Macintosh) to display the Coded Design (Figure 11.10).

Figure 11.10 Coding for Eight Factor L12 Design
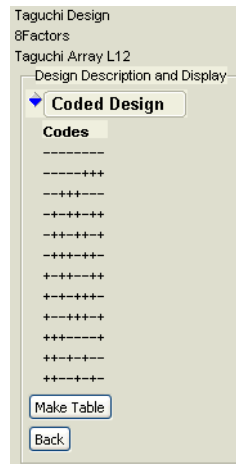
The Coded Design shows the pattern of high and low values for the factors in each run. For more details on the coded design, see "Understanding Design Codes," p. 104.

Make the Design Table

When you click **Make Table**, a table similar to that shown in Figure 11.11 appears. In the data table, each row represents a run. In the values for the Pattern variable, plus signs designate high levels and minus signs represent low levels.

Figure 11.11 Taguchi Design Table for Eight Factor L12 Design

		X1	X2	X3	X4	X5	X6	X7	X8	Pattern	run 1	run 2	Mean	SN Ratio
	1	1	1	1	1	1	1	1	1	--------	▪	▪	▪	▪
	2	1	1	1	1	1	2	2	2	-----+++	▪	▪	▪	▪
	3	1	1	2	2	2	1	1	1	--+++---	▪	▪	▪	▪
	4	1	2	1	2	2	1	2	2	-+-++-++	▪	▪	▪	▪
	5	1	2	2	1	2	2	1	2	-++-++-+	▪	▪	▪	▪
	6	1	2	2	2	1	2	2	1	-+++-++-	▪	▪	▪	▪
	7	2	1	2	2	1	1	2	2	+-++--++	▪	▪	▪	▪
	8	2	1	2	1	2	2	2	1	+-+-+++-	▪	▪	▪	▪
	9	2	1	1	2	2	2	1	2	+--+++-+	▪	▪	▪	▪
	10	2	2	2	1	1	1	1	2	+++---+	▪	▪	▪	▪
	11	2	2	1	2	1	2	1	1	++-+-+--	▪	▪	▪	▪
	12	2	2	1	1	2	1	2	1	++--+-+-	▪	▪	▪	▪

Taguchi Array L12
Design Taguchi Array
Model

Columns (13/0)

X1 ✳
X2 ✳
X3 ✳
X4 ✳
X5 ✳
X6 ✳
X7 ✳
X8 ✳
Pattern
run 1
run 2
Mean ✚
SN Ratio ✚

Chapter **12**

Augmented Designs

If you treat experimentation as an iterative process, you can master the temptation to assume that one successful screening experiment has optimized your process. You can also avoid disappointment if a screening experiment leaves behind some ambiguities. The augment designer helps facilitate experimentation as an iterative process.

The augment designer modifies an existing design data table, supporting your iterative process. It gives the following five choices:

- replicate the design a specified number of times
- add center points
- create a foldover design
- add axial points together with center points to transform a screening design to a response surface design
- add runs to the design using a model that can have more terms than the original model

This chapter provides an overview of the augment designer. It also presents a case study of design augmentation.

Contents

A *D*-Optimal Augmentation of the Reactor Example

This example, adapted from Meyer, *et al.* (1996), demonstrates how to use the augment designer in JMP to resolve ambiguities left by a screening design. In this study, a chemical engineer investigates the effects of five factors on the percent reaction of a chemical process.

To begin, open Reactor 8 Runs.jmp found in the Design Experiment Sample Data folder installed with JMP. Then select **Augment Design** from the **DOE** menu. When the initial launch dialog appears:

1 Select Percent Reacted and click **Y, Response**.
2 Select all other variables except Pattern and click **X, Factor**.
3 Click **OK** on the launch dialog to see the Augment Design dialog in Figure 12.1.

Note: You can check Group New Runs into Separate Blocks to add a blocking factor to any design. However, the purpose of this example is to estimate all two-factor interactions in 16 runs, which can't be done when there is the additional blocking factor in the model.

Figure 12.1 Augment Design Dialog for the Reactor Example
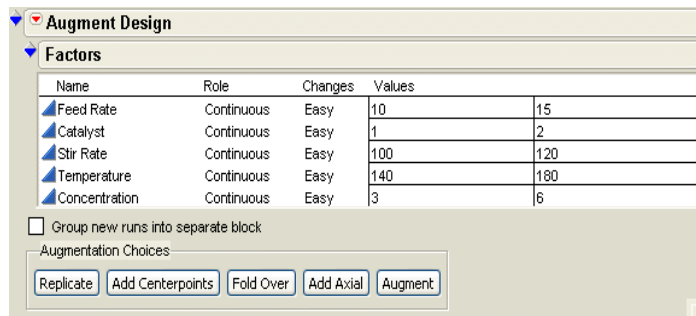
4 Now click **Augment** on the Augment Design dialog to see the display in Figure 12.2.

This model shown in Figure 12.2 is the result of the model stored with the data table when it was created by the Custom designer. However, the augmented design is to have 16 runs in order to estimate all two-factor interactions.

Figure 12.2 Initial Augmented Model

To continue with the augmented reactor design:

5 Choose **2nd** from the Interactions menu as shown in Figure 12.3. This adds all the two-factor inter-
   actions to the model. The Minimum number of runs given for the specified model is 16, as shown
   in the Design Generation text edit box.

Figure 12.3 Augmented Model with All Two-Factor Interactions

6 Click **Make Design**.

JMP now computes *D*-optimally augmented factor settings, similar to the design shown in Figure 12.4.

Figure 12.4 D-Optimally Augmented Factor Settings

Run	Feed Rate	Catalyst	Stir Rate	Temperature	Concentration	Percent Reacted
1	10	1	100	180	6	44
2	10	1	120	180	3	66
3	10	2	100	140	6	70
4	10	2	120	140	3	54
5	15	1	100	140	3	53
6	15	1	120	140	6	55
7	15	2	100	180	3	93
8	15	2	120	180	6	82
9	15	1	120	140	3	.
10	15	1	100	180	3	.
11	10	2	100	180	3	.
12	10	1	100	140	3	.
13	10	1	120	140	6	.
14	15	2	120	140	6	.
15	15	2	100	140	3	.
16	15	2	120	180	3	.

Note: The resulting design is a function of an initial random number seed. To reproduce the exact factor settings table in Figure 12.4, (or the most recent design you generated), choose **Set Random Seed** from the popup menu on the Augment Design title bar. A dialog shows the most recently used random number. Click **OK** to use that number again, or **Cancel** to generate a design based on a new random number. The dialog in Figure 12.5 shows the random number (12834729) used to generate the runs in Figure 12.4.

Figure 12.5 Specifying a Random Number
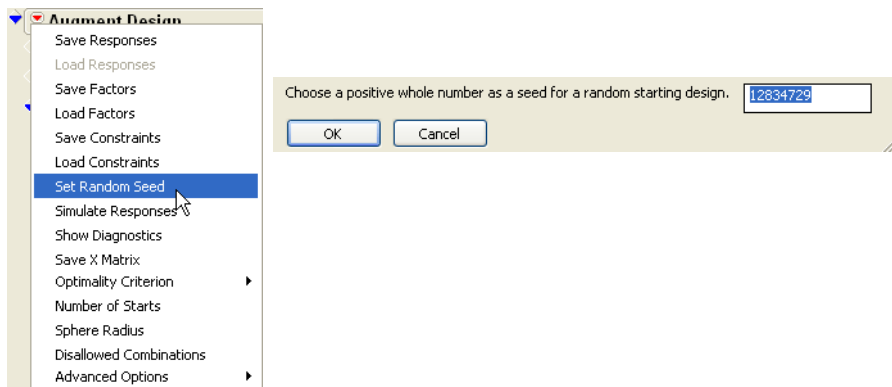
7 Click **Make Table** to generate the JMP table with *D*-Optimally augmented runs.

Analyze the Augmented Design

Suppose you have already run the experiment on the augmented data and recorded results in the Percent Reacted column of the data table.

1 To see these results, open Reactor Augment Data.jmp found in the Design Experiment Sample Data folder installed with JMP.

It is desirable to maximize Percent Reacted, however its column in this sample data table has a response limits column property set to **Minimize**.

2 Click the asterisk next to the Percent Reacted column name in the Columns panel of the data table and select **Response Limits**, as shown on the left in Figure 12.6.

3 In the Column Info dialog that appears, change the response limit to **Maximize**, as shown on the right in Figure 12.6.

