A/B Testing and Beyond

Designed Experiments for Data Scientists

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Week 7

Tuesday October 16th, 2018

Outline

- Recap
- 2^{k-p} Fractional Factorial Experiments
  - Recap
  - The Chehalem Example
- Response Surface Experiments
  - The Lyft Example

RECAP

Recap

- Designing and Analyzing Factorial Experiments
  - Continuous Responses
  - Binary Responses
- Two-Level Factorial Experiments
  - 2^k Factorial Experiments

TWO-LEVEL FACTORIAL EXP'S

Two-Level Factorial Experiments

- When investigating k factors, two-level factorial experiments are the smallest possible factorial experiments

- Such experiments are typically used for factor screening

- Pareto Principle: only *a vital few* factors are important relative to the *trivial many*

- The purpose of a screening experiment is to identify this small number of influential factors

TWO-LEVEL FACTORIAL EXP'S

Two-Level Factorial Experiments

Here we discuss two particular types of two-level factorial experiments for investigating k factors:

- 2^k factorial experiments
  - These investigate each of the unique 2^k conditions
- 2^{k-p} fractional factorial experiments
  - These investigate just a *fraction* of the unique 2^k conditions

2^k FACTORIAL EXPERIMENTS

Designing 2^k Factorial Experiments

Step 1: Choose k factors that are expected to influence the response in some way

Step 2: Choose two levels for each factor to experiment with

- It's important to choose levels that provide the largest opportunity for an influential factor to be noticed
- Levels should be chosen that are quite different from one another; even a very influential factor may not appear to be influential if the factor levels are too similar.

2^k FACTORIAL EXPERIMENTS

Designing 2^k Factorial Experiments

Step 3: The experimental conditions are defined to be the unique combination of these factors' levels

- There will be 2^k of them

Step 4: Assign experimental units to each of the 2^k conditions

- For ease of notation, we assume that the experiment is balanced and n units are assigned to each condition
- The sample size n can be determined by power analyses based on two-sample tests that account for the multiple comparison problem

2^k FACTORIAL EXPERIMENTS

Designing 2^k Factorial Experiments

- Using the ± 1 coding, each experimental condition can be identified by a unique combination of plus and minus ones
- The design of the experiment can be displayed in what is known as a design matrix
- Using the data collected from such a study we fit a linear or logistic regression model
- Let's review some design matrices

2^k FACTORIAL EXPERIMENTS

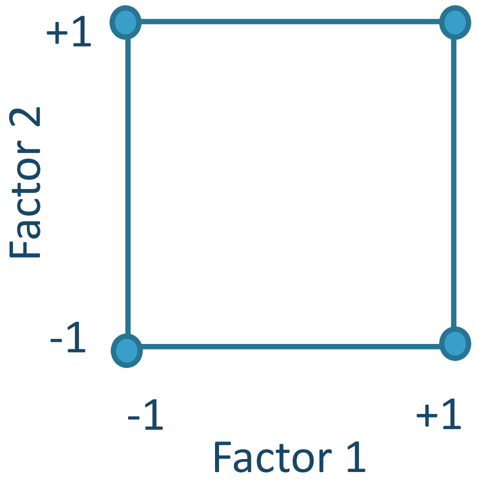
A 2^1 Factorial Experiment (i.e., an A/B test)

Condition	Factor 1
1	-1
2	+1

2^k FACTORIAL EXPERIMENTS

A 2^2 Factorial Experiment

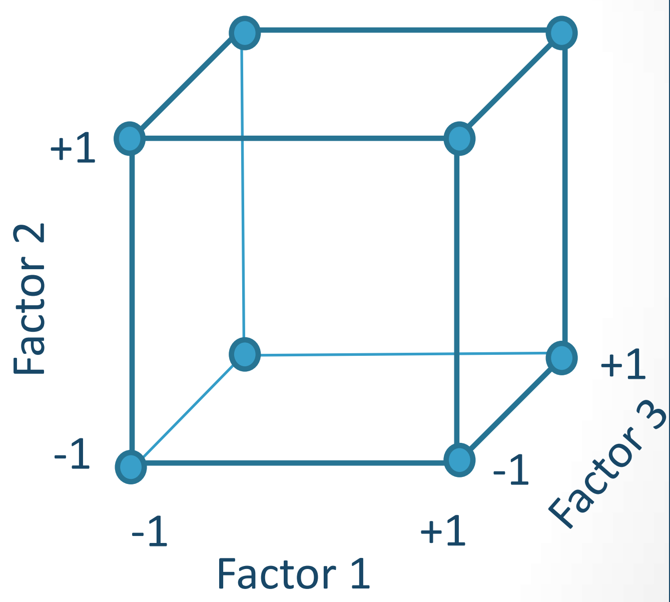
Condition	Factor 1	Factor 2
1	-1	-1
2	+1	-1
3	-1	+1
4	+1	+1



2^k FACTORIAL EXPERIMENTS

A 2^3 Factorial Experiment

Condition	Factor 1	Factor 2	Factor 3
1	-1	-1	-1
2	+1	-1	-1
3	-1	+1	-1
4	+1	+1	-1
5	-1	-1	+1
6	+1	-1	+1
7	-1	+1	+1
8	+1	+1	+1



2^k FACTORIAL EXPERIMENTS

Analyzing 2^k Factorial Experiments

- Using the data collected from such a study we fit a linear or logistic regression model
- Apart from this difference, the models are similar in that
  - they are based on exactly the same linear predictor
  - we can evaluate the significance of main and interaction effects by performing tests concerning individual or multiple β's (although the specific tests that are used differ in the two settings)

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

- 2^k factorial experiments are a useful special case of a general factorial experiment
  - They minimize the number of levels being investigated, and hence reduces the overall number of experimental conditions
- BUT they still investigate **all possible** combinations of the factor levels – which can be a lot!
  - With $k = 8$ factors the 2^k factorial experiment has 256 conditions

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

- Alternatively we could use a 2^{k-p} fractional factorial experiment which also investigates k factors, but with just a fraction of the conditions
- Rather than performing 2^k conditions, we perform 2^{k-p} specially selected conditions which still allow us to estimate main effects and potentially important interaction effects
- **With these experiments we can investigate a relatively large number of factors with a relatively small number of conditions**
- However, we sacrifice the ability to separately estimate *all* main and interaction effects

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

Motivation: the linear predictor for a 2^k factorial experiment consists of

- $\binom{k}{1} = k$ main effect terms
- $\binom{k}{2}$ two-factor interaction terms
- $\vdots$
- $\binom{k}{k} = 1$ k-factor interaction term

That's a total of $\sum_{i=1}^{k} \binom{k}{i} = 2^k - 1$ terms

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

- Of these $2^k - 1$ terms, only $k + \binom{k}{2}$ of them are main effects and two factor interactions – the remaining correspond to higher order interaction terms

- If $k = 8$, there are 8 main effects, 28 two-factor interactions and 219 higher order interactions, many of which are likely to be insignificant

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

- Principle of effect sparsity: in the presence of several factors, variation in the response is likely to be driven by a **small number of main effects and low-order interactions**
- Thus, it is typically a waste of resources to estimate these higher order interaction terms
- It is a better use of these resources is to estimate the main effects and low-order interactions of a larger number of factors
- So how do we do this?

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

First let's discuss p:

- Investigating k factors in a full factorial experiments takes 2^k conditions
- If we'd like to investigate k factors in half as many conditions, we use a 2^{k-1} experiment
- If we'd like to investigate k factors with just a quarter of the conditions, we use a 2^{k-2} experiment
- In general, if we'd like to investigate k factors in $(1/2)^p$ as many conditions, we use a 2^{k-p} experiment

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

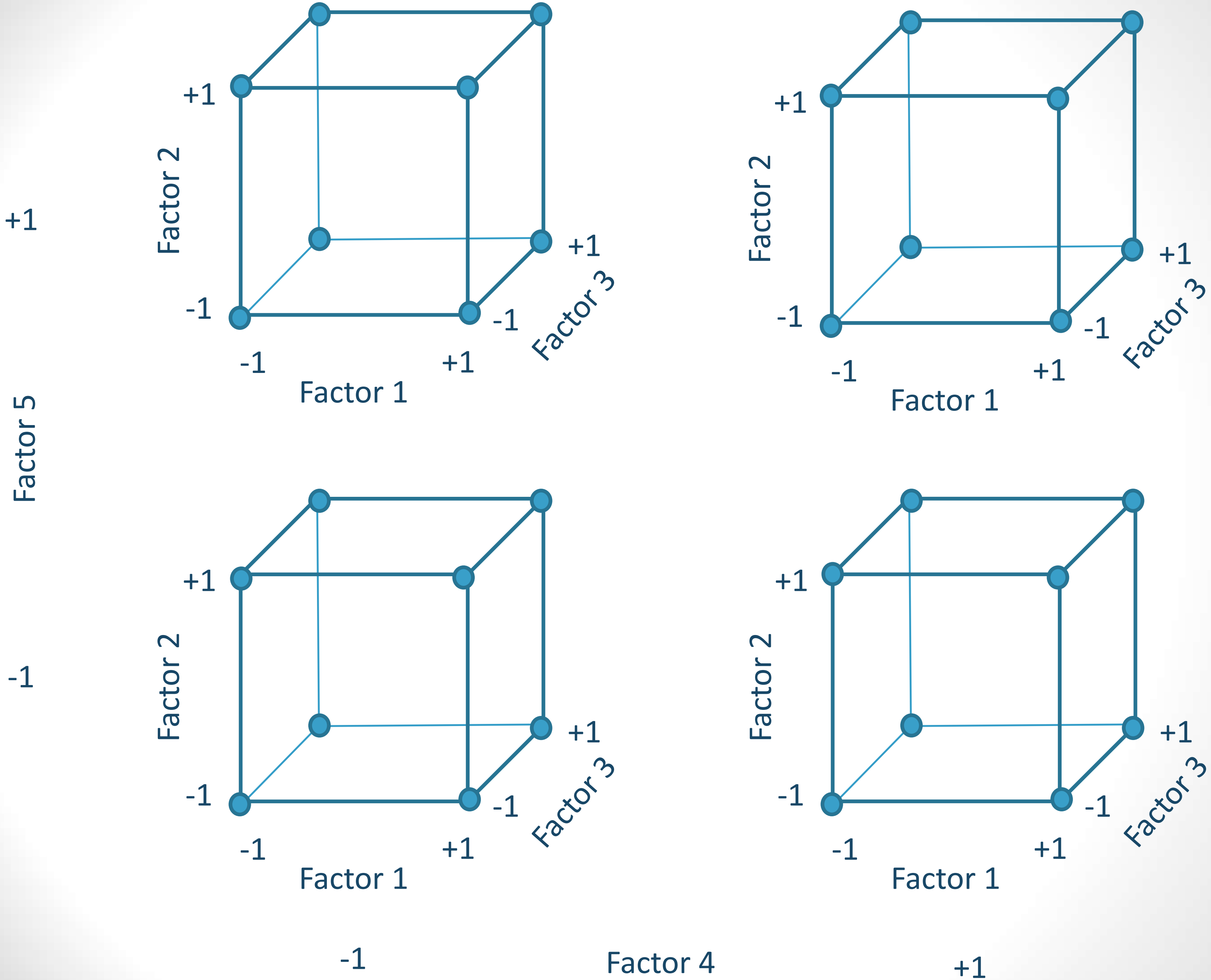
- If a full factorial approach requires 2^k conditions and we only want 2^{k-p}, we need to choose **which** 2^{k-p} conditions to experiment with

- For instance, if $k = 5$ and $p = 2$, then the goal is to investigate 5 factors in $2^3 = 8$ conditions (where normally 32 conditions would be required with the full factorial approach).

