Response Surface Designs

Designs for continuous variables

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ENSAI 3e Année
2016-2017

References

This course in mainly based on:

1. the book of Gary W. Oehlert, **A First Course in Design and Analysis of Experiments**, 2010. Freely available at **http://users.stat.umn.edu/~gary/Book.html**.
2. the book of Douglas C. Montgomery, **Design and Analysis of Experiments**, 7th Edition, Wiley, 2009.
3. the book of Samuel D. Silvey, **Optimal Design**, Chapman and Hall, 1980.

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Introduction

Setting

Many experiments have the goals of **describing** how the response **varies** as a function of the treatments and determining treatments that give **optimal responses**, perhaps **maxima** or **minima**.

Factorial-treatment structures can be used for these kinds of experiments, but when treatment factors can be varied across a **continuous range of values**, **other treatment designs** may be **more efficient**.

Response surface methods are designs and models for working Response with **continuous treatments** when finding **optima** or **describing the response** surface methods is the goal.

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Introduction

Visualizing the Response

In some experiments, the treatment factors can vary continuously.

When we bake a cake, we bake for a certain **time** x_1 at a certain **temperature** x_2; time and temperature can **vary continuously**. We could, in principle, bake cakes for **any time and temperature combination**. Assuming that all the cake batters are the same, the **quality** of the cakes y will depend on the time and temperature of baking.

Introduction

Visualizing the Response

Response is a **function of continuous design variables**. We express this as

$$y_{ij} = f(x_{1,i}, x_{2,i}) + \varepsilon_{ij},$$

meaning that the **response** y is some **function** f of the **design variables** x_1 and x_2, plus **experimental error**. Here j indexes the replication at the i^{th} unique set of design variables.

Introduction

Visualizing the Response

One **common goal** when working with response surface data is to find the settings for the design variables that **optimize** (maximize or minimize) the response.

Often there are **complications**.

1) For example, there may be **several responses**, and we must seek some kind of **compromise optimum** that makes all responses good but does not exactly optimize any single response.

Introduction

Visualizing the Response

2) Alternatively, there may be **constraints** on the **design variables**, so that the goal is to optimize a response, subject to the design variables meeting some constraints.

A **second goal** for response surfaces is to understand **"the lie of the land"**.

Where are the hills, valleys, ridge lines, and so on that make up the **topography** of the **response surface**? At any give design point, how will the **response change** if we alter the design variables in a **given direction**?

Introduction

Visualizing the Response

We can **visualize** the function f as a **surface of heights** over the x_1, x_2 plane, like a relief map showing mountains and valleys.

1) A **perspective plot** shows the **surface** when viewed **from the side**; Figure 1 is a perspective plot of a fairly complicated surface that is wiggly for low values of x_2, and flat for higher values of x_2.

2) A **contour plot** shows the **contours of the surface**, that is, **curves** of x_1, x_2 pairs that have the **same response value.** Figure 2 is a contour plot for the same surface as Figure 1.

Introduction

Visualizing the Response

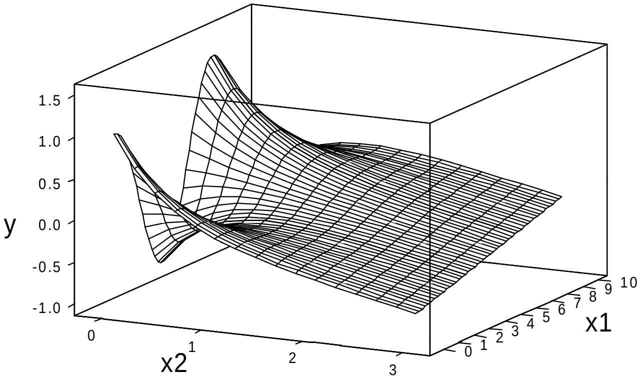

Figure 1: Sample perspective plot, using Minitab.

Introduction

Visualizing the Response

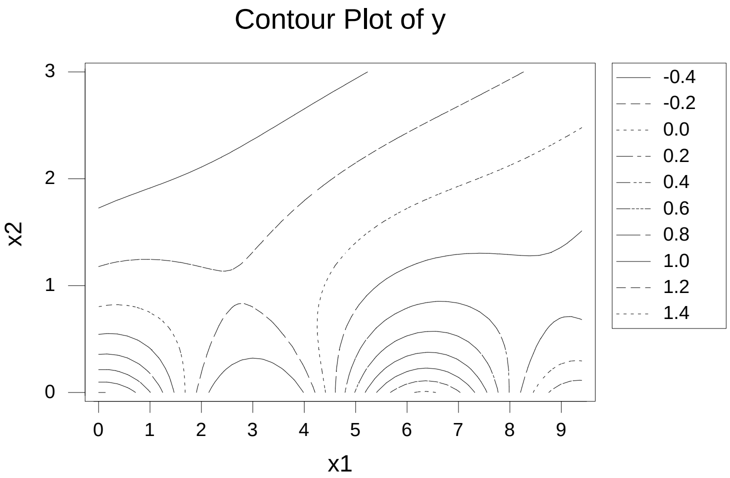

Figure 2: Sample contour plot, using Minitab.

Introduction

Visualizing the Response

Graphics and **visualization** techniques are some of our **best tools** for understanding **response surfaces.**

Unfortunately, response surfaces are difficult to **visualize** when there are three design variables, and become almost **impossible for more than three.**

We thus work with **models** for the **response** function f.

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First-Order Models

Introduction

All models are wrong; some models are useful.
George Box.

We often **don't know anything** about the shape or form of the function f, so **any mathematical model** that we assume for f is surely **wrong.**

On the other hand, experience has shown that simple models using **low-order polynomial** terms in the design variables are **generally sufficient** to **describe** sections of a **response surface.**

First-Order Models

Introduction

In other words, we know that the **polynomial models** described below are almost surely **incorrect**, in the sense that the response surface f is **unlikely** to be a **true polynomial**.

But in a “small” region, **polynomial models** are usually a **close enough approximation** to the response surface that we can make **useful inferences** using polynomial models.

First-Order Models

Introduction

We will consider **first-order models** and **second-order models** for response surfaces. A **first-order model** with q variables takes the form

$$
\begin{aligned}
y_{ij} &= \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \quad + \beta_q x_{qi} + \varepsilon_{ij} \\
&= \beta_0 + \sum_{k=1}^{q} \beta_k x_{ki} + \varepsilon_{ij} \\
&= \beta_0 + \boldsymbol{x}_{\boldsymbol{i}}' \boldsymbol{\beta} + \varepsilon_{ij},
\end{aligned}
$$

where $\boldsymbol{x_i} = (x_{1i}, x_{2i}, \ldots, x_{qi})'$ and $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_q)'$. The first-order model is an **ordinary multiple-regression model**, with design variables as predictors and β_k's as regression coefficients.

First-Order Models

Introduction

First-order models describe inclined planes: **flat surfaces**, possibly tilted.

These models are **appropriate** for describing **portions** of a response surface that are **separated** from maxima, minima, ridge lines, and other **strongly curved regions.** For example, the side slopes of a hill might be reasonably approximated as inclined planes.

First-Order Models

Local approximation

These **approximations** are **local**, in the sense that you need different inclined planes to describe different parts of the mountain.

First-order models can approximate f reasonably well as long as the **region of approximation** is **not too big** and f is **not too curved** in that region.