Figure 12.6 Change the Response Limits Column Property for the Percent Reacted Column
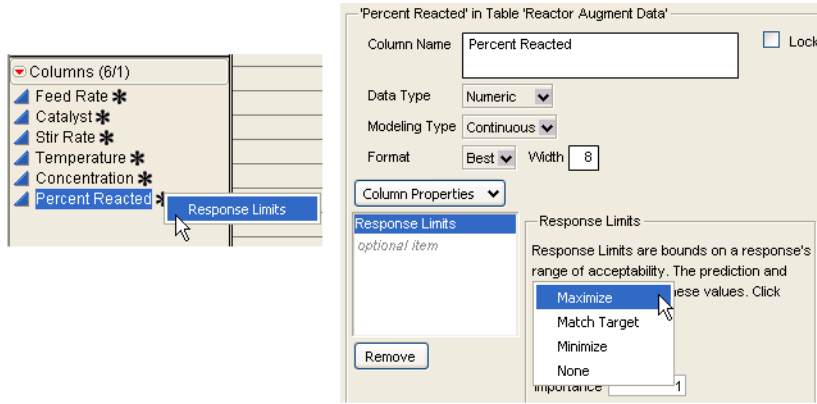
You are now ready to run the analysis.

4 To start the analysis, click the red triangle for **Model** in the upper left of the data table and select **Run Script** from the menu, as shown in Figure 12.7.

Figure 12.7 Completed Augmented Experiment (Reactor Augment Data.jmp)

The **Model** script, stored as a table property with the data, contains the JSL commands that display the Fit Model dialog with all main effects and two-factor interactions as effects.

5 Change the fitting personality on the Fit Model dialog from **Standard Least Squares** to **Stepwise**, as shown in Figure 12.8.

Figure 12.8 Fit Model Dialog for Stepwise Regression on Generated Model
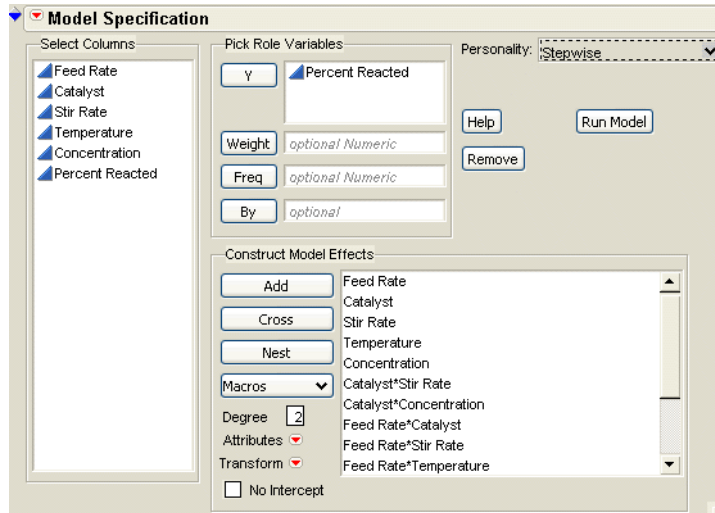
6   When you click **Run Model**, the stepwise regression control panel appears. Click the check boxes for all the main effect terms.

Important: Choose **Mixed** from the **Direction** menu and make sure **Prob to Enter** is 0.050 and **Prob to Leave** is 0.100. These are not the default values. You should see the dialog shown in Figure 12.9.

Figure 12.9 Initial Stepwise Model

7 Click **Go** to start the stepwise regression and watch it continue until all terms are entered into the model that meet the **Prob to Enter** and **Prob to Leave** criteria in the Stepwise Regression Control panel.

Figure 12.10, shows the result of this example analysis. Note that Feed Rate is out of the model while the Catalyst*Temperature, Stir Rate*Temperature, and the Temperature*Concentration interactions have entered the model.

Figure 12.10 Completed Stepwise Model
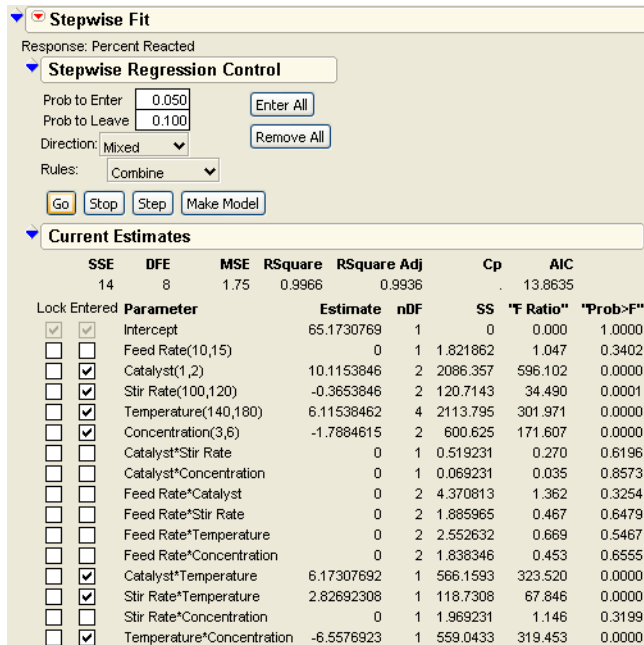
8 After Stepwise is finished, click **Make Model** on the Stepwise control panel to generate this reduced model, as shown in Figure 12.11.

9 Click **Run Model** and fit the reduced model to do additional diagnostic work, make predictions, and find the optimal factor settings.

Figure 12.11 New Prediction Model Dialog

The Analysis of Variance and Lack of Fit Tests in Figure 12.12, indicate a highly significant regression model with no evidence of Lack of Fit.

Figure 12.12 Prediction Model Analysis of Variance and Lack of Fit Tests

The Sorted Parameter Estimates table in Figure 12.13, shows that Catalyst has the largest main effect. However, the significance of the two-factor interactions are of the same order of magnitude as the main effects. This is the reason that the initial screening experiment, shown in the chapter "Screening Designs," p. 89, had ambiguous results.

Figure 12.13 Prediction Model Estimates Plot
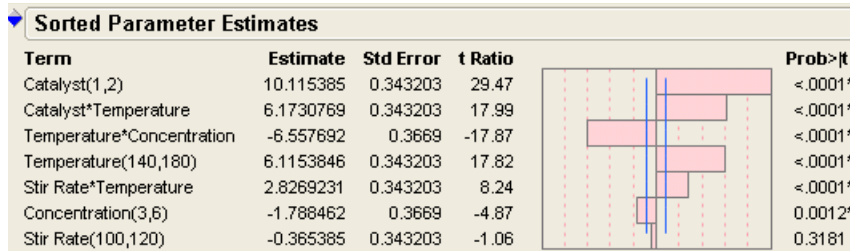
10 Chose **Maximimize Desirability** from the menu on the Prediction Profiler title bar.

The prediction profile plot at the bottom in Figure 12.14, shows that maximum occurs at the high levels of Catalyst, Stir Rate, and Temperature and the low level of Concentration. At these extreme settings, the estimate of Percent Reacted increases from 65.17 to 98.38.

Figure 12.14 Maximum Percent Reacted
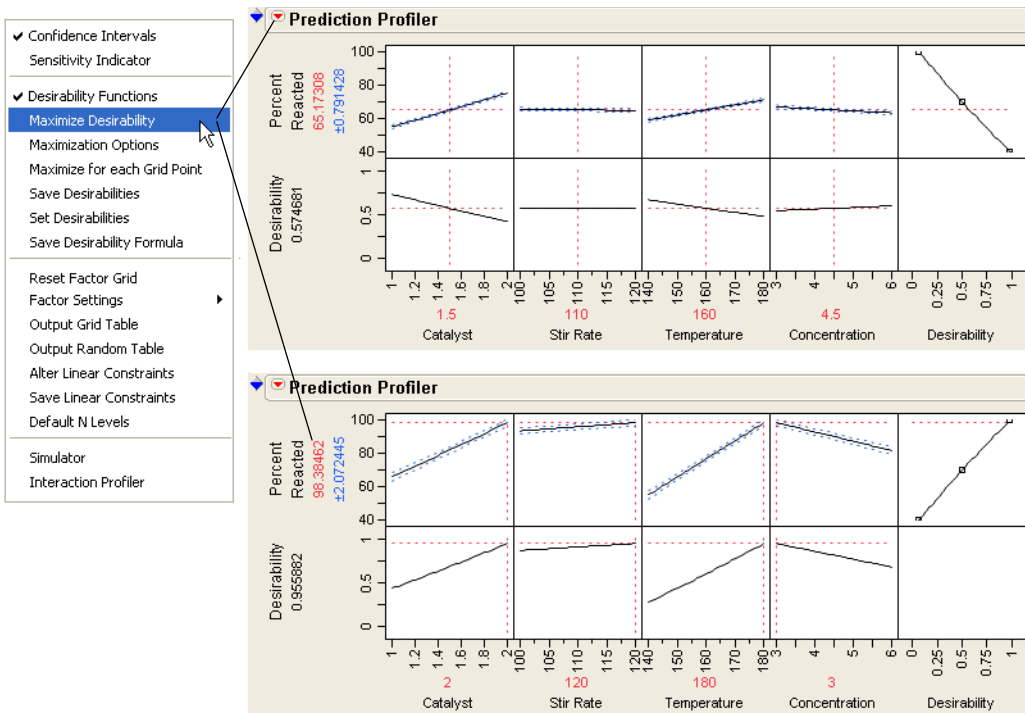
To summarize, compare the analysis of 16 runs with the analyses of reactor data from previous chapters:

- "Screening Designs," p. 89, the analysis of a screening design with only 8 runs produced a model with the five main effects and two interaction effects with confounding. None of the factors effects were significant, although the Catalyst factor was large enough to encourage collecting data for further runs.