- The question is, among these 32 conditions, which 8 do we choose to for the 2^{5-2} fractional design?

Condition	A	B	C	D	E
1	-1	-1	-1	-1	-1
2	+1	-1	-1	-1	-1
3	-1	+1	-1	-1	-1
4	+1	+1	-1	-1	-1
5	-1	-1	+1	-1	-1
6	+1	-1	+1	-1	-1
7	-1	+1	+1	-1	-1
8	+1	+1	+1	-1	-1
9	-1	-1	-1	+1	-1
10	+1	-1	-1	+1	-1
11	-1	+1	-1	+1	-1
12	+1	+1	-1	+1	-1
13	-1	-1	+1	+1	-1
14	+1	-1	+1	+1	-1
15	-1	+1	+1	+1	-1
16	+1	+1	+1	+1	-1

Condition	A	B	C	D	E
17	-1	-1	-1	-1	+1
18	+1	-1	-1	-1	+1
19	-1	+1	-1	-1	+1
20	+1	+1	-1	-1	+1
21	-1	-1	+1	-1	+1
22	+1	-1	+1	-1	+1
23	-1	+1	+1	-1	+1
24	+1	+1	+1	-1	+1
25	-1	-1	-1	+1	+1
26	+1	-1	-1	+1	+1
27	-1	+1	-1	+1	+1
28	+1	+1	-1	+1	+1
29	-1	-1	+1	+1	+1
30	+1	-1	+1	+1	+1
31	-1	+1	+1	+1	+1
32	+1	+1	+1	+1	+1



+1
Factor 5
-1
Factor 2
+1
-1
Factor 1
-1
+1
Factor 3
-1
+1
Factor 4
-1
+1

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

- To answer this, we consider an extended version of the design matrix associated with a full 2^3 factorial experiment

Condition	A	B	C	AB	AC	BC	ABC
1	-1	-1	-1	+1	+1	+1	-1
2	+1	-1	-1	-1	-1	+1	+1
3	-1	+1	-1	-1	+1	-1	+1
4	+1	+1	-1	+1	-1	-1	-1
5	-1	-1	+1	+1	-1	-1	+1
6	+1	-1	+1	-1	+1	-1	-1
7	-1	+1	+1	-1	-1	+1	-1
8	+1	+1	+1	+1	+1	+1	+1

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

- When it comes to fitting a regression model, each column in this matrix is used to estimate the corresponding effect a particular effect
- For instance:
  - the AB column is used to estimate β_{AB}, the interaction effect between factors A and B
  - the ABC column is used to estimate β_{ABC}, the interaction effect between factors A, B and C
- Now recall the effect sparsity principle: if an interaction is likely to be negligible, why not use its column to dictate the levels of an extra factor?

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

For example:

- Let's use the ± 1's in the ABC column as a prescription for when to run D at its low and high levels

- Let's use the ± 1's in the BC column as a prescription for when to run E at its low and high levels

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

Condition	A	B	C	AB	AC	E=BC	D=ABC
1	-1	-1	-1	+1	+1	+1	-1
2	+1	-1	-1	-1	-1	+1	+1
3	-1	+1	-1	-1	+1	-1	+1
4	+1	+1	-1	+1	-1	-1	-1
5	-1	-1	+1	+1	-1	-1	+1
6	+1	-1	+1	-1	+1	-1	-1
7	-1	+1	+1	-1	-1	+1	-1
8	+1	+1	+1	+1	+1	+1	+1

- Here we say that D and ABC are aliased and E and BC are aliased
- 'D=ABC' and 'E=BC' are called the design generators

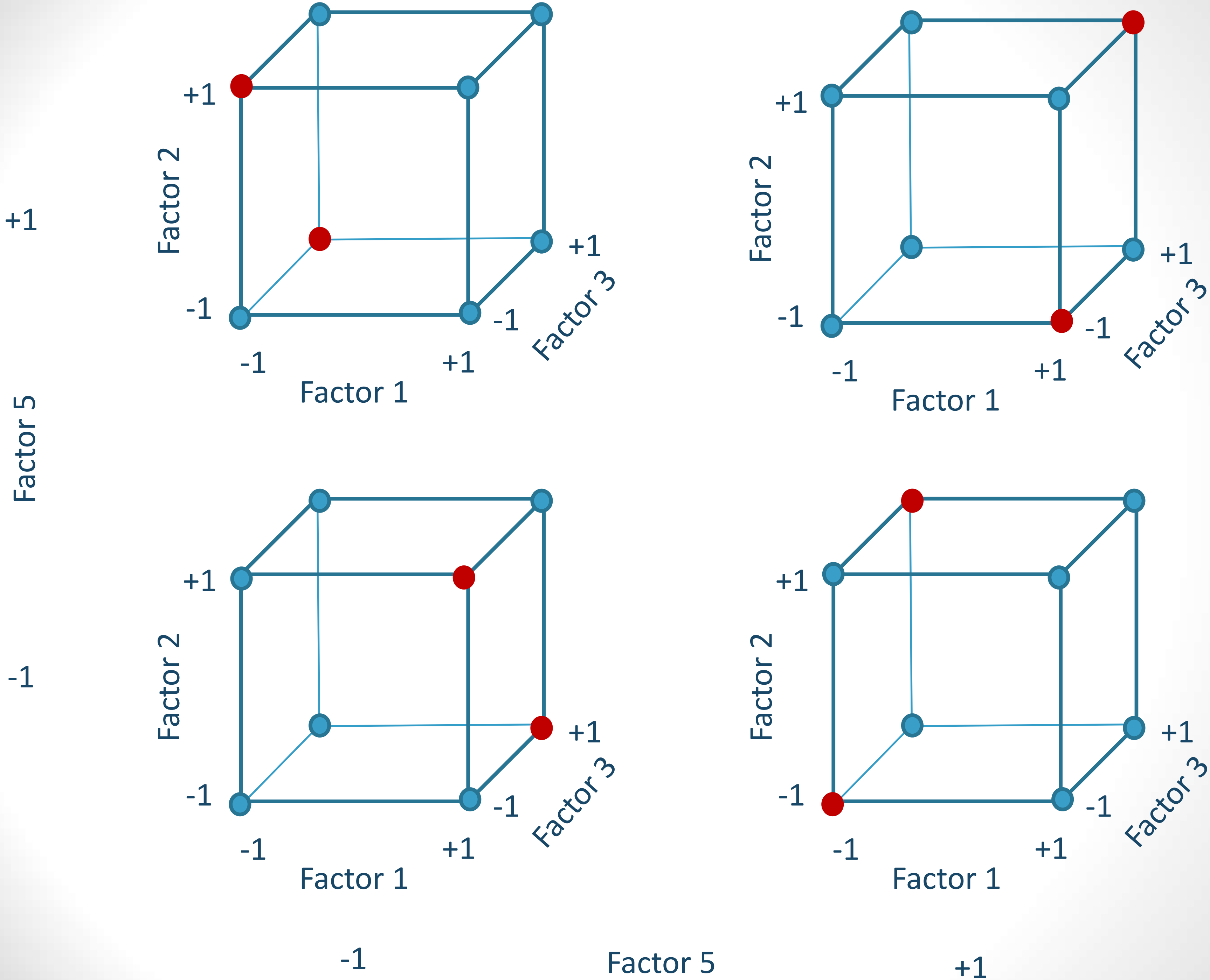
2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

The design matrix indicating the levels of factors A, B, C, D, and E in each condition is shown below

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

These are a subset of the 32 conditions required in a full 2^5 factorial experiment



+1
Factor 2
-1
-1
+1
Factor 1
+1
-1
Factor 3
+1
Factor 2
-1
-1
+1
Factor 1
+1
-1
Factor 3
+1
Factor 2
-1
-1
+1
Factor 1
+1
-1
Factor 3
+1
Factor 2
-1
-1
+1
Factor 1
+1
-1
Factor 3
+1
-1
Factor 5
-1
Factor 5
+1

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

- When two terms are aliased, their effects become confounded
- For instance the D=ABC column estimates the ABC interaction **and** the main effect of D
- So the coefficient β_{ABC} quantifies the joint effects of the ABC interaction and the main effect of factor D
- Thus, we cannot separately estimate the main effect of D from the ABC interaction effect

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

- Thus confounding results from aliasing a new main effect with an existing interaction
- As such, it is important to think carefully about **which** interaction to choose as an alias
- It is best to avoid aliasing a new factor with an interaction that is likely to be significant (since separately estimating significant effects is desirable)
- So high order interaction terms (that are unlikely to be significant) are good choices for aliases

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

- This notion is quantified by the resolution of the fractional factorial design
- A design is of resolution R if main effects are aliased with interaction effects involving at least $R-1$ factors
- In the design we've been discussing main effects are aliased with two- and three-factor interactions
- Thus it is a resolution III experiment denoted by

$$2_{III}^{5-2}$$

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

- In general, higher resolution designs are to be preferred over lower resolution designs.
- For instance, resolution IV and V designs are to be preferred over a resolution III designs
- In these cases main effects will not be confounded with two-factor interactions
- Since two-factor interactions are typically important, it is best if their effects are not confounded with main effects

2^{k-p} FRACTIONAL FACTORIAL

Designing 2^{k-p} Fractional Factorial Experiments

- The resolution of a fractional factorial experiment is determined by two things:
  1. The degree of fractionation desired (i.e., the size of p relative to k)
  2. The design generators chosen for aliasing
- The degree of fractionation is typically determined by resource constraints – how many conditions can you manage?
- Given the degree of fractionation (p) we typically choose design generators to maximize resolution

2^{k-p} FRACTIONAL FACTORIAL

Analyzing 2^{k-p} Fractional Factorial Experiments

- The analysis of these fractional factorial experiments is based on regression models
  - Linear regression (if Y is continuous)
  - Logistic regression (if Y is binary)

- In fact, the analysis is not very different from what we saw in the credit card example
  - We perform individual and simultaneous hypothesis tests to compare full and reduced models
  - This allows us to evaluate the significance of various main and interaction effects

2^{k-p} FRACTIONAL FACTORIAL

Analyzing 2^{k-p} Fractional Factorial Experiments

The wrinkle:

- Here the effects estimated in these models are confounded with other effects
- So we can't be 100% certain that a given effect is due to say a main effect, or perhaps the interaction it is aliased with
- But, if the resolution is high, we hope that important effects are aliased with high-order interactions (that are likely negligible)
- This provides confidence that significant effects are not due to the high-order interactions

2^{k-p} FRACTIONAL FACTORIAL

Example: The Chehalem Experiment

Chehalem is a winery in Newberg Oregon that regularly uses experiments to develop and refine wine recipes. Montgomery (2017) discusses a 2_{IV}^{8-4} fractional factorial experiment that was used to investigate $k = 8$ factors with just 16 conditions.