A first-order model would be a reasonable approximation for the part of the surface in Figures 1 or 2 where x_2 is large; a first-order model would work poorly where x_2 is small.

First-Order Models

Steepest ascent

Bearing in mind that these models are only approximations to the true response, **what can these models tell us about the surface**?

First-order models can tell us **which way** is **up** (or **down**). Suppose that we are at the design variables $\boldsymbol{x}$, and we want to know in **which direction** to move to **increase** the **response** the **most.**

This is the direction of **steepest ascent.**

First-Order Models

Steepest ascent and descent

It turns out that we should take a **step proportional** to β, so that our **new design variables** are $x + r\beta$, for some $r > 0$.

If we want the direction of **steepest descent**, then we **move to** $x - r\beta$, for some $r > 0$.

Note that this direction of steepest ascent is **only approximately correct**, even in the region where we have fit the first-order model. As we move outside that region, the **surface may change** and a **new direction** may be **needed**.

First-Order Models

Introduction

Contours or **level curves** are sets of design variables that have the **same expected response.**

For a **first-order surface**, design points $\boldsymbol{x}$ and $\boldsymbol{x} + \boldsymbol{\delta}$ are on the **same contour if** $\sum \beta_k \delta_k = 0$.

First-order model contours are straight **lines** for $q = 2$, **planes** for $q = 3$, and so on. Note that directions of **steepest ascent** are **perpendicular** to **contours.**

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First-Order Designs

Three basic needs

We have **three basic needs** from a response surface design.

1) We must be able to **estimate** the **parameters** of the **model.**

2) We must be able to **estimate pure error** and **lack of fit.** As described below, pure error and lack of fit are our **tools** for **determining** if the **first-order** model is an **adequate approximation** to the **true mean structure** of the data.

3) We need the **design** to be **efficient**, **both** from a **variance of estimation** point of view and a **use of resources** point of view.

First-Order Designs

Pure error and lack of fit

The concept of **pure error** needs a little **explanation.**

Data might **not fit** a **model** because of **random error** (the ε_{ij} sort of error); this is **pure error.**

Data also might **not fit** a **model** because the **model is misspecified** and does not truly describe the mean structure; this is **lack of fit.**

First-Order Designs

Need to detect lack of fit

Our **models** are **approximations**, so we need to **know when** the **lack of fit** becomes **large relative to pure error.**

This is **particularly true** for **first-order models**, which we will then **replace** with **second-order models.**

It is also **true** for **second-order models**, though we are **more likely** to **reduce our region** of modeling rather than move to higher orders.

First-Order Designs

When can there be LoF?

We do not have lack of fit for factorial models when the **full factorial model** is fit.

In that situation, we have fit a degree of freedom for every factor-level combination—in effect, a mean for each combination. There can be **no lack of fit** in that case because **all means** have been **fit exactly**.

We can get **lack of fit** when our models contain **fewer degrees of freedom** than the **number of distinct design points** used; in particular, **first-** and **second-order** models may **not fit** the **data**.

First-Order Designs

Coding the variables

Response surface **designs** are usually given in terms of **coded variables.**

Coding simply means that the design **variables** are **rescaled** so that **0** is in the **center** of the design, and $\pm$**1** are **reasonable steps up** and **down** from the center.

For example, if cake baking **time** should be **about 35 minutes**, give or take a couple of minutes, we might **rescale time** by $\boldsymbol{(x_1 - 35)/2}$, so that **33** minutes is a $\boldsymbol{-1}$, **35** minutes is a **0**, and **37** minutes is a **1**.

First-Order Designs

Standard first order designs

First-order designs collect data to fit **first-order models.**

The **standard first-order design** is a $\mathbf{2^q}$ factorial with ***center points***. The (coded) low and high **values** for each **variable** are $\pm\mathbf{1}$; the **center points** are $\boldsymbol{m}$ **observations** taken with all variables at **0**.

This design has $\mathbf{2^q + m}$ **points.** We may also use any $\mathbf{2^{q-k}}$ **fraction** with **resolution III** or **greater**.

First-Order Designs

One stone two birds

The **replicated center points** serve **two uses.**

1) The **variation** among the **responses** at the **center point** provides an **estimate of pure error.**

2) The **contrast** between the **mean** of the **center points** and the **mean** of the **factorial points** provides a **test for lack of fit.**

First-Order Designs

Test for lack of fit

The **contrast** between the **mean** of the **center points** and the **mean** of the **factorial points** has:

1) an **expected value zero**, when the data follow a **first-order model**,

2) an **expectation** that **depends** on the **pure quadratic terms**, when the data follow a **second-order model.**

First-Order Designs

Example 1: Cake baking

Our cake mix recommends **35** minutes at **350** °F, but we are going to try to find a time and temperature that suit our palate better.

We begin with a **first-order design** in baking time and temperature, so we use a $\mathbf{2^2}$ factorial with **three center points.** We use the coded values:

1) -1, 0, 1 for 33, **35**, and 37 minutes for time, and

2) -1, 0, 1 for 340, **350**, and 360 degrees for temperature.

First-Order Designs

Example 1: Cake baking

We will thus have

1) **three cakes** baked at the **package-recommended time** and temperature (our **center point**),

2) and **four cakes** with time and temperature **spread around the center.**

First-Order Designs

Example 1: Cake baking

Our response is an average palatability score, with higher values being desirable:

x_1	x_2	y
-1	-1	3.89
1	-1	6.36
-1	1	7.65
1	1	6.79
0	0	8.36
0	0	7.63
0	0	8.12

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First-Order Analysis

Possible Goals for a First-Order Design analysis

Here are three **possible goals** when analyzing data **from** a **first-order design**:

- Determine **which** design **variables affect** the **response.**
- Determine **whether** there is **lack of fit.**
- Determine the **direction** of **steepest ascent.**

Some experimental situations can involve a sequence of designs and all these goals.

First-Order Analysis

Fitting First-Order Models

In all cases, **model fitting** for **response surfaces** is done using **multiple linear regression.**

The **model variables** (x_1 through x_q for the first-order model) are the "**independent**" or "**predictor**" variables of the **regression.** The **estimated** regression **coefficients** are estimates of the model parameters β_k.

First-Order Analysis

Fitting First-Order Models

For **first-order models** using data from 2^q factorials **with or without** center points, the **estimated regression slopes** using coded variables are equal to the ordinary **main effects** for the **factorial model**.

Let $\boldsymbol{b} = \hat{\beta}$ be the vector of estimated coefficients for first-order terms (an estimate of β).

First-Order Analysis

Model Testing

Model testing is done with ***F*-tests** on mean squares from the ANOVA of the regression; each term has its own line in the **ANOVA table**.

Predictor variables are **orthogonal** to each other in **many designs** and models, but **not** in **all cases**, and certainly not when there is missing data; so it seems easiest just to treat all testing situations as if the model **variables** were **nonorthogonal**.

First-Order Analysis

Improvement sum of squares

To **test** the **null hypothesis** that the **coefficients** for a **set** of **model terms** are all **zero**, get:

1) the **error sum of squares** for the **full model** and
2) the **error sum of squares** for the **reduced model** that does not contain the model terms being tested.

The **difference** in these **error sums of squares** is the **improvement sum of squares** for the model terms under test.