- "Full Factorial Designs," p. 129, a full factorial of the five two-level reactor factors, 32 runs, was first subjected to a stepwise regression. This approach identified three main effects (Catalyst,

Temperature, and Concentration) and two interactions (Temperature*Catalyst, Contentration*Temperature) as significant effects.

• By using a D-optimal augmentation of 8 runs to produce 8 additional runs, a stepwise analysis returned the same results as the analysis of 32 runs. The bottom line is that only half as many runs yielded the same information. Thus, using an iterative approach to DOE can save time and money.

Creating an Augmented Design

The augment designer modifies an existing design data table. It gives the following five choices:

Replicate   replicates the design a specified number of times. See "Replicate a Design," p. 233.

Add Centerpoints   adds center points. See "Add Center Points," p. 235.

Fold Over   creates a foldover design. See "Creating a Foldover Design," p. 236.

Add Axial   adds axial points together with center points to transform a screening design to a response surface design. See "Adding Axial Points," p. 237.

Augment   adds runs to the design (augment) using a model, which can have more terms than the original model. See "Adding New Runs and Terms," p. 238.

Replicate a Design

Replication provides a direct check on the assumption that the error variance is constant. It also reduces the variability of the regression coefficients in the presence of large process or measurement variability.

To replicate the design a specified number of times:

1   Open a data table that contains a design you want to augment. This example uses Reactor 8 Runs.jmp from the Design Experiment Sample Data folder installed with JMP.

2   Select **DOE > Augment Design** to see the initial dialog for specifying factors and responses.

3   Select Percent Reacted and click **Y, Response**.

4   Select all other variables (except Pattern) and click **X, Factor** to identify the factors you want to use for the augmented design (Figure 12.15).

Figure 12.15 Identify Response and Factors
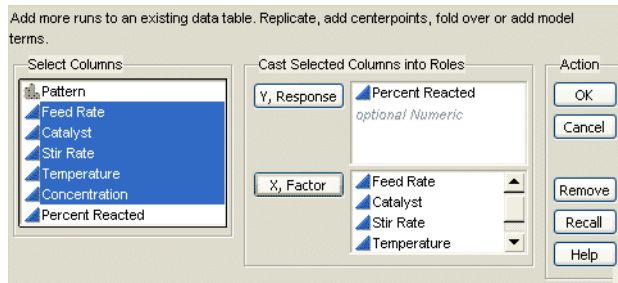
5   Click **OK** to see the Augment Design panel shown in Figure 12.16.

6 If you want the original runs and the resulting augmented runs to be identified by a blocking factor, check the box beside **Group New Runs into Separate Block** on the Augment Design panel.

Figure 12.16 Choose an Augmentation Type
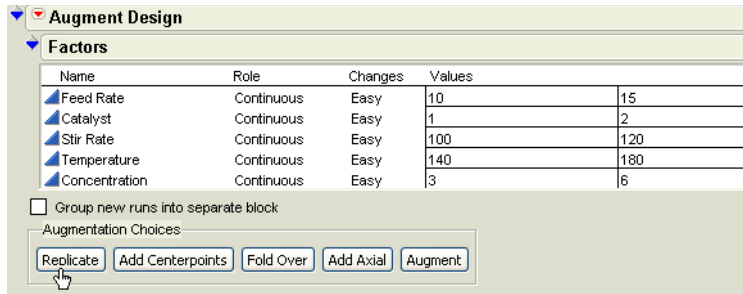
7 Click the **Replicate** button to see the dialog shown on the left in Figure 12.17. Enter the number of times you want JMP to perform each run, then click **OK**.

Note: Entering 2 specifies that you want each run to appear twice in the resulting design. This is the same as one replicate (Figure 12.17).

---

8 View the design, shown on the right in Figure 12.17.

Figure 12.17 Reactor Data Design Augmented With Two Replicates

9 Click the disclosure icons next to Prediction Variance Profile and Prediction Variance Surface to see the profile and surface plots shown in Figure 12.18.

Figure 12.18 Prediction Profiler and Surface Plot
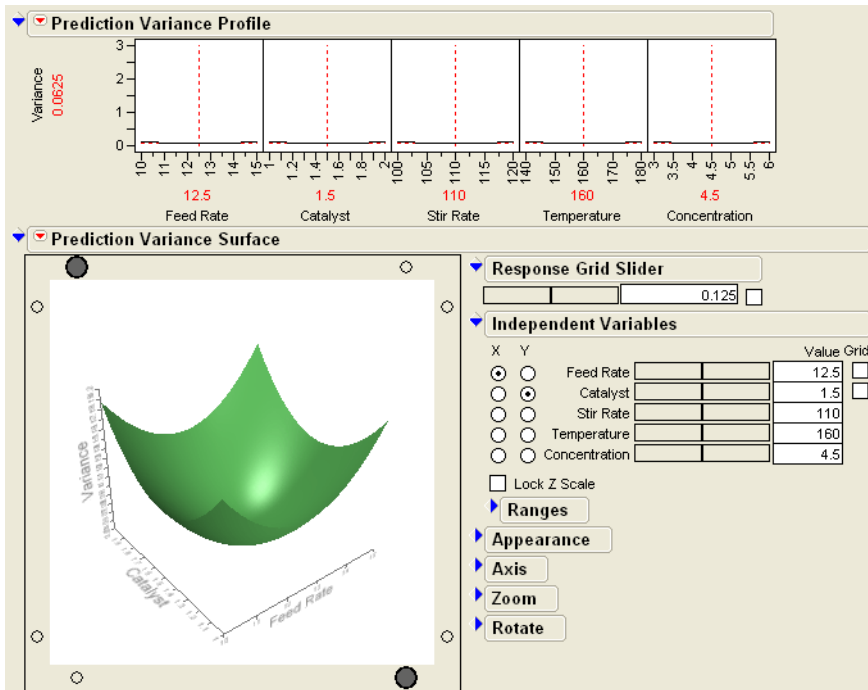
10 Click **Make Table** to produce the design table shown in Figure 12.19.

Figure 12.19 The Replicated Design

	Feed Rate	Catalyst	Stir Rate	Temperature	Concentration	Percent Reacted
1	10	1	100	180	6	44
2	10	1	120	180	3	66
3	10	2	100	140	6	70
4	10	2	120	140	3	54
5	15	1	100	140	3	53
6	15	1	120	140	6	55
7	15	2	100	180	3	93
8	15	2	120	180	6	82
9	10	1	100	180	6	.
10	10	1	120	180	3	.
11	10	2	100	140	6	.
12	10	2	120	140	3	.
13	15	1	100	140	3	.
14	15	1	120	140	6	.
15	15	2	100	180	3	.
16	15	2	120	180	6	.

Augmented Design
Design   Augmented Design
Model

Columns (6/0)
Feed Rate ✱
Catalyst ✱
Stir Rate ✱
Temperature ✱
Concentration ✱
Percent Reacted ✱

Rows
All rows   16
Selected   0
Excluded   0
Hidden   0
Labelled   0

Add Center Points

Adding center points is useful to check for curvature and reduce the prediction error in the center of the factor region. Center points are usually replicated points that allow for an independent estimate of pure error, which can be used in a lack-of-fit test.

To add center points:

1 Open a data table that contains a design you want to augment. This example uses Reactor 8 Runs.jmp found in the Design Experiment Sample Data folder installed with JMP.