The goal of the experiment was to evaluate and quantify the influence of several factors on the quality of the wine. The response variable here is a tasting score provided subjectively by $n = 5$ taste-testers.

2^{k-p} FRACTIONAL FACTORIAL

Example: The Chehalem Experiment

Factor	Low (-)	High (+)
Pinot Noir clone (A)	Pommard	Wadenswil
Oak type (B)	Allier	Troncais
Age of barrel (C)	Old	New
Yeast/Skin contact (D)	Champagne	Montrachet
Stems (E)	None	All
Barrel toast (F)	Light	Medium
Whole cluster (G)	None	10%
Fermentation Temperature (H)	Low (75˚F max)	High (92˚F max)

Condition	A	B	C	D	E	F	G	H	Avg. Rating
1	-1	-1	-1	-1	-1	-1	-1	-1	9.6
2	+1	-1	-1	-1	-1	+1	+1	+1	10.8
3	-1	+1	-1	-1	+1	-1	+1	+1	12.6
4	+1	+1	-1	-1	+1	+1	-1	-1	9.2
5	-1	-1	+1	-1	+1	+1	+1	-1	9.0
6	+1	-1	+1	-1	+1	-1	-1	+1	15.0
7	-1	+1	+1	-1	-1	+1	-1	+1	5.0
8	+1	+1	+1	-1	-1	-1	+1	-1	15.2
9	-1	-1	-1	+1	+1	+1	-1	+1	2.2
10	+1	-1	-1	+1	+1	-1	+1	-1	7.0
11	-1	+1	-1	+1	-1	+1	+1	-1	8.8
12	+1	+1	-1	+1	-1	-1	-1	+1	2.8
13	-1	-1	+1	+1	-1	-1	+1	+1	4.6
14	+1	-1	+1	+1	-1	+1	-1	-1	2.4
15	-1	+1	+1	+1	+1	-1	-1	-1	9.2
16	+1	+1	+1	+1	+1	+1	+1	+1	12.6

2^{k-p} FRACTIONAL FACTORIAL

Example: The Chehalem Experiment

- Because the response variable is continuous we use linear regression for this analysis
- Because only 2^4=16 conditions were used, we can only fit a model with 16 regression coefficients
- In the context of a full 2^4 factorial experiment this corresponds to a model with
  - 4 main effects
  - 6 two-factor interactions
  - 4 three-factor interactions
  - 1 four-factor interaction

```
Coefficients:
                Estimate Std. Error t value  Pr(>|t|)
(Intercept)  8.5000    0.2658    31.985   < 2e-16 ***
A            0.8750    0.2658     3.293   0.001619 **
B            0.9250    0.2658     3.481   0.000906 ***
C            0.6250    0.2658     2.352   0.021772 *
D           -2.3000    0.2658    -8.655   2.27e-12 ***
A:B         -0.3500    0.2658    -1.317   0.192532
A:C          1.3000    0.2658     4.892   7.07e-06 ***
B:C          0.4500    0.2658     1.693   0.095261 .
A:D         -0.8750    0.2658    -3.293   0.001619 **
B:D          1.2250    0.2658     4.610   1.98e-05 ***
C:D          0.3750    0.2658     1.411   0.163063
A:B:C        1.5750    0.2658     5.927   1.35e-07 ***
A:B:D       -0.3000    0.2658    -1.129   0.263168
A:C:D       -1.0000    0.2658    -3.763   0.000367 ***
B:C:D        1.1000    0.2658     4.139   0.000104 ***
A:B:C:D      0.4750    0.2658     1.787   0.078613 .
---
Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
Residual standard error: 2.377 on 64 degrees of freedom
Multiple R-squared: 0.7873,Adjusted R-squared: 0.7374
F-statistic: 15.79 on 15 and 64 DF, p-value: 4.547e-16
```

2^{k-p} FRACTIONAL FACTORIAL

Example: The Chehalem Experiment

- Notice this output does not involve the factors E, F, G or H – it only directly references factors A, B, C and D

- However, because of the confounding associated with the aliasing in this experiment
  - BCD interaction estimate corresponds to E's main effect
  - ACD interaction estimate corresponds to F's main effect
  - ABC interaction estimate corresponds to G's main effect
  - ABD interaction estimate corresponds to H's main effect

```
Coefficients:
             Estimate Std. Error  t value   Pr(>|t|)
(Intercept) 8.5000    0.2658     31.985    < 2e-16 ***
A            0.8750    0.2658      3.293    0.001619 **
B            0.9250    0.2658      3.481    0.000906 ***
C            0.6250    0.2658      2.352    0.021772 *
D           -2.3000    0.2658     -8.655    2.27e-12 ***
E            1.1000    0.2658      4.139    0.000104 ***
F           -1.0000    0.2658     -3.763    0.000367 ***
G            1.5750    0.2658      5.927    1.35e-07 ***
H           -0.3000    0.2658     -1.129    0.263168
A:B         -0.3500    0.2658     -1.317    0.192532
A:C          1.3000    0.2658      4.892    7.07e-06 ***
A:D         -0.8750    0.2658     -3.293    0.001619 **
A:E          0.4750    0.2658      1.787    0.078613 .
A:F          0.3750    0.2658      1.411    0.163063
A:G          0.4500    0.2658      1.693    0.095261 .
A:H          1.2250    0.2658      4.610    1.98e-05 ***
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Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
Residual standard error: 2.377 on 64 degrees of freedom
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F-statistic: 15.79 on 15 and 64 DF, p-value: 4.547e-16
```

2^{k-p} FRACTIONAL FACTORIAL

Example: The Chehalem Experiment

- All of the main effects – except H (fermentation temperature) – are significant
- Factors D, E, F, G (yeast/skin contact, stems, barrel toast, whole cluster) are most influential
- AC, AH and AD interactions are also significant
- Because of aliasing and confounding, it is equivalent to conclude that the DF, FG and EG interactions are significant
- Because factors D, E, F and G are most influential, it is likely that the DF, FG and EG interactions are responsible for the significant effect

2^{k-p} FRACTIONAL FACTORIAL

Example: The Chehalem Experiment

- Note that partial *F*-test of

$$H_0: \beta_H = \beta_{AB} = \beta_{AE} = \beta_{AF} = \beta_{AG} = 0$$

which compares the full model above to the one that is reduced by H_0 has an associated p-value of

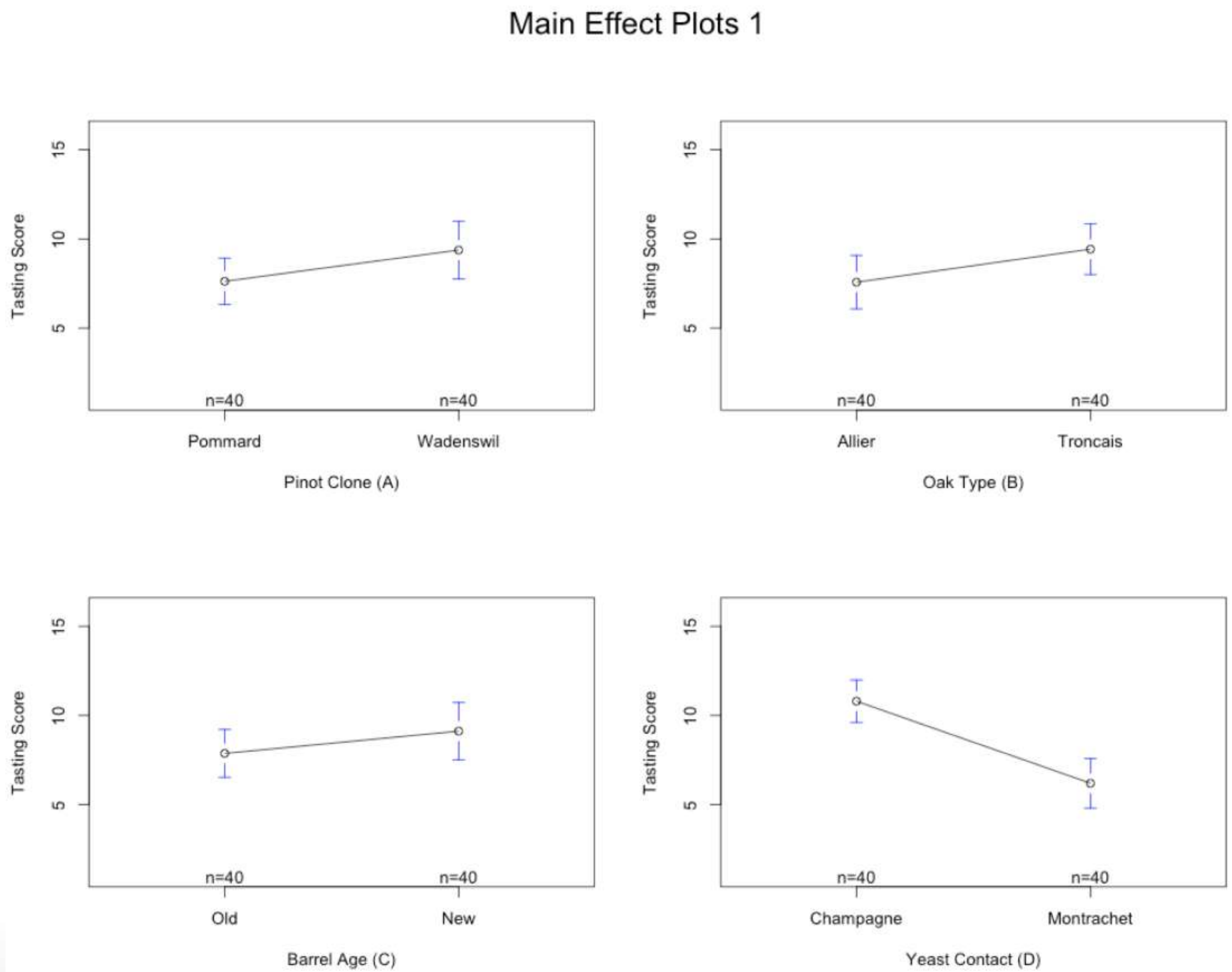
$$P(T \geq 2.2124) = 0.06375$$

where $T \sim F(5, 64)$

- Thus we do not reject H_0 and we conclude that all factors other than H are significantly influential, and the DF, FG and EG interactions are statistically significant