First-Order Analysis

Test's statistic

The **improvement mean square** is the **improvement sum of squares divided** by its **degrees of freedom** (the number of model terms in the multiple regression being tested).

This **improvement mean square** is **divided** by the **error mean square** from the full model to obtain an ***F*-test** of the null hypothesis.

First-Order Analysis

Sequential ANOVA. t-tests

The **sum of squares for improvement** can also be computed from a **sequential** (Type I) **ANOVA** for the model, provided that the **terms** being **tested** are the **last terms entered** into the model.

The ***F*-test** of $\beta_k = 0$ (with one numerator degree of freedom) is **equivalent** to the ***t*-test** for β_k that is printed by most regression software.

First-Order Analysis

Noise variables

In many response surface experiments, **all variables** are **important**, as there has been **preliminary screening** to find important variables **prior** to **exploring** the **surface.**

However, inclusion of **noise variables** into models can **alter** subsequent **analysis.**

It is worth noting that **variables** can **look inert** in **some parts** of a response surface, and **active** in **other parts.**

First-Order Analysis

Steepest ascent and inert variables

The direction of **steepest ascent** in a first-order model is **proportional** to the coefficients β. Our **estimated** direction of **steepest ascent** is then proportional to $\boldsymbol{b}$.

Inclusion of **inert variables** in the computation of this direction **increases** the **error** in the direction of the active variables. This effect is worst when the active variables have relatively small effects.

The net effect is that our response will not increase as quickly as possible per unit change in the design variables, because the direction could have a nonnegligible component on the inert axes.

Residual variation's decomposition

Possible Goals for a First-Order Design analysis

Residual variation can be divided into **two parts**: **pure error** and **lack of fit.**

1) **Pure error** is variation among responses that have the same explanatory variables (and are in the same blocks, if there is blocking). We use **replicated points**, usually center points, to get an **estimate of pure error.**

2) All the **rest of residual variation** that is not pure error is **lack of fit.**

Residual variation's decomposition

Possible Goals for a First-Order Design analysis

Thus we can make the **decompositions**:

$$\begin{aligned} SS_{\text{Tot}} &= SS_{\text{Model}} + SS_{\text{LoF}} + SS_{\text{PE}} \\ n-1 &= df_{\text{Model}} + df_{\text{LoF}} + df_{\text{PE}}. \end{aligned}$$

First-Order Analysis

Testing lack of fit

The **mean square for pure error estimates** σ^2, the **variance** of ε.

If the model we have fit has:

1) the **correct mean structure**, then the **mean square for lack of fit also estimates** σ^2, and the ***F*-ratio** $MS_{\text{LoF}}/MS_{\text{PE}}$ will have an ***F*-distribution** with df_{LoF} and df_{PE} degrees of freedom.

2) the **wrong mean structure** -for example, if we fit a first-order model and a second-order model is correct- then the **expected value** of $\boldsymbol{MS_{\text{LoF}}}$ is **larger** than σ^2.

First-Order Analysis

Testing for lack of fit

Thus we can **test for lack of fit** by comparing the F-ratio $\boldsymbol{MS}_{\textbf{LoF}}/\boldsymbol{MS}_{\textbf{PE}}$ to an ***F*-distribution** with df_{LoF} and df_{PE} degrees of freedom.

Example

For a 2^q factorial design with m center points, there are $2^q + m - 1$ degrees of freedom, with q for the model, $m - 1$ for pure error, and all the rest for lack of fit.

First-Order Analysis

Cannot use model if significant lack of fit

Quantities in the analysis of a first-order model are **not** (very) **reliable** when there is **significant lack of fit.**

Because the **model** is **not tracking** the **actual mean structure** of the **data**, the importance of a variable in the first-order model **may not relate** to the **variable's importance** in the **mean structure** of the data.

Likewise, the direction of **steepest ascent** from a first-order model may be **meaningless** if the the model is not describing the true mean structure.

First-Order Analysis

Example 2: Cake baking, continued

Example 1 was a $\mathbf{2^2}$ design with **three center points.**

Our **first-order model** includes a **constant** and **linear terms** for time and temperature. With **seven data points**, there will be **4 residual degrees of freedom.**

The only **replication** in the design is at the **three center points**, so we have **2 degrees of freedom** for **pure error.** The remaining **2 residual degrees of freedom** are **lack of fit.**

First-Order Analysis

Example 2: Cake baking, continued

```
Estimated Regression Coefficients for y

Term        Coef   StDev      T      P
Constant  6.9714  0.5671 12.292  0.000
x1        0.4025  0.7503  0.536  0.620 (A)
x2        1.0475  0.7503  1.396  0.235 (A)

S = 1.501 R-Sq = 35.9% R-Sq(adj) = 3.8%
```

Listing 1: Minitab output for first-order model of cake baking data.

First-Order Analysis

Example 2: Cake baking, continued

```
Analysis of Variance for y

Source            DF  Seq SS  Adj SS  Adj MS      F      P
  Regression       2  5.0370  5.0370  2.5185   1.12  0.411
  Linear           2  5.0370  5.0370  2.5185   1.12  0.411
Residual Error    4  9.0064  9.0064  2.2516
  Lack-of-Fit     2  8.7296  8.7296  4.3648  31.53  0.031  (B)
  Pure Error      2  0.2769  0.2769  0.1384
Total 6 14.0435
```

Listing 1 : Minitab output for first-order model of cake baking data.

First-Order Analysis

Example 2: Cake baking, continued

Listing 1 shows results for this analysis.

Using the 4-degree-of-freedom residual mean square, **neither time nor temperature** has an ***F*-ratio much bigger than one**, so **neither appears to affect the response**, see (A).

However, look at the **test for lack of fit**, see (B). This test has an ***F*-ratio of 31.5** [1], indicating that the **first-order model** is **missing** some of the **mean structure.**

1. and p-value of .03. Yet that p-value cannot be used since the **Gaussian** linear model **assumptions cannot be checked** with such a **low sample size** of $n = 7$.

First-Order Analysis

Example 2: Cake baking, continued

The **2 degrees of freedom** for **lack of fit** are the **interaction** in the **factorial points** and the **contrast** between the **factorial points** and the **center points.**

The sums of squares for these contrasts are 2.77 and 5.96, so **most** of the **lack of fit** is **due to** the **center points not lying** on the **plane fit** from the **factorial points.**

In fact, the **center points** are about **1.86 higher** on average than what the **first-order model predicts.**

First-Order Analysis

Example 2: Cake baking, continued

The direction of **steepest ascent** in this model is proportional to $\mathbf{(.40, 1.05)}$, the estimated β_1 and β_2.

That is, the model says that a **maximal increase in response** can be obtained by **increasing x_1 by .38** (coded) units **for every increase** of **1** (coded) unit in x_2.

However, we have already seen that there is **significant lack of fit** using the **first-order model** with these data, so this **direction of steepest ascent** is **not reliable**.

Contents

Second-Order Models

Definition

We use **second-order models** when the portion of the **response surface** that we are describing **has curvature.**

A **second-order model contains**:

1) all the terms in the **first-order model**, plus

2) **all quadratic terms** like $\beta_{11} x_{1i}^2$ and

3) **all cross product terms** like $\beta_{12} x_{1i} x_{2i}$.