2 Select **DOE > Augment Design**.

3 In the initial Augment Design dialog, identify the response and factors you want to use for the augmented design (see Figure 12.15) and click **OK**.

4 If you want the original runs and the resulting augmented runs to be identified by a blocking factor, check the box beside **Group New Runs into Separate Block** (Figure 12.16).

5 Click the **Add Centerpoints** button and type the number of center points you want to add. For this example, add two center points, and click **OK**.

6 Click **Make Table** to see the data table in Figure 12.20.

The table shows two center points appended to the end of the design.

Figure 12.20 Design with Two Center Points Added

Creating a Foldover Design

A foldover design removes the confounding of two-factor interactions and main effects. This is especially useful as a follow-up to saturated or near-saturated fractional factorial or Plackett-Burman designs.

To create a foldover design:

1 Open a data table that contains a design you want to augment. This example uses Reactor 8 Runs.jmp, found in the Design Experiment Sample Data folder installed with JMP.

2 Select **DOE > Augment Design**.

3 In the initial Augment Design dialog, identify the response and factors you want to use for the augmented design (see Figure 12.15) and click **OK**.

4 Check the box to the left of **Group New Runs into Separate Block** (Figure 12.16). This identifies the original runs and the resulting augmented runs with a blocking factor.

5 Click the **Fold Over** button. A dialog appears that lists all the design factors.

6 Choose (select) which factors to fold. The default, if you choose no factors, is to fold on all design factors. If you choose a subset of factors to fold over, the remaining factors are replicates of the original runs. The example in Figure 12.21 folds on all five factors and includes a blocking factor.

7 Click **Make Table**. The design data table that results lists the original set of runs as block 1 and the

new (foldover) runs are block 2.

Figure 12.21 Listing of a Foldover Design On All Factors

		Feed Rate	Catalyst	Stir Rate	Temperature	Concentration	Block	Percent Reacted
	1	10	1	100	180	6	1	44
	2	10	1	120	180	3	1	66
	3	10	2	100	140	6	1	70
	4	10	2	120	140	3	1	54
	5	15	1	100	140	3	1	53
	6	15	1	120	140	6	1	55
	7	15	2	100	180	3	1	93
	8	15	2	120	180	6	1	82
	9	15	2	120	140	3	2	.
	10	15	2	100	140	6	2	.
	11	15	1	120	180	3	2	.
	12	15	1	100	180	6	2	.
	13	10	2	120	180	6	2	.
	14	10	2	100	180	3	2	.
	15	10	1	120	140	6	2	.
	16	10	1	100	140	3	2	.

Columns on the left panel:
- Augmented Design
- Design — Augmented Design
- Model
- Columns (7/0)
  - Feed Rate ✳
  - Catalyst ✳
  - Stir Rate ✳
  - Temperature ✳
  - Concentration ✳
  - Block ✳
  - Percent Reacted ✳
- Rows
  - All rows — 16
  - Selected — 0
  - Excluded — 0
  - Hidden — 0
  - Labelled — 0

Adding Axial Points

You can add axial points together with center points, which transforms a screening design to a response surface design. To do this:

1 Open a data table that contains a design you want to augment. This example uses Reactor 8 Runs.jmp, from the Design Experiment Sample Data folder installed with JMP.

2 Select **DOE > Augment Design**.

3 In the initial Augment Design dialog, identify the response and factors you want to use for the augmented design (see Figure 12.15) and click **OK**.

4 If you want the original runs and the resulting augmented runs to be identified by a blocking factor, check the box beside **Group New Runs into Separate Block** (Figure 12.16).

5 Click **Add Axial**.

6 Enter the axial values in units of the factors scaled from –1 to +1, then enter the number of center points you want. When you click **OK**, the augmented design includes the number of center points specified and constructs two axial points for each variable in the original design.

Figure 12.22 Entering Axial Values

Axial values dialog
Please supply an axial value.   1
Please supply the number of center points desired.   2

OK
Cancel

7 Click **Make Table**. The design table appears. Figure 12.23 shows a table augmented with two center points and two axial points for five variables.

Figure 12.23 Design Augmented With Two Center and Ten Axial Points

Adding New Runs and Terms

A powerful use of the augment designer is to add runs using a model that can have more terms than the original model. For example, you can achieve the objectives of response surface methodology by changing a linear model to a full quadratic model and adding the necessary number of runs. Suppose you start with a two-factor, two-level, four-run design. If you add quadratic terms to the model and five new points, JMP generates the 3 by 3 full factorial as the optimal augmented design.

D-optimal augmentation is a powerful tool for sequential design. Using this feature you can add terms to the original model and find optimal new test runs with respect to this expanded model. You can also group the two sets of experimental runs into separate blocks, which optimally blocks the second set with respect to the first.

To add new runs and terms to the original model:

1 Open a data table that contains a design you want to augment. This example uses Reactor Augment Data.jmp, from the Design Experiment Sample Data folder installed with JMP.

2 Select **DOE > Augment Design**.

3 In the initial Augment Design dialog, identify the response and factors you want to use for the augmented design (see Figure 12.15) and click **OK**.

4 If you want the original runs and the resulting augmented runs to be identified by a blocking factor, check the box beside **Group New Runs into Separate Block** (not used in this example).

5 Click the **Augment** button. The original number of runs (Figure 12.24) appear in the Factor Design panel.

Figure 12.24 Viewing the Existing Design

6 In the Design Generation panel, enter the number of total runs you want this design to contain. The number you enter is the original number of runs plus the number of additional runs you want.

7 Click the **Make Design** button. The new number of runs (Figure 12.25) appear in the Design panel.

Figure 12.25 24 Total Runs

8 If desired, view the prediction variance profile and the prediction variance surface.

9 Click **Make Table** to create the augmented design JMP table (Figure 12.26) with the additional
   runs.

Figure 12.26 The Augmented Design Table with New Runs

additional
runs

Technical Note: The Augment designer does not support designs that have terms whose estimability has been set to If Possible instead of Necessary, as is done in some screening designs that have fewer runs than terms.

Special Augment Design Commands

After you select **DOE > Augment Design** and identify factors and responses, the window in Figure 12.27 appears. Click the red triangle icon on the Augment Design title bar to see a list of commands. Most of these commands are for saving and loading information about variables; they are available in all designs and more information is in "Special Custom Design Commands," p. 74. The following sections describe commands found in this menu that are specific to augment designs.

Figure 12.27 Click the Red Triangle Icon to Reveal Commands
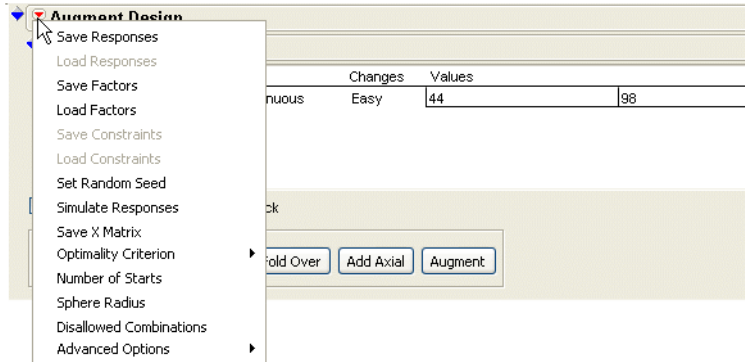
Save the Design (X) Matrix

To create a script and save it as a table property in the JMP design data table, click the red triangle icon in the Augment Design title bar (Figure 12.27) and select **Save X Matrix**. The script is saved as a table property called **Design Matrix**. When you run this script, JMP creates a global matrix called X and displays its number of rows in the log. If you do not have the log visible, select **View > Log** or **Window > Log** on the Macintosh.

Modify the Design Criterion (*D*- or *I*- Optimality)

To modify the design optimality criterion, click the red triangle icon in the Augment Design title bar (Figure 12.28) and select **Optimality Criterion**, then choose **Make D-Optimal Design** or **Make I-Optimal Design**. The default criterion for **Recommended** is *D*-optimal for all design types unless you have used the **RSM** button in the Model panel to add effects that make the model quadratic.