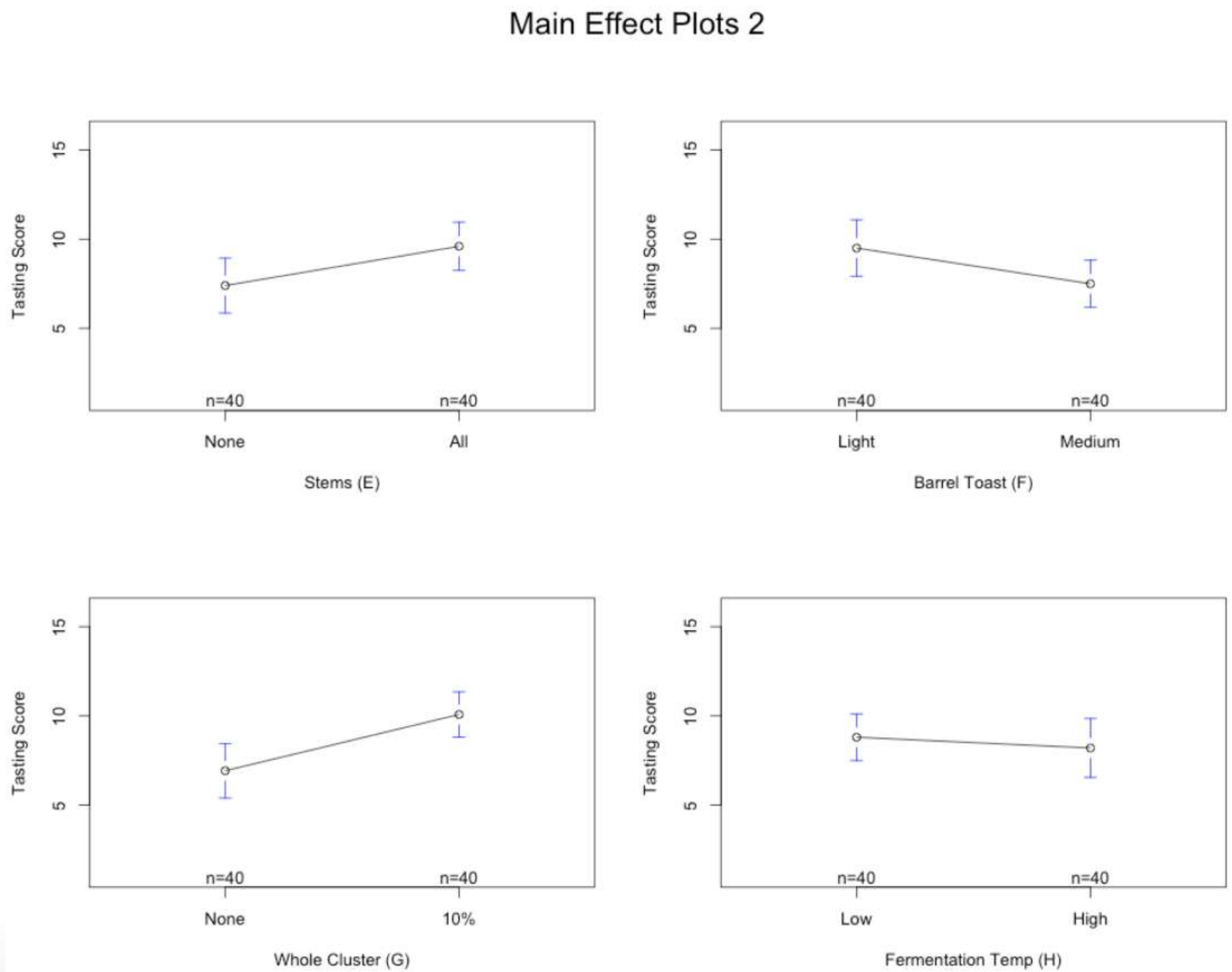
2^{k-p} FRACTIONAL FACTORIAL

Example: The Chehalem Experiment



2^{k-p} FRACTIONAL FACTORIAL

Example: The Chehalem Experiment



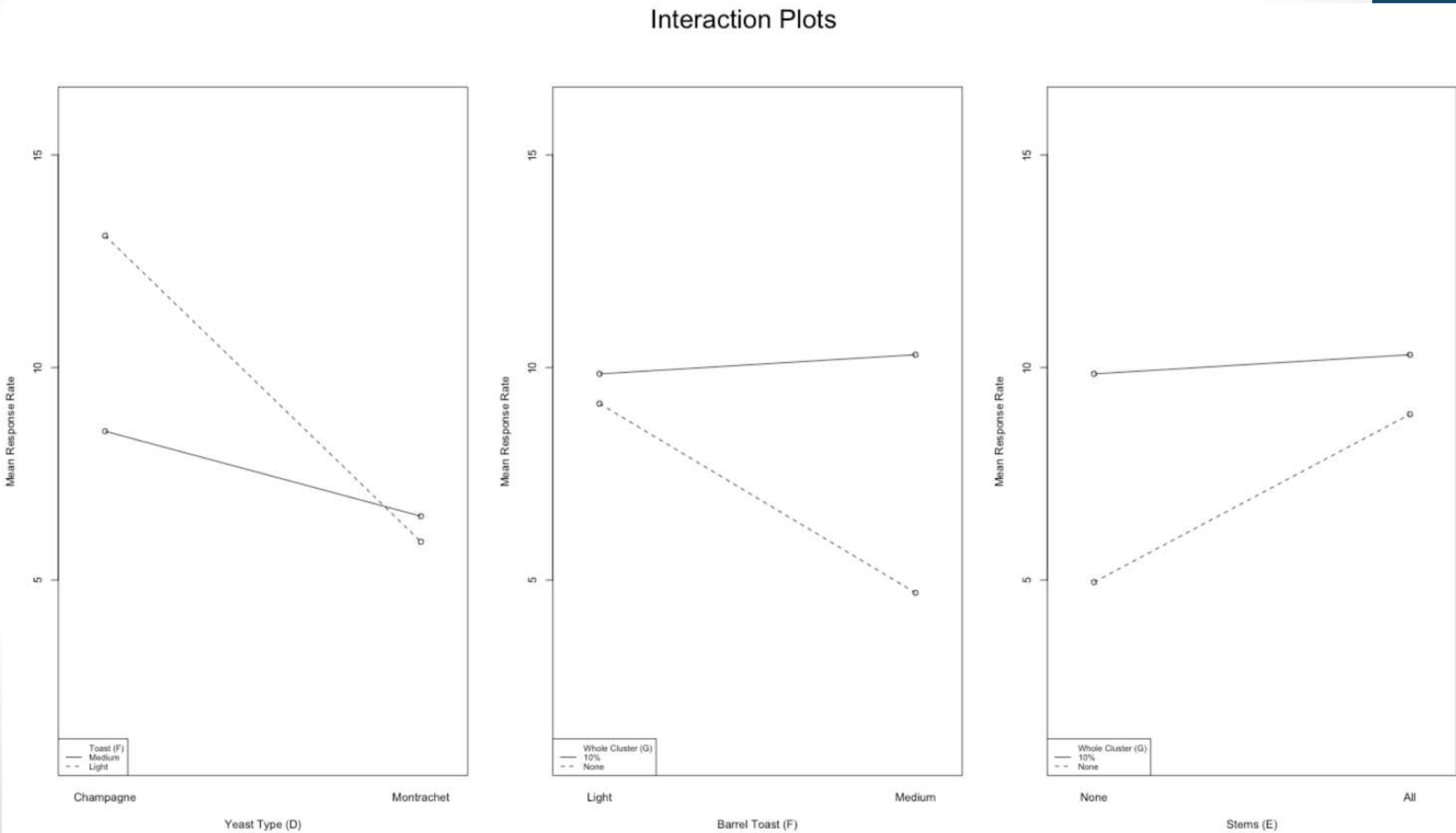
2^{k-p} FRACTIONAL FACTORIAL

Example: The Chehalem Experiment

- The main effect plots suggest that:
  - yeast type (D) and the amount of whole clusters (G) used during fermentation are most important, with no whole clusters and Montrachet yeast producing a better tasting Pinot Noir
  - medium barrel toast (F) and no stems (E) also seem to correspond to a better tasting wine

2^{k-p} FRACTIONAL FACTORIAL

Example: The Chehalem Experiment



2^{k-p} FRACTIONAL FACTORIAL

Example: The Chehalem Experiment

- The interaction effect plots suggest that:
  - If yeast type is Montrachet, the level of barrel toasting doesn't matter much, but if yeast type is Champagne, a medium barrel toast is best.
  - If barrel toast is chosen to be medium, then not including any whole-clusters is best
  - If using none of the stems, then it is also best not to include any whole-clusters

Response Surface Methodology

Response Surface Methodology

Recall the goal of screening experiments:

- Identify which, among a large number of factors, are the ones that influence the response

We used 2-level designs to achieve this goal

- 2^k full factorial
- 2^{k-p} fractional factorial

What next?

Response Surface Methodology

Once we’ve identified which factors are influential, follow-up experiments can tell us how they influence the response

When response optimization is the goal, follow-up experiments can help us identify optimal settings for each of the important factors

i.e., find factor levels that maximize/minimize the metric of interest

Response Surface Methodology

This can be achieved by fitting response surfaces

Suppose a response Y depends on k factors $x_1, x_2, \dots, x_k$ through some unknown functional relationship:

$$Y = f(x_1, x_2, \dots, x_k)$$

We refer to this relationship as a response surface, and through response surface designs we fit models which attempt to approximate $f(\cdot)$

Response Surface Methodology

We rely on Taylor's Theorem and use first and second-order models as an approximation of the true response surface $f(\cdot)$

The linear predictors in such models include

- Main effects
- Two-way interaction effects
- Quadratic effects

Response Surface Methodology

- Main effects only:

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k$$

- Main effects plus two-way interactions

$$\beta_0 + \sum_{j=1}^{k} \beta_j x_j + \sum_{j<l} \beta_{jl} x_j x_l$$

- Main effects, two-way interactions and quadratic effects:

$$\beta_0 + \sum_{j=1}^{k} \beta_j x_j + \sum_{j<l} \beta_{jl} x_j x_l + \sum_{j=1}^{k} \beta_{jj} x_j^2$$