Second-Order Models

Definition

Specifically, it takes the form

$$
\begin{aligned}
y_{ij} &= \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \cdots + \beta_q x_{qi} + \\
&\quad \beta_{11} x_{1i}^2 + \beta_{22} x_{2i}^2 + \cdots + \beta_{qq} x_{qi}^2 + \\
&\quad \beta_{12} x_{1i} x_{2i} + \beta_{13} x_{1i} x_{3i} + \cdots + \beta_{1q} x_{1i} x_{qi} + \\
&\quad \beta_{23} x_{2i} x_{3i} + \beta_{24} x_{2i} x_{4i} + \cdots + \beta_{2q} x_{2i} x_{qi} + \\
&\quad \cdots + \beta_{(q-1)q} x_{(q-1)i} x_{qi} + \varepsilon_{ij} \\
&= \beta_0 + \sum_{k=1}^{q} \beta_k x_{ki} + \sum_{k=1}^{q} \beta_{kk} x_{ki}^2 + \\
&\quad \sum_{k=1}^{q-1} \sum_{l=k+1}^{q} \beta_{kl} x_{ki} x_{li} + \varepsilon_{ij}.
\end{aligned}
$$

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Second-Order Models

Definition

It can also take the matrix form

$$y_{ij} = \beta_0 + \boldsymbol{x_i}'\boldsymbol{\beta} + \boldsymbol{x_i}'\boldsymbol{\mathcal{B}}\boldsymbol{x_i} + \varepsilon_{ij},$$

where $\boldsymbol{x_i} = (x_{1i}, x_{2i}, \ldots, x_{qi})'$, $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_q)'$, and $\boldsymbol{\mathcal{B}}$ is a $q \times q$ matrix with $\mathcal{B}_{kk} = \beta_{kk}$ and $\mathcal{B}_{kl} = \mathcal{B}_{lk} = \beta_{kl}/2$ for $k < l$.

Note that the model only includes the kl cross product for $k < l$; the matrix form with $\boldsymbol{\mathcal{B}}$ includes both kl and lk, so the coefficients are halved to take this into account.

Second-Order Models

Shapes of quadratic surfaces

Second-order models describe **quadratic surfaces**, and quadratic surfaces can take **several shapes.**

Figure 3 shows **four** of the **shapes** that a **quadratic surface** can take:

First, we have a simple **minimum** (a) and **maximum** (b). Then we have a **ridge** (c); the surface is curved (here a maximum) in one direction, but is fairly constant in another direction. Finally, we see a **saddle point** (d); the surface curves up in one direction and curves down in another.

Second-Order Models

Shapes of quadratic surfaces

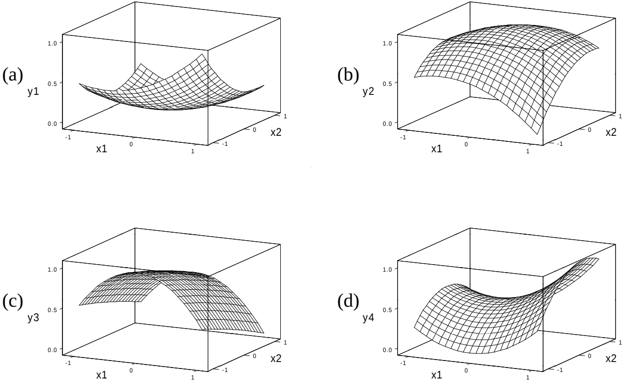

Figure 3: Sample second-order surfaces: (a) minimum, (b) maximum, (c) ridge, and (d) saddle, using Minitab.

Second-Order Models

Canonical variables

Second-order models are easier to understand if we change from the original design variables x_1 and x_2 to **canonical variables** v_1 and v_2.

Canonical variables will be defined shortly, but for now consider that they **shift the origin** (the zero point) and **rotate the coordinate axes to match** the second-order surface.

Second-Order Models

Canonical variables

The second-order model is very simple when expressed in canonical variables:

$$f_v(\boldsymbol{v}) = f_v(\mathbf{0}) + \sum_{k=1}^{q} \lambda_k v_k^2.$$

where $v = (v_1, v_2, \ldots, v_q)'$ is the design variables expressed in canonical coordinates; $f_v(\boldsymbol{v})$ is the response as a function of the canonical variables; and λ_k's are numbers computed from the $\mathcal{B}$ matrix.

Second-Order Models

Stationary point

The $\boldsymbol{x}$ value that maps to $\mathbf{0}$ in the canonical variables is called the **stationary point** and is denoted by $\boldsymbol{x_0}$; thus $f_v(\mathbf{0}) = f(\boldsymbol{x_0})$.

The key to understanding canonical variables is the stationary point of the second-order surface.

The stationary point is that **combination** of **design variables** where the surface is at either a **maximum** or a **minimum** in **all directions.**

Second-Order Models

Stationary point

1) If the stationary point is a **maximum in all directions**, then the stationary point is the **maximum response** on the **whole modeled surface.**

2) If the stationary point is a **minimum in all directions**, then it is the **minimum response** on the **whole modeled surface.**

Second-Order Models

Stationary point

3) If the stationary point is a **maximum in some directions** and a **minimum in other directions**, then the stationary point is a **saddle point**, and **the modeled surface** has **no overall maximum or minimum.**

4) If a **ridge surface** is absolutely level in some direction, then it does not have a unique stationary point; this **rarely happens** in practice.

Second-Order Models

First canonical axis

The stationary point will be the origin (0 point) for our canonical variables.

Now imagine yourself **situated at the stationary point** of a second-order surface.

The **first canonical axis** is the direction in which you would **move** so that a step of unit length **yields a response as large as possible** (either increase the response as much as possible or decrease it as little as possible).

Second-Order Models

Second canonical axis

The **second canonical axis** is the direction, among all those directions **perpendicular to the first canonical axis**, that **yields a response as large as possible.**

There are **as many canonical axes** as there are **design variables. Each additional canonical axis** that we find must be **perpendicular** to all those we have already found.

Figure 4 shows contours, stationary points, and canonical axes for the four sample second-order surfaces.

Second-Order Models

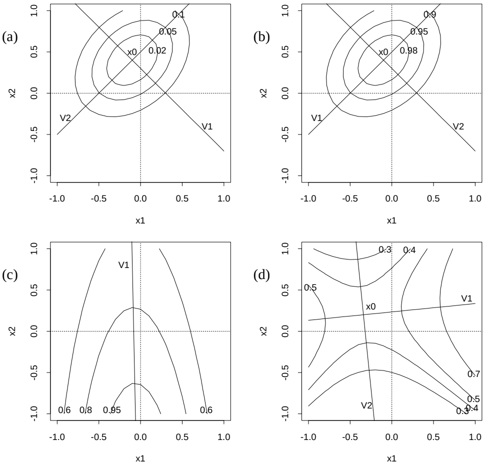

Figure 4: Contours, stationary points, and canonical axes for Figure 3.

Second-Order Models

Contours

As shown in this figure (a) and (b), **contours** for surfaces with **maxima** or **minima** are **ellipses**. The stationary point $\boldsymbol{x_0}$ is the center of these ellipses, and the canonical axes are the major and minor axes of the elliptical contours.

For the **ridge** system (c), we still have **elliptical contours**, but they are very long and skinny, and the stationary point is outside the region where we have fit the model. If the is **absolutely flat**, then the contours are **parallel lines**.