Figure 12.28 Change the Optimality Criterion
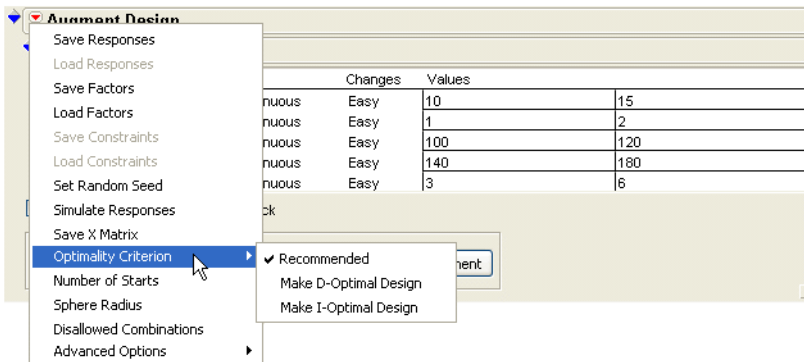
Select the Number of Random Starts

To override the default number of random starts, click the red triangle icon in the Augment Design title bar (Figure 12.28) and select **Number of Starts**. The window in Figure 12.29 appears with an edit box for you to enter the number of random starts for the design you want to build. The number you enter overrides the default number of starts, which varies depending on the design.

Figure 12.29 Changing the Number of Starts

Choose a positive whole number for the number of random starting designs. [1]

[OK]   [Cancel]
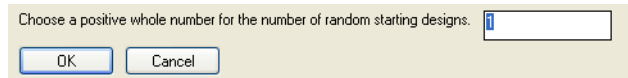
For additional information on the number of starts, see "Why Change the Number of Starts?," p. 79.

Specify the Sphere Radius Value

Augment designs can be constrained to a hypersphere. To edit the sphere radius for the design in units of the coded factors (–1, 1), click the red triangle icon in the Augment Design title bar (Figure 12.27) and select **Sphere Radius**. Enter the appropriate value and click **OK**.

Or, use JSL and submit the following command before you build a custom design:

```
DOE Sphere Radius = 1.0;
```

In this statement you can replace 1.0 with any positive number.

Disallow Factor Combinations

In addition to linear inequality constraints on continuous factors and constraining a design to a hypersphere, you can define general factor constraints on the factors. You can disallow any combination of levels of categorical factors if you have not already defined linear inequality constraints.

For information on how to do this, see "Disallowed Combinations: Accounting for Factor Level Restrictions," p. 80.

Chapter **13**

Prospective Power and Sample Size

Use the **DOE > Sample Size and Power** command to answer the question "How many runs do I need?" The important quantities are sample size, power, and the magnitude of the effect. These depend on the significance level—alpha—of the hypothesis test for the effect and the standard deviation of the noise in the response. You can supply either one or two of the three values. If you supply only one of these values, the result is a plot of the other two. If you supply two values, JMP computes the third.

Using the **Sample Size and Power** command when doing a prospective analysis helps answer the question, "Will I detect the group differences I am looking for, given my proposed sample size, estimate of within-group variance, and alpha level?" In this type of analysis, you must give JMP an estimate of the group means and sample sizes in a data table as well as an estimate of the within-group standard deviation (σ).

The sample size and power computations determine how large a sample is needed to be reasonably likely that an experiment or sample will yield a significant result, given that the true effect size is at least a certain size. It requires that you enter any two of three quantities, difference to detect, sample size, and power, and computes the third for the following cases:

- difference between one sample's mean and a hypothesized value
- difference between two samples means
- differences in the means among *k* samples
- difference between a standard deviation and a hypothesized value
- difference between one sample proportion and a hypothesized value
- difference between two sample proportions
- difference between counts per unit in a Poisson-distributed sample and a hypothesized value.

The calculations assume that there are equal numbers of units in each group. You can apply this platform to more general experimental designs, if they are balanced, and a number-of-parameters adjustment is specified.

Contents

Prospective Power Analysis

The following five values have an important relationship in a statistical test on means:

Alpha   Alpha is the significance level that prevents declaring a zero effect significant more than alpha portion of the time.

Error Standard Deviation   Error Standard Deviation is the unexplained random variation around the means. An estimate of the Error Standard Deviation could be the root mean square error (RMSE) from a previous model fit.

Sample Size   Sample size is how many experimental units (runs, or samples) are involved in the experiment.

Power   Power is the probability of declaring a significant result.

Effect Size   Effect size is how different the means are from each other or from the hypothesized value.

The **Sample Size and Power** command in JMP helps estimate in advance either the sample size needed, power expected, or the effect size expected in the experimental situation where there is a single mean or proportion comparison, a two sample or proportion comparison, when comparing k sample means, or when comparing counts per unit.

When you select **DOE > Sample Size and Power**, the panel shown in Figure 13.1 appears with button selections for experimental situations. The following sections describe each of these selections and explains how to enter estimated parameter values and the desired computation.

Figure 13.1 Sample Size and Power Choices
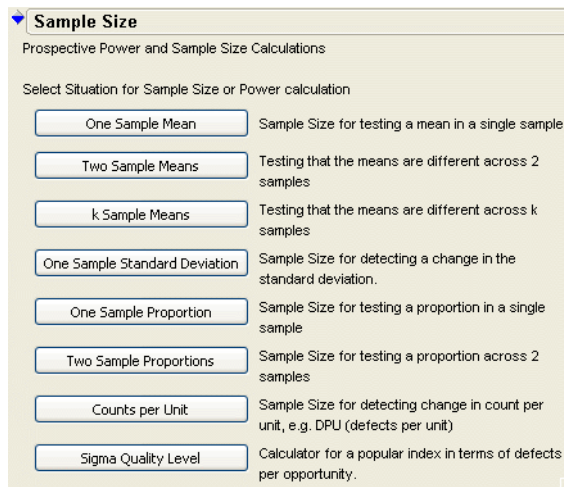
One-Sample and Two-Sample Means

After you click either **One Sample Mean**, or **Two Sample Means** in the initial Sample Size selection list (Figure 13.1), the Power and Sample Size dialog in Figure 13.2 appears and asks for the anticipated experimental values. As an example, consider the two-sample situation.

Figure 13.2 Initial Power and Sample Size Dialogs for Single Mean (left) and Two Means (right)
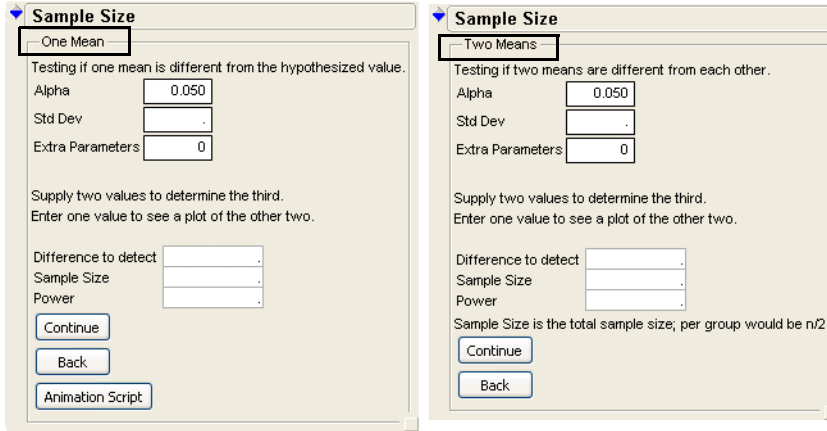
The dialogs are the same except the One Mean dialog has a button at the bottom that accesses an animation script.

The choice in the initial Power and Sample Size dialog always requires values for **Alpha** and the error standard deviation (**Std Dev**), and one or two of the other three values: **Difference to detect**, **Sample Size**, and **Power**. The power and sample size platform then calculates the missing item. If there are two unspecified fields, the power and sample size platform constructs a plot that shows the relationship between those two values:

- power as a function of sample size, given specific effect size
- power as a function of effect size, given a sample size
- effect size as a function of sample size, for a given power.

The Power and Sample Size dialog asks for these values:

    Alpha   Alpha is the significance level, usually 0.05. This implies willingness to accept (if the true difference between groups is zero) that 5% (alpha) of the time a significant difference will be incorrectly declared.

    Std Dev   Std Dev (error standard deviation) is the true residual error. Even though the true error is not known, the power calculations are an exercise in probability that calculates what might happen if the true value is the one you specify. An estimate of the Error Standard Deviation could be the root mean square error (RMSE) from a previous model fit.

    Extra Parameters   Extra Parameters is only for multi-factor designs. Leave this field zero in simple cases. In a multi-factor balanced design, in addition to fitting the means described in the situation, there are other factors with the extra parameters that can be specified here. For example, in a three-factor two-level design with all three two-factor interactions, the number of extra parameters is five—two parameters for the extra main effects, and three parameters for the interactions.