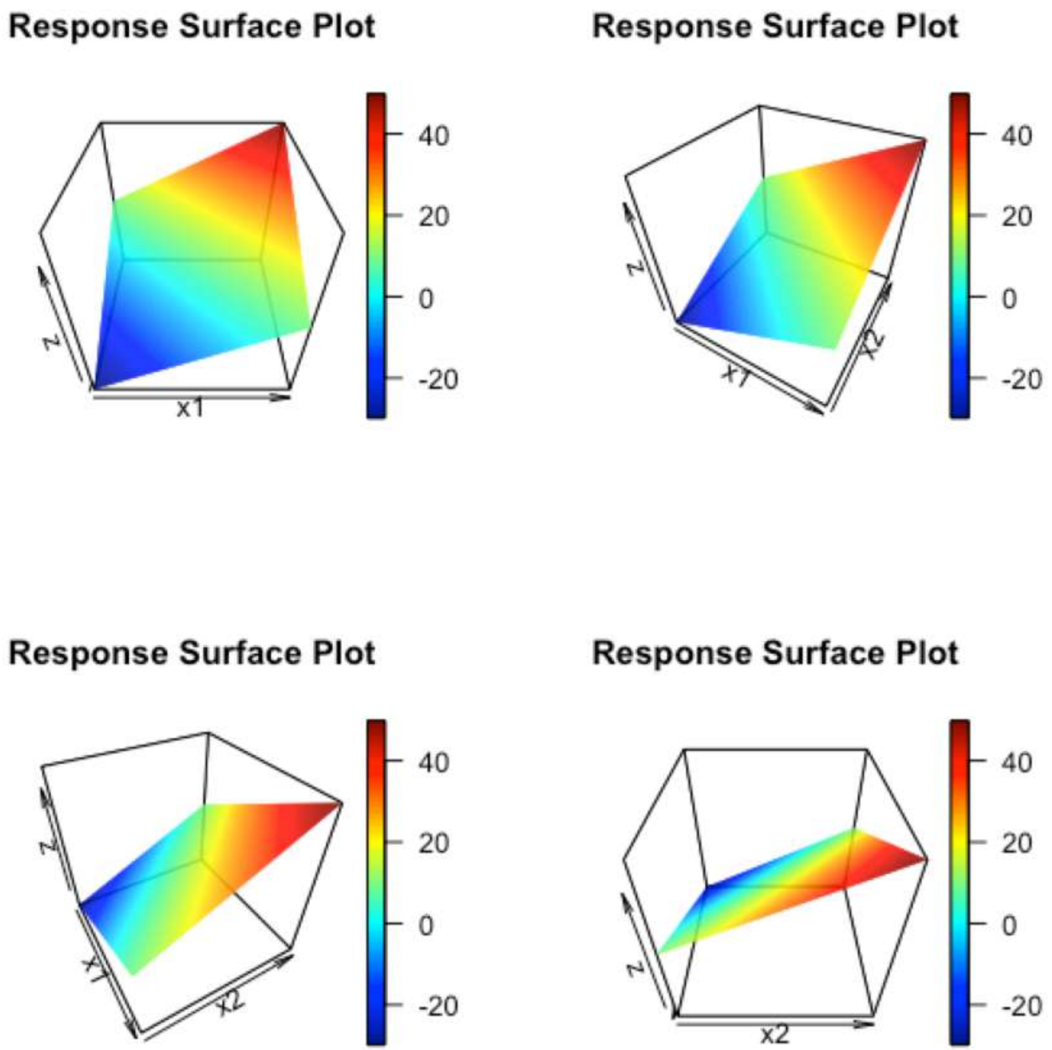
Response Surface Methodology

In three dimensions (i.e, Y, x_1, x_2) these response surfaces can be visualized using either 2D contour plots or 3D surface plots

- First order: plane
- First order + interaction: twisted plane
- Second order: surface with curvature