For the **saddle** point (d), contours are **hyperbolic** instead of elliptical. The stationary point is in the center of the hyperbolas, and the canonical axes are the axes of the hyperbolas.

Second-Order Models

Algebraic description

This **description** of second-order surfaces has been **geometric**; pictures are an **easy way** to **understand** these surfaces.

It is **difficult to calculate** with pictures, though, so we also have an **algebraic description** of the second-order surface. Recall that the matrix form of the response surface is written

$$f(\boldsymbol{x}) = \beta_0 + \boldsymbol{x}'\boldsymbol{\beta} + \boldsymbol{x}'\boldsymbol{\mathcal{B}}\boldsymbol{x}.$$

Second-Order Models

Algebraic description

Our **algebraic description** of the surface depends on the following facts:

1) The **stationary point** for this quadratic surface **is at**

$$\boldsymbol{x}_0 = -\frac{1}{2}\mathcal{B}^{-1}\beta,$$

where $\mathcal{B}^{-1}$ is the matrix inverse of $\mathcal{B}$.

2) For the $q \times q$ symmetric matrix $\mathcal{B}$, we can find a $q \times q$ matrix H such that $H'H = HH' = I_q$ and $H'\mathcal{B}H = \boldsymbol{\Lambda}$, where I_q is the $q \times q$ identity matrix and $\boldsymbol{\Lambda}$ is a matrix with elements $\lambda_1, \ldots, \lambda_q$ on the diagonal and zeroes off the diagonal.

Second-Order Models

Change of coordinates

The numbers λ_k are the **eigenvalues** of $\mathcal{B}$, and the columns of H are the corresponding **eigenvectors.**

We saw in Figure 4 that the stationary point and canonical axes give us a **new coordinate system** for the design variables. We get the new coordinates $\boldsymbol{v}' = (v_1, v_2, \ldots, v_q)$ **via**

$$\boldsymbol{v} = H'(\boldsymbol{x} - \boldsymbol{x_0}).$$

Subtracting $\boldsymbol{x_0}$ shifts the origin, and multiplying by H' rotates to the canonical axes.

Second-Order Models

Change of coordinates

Finally, the **payoff**: in the canonical coordinates, we can express the response surface as

$$f_v(\boldsymbol{v}) = f_v(\boldsymbol{0}) + \sum_{k=1}^{q} \lambda_k v_k^2,$$

where

$$f_v(\boldsymbol{0}) = f(\boldsymbol{x_0}) = \beta_0 + \frac{1}{2}\boldsymbol{x_0}'\beta.$$

That is, when looked at in the canonical coordinates, the **response surface** is a **constant** plus a simple **squared term** from **each** of the **canonical variables** v_i.

Second-Order Models

Shape analysis

1) If all of the λ_k's are positive, $\boldsymbol{x_0}$ is a minimum.

2) If all of the λ_k's are negative, $\boldsymbol{x_0}$ is a maximum.

3) If all of the λ_k's are of the same sign, but some are near zero in value, we have a ridge system.

4) If some λ_k's are negative and λ_k's some are positive, $\boldsymbol{x_0}$ is a saddle point.

Second-Order Models

Shape analysis

The λ_k's for our four examples in Figure 4 are

1) $(.31771, .15886)$ for the surface with a **minimum**,

2) $(-.31771, -.15886)$ for the surface with a **maximum**,

3) $(-.021377, -.54561)$ for the surface with a **ridge**,

4) and $(.30822, -.29613)$ for the surface with a **saddle point.**

Second-Order Models

Higher order models

In principal, we could also use **third-** or **higher-order models**.

This is **rarely done**, as second-order models are generally sufficient.

Contents

Second-Order Designs

Central Composite Designs

There are **several choices** for second-order designs.

One of the most **popular** is the **central composite design** (CCD).

A CCD is composed of **factorial** points, **axial** points, and **center** points.

Second-Order Designs

Central Composite Designs

1) **Factorial** points are the points from a $\mathbf{2^q}$ design with **levels coded** as ± 1 or the points in a $\mathbf{2^{q-k}}$ fraction with resolution **V** or greater.

2) **Center** points are again m points at the **origin.**

3) **Axial** points have one design variable at $\pm\alpha$ and all other design variables at 0; there are $2q$ axial points.

Figure 5 shows a CCD for $q = 3$.

Second-Order Designs

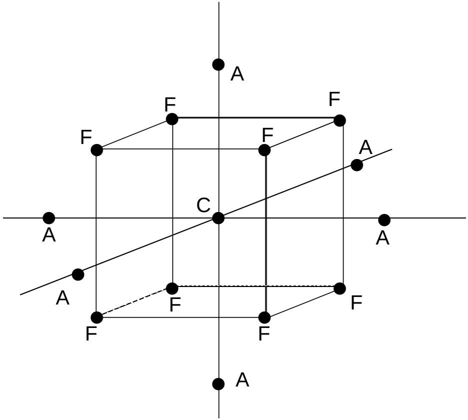

Figure 5: A central composite design in three dimensions, showing center (C), factorial (F), and axial (A) points.

Second-Order Designs

From factorial to CCD

One of the reasons that **CCD's** are **so popular** is that

1) you can **start** with a first-order design using a **2^q factorial** and

2) then **augment it** with **axial points**

3) and perhaps **more center points** to get a **second-order design.**

Second-Order Designs

From factorial to CCD

For example, we may find **lack of fit** for a **first-order model** fit to data from a first-order design.

Augment the first-order design by adding axial points and center points to get a **CCD**, which is a second-order design and can be used to fit a **second-order model**.

We consider such a **CCD** to have been **run** in **two incomplete blocks**.

Second-Order Designs

Orthogonal blocking

We get to **choose** α and the **number** of **center points** ***m***.

Suppose that we run our CCD in incomplete blocks, with the **first block** having the **factorial points** and **center points**, and the **second block** having **axial points** and **center points**.

Block effects should be **orthogonal** to **treatment effects**, **so that blocking does not affect the shape of our estimated response surface**.

Second-Order Designs

Orthogonal blocking

We can achieve this **orthogonality** by choosing

1) α and

2) the number of **center points** in the **factorial** and **axial blocks**

as shown in Table 1 (Box and Hunter 1957).

When blocking the CCD, factorial points and axial points will be in different blocks. The factorial points may also be blocked using the **confounding schemes** of **regular fractional factorial designs**.

Second-Order Designs

q	2	3	4	5	5
rep	1	1	1	1	$\frac{1}{2}$
Number of blocks in factorial	1	2	2	4	1
Center points per factorial block	3	2	2	2	6
α for axial points	1.414	1.633	2.000	2.366	2.000
Center points for axial block	3	2	2	4	1
Total points in design	14	20	30	54	33

Table 1: Design parameters for Central Composite Designs with orthogonal blocking.

Second-Order Designs

q	6	6	7	7
rep	1	$\frac{1}{2}$	1	$\frac{1}{2}$
Number of blocks in factorial	8	2	16	8
Center points per factorial block	1	4	1	1
α for axial points	2.828	2.366	3.364	2.828
Center points for axial block	6	2	11	4
Total points in design	90	54	169	80

Table 1: Design parameters for Central Composite Designs with orthogonal blocking.

Second-Order Designs

Orthogonal blocking

Table 1 deserves some explanation.

