Part 4-1 Response Surface Methodology

Christian Leonard Quale

University of Edinburgh

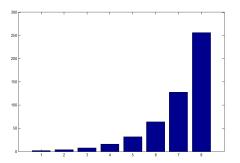
January, 2013

Response Surface Methodology - Why?

Necessity:

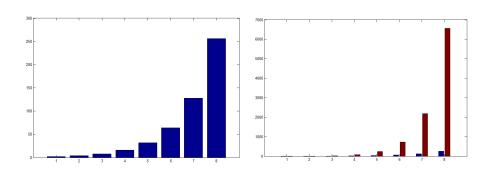
Response Surface Methodology - Why?

Necessity:



Response Surface Methodology - Why?

Necessity:



Create specialised experimental models

- ► Create specialised experimental models
- ► Perform a regression on results

- ► Create specialised experimental models
- ▶ Perform a regression on results
- Create a simplified mathematical model:

- Create specialised experimental models
- ► Perform a regression on results
- Create a simplified mathematical model:

$$Y = a_0 + a_1X1 + a_2X2 + a_3X1X2 + a_4X1^2 + a_5X2^2 + Error$$

Theoretical Model:

$$Y = \frac{15.0X1^2}{1.0 + 1.5e^{2.5X2}}$$

Theoretical Model:

$$Y = \frac{15.0X1^2}{1.0 + 1.5e^{2.5X2}}$$

Quadratic Approximation:

$$Y = a_0 + a_1X1 + a_2X2 + a_3X1X2 + a_4X1^2 + a_5X2^2$$

Theoretical Model:

$$Y = \frac{15.0X1^2}{1.0 + 1.5e^{2.5X2}}$$

Quadratic Approximation:

$$Y = a_0 + a_1 X 1 + a_2 X 2 + a_3 X 1 X 2 + a_4 X 1^2 + a_5 X 2^2$$

$$a_0 = 14.92$$
 $a_1 = 7.65$ $a_2 = -16.76$ $a_3 = 0.77$ $a_4 = -6.53$ $a_5 = 6.31$

$$2 < X1 < 3$$
 $0 < X2 < 1$

Quadratic Approximation:

$$14.92 + 7.65X1 - 16.76X2 + 0.77X1X2 - 6.53X1^2 + 6.31X2^2$$

$$2 \le X1 \le 3$$

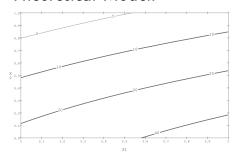
$$0 \le X2 \le 1$$

Quadratic Approximation:

$$14.92 + 7.65X1 - 16.76X2 + 0.77X1X2 - 6.53X1^2 + 6.31X2^2 \\$$

$$0 \le X2 \le 1$$

Theoretical Model:



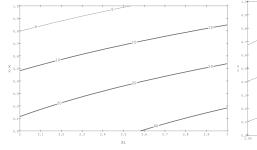
Quadratic Approximation:

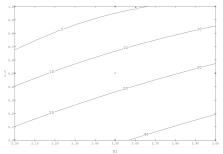
$$14.92 + 7.65X1 - 16.76X2 + 0.77X1X2 - 6.53X1^2 + 6.31X2^2$$

$$0 \le X2 \le 1$$

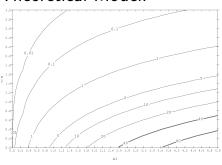
Theoretical Model:

Approximation:

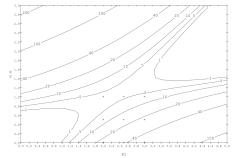




Theoretical Model:



Approximation:



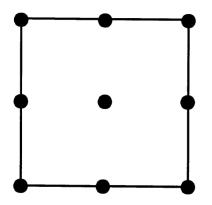
Based on Fractional Factorial Designs

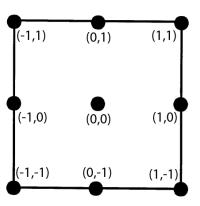
- Based on Fractional Factorial Designs
- Creates a new design suitable for regression

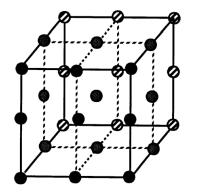
- Based on Fractional Factorial Designs
- Creates a new design suitable for regression
- Software kindly designs experimental models for us

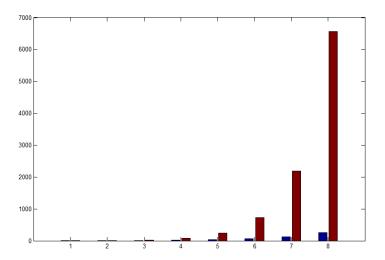
- Based on Fractional Factorial Designs
- Creates a new design suitable for regression
- Software kindly designs experimental models for us

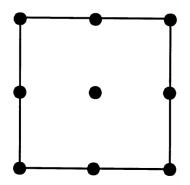
Good basis for regressions: Rotatable Designs