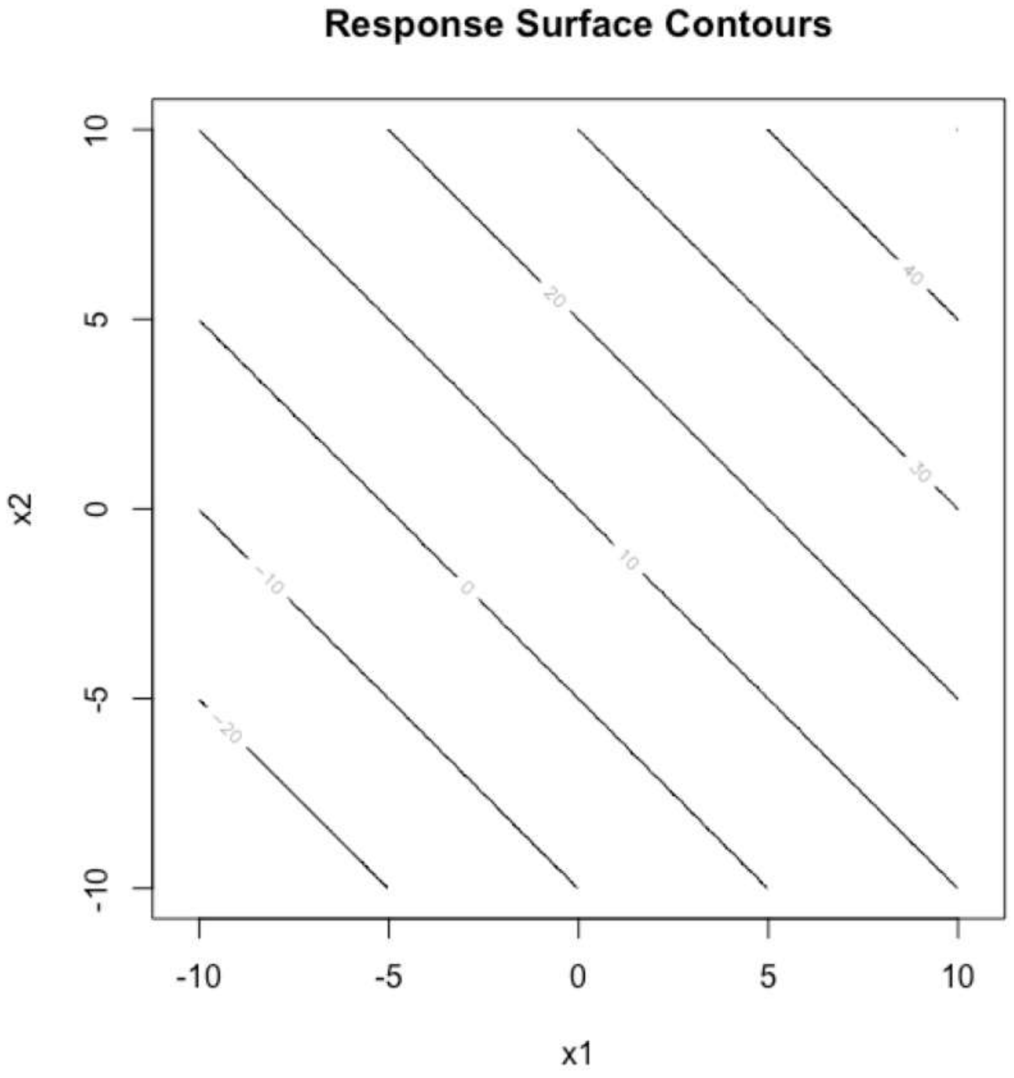
Response Surface Methodology

First-order response surfaces



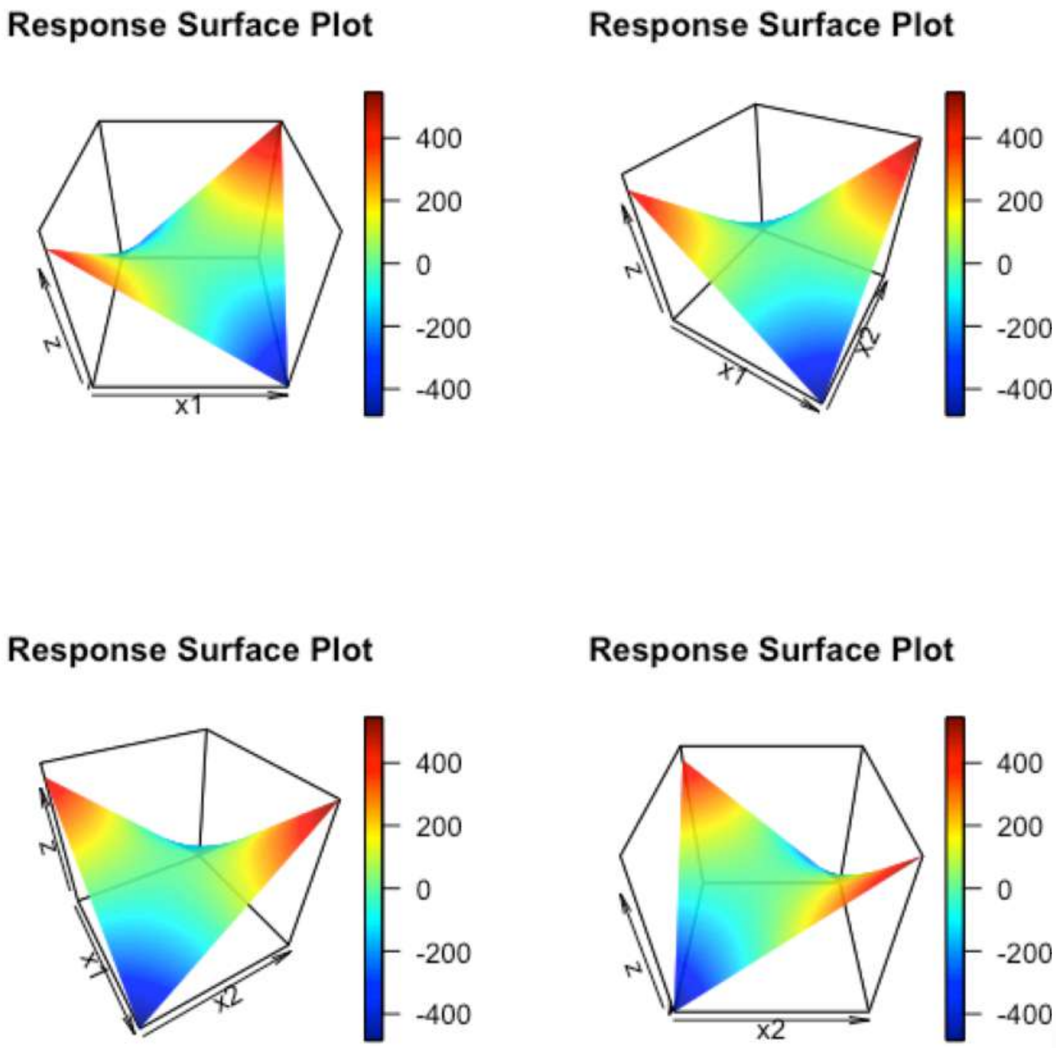
Response Surface Methodology

First-order response surfaces



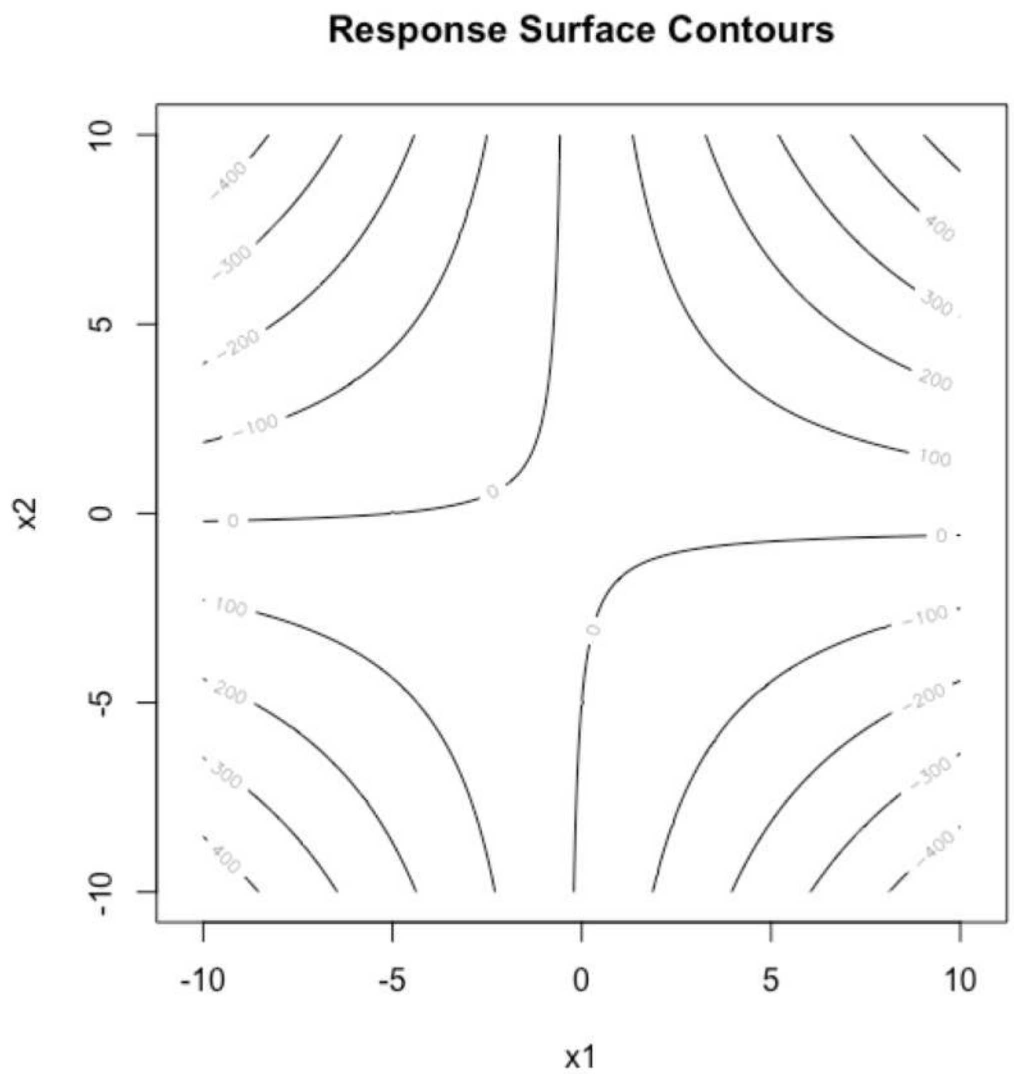
Response Surface Methodology

First-order response surfaces with interaction



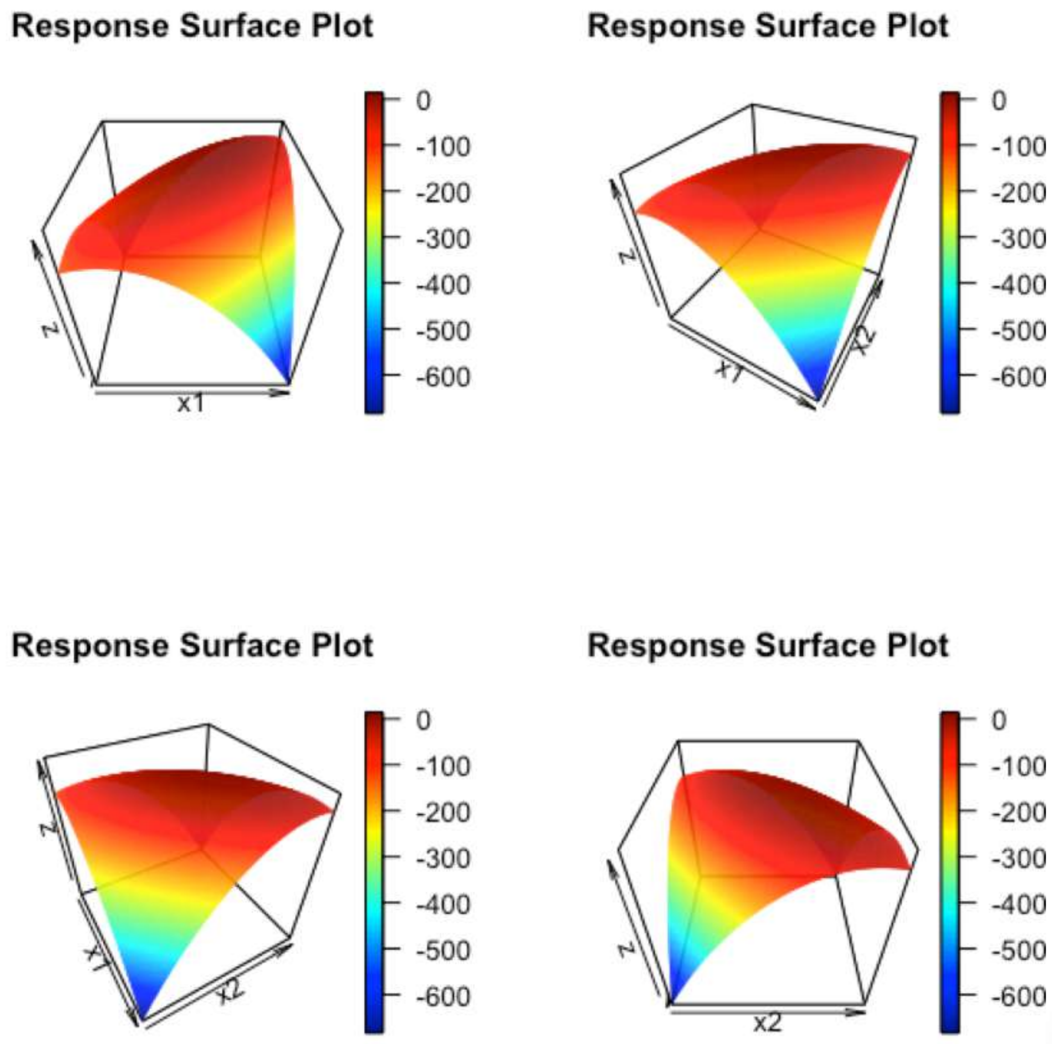
Response Surface Methodology

First-order response surfaces with interaction



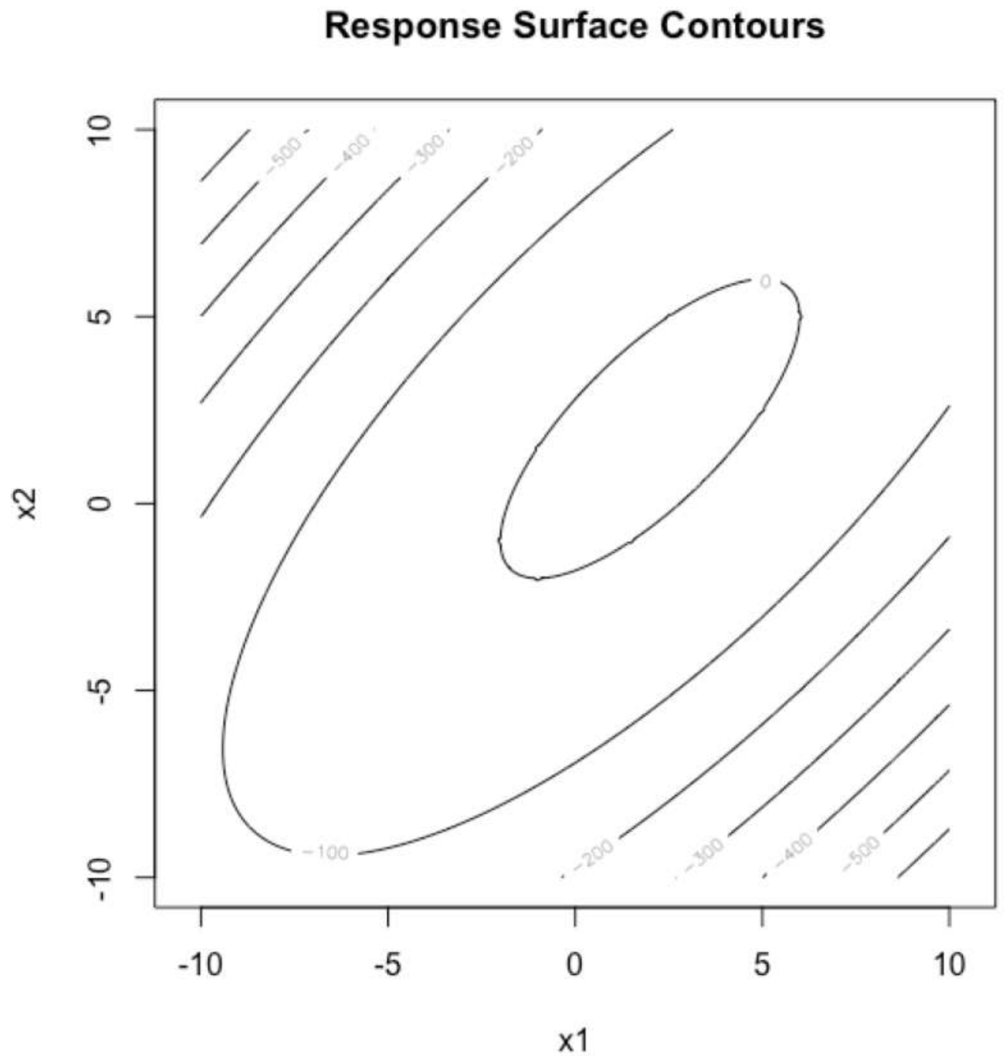
Response Surface Methodology

Second-order response surfaces



Response Surface Methodology

Second-order response surfaces



Response Surface Methodology

We estimate these surfaces by estimating the β's in the corresponding linear predictors

The surface (model) we pick depends on our goal:

- Factor screening: first order
- Response optimization: second order

Note that these approximations of $f(\cdot)$ are unlikely to be good over the hole region of the x's, but in a relatively small design region they should be fine

Response Surface Methodology

We’ve seen that our two-level designs are sufficient for estimating first order models.

However, they would not provide enough independent degrees of freedom to estimate a full second-order model.

For this we use response surface designs.

Such designs explore each factor at several (i.e., more than two) levels

Response Surface Methodology

Central Composite Designs

While many response surface designs exist, we will focus on one of the most common ones: the central composite design (CCD).