The table gives the **maximum number** of **blocks** into which the **factorial portion** can be **confounded**, while **main effects** and **two-way** interactions are **confounded only** with **three-way** and **higher-order** interactions (is still resolution V).

The table also gives the **number of center points** for **each of these blocks**. If fewer blocks are desired, the center points are added to the combined blocks.

Second-Order Designs

Orthogonal blocking

For example, the 2^5 can be run in **four blocks**, with **two center points per block.**

If we instead **use two blocks**, then **each** should have **four center points**; with only **one block**, use all **eight center points.**

The **final block** consists of **all axial points** and **additional center points.**

Second-Order Designs

Rotatable Designs: Definition

There are a couple of heuristics for choosing α and the number of center points when the CCD is not blocked, but these are just guidelines and not overly compelling.

If the **precision** of the estimated response surface at some point ***x* depends only** on the **distance** from ***x* to the origin**, not on the direction, then the design is said to be **rotatable**.

Second-Order Designs

Rotatable CCD

Thus **rotatable** designs do **not favor one direction** over another when we explore the surface. This is **reasonable** when we **know little** about the surface **before experimentation.**

We get a **rotatable** design by choosing

1) $\alpha = 2^{q/4}$ for the **full factorial** or

2) $\alpha = 2^{(q-k)/4}$ for a **fractional factorial.**

Some of the **blocked CCD's** given in **Table 1** are **exactly rotatable**, and **all** are **nearly rotatable**.

Second-Order Designs

Rotatability

Rotatable designs are **nice**, and I would probably **choose one as a default.** However, I **don't obsess on rotatability**, for a couple of reasons.

1) **Rotatability depends on the coding we choose.** The **property** that the **precision** of the estimated surface **does not depend** on **direction disappears** when we **go back** to the original, **uncoded variables.** It also disappears if we keep the same design points in the original variables but then express them with a different coding.

Second-Order Designs

Rotatability

2) **Rotatable** designs use **five levels of every variable**, and this may be **logistically awkward.** Thus choosing $\alpha = 1$ so that all variables have only three levels may make a more practical design.

3) Using $\alpha = \sqrt{q}$ so that all the **noncenter points** are on the **surface of a sphere** (only rotatable for $q = 2$) gives a **better design** when we are only interested in the **response surface within that sphere.**

Second-Order Designs

Uniform Precision: Definition

A **second-order design** has **uniform precision** if the **precision** of the fitted surface is the **same**

- **at the origin** and

- at a **distance of 1 from the origin.**

Second-Order Designs

Uniform Precision: Why ?

Uniform precision is a **reasonable criterion**, because we are **unlikely to know** just **how close to the origin** a **maximum** or **other** surface **feature** may be;

- (relatively) too **many center points** give us much **better precision near** the **origin**, and

- too **few** give us **better precision away** from the **origin.**

Second-Order Designs

Uniform Precision: How ?

It is impossible to achieve this exactly.

Table 2 shows the **number of center points** to get **as close as possible** to **uniform precision** for **rotatable CCD's.**

q	2	3	4	5	5	6	6	7	7
Replication	1	1	1	1	$\frac{1}{2}$	1	$\frac{1}{2}$	1	$\frac{1}{2}$
Number of center points	5	6	7	10	6	15	9	21	14

Table 2: Parameters for rotatable, uniform precision Central Composite Designs.

Second-Order Designs

Example 3: Cake baking, continued

We saw in Example 2 that the **first-order model** was a **poor fit**.

In particular, the **contrast** between the **factorial** points and the **center points** indicated **curvature** of the response surface.

We will **need** a **second-order model** to fit the curved surface, so we will need a second-order design to collect the data for the fit.

Second-Order Designs

Example 3: Cake baking, continued

We **already** have **factorial points** and **three center points.**

Looking in Table 1, we see that **adding**

1) **three more center points** and

2) **axial points** at $\alpha = 1.414$

will give us a design with **two blocks** with **blocks orthogonal to treatments.**

This design is also **rotatable**, but **not uniform precision.**

Second-Order Designs

Example 3: Cake baking, continued

Here is the **complete design.** The **first block** made of the **initial measurements**:

Block	x_1	x_2	y
1	-1	-1	3.89
1	1	-1	6.36
1	-1	1	7.65
1	1	1	6.79
1	0	0	8.36
1	0	0	7.63
1	0	0	8.12

Second-Order Designs

Example 3: Cake baking, continued

The **second block** including responses for the **seven additional cakes** we bake **to complete the CCD**:

Block	x_1	x_2	y
2	1.414	0	8.40
2	−1.414	0	5.38
2	0	1.414	7.00
2	0	−1.414	4.51
2	0	0	7.81
2	0	0	8.44
2	0	0	8.06

Second-Order Designs

Full or Fractions of 3^q Factorials

There are several other second-order designs in addition to central composite designs.

The simplest are **3^q factorials** and **fractions** with **resolution V** or greater.

These designs are **not much used** for $q \geqslant 3$, as they require **large numbers** of design **points**.

Second-Order Designs

Box-Behnken Designs

Box-Behnken designs are **rotatable**, second-order designs that are **incomplete 3^q** factorials, but **not ordinary fractions.**

Box-Behnken designs are formed by **combining incomplete block designs** with **factorials.**

For q factors, find an incomplete block design for q treatments in blocks of size two. (Blocks of other sizes may be used, we merely illustrate with two.)

Second-Order Designs

Box-Behnken Designs

Associate the “treatment” letters A, B, C, and so on with “factor” letters A, B, C, and so on.

When **two factor letters** appear **together** in a **block**,

- use **all combinations** where those factors are at the **$\pm$1 levels**, and

- **all other factors** are at **0**.

The **combinations from all blocks** are then **joined** with some **center points** to form the **Box-Behnken design.**

Second-Order Designs

Box-Behnken Designs

For example, for $q = 3$, we can use the **BIBD** with **three blocks** and (A, B), (A, C), and (B, C) as assignment of treatments to blocks. From the three blocks, we get the **combinations**:

A	B	C
x_1	x_2	x_3
-1	-1	0
-1	1	0
1	-1	0
1	1	0

A	B	C
x_1	x_2	x_3
-1	0	-1
-1	0	1
1	0	-1
1	0	1

A	B	C
x_1	x_2	x_3
0	-1	-1
0	-1	1
0	1	-1
0	1	1

Second-Order Designs

Box-Behnken Designs

To this we **add some center points**, say five, to form the **complete design.**

This design takes **only 17 points**, **instead** of the **27** (plus some for replication) needed in the **full factorial.**

Contents

Second-Order Analysis

Analysis' Goals

Here are **three** possible **goals** for the analysis of **second-order models**:

•Determine which design **variables affect** the **response.**

•Determine **whether** there is **lack of fit.**

•Determine the **stationary point** and **surface type.**

Second-Order Analysis

Inferring

As with first-order models,

- **fitting** is done with **multiple linear regression**, and

- **testing** is done with ***F*-tests**.

Let ***b*** be the estimated coefficients for first-order terms, and let ***B*** be the estimate of the second-order terms.

The goal of determining which variables affect the response is a bit more complex for second-order models.

Second-Order Analysis

Testing a variable

To **test** that a **variable** –say variable 1– has **no effect** on the response, we must test that its

- **linear**,

- **quadratic**, and

- **cross product** coefficients

are all zero: $\beta_1 = \beta_{11} = \cdots = \beta_{1q} = 0$.