In practice, it isn't very important what values you enter here unless the experiment is in a range where there is very few degrees of freedom for error.

Difference to Detect   Difference to detect is the smallest detectable difference (how small a difference you want to be able to declare statistically significant). For single sample problems this is the difference between the hypothesized value and the true value.

Sample Size   Sample size is the total number of observations (runs, experimental units, or samples). Sample size is not the number per group, but the total over all groups. Computed sample size numbers can have fractional values, which you need to adjust to real units. This is usually done by increasing the estimated sample size to the smallest number evenly divisible by the number of groups.

Power   Power is the probability of getting a statistic that will be declared statistically significant. Bigger power is better, but the cost is higher in sample size. Power is equal to alpha when the specified effect size is zero. You should go for powers of at least 0.90 or 0.95 if you can afford it. If an experiment requires considerable effort, plan so that the experimental design has the power to detect a sizable effect, when there is one.

Continue   Evaluates at the entered values.

Back   Goes back to the previous dialog.

Animation Script   The **Animation Script** button runs a JSL script that displays an interactive plot showing power or sample size. See the section, "Power and Sample Size Animation for a Single Sample," p. 250, for an illustration of this animation script.

Single-Sample Mean

Suppose there is a single sample and the goal is to detect a difference of 1.5 where the error standard deviation is 2, as shown in the left-hand dialog in Figure 13.3. To calculate the power when the sample size is 20, leave **Power** missing in the dialog and click **Continue**. The dialog on the right in Figure 13.3, shows the power is calculated to be 0.0.8888478174 (round to 0.89).

Figure 13.3 A One-Sample Example

To see a plot of the relationship of power and sample size, leave both Sample Size and Power empty in the dialog and click **Continue**.

The plots in Figure 13.4, show a range of sample sizes for which the power varies from about 0.1 to about 0.95. The plot on the right in Figure 13.4 shows using the crosshair tool to illustrate the example in Figure 13.3.

Figure 13.4 A One-Sample Example Plot
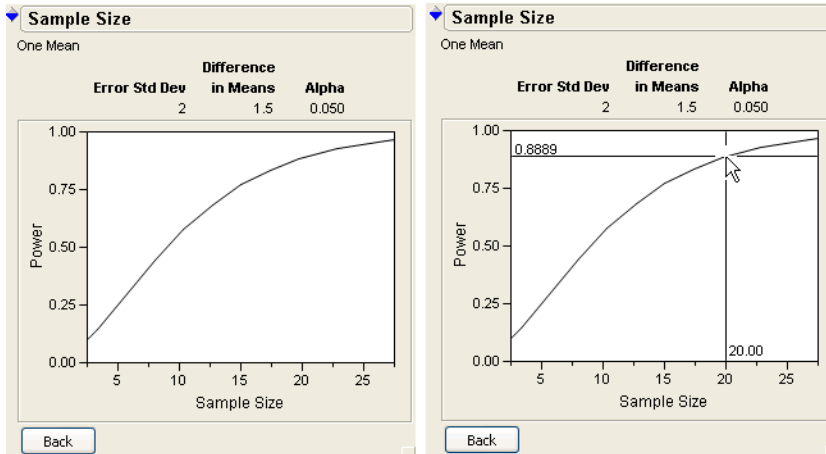
When only Sample Size is specified (Figure 13.5) and Difference to Detect and Power are empty, a plot of power by difference appears.

Figure 13.5 Plot of Power by Difference to Detect for a Given Sample Size
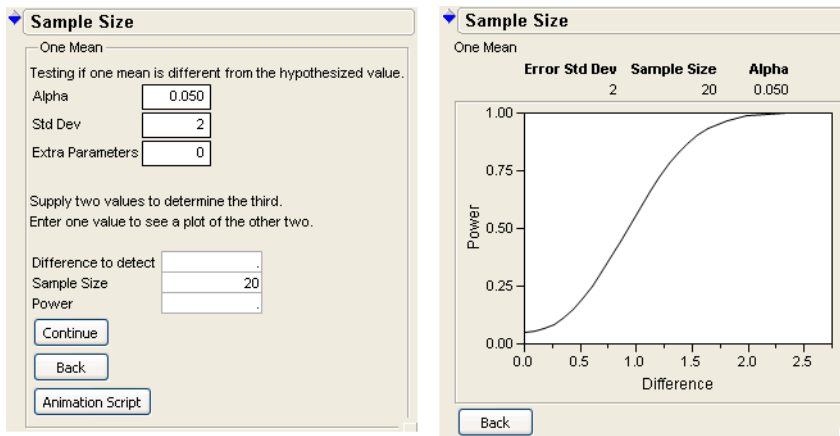
Power and Sample Size Animation for a Single Sample

The **Animation Script** button on the Power and Sample Size dialog for the single mean displays an interactive plot that illustrates the effect that changing the sample size has on power. The example in Figure 13.6 shows a Sample Size of 20, Alpha is 0.05, and the Difference to Detect is set to 1.5. The

initial animation shows a normal curve positioned with mean at zero (representing the estimated mean and the true mean), and another with mean at 1.5 (the difference to be detected). The probability of committing a Type II error (not detecting a difference when there is a difference), often represented as β in literature, is shaded in blue on this plot.

Select and drag the square handles to see the changes in statistics based on the positions of the curves. To change the values of Sample Size and Alpha, click on their values beneath the plot.

Figure 13.6 Example of Animation Script to Illustrate Power
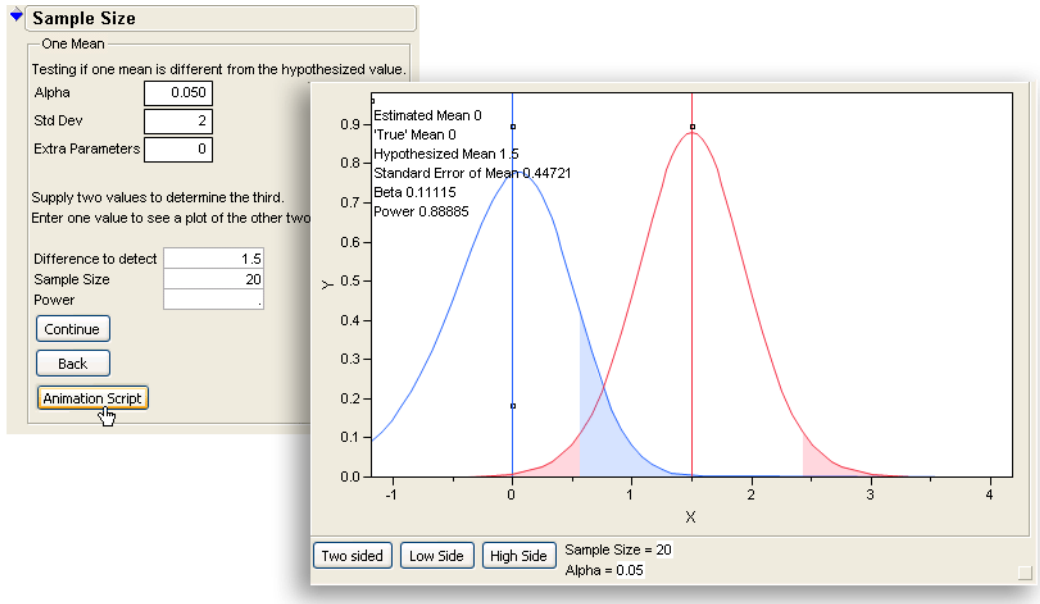
Two-Sample Means

Choose Two Sample Means from the Power and Sample Size options (see Figure 13.1). The dialogs work similarly for one and two samples; the Difference to Detect is the difference between two means. Suppose the standard deviation is 2 (as before), the desired detectable difference is 1.5, and the sample size is 30 (15 per group).

Leave Power blank and click Continue to see the power calculation, 0.509347, as shown in the dialog on the left in Figure 13.7. This result is considerably lower than in the single sample (0.89) because each mean has only half the sample size. The comparison is between two random samples instead of one sample and an hypothesized mean.

To have a greater power requires a larger sample. To find out how large, leave both Sample Size and Power blank and examine the resulting plot, shown on the right in Figure 13.7. The crosshair tool estimates that a sample size of about 78 is needed to obtain a power of 0.9.