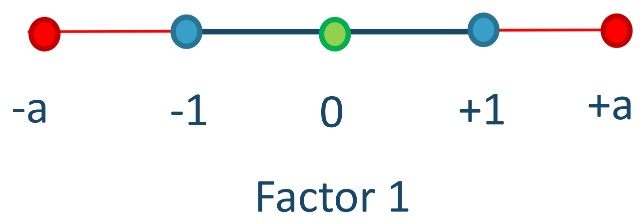
This design involves:

- Ordinary two-level factorial conditions
- Axial conditions
- Center point condition ($x_1 = x_2 = \cdots = x_k = 0$)

Response Surface Methodology

Central Composite Designs

CCD with $k = 1$



Response Surface Methodology

Central Composite Designs

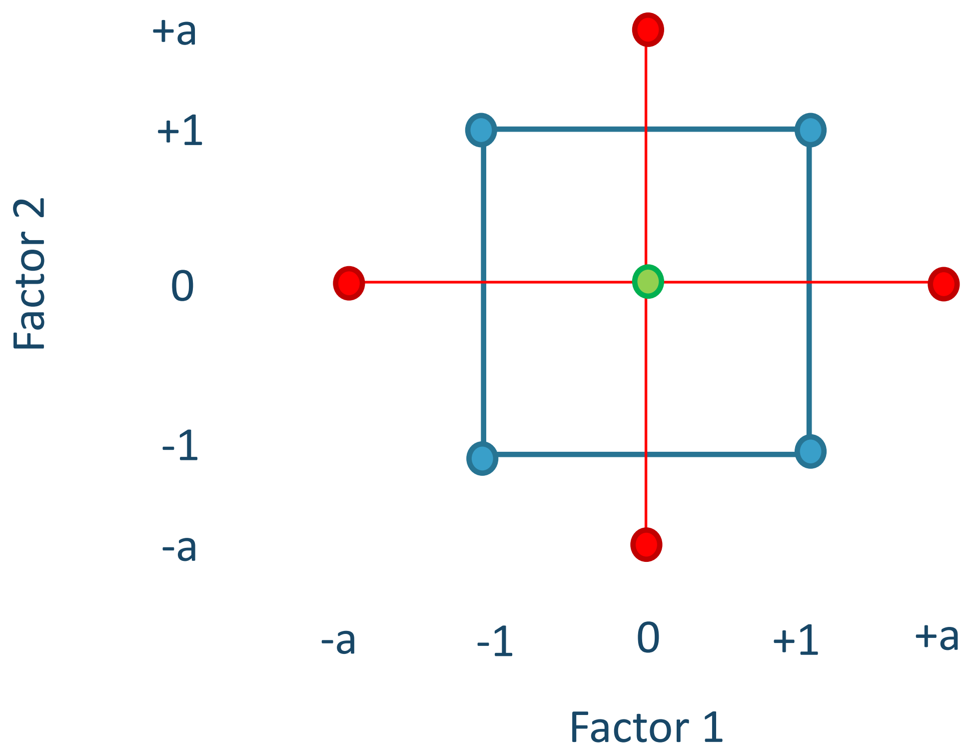
CCD with $k = 1$

Condition	Factor 1
1	-1
2	+1
3	-a
4	+a
5	0

Response Surface Methodology

Central Composite Designs

CCD with $k = 2$ factors



Response Surface Methodology

Central Composite Designs

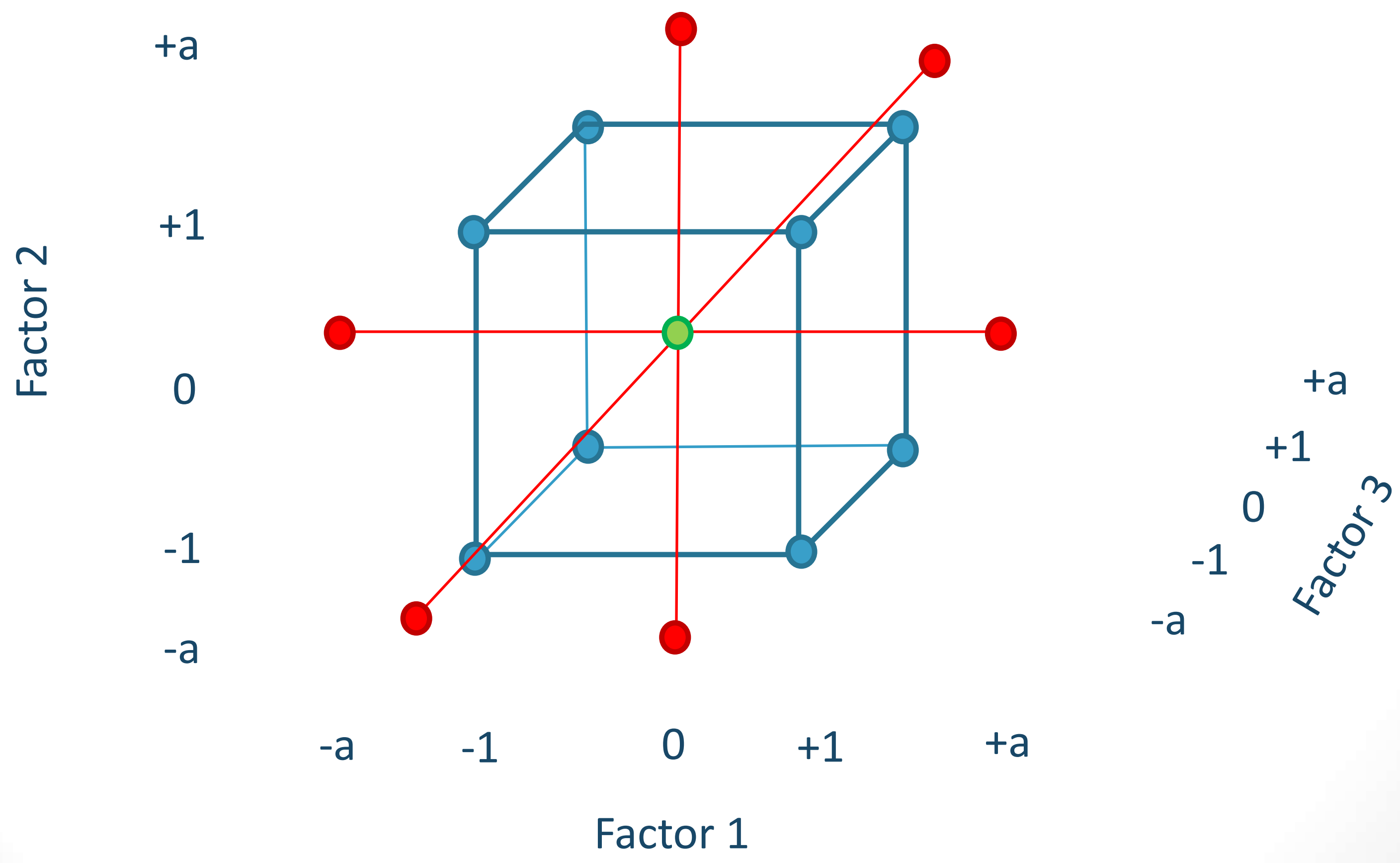
CCD with $k = 2$ factors

Condition	Factor 1	Factor 2
1	-1	-1
2	+1	-1
3	-1	+1
4	+1	+1
6	-a	0
7	+a	0
8	0	-a
9	0	+a
10	0	0

Response Surface Methodology

Central Composite Designs

CCD with $k = 3$ factors



Response Surface Methodology

Central Composite Designs

CCD with $k = 3$ factors

Condition	Factor 1	Factor 2	Factor 3
1	-1	-1	-1
2	+1	-1	-1
3	-1	+1	-1
4	+1	+1	-1
5	-1	-1	+1
6	+1	-1	+1
7	-1	+1	+1
8	+1	+1	+1
9	-a	0	0
10	+a	0	0
11	0	-a	0
12	0	+a	0
13	0	0	-a
14	0	0	+a
15	0	0	0

Response Surface Methodology

Central Composite Designs

As we can see, CCDs involving k factors have

- 2^k factorial conditions
- $2k$ axial conditions
- *1* center point condition

For a total of

$$2^k + 2k + 1$$

experimental conditions

Note, these designs are no longer orthogonal

Response Surface Methodology

The data arising from such a study allows us to fit a full second-order model which is a convex surface that can be optimized

The stationary point is the point

$$x^* = (x_1^*, x_2^*, \ldots, x_k^*)$$

in the design space at which the response surface achieves its maximum / minimum value

This can be found by gradient ascent / descent

Response Surface Methodology

The stationary point tells us exactly which level each factor must be held at in order to optimize the response.

HOWEVER

The values of the x's in our model are recorded in the coded units.

Thus, for the stationary point to be useful, we must convert its coordinates back to the natural units.

Response Surface Methodology

Recall:

$$x_C = \frac{x_N - (x_H + x_L)/2}{(x_H - x_L)/2}$$

Rearranging and solving for x_N yields:

$$x_N = \frac{x_C(x_H - x_L) + (x_H + x_L)}{2}$$

which can be used to calculate the stationary point in the natural units.

Response Surface Methodology

But what about factors that are categorical?

Everything that we have discussed thus far pertains only to quantitative factors (i.e., factors whose levels are numeric).

In the presence of one or more categorical factors we fit different response surfaces at each factorial combination of these chosen levels.

The surface with the most optimal optimum is the 'winner'.

Response Surface Methodology

Example: Ride sharing

Suppose you are data scientist at a ride-sharing company such as Lyft or Uber and you are interested in designing a promotional offer that maximizes ride bookings during an experimental period.

Previous screening studies evaluated the influence of the following five factors on ride bookings:

- Discount amount
- Discount duration
- Method of dissemination
- Ride Type
- Time of Day

Response Surface Methodology

Example: Ride sharing

It was found that the most important factors were discount amount (x_1) and discount duration (x_2). To find optimal values of these factors, a follow-up two-factor central composite design was run in order to fit a second-order response surface model.