This is a $\boldsymbol{q+1}$**-degree-of-freedom null hypothesis** which we must test using an F-test.

Second-Order Analysis

Lack of Fit

Testing for **lack of fit** in the second-order model is **completely analogous** to the **first-order model.**

Compute an **estimate** of **pure error** variability from the replicated points; all other **residual variability** is **lack of fit.** Significant lack of fit indicates that our **model** is **not capturing** the **mean structure** in our region of experimentation.

Second-Order Analysis

Remedial

When we have **significant lack of fit**, we should **first** consider whether a **transformation of the response** will improve the quality of the fit. For example, a second-order model may be a good fit for the **log** of the response.

Alternatively, we can investigate **higher-order models** for the mean or **obtain data** to **fit** the second-order model in a **smaller region**.

Second-Order Analysis

Canonical Analysis

Canonical Analysis is

- the determination of the **type** of second-order **surface**,

- the location of its **stationary point**, and

- the **canonical directions.**

These quantities are **functions** of the **estimated coefficients** ***b*** and ***B*** computed in the multiple regression.

Second-Order Analysis

Estimates

We **estimate** the **stationary point** as

$$\hat{\boldsymbol{x}}_{\boldsymbol{0}} = -\boldsymbol{B}^{-1}\boldsymbol{b}/2,$$

and the **eigenvectors** and **eigenvalues** of $\mathcal{B}$ are estimated by the **eigenvectors** and **eigenvalues** of $\boldsymbol{B}$ using special software.

Second-Order Analysis

Precision of Estimation

The **results** of a **canonical analysis** have an **aura of precision** that is **often not justified**.

Many software packages can compute and print the estimated stationary point, but **few give** a **standard error** for this estimate.

In fact, the **standard error** is **difficult** to **compute** and tends to be rather **large**. Likewise, there can be **considerable error** in the **estimated canonical directions**.

Second-Order Analysis

Example 4: Cake baking, continued

We now **fit a second-order model** to the data from the blocked central composite design of Example 3.

This **model** will have

- **linear** terms,

- **quadratic** terms,

- a **cross product** term, and

- a **block** term.

Listing 2 shows the results.

Second-Order Analysis

Example 4: Cake baking, continued

```
Estimated Regression Coefficients for y

Term        Coef  StDev       T     P
Constant   8.070 0.1842  43.809 0.000  (A)
Block     -0.057 0.1206  -0.473 0.651
x1         0.735 0.1595   4.608 0.002
x2         0.964 0.1595   6.042 0.001
x1*x1     -0.628 0.1661  -3.779 0.007
x2*x2     -1.195 0.1661  -7.197 0.000
x1*x2     -0.832 0.2256  -3.690 0.008

S = 0.4512 R-Sq = 95.0% R-Sq(adj) = 90.8%
```

Listing 2: Minitab output for second-order model of cake baking data.

Second-Order Analysis

Example 4: Cake baking, continued

```
Analysis of Variance for y

Source            DF   Seq SS   Adj SS    Adj MS      F      P
Blocks             1   0.0457   0.0455   0.04546   0.22  0.651
Regression         5  27.2047  27.2047   5.44094  26.72  0.000
  Linear           2  11.7562  11.7562   5.87808  28.87  0.000
  Square           2  12.6763  12.6763   6.33816  31.13  0.000
  Interaction      1   2.7722   2.7722   2.77223  13.62  0.008
Residual Error     7   1.4252   1.4252   0.20359
B)Lack-of-Fit      3   0.9470   0.9470   0.31567   2.64  0.186
  Pure Error       4   0.4781   0.4781   0.11953
Total             13  28.6756
```

Listing 2 : Minitab output for second-order model of cake baking data.

Second-Order Analysis

Example 4: Cake baking, continued

At (A) we see that all **first-** and **second-order** terms are **significant**, so that no variables need to be deleted from the model.

We also see that **lack of fit** is **not significant** B), so the second-order model should be a **reasonable approximation** to the **mean structure** in the **region of experimentation.**

Second-Order Analysis

Example 4: Cake baking, continued

Figure 6 shows a **contour plot** of the fitted second-order model.

We see that the **optimum** is at about .4 coded time units above 0, and .2 coded temperature units above zero, corresponding to 35.8 minutes and 352°.

We also see that the **ellipse slopes northwest to southeast**, meaning that we can **trade time** for **temperature** and still get a cake that we like.

Second-Order Analysis

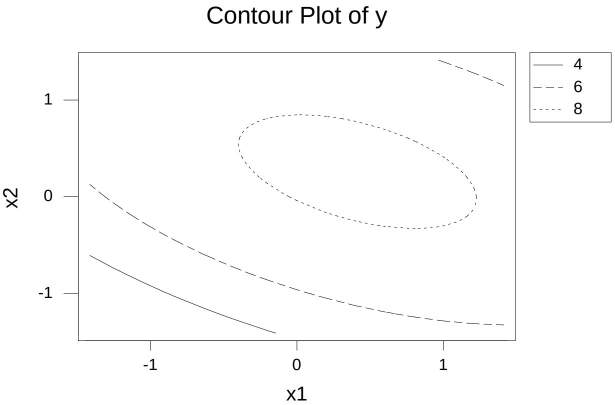

Figure 6: Contour plot of fitted second-order model for cake baking data, using Minitab.

Second-Order Analysis

Example 4: Cake baking, continued

Listing 3 shows a canonical analysis for this surface.

The **estimated coefficients** are at (A) ($\hat{\beta}_0$), (B) ($\boldsymbol{b}$), and (C) ($\boldsymbol{B}$).

The **estimated stationary point** and its **response** are at (D) and (E); I guessed (.4, .2) for the **stationary point** from Figure 6 –it was actually (.42, .26).

Second-Order Analysis

Example 4: Cake baking, continued

The **estimated eigenvectors** and **eigenvalues** are at (F) and (G). **Both eigenvalues** are **negative**, indicating a **maximum.**

The **smallest decrease** is associated with the **first eigenvector** $(-.884, .467)$, so increasing the temperature by .53 coded units for every decrease in 1 coded unit of time keeps the response as close to maximum as possible.

Second-Order Analysis

Example 4: Cake baking, continued

```
component:      b0                  (A)
(1)              8.07
component:       b                  (B)
(1)              0.73515 0.964
component:       B                  (C)
(1,1)           -0.62756 -0.41625
(2,1)           -0.41625 -1.1952
component:      x0                  (D)
(1,1)            0.41383
(2,1)            0.25915
```

Listing 3: MacAnova output for canonical analysis of cake baking data.

Second-Order Analysis

Example 4: Cake baking, continued

```
component:     y0                  (E)
(1,1)           8.347
component:      H                  (F)
(1,1)          -0.88413 -0.46724
(2,1)           0.46724 -0.88413
component:  lambda                 (G)
(1)            -0.40758 -1.4152
```

Listing 3: MacAnova output for canonical analysis of cake baking data.

Contents

Mixture Experiments

Introduction

Mixture experiments are a **special case** of **response surface** experiments in which the response depends on the **proportions** of the **various components**, but **not on absolute amounts**.

For example, the taste of a punch depends on the proportion of ingredients, not on the amount of punch that is mixed, and the strength of an alloy may depend on the proportions of the various metals in the alloy, but not on the total amount of alloy produced.