Figure 13.7 Plot of Power by Sample Size to Detect for a Given Difference
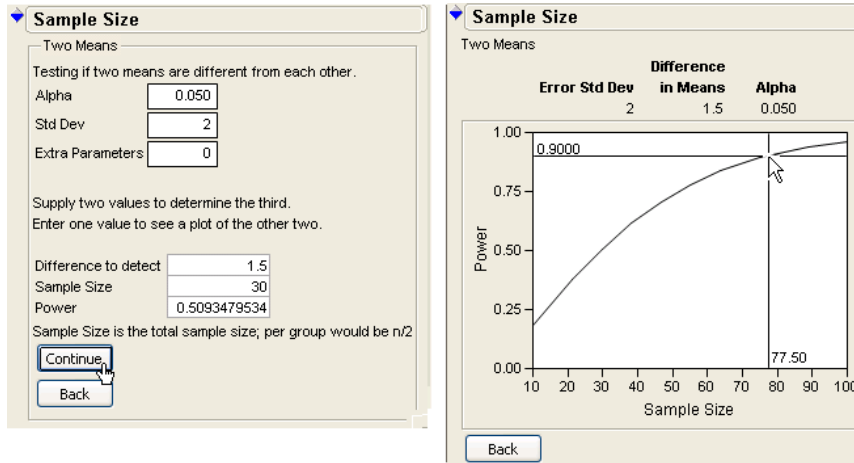
k-Sample Means

The **k-Sample Means** situation can compare up to 10 means. The next example considers a situation where 4 levels of means are expected to be about 10 to 13, and the standard deviation is 0.9. When a sample size of 16 is entered the power calculation is 0.95, as shown in the dialog on the left in Figure 13.8.

If both Sample Size and Power are left blank, the power and sample size calculations produce the power curve shown on the right in Figure 13.8. This confirms that a sample size of 16 looks acceptable.

Notice that the difference in means is 2.236, calculated as square root of the sum of squared deviations from the grand mean. In this case it is the square root of $(-1.5)^2 + (-0.5)^2 + (0.5)^2 + (1.5)^2$, which is the square root of 5.

Figure 13.8 Prospective Power for k-Means and Plot of Power by Sample Size
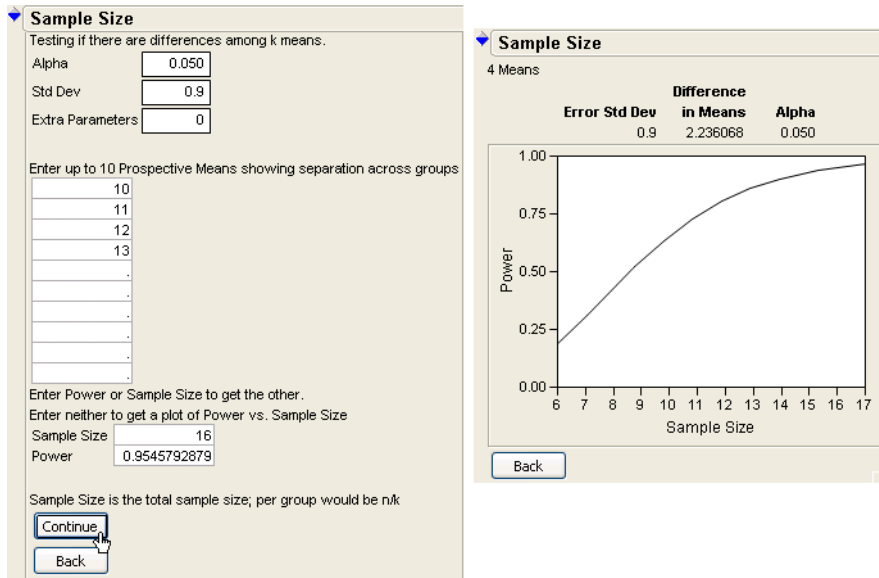
One Sample Standard Deviation

The **One-Sample Standard Deviation** choice on the Power and Sample Size dialog (Figure 13.1) determines sample size for detection of a change in standard deviation. The usual purpose of this option is to compute a large enough sample size to guarantee that the risk of accepting a false hypothesis (β) is small.

In the dialog, specify

Alpha   Alpha is the significance level, usually 0.05. This implies willingness to accept (if the true difference between standard deviation and the hypothesized standard deviation is zero) that 5% (alpha) of the time a significant difference will be incorrectly declared.

Hypothesized Standard Deviation   Hypothesized or baseline standard deviation to which the sample standard deviation is compared.

Alternative Standard Deviation   Select **Larger** or **Smaller** from the menu to indicate the direction of the change you want to detect.

In the lower part of the dialog you enter two of the items and the Power and Sample Size calculations determines the third.

The examples throughout the rest of this chapter use engineering examples from the online manual of The National Institute of Standards and Technology (NIST). You can access the NIST manual examples at http://www.itl.nist.gov/div898/handbook.

One example from the NIST manual states a problem in terms of the variance and difference to detect. The variance for resistivity measurements on a lot of silicon wafers is claimed to be 100 ohm-cm and

the buyer is unwilling to accept a shipment if the variance is greater than 155 ohm-cm for a particular lot (55 ohm-cm above the baseline of 100 ohm-cm).

The hypothesis to be tested is:

Ho: $v_1 = v_2$, where v_1 is the hypothesized variance, and $v_2 = v_1$ plus the difference to detect.

In JMP, the computations use the standard deviation. The hypothesis is stated:

Ho: $s_1 = s_2$, where s_1 is the hypothesized standard deviation, and $s_2 = s_1$ plus the difference to detect.

In this example the hypothesized standard deviation, s_1, is 10 (the square root 100) and s_2 is 12.4499 (the square root of $100 + 55 = 155$). The difference to detect is $12.4499 - 10 = 2.4499$.

You want to detect an increase in the standard deviation of 2.4499 for a known hypothesized standard deviation of 10, with an alpha of 0.05 and power of 0.99.

Enter these items as shown in Figure 13.9. When you click **Continue**, the computed result shows that you need a sample size of 171 (sample size rounded up the next whole number).

If you select **Smaller** from the **Alternative Standard Deviation** menu (you want to detect a change to a smaller standard deviation), enter a negative amount in the **Difference to Detect** box.

Figure 13.9 Dialog To Compare Single-Direction One-Sample Standard Deviation
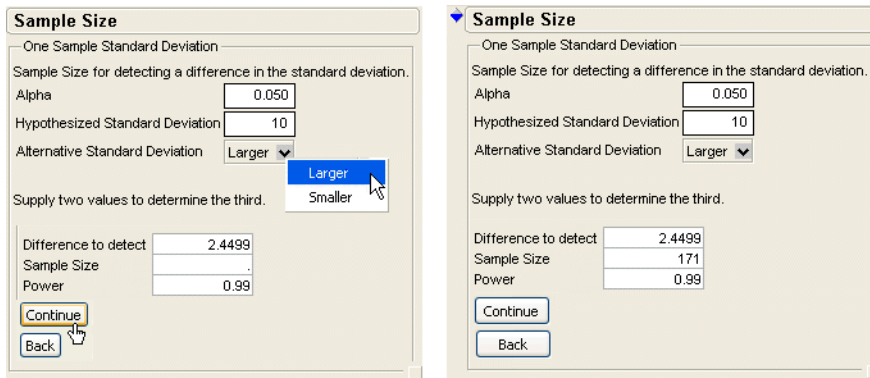
One-Sample and Two-Sample Proportions

The dialogs and computations to test power and sample sizes for proportions are similar to those for testing sample means. You enter a baseline **Proportion** (known or hypothesized proportion) and choose an **Alpha** level. Then, for the one-sample proportion case, enter the **Sample Size** to obtain the estimated **Power** or enter the **Power** to obtain the estimated **Sample Size**. You can also see a plot of **Sample Size** versus **Power** by leaving the two fields blank and clicking **Continue**. For the two-sample proportion case, either the two sample sizes or the desired **Power** must be entered. (See Figure 13.10 and Figure 13.11). The sampling distribution for proportions is actually binomial, but the computations to determine sample size and test proportions use exact methods described in Agresti and Coull (1998).

One Sample Proportion

The **One Sample Proportion** choice on the Power and Sample Size dialog (Figure 13.10) determines either a difference in proportion, the power, or the sample size, for detection of a change in proportion in a single sample from a known or hypothesized proportion. If you supply two of these quantities, the third is computed, or if you enter any one of the quantities, you see a plot of the other two.

Often, there is a known proportion of defects (or other proportion of interest) and you want a large enough sample size to guarantee that the risk of accepting a false hypothesis (β) is small. That is, you want to detect, with reasonable certainty, a given increase in the proportion of defects.

For the one sample proportion, the hypothesis supported is

$$H_0: p = p_0$$

and the two-sided alternative is

$$H_a: p \neq p_0$$

where p is the true proportion and p_0 is the null proportion to test against.