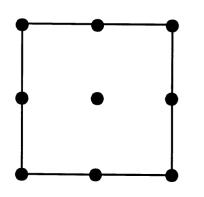


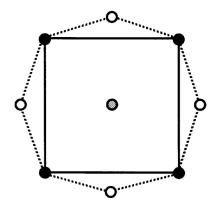


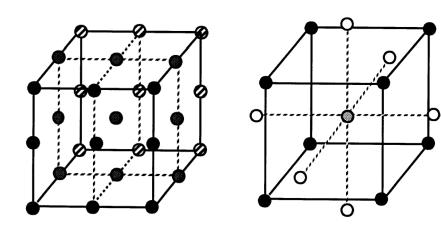


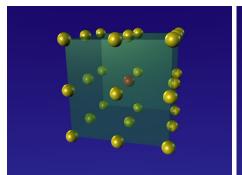


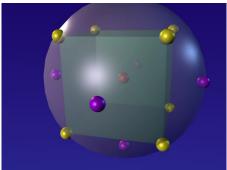


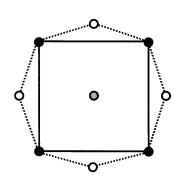


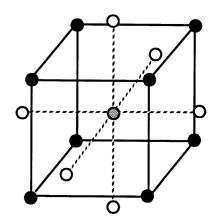






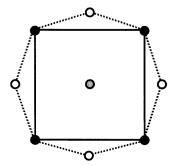




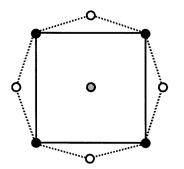


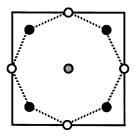
▶ Need access to 5 levels

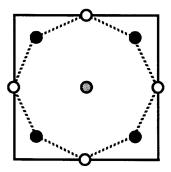
- ▶ Need access to 5 levels
- Need access above and below previously defined Max/Min points

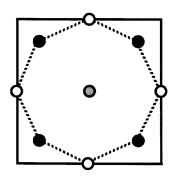


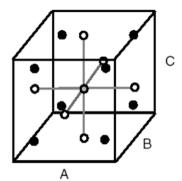
Central Composite Circumscribed Design

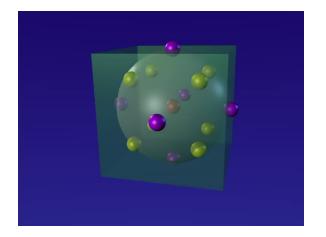






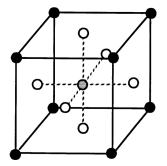


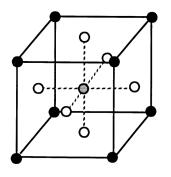


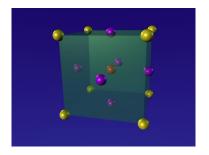


► Still need access to 5 levels

- ▶ Still need access to 5 levels
- ► Fails to test extremities







Kind of like CCC/CCI Designs...

Kind of like CCC/CCI Designs...

Only requires three levels.

Kind of like CCC/CCI Designs...

Only requires three levels.

One Major disadvantage:

Kind of like CCC/CCI Designs...

Only requires three levels.

One Major disadvantage: Not orthogonal!

Kind of like CCC/CCI Designs...

Only requires three levels.

One Major disadvantage: Not orthogonal!

Wait, what? Orthogonal?

► Blockable

- ► Blockable
- ► Can be run in batches

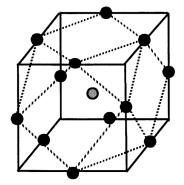
- Blockable
- Can be run in batches
- Divide experiments into groups

- ► Blockable
- Can be run in batches
- Divide experiments into groups

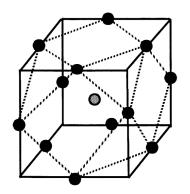
...even more options?

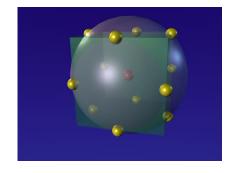
Box Behnken Design

Box Behnken Design



Box Behnken Design





D-Optimal Designs

D-Optimal Designs

The computer sorts out everything!

D-Optimal Designs

The computer sorts out everything!

Tell it how many runs you can afford, what regions you are interested in, and what model you prefer, and it will automatically design and optimal set of experimental runs for you.

How to choose?

► How close is the corner of the optimum operating region to the corner of the design region?

- ► How close is the corner of the optimum operating region to the corner of the design region?
- ▶ Do I care about orthogonality or rotatability?

- ► How close is the corner of the optimum operating region to the corner of the design region?
- ▶ Do I care about orthogonality or rotatability?
- ▶ Is it possible to experiment outside of the design-factor range?

- ► How close is the corner of the optimum operating region to the corner of the design region?
- ▶ Do I care about orthogonality or rotatability?
- ▶ Is it possible to experiment outside of the design-factor range?
- ▶ How many runs can I afford?

- ► How close is the corner of the optimum operating region to the corner of the design region?
- ▶ Do I care about orthogonality or rotatability?
- ▶ Is it possible to experiment outside of the design-factor range?
- ▶ How many runs can I afford?
- ▶ What is my personal preference?

▶ The ultimate goal is to create an RSM model.

- ▶ The ultimate goal is to create an RSM model.
- ► In the process of doing this we choose an experimental design to create a good RSM model.

- ► The ultimate goal is to create an RSM model.
- ► In the process of doing this we choose an experimental design to create a good RSM model.
- ► Different designs are all different, but valid, ways of gathering data for this model.

- ▶ The ultimate goal is to create an RSM model.
- ► In the process of doing this we choose an experimental design to create a good RSM model.
- ► Different designs are all different, but valid, ways of gathering data for this model.
- Once a good model exists, no more experiments are necessary. The magic of statistics lets you predict the likely outcome of any combination of factors without running an experiment.