The CCD used low and high values of x_1 and x_2 respectively given by 25%/75% and 1 day/7days

- 4 factorial conditions
- 1 center point condition
- 4 axial conditions

each with $n = 500$ users

Response Surface Methodology

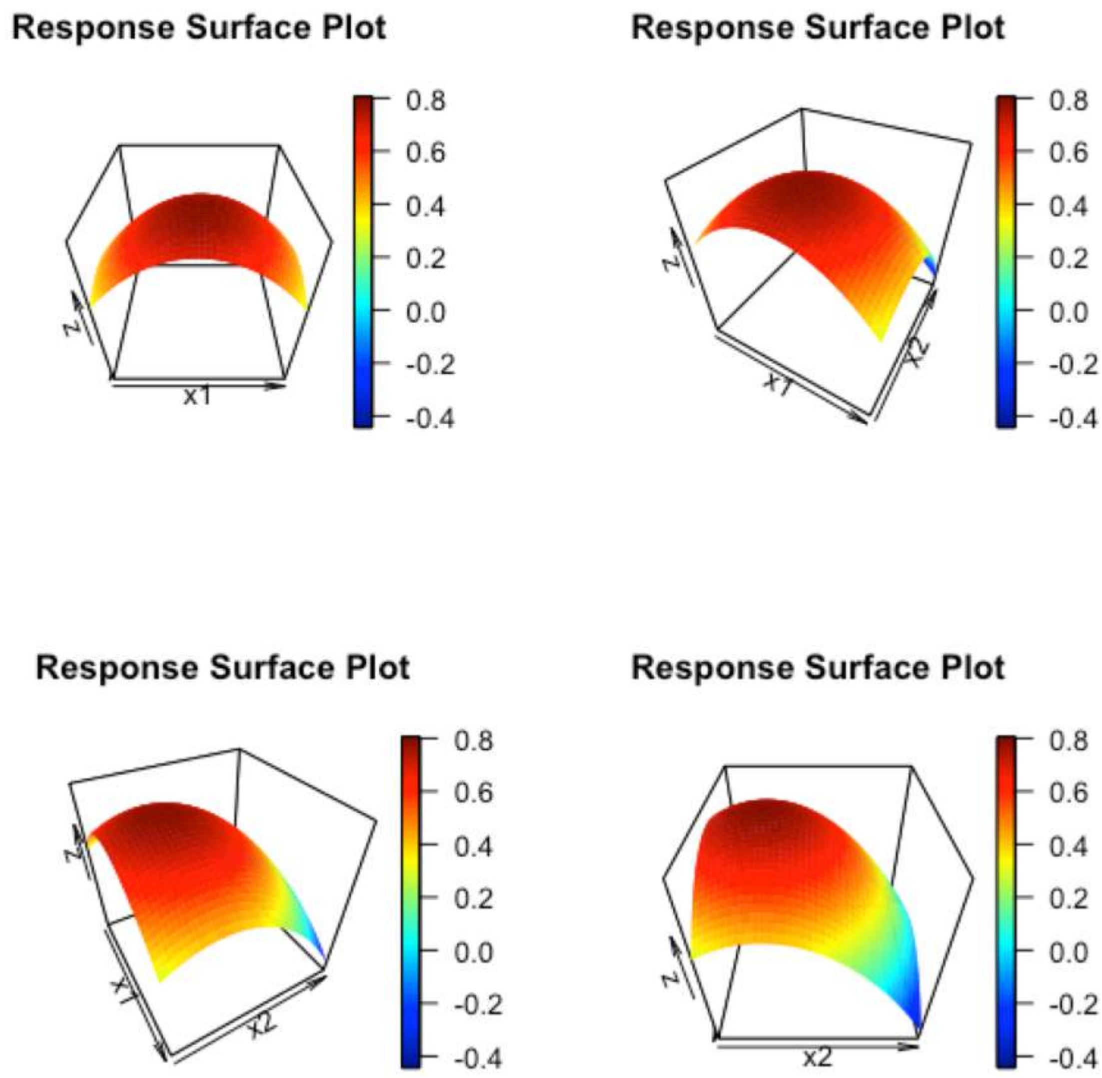
Example: Ride sharing

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)    
(Intercept)  0.720000   0.005656 127.293 1.07e-06 ***
X1           0.009053   0.002000   4.527   0.0202 *  
X2          -0.185674   0.002000 -92.847 2.75e-06 ***
X1X2         0.007500   0.002828   2.652   0.0769 .  
X1q         -0.101250   0.003316 -30.531 7.72e-05 ***
X2q         -0.098750   0.003316 -29.777 8.32e-05 ***
---
Signif.codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.005656 on 3 degrees of freedom
Multiple R-squared:  0.9997, Adjusted R-squared:  0.9992
F-statistic:  1952 on 5 and 3 DF,  p-value: 1.828e-05
```

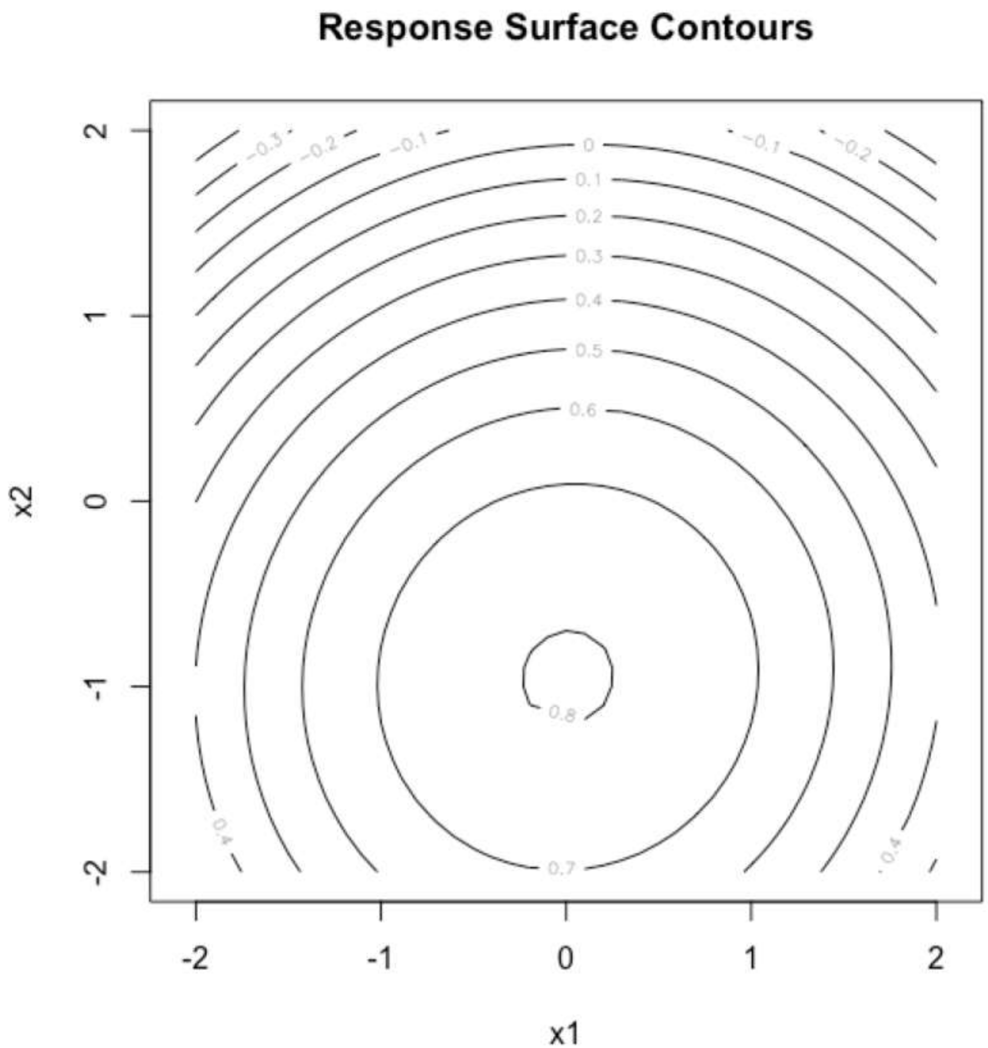
Response Surface Methodology

Example: Ride sharing



Response Surface Methodology

Example: Ride sharing



Response Surface Methodology

Example: Ride sharing

The stationary point is located (in coded units) at

$$x_1 = 0.00990,\ x_2 = \text{-}0.93974$$

and achieves a maximum booking rate of 0.8072879 with a 95% PI of (0.7853, 0.8293).

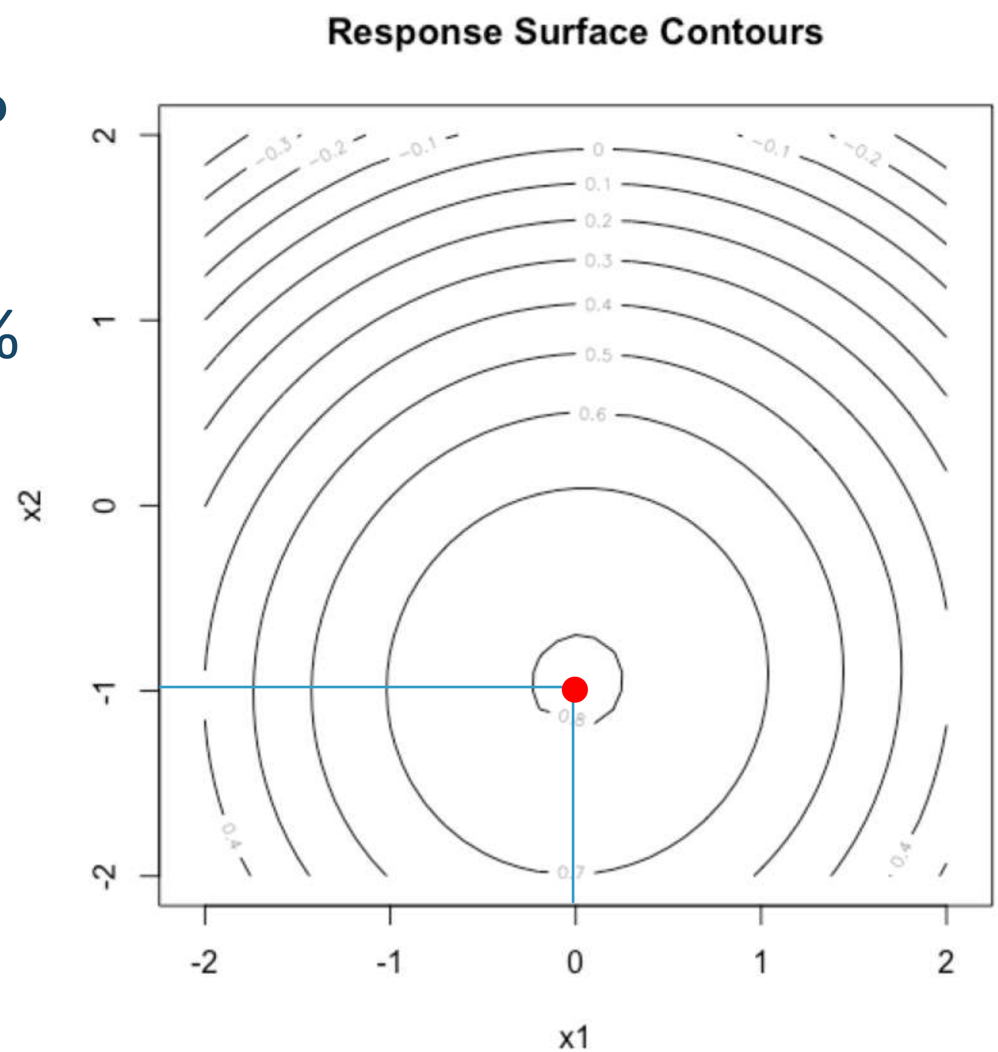
In the natural units this corresponds to a discount rate of 50.24% that lasts for 1.18 days which yields an 80.72% booking rate.

Response Surface Methodology

Example: Ride sharing

What about a 50% discount for 1 day?

Book rate = 80.69%



A BRIEF SUMMARY (OF EVERYTHING)

A Brief Summary (of Everything)

- Designed Experiments are a useful tool for data scientists – in fact they are becoming a required tool

- They facilitate the identification, quantification, and understanding of causal relationships between a response and one or more factors

- Although A/B testing is common in the world of data science, there are many more informative, efficient, and useful approaches that may be applied – an effective data scientist will be familiar with these experimentation alternatives

DATA INSTITUTE
UNIVERSITY OF SAN FRANCISCO

THANK YOU!!