In the top portion of the dialog, specify Alpha and the following quantity:

Proportion   True proportion, which could be known or hypothesized.

In the bottom portion of the dialog, enter two of the following quantities to see the third, or a single quantity to see a plot of the other two.

Null Proportion   Proportion to test against.

Sample Size   Desired sample size, or blank for computation.

Power   Desired power, or blank for computation.

For example, suppose an assembly line has a known proportion of defects of 0.3 and you want to know the power to detect when the proportion is different from 0.5 in a sample of 25. That is, you want to be able to detect a change of 0.2 in the proportion of defects, for an alpha level of 0.05 in a sample size of 25.

Click **Continue** to see the Power computation of approximately 0.7.

Figure 13.10 Power and Sample Dialog for One-Sample Proportions
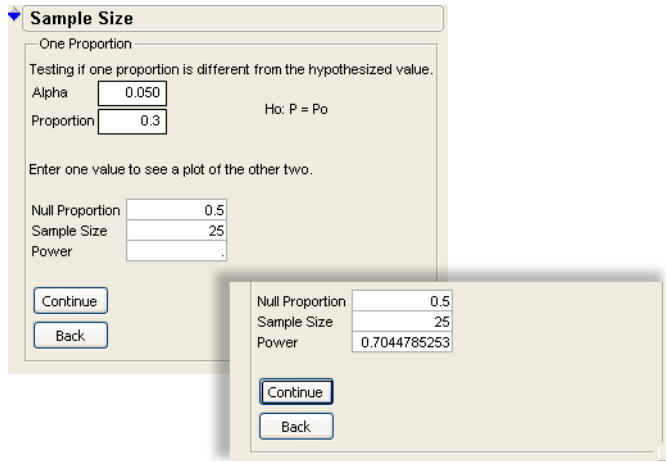
Two Sample Proportions

The **Two Sample Proportions** choice computes the power or sample size needed to detect the difference between two proportions, p_1 and p_2.

For the two sample proportion, the hypothesis supported is

$$H_0: p_1 - p_2 = D_0$$

and the two-sided alternative is

$$H_a: p_1 - p_2 \neq D_0$$

where $p1$ and $p2$ are the true proportions from two populations, and D_0 is the hypothesized difference in proportions.

If you enter any two of the three quantities (Null Difference in Proportion, Sample Size 1 and Sample Size 2, or Power), the third is computed.

As an example, suppose **Proportion 1** is 0.2, **Proportion 2** is 0.4. You want to know the power for a sample size of 50 (25 in each group) to detect a difference of 0.175.

In the Two Proportions dialog, enter:

1   0.2 as **Proportion 1**.
2   0.4 as **Proportion 2**.
3   Enter 0.175 as the **Null difference in Proportion**.
4   Enter 25 as **Sample Size 1** and 25 as **Sample Size 2** (for a total sample size of 50).
5   Leave **Power** blank.

The completed dialog should look like the one on the left in Figure 13.11.

6   Click **Continue** to see the right dialog in Figure 13.11, which shows the power calculation of approximately 0.83.

Suppose you want to know the sample size needed to obtain a power of 0.9, that detects the same difference (0.175) and given the same observed proportions (0.2 and 0.4).

7   Enter the power you want (0.9) and leave the two sample size edit boxes blank.

8   Click **Continue** to see the results on the lower right in Figure 13.11.

Equal sample sizes are computed (rounded to the next whole number). In this example, you need 30 in each group to obtain a power of 0.9 when detecting a difference in proportions of 0.175.

Note: The computations for finding two sample sizes may take a little time so be patient.

Figure 13.11 Difference Between Two Proportions

Counts per Unit

The **Counts per Unit** selection from the Power and Sample size selection list calculates sample size for the Poisson-distributed counts typical when you can measure more than one defect per unit. A unit can be an area and the counts can be fractions or large numbers.

Although the number of defects observed in an area of a given size is often assumed to have a Poisson distribution, the area and count are assumed to be large enough to support a normal approximation.

Questions of interest are:

• Is the defect density within prescribed limits?

• Is the defect density greater than or less than a prescribed limit?

In the Counts per Unit dialog, enter Alpha and the Baseline Count per Unit. Then enter two of the remaining fields to see the calculation of the third. The test is for one-sided (one-tailed) change. Enter the Difference to Detect in terms of the Baseline Count per Unit (defects per unit). The computed sample size is expressed in those units, rounded to the next whole number.

As an example, consider a wafer manufacturing process with a target of 4 defects per wafer and you want to verify that a new process meets that target within a difference of 2 defects per wafer. In the Counts per Unit dialog:

9 Enter an Alpha of 0.1 to be the chance of failing the test if the new process is as good as the target.

10 Enter 4 as the Baseline Counts per Unit, indicating the target of 4 defects per wafer.

11 Enter 2 as the Difference to detect.

12 Enter a power of 0.9, which is the chance of detecting a change larger than 2 (6 defects per wafer). In this kind of situation, alpha is sometimes called the *producer's risk* and beta is called the *consumer's risk*.

13 Click **Continue** to see the results in Figure 13.12, showing a computed sample size of 9 (rounded to the next whole number).

The process meets the target if there are less than 54 defects (6 defects per wafer in a sample of 9 wafers).

Figure 13.12 Dialog For Counts Per Unit Example
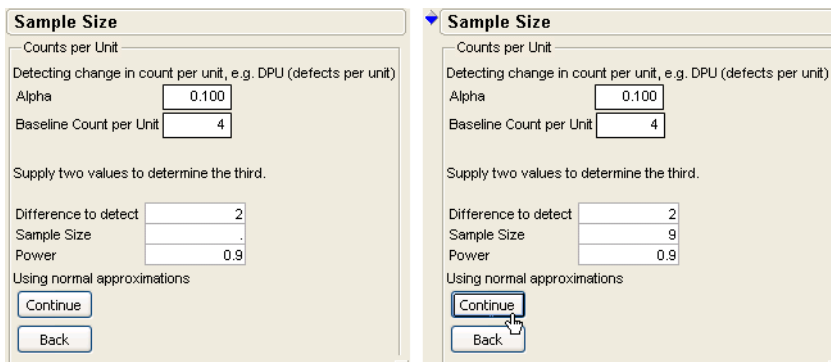
Sigma Quality Level

The Sigma Quality Level feature is a simple statistic that puts a given defect rate on a six sigma scale. For example, on a scale of one million opportunities, 3.397 defects results in a '6-sigma process. The computation that gives the Sigma Quality Level statistic is

Sigma Quality Level = NormalQuantile(1 – defects/opportunities) + 1.5

Select **DOE > Sample Size and Power** and then click the **Sigma Quality Level** button to see the Sample Size dialog:

Enter any two of the three quantities on the dialog:

- number of defects
- number of opportunities
- Sigma quality level

When you click **Continue**, the sigma quality calculator computes the missing quantity.

As an example, use the Sample Size and Power feature to compute the Sigma quality level for 50 defects in 1,000,000 opportunities:

1 Select **DOE > Sample Size and Power**.
2 Then, click the **Sigma Quality Level** button.
3 Enter 50 for the Number of Defects and 1,000,000 as the Number of Opportunities, as shown in the window to the left in Figure 13.13.
4 Click **Continue**. The results, as shown in the window on the right in Figure 13.13, are a Sigma quality level for 5.39 defects in 1,000,000 opportunities.

Figure 13.13 Sigma Quality Level Example 1

If you want to know how many defects reduce the Sigma Quality Level to 'six-sigma' for 1,000,000 opportunities, enter 6 as the Sigma Quality Level and leave the Number of Defects blank (dialog on the left in Figure 13.14). The computation (dialog on the right in Figure 13.14) shows that the Number of Defects cannot be more than approximately 3.4.

Figure 13.14 Sigma Quality Level Example 2
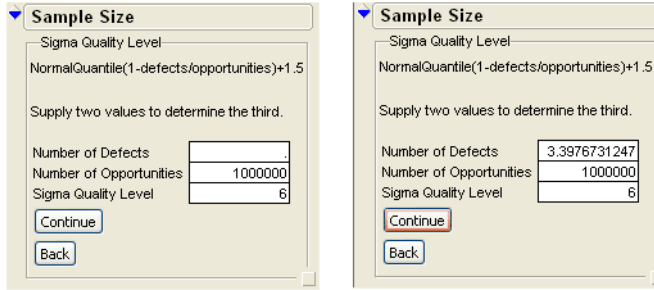
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