Mixture Experiments

Simplex

The **design variables** $x_1, x_2, \ldots, x_q$ in a mixture experiment are **proportions**, so they must be nonnegative and add to one:

$$x_k \geqslant 0, \qquad k = 1, 2, \ldots, q$$

and

$$x_1 + x_2 + \cdots + x_q = 1.$$

This design space is called a **simplex** in q dimensions.

Mixture Experiments

Temp

In **two dimensions**, the design space is the **segment** from (1,0) to (0,1); in **three dimensions**, it is bounded by the **equilateral triangle** (0,0,1), (0,1,0), and (1,0,0); and so on.

Note that a point in the simplex in q dimensions is determined by any $q-1$ of the coordinates, with the remaining coordinate determined by the constraint that the coordinates add to one.

Mixture Experiments

Example 5: Fruit punch

Cornell (1985) gave an example of a **three-component** fruit punch **mixture experiment**, where the goal is to find the **most appealing mixture** of **watermelon juice** (x_1), **pineapple juice** (x_2), and **orange juice** (x_3).

Appeal depends on the recipe, **not on the quantity** of punch produced, so it is the **proportions** of the constituents **that matter.**

Mixture Experiments

Example 5: Fruit punch

Six different punches are produced, and **eighteen judges** are assigned at **random** to the punches, **three to a punch.** The recipes and results are given in Table 3.

x_1	x_2	x_3	Appeal		
1	0	0	4.3	4.7	4.8
0	1	0	6.2	6.5	6.3
.5	.5	0	6.3	6.1	5.8
0	0	1	7.0	6.9	7.4
.5	0	.5	6.1	6.5	5.9
0	.5	.5	6.2	6.1	6.2

Table 3: Blends of fruit punch.

Mixture Experiments

Model

As in ordinary response surfaces, we have some **response** y that we wish to **model** as a **function** of the **explanatory variables**:

$$y_{ij} = f(x_{1i}, x_{2i}, \ldots, x_{qi}) + \varepsilon_{ij}.$$

We use a **low-order polynomial** for this model, not because we believe that the function really is polynomial, but rather because we usually don't know what the correct model form is; we are willing to **settle for a reasonable approximation** to the underlying function.

Mixture Experiments

Model Purposes

We can use this model for various purposes:

- To **predict** the **response** at any combination of design variables,

- To find **combinations** of design variables that give **best response**, and

- To measure the **effects** of **various factors** on the **response**.

Contents

Designs for mixtures

Simplex Lattice Design

A $\{q, m\}$ **simplex lattice** design for q components consists of all **design points** on the **simplex** where **each component** is of the form r/m, for some integer $r = 0, 1, 2, \ldots, m$.

For example, the $\{3, 2\}$ simplex lattice consists of the **six combinations** $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, $(1/2, 1/2, 0)$, $(1/2, 0, 1/2)$, and $(0, 1/2, 1/2)$.

Designs for mixtures

A $\{3,2\}$ Simplex Lattice

The **fruit punch** experiment in Example 5 is a **$\{3,2\}$ simplex lattice.**

The $\{3,3\}$ simplex lattice has the **ten combinations** $(1,0,0)$, $(0,1,0)$, $(0,0,1)$, $(2/3,1/3,0)$, $(2/3,0,1/3)$, $(1/3,2/3,0)$, $(0,2/3,1/3)$, $(1/3,0,2/3)$, $(0,1/3,2/3)$, and $(1/3,1/3,1/3)$.

Designs for mixtures

Which m ?

In general, ***m*** needs to be

- at least **as large as *q*** to get any points in the **interior of the simplex**, and

- **larger still** to get **more points** into the **interior of the simplex.**

Figure 7(a) illustrates a $\{3, 4\}$ simplex lattice.

Designs for mixtures

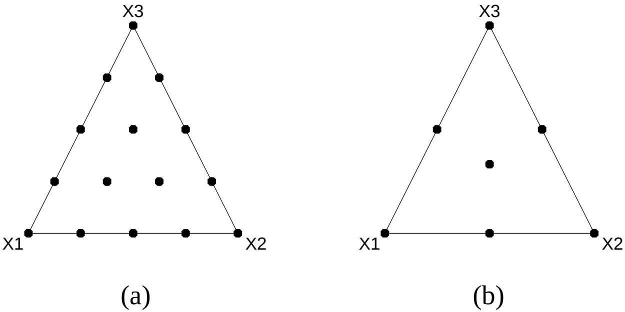

Figure 7: (a) {3,4} simplex lattice and (b) three variable simplex centroid designs.

Designs for mixtures

Simplex centroid designs

The **second class** of models is the **simplex centroid designs.**

These designs have $2^q - 1$ design points for q factors.

The design points are the **pure design mixtures**, all the $1/2 - 1/2$ two-component mixtures, all the $1/3 - 1/3 - 1/3$ three component mixtures, and so on, through the **equal mixture** of all q components.

Designs for mixtures

Simplex centroid designs

Alternatively, we may describe this design as

- all the **permutations** of $(1, 0, \ldots, 0)$,

- all the **permutations** of $(1/2, 1/2, \ldots, 0)$,

- all the **permutations** of $(1/3, 1/3, 1/3, \ldots, 0)$, and

- so on

- to the **point** $(1/q, 1/q, \ldots, 1/q)$.

A simplex centroid design **only** has **one point** in the **interior** of the simplex; all the **rest** are on the **boundary**.

Figure 7(b) illustrates a simplex centroid in three factors.

Designs for mixtures

Complete mixtures

Mixtures in the **interior** of the **simplex**—that is, mixtures which include at least some of each component—are called **complete mixtures.**

We sometimes **need** to do our experiments with **complete mixtures**.

This may arise for several reasons, for example, **all components** may **need** to be present for a chemical **reaction** to **take place.**

Designs for mixtures

Factorial ratios

Factorial ratios provide one class of designs for **complete mixtures**.

This design is a **factorial** in the **ratios** of the first $q - 1$ components to the last component.

We may want to reorder our components to obtain a convenient "last" component.

Designs for mixtures

Factorial ratios

The **design points** will have

- **ratios $\boldsymbol{x_k/x_q}$** that take a **few fixed values** (the factorial levels) for each k, and

- we then **solve** for the actual **proportions** of the components.

For example, if $x_1/x_3 = 4$ and $x_2/x_3 = 2$, then $x_1 = 4/7$, $x_2 = 2/7$, and $x_3 = 1/7$.

Only complete mixtures occur in a factorial ratios design with all ratios greater than 0.

Designs for mixtures

Example 6: Harvey Wallbangers

Sahrmann, Piepel, and Cornell (1987) ran an experiment to find the **best proportions** for

- **orange juice** (O),

- **vodka** (V), and

- **Galliano** (G)

in a mixed drink called a **Harvey Wallbanger**.

Designs for mixtures

Example 6: Harvey Wallbangers

Only complete mixtures are considered, because it is the **mixture of these three ingredients** that **defines** a **Wallbanger** (as opposed to say, orange juice and vodka, which is a drink called a screwdriver).

Furthermore, preliminary screening established some approximate limits for the various components.

Designs for mixtures

Example 6: Harvey Wallbangers

The authors used a **factorial ratios** model, with **three levels** of the **ratio** V/G (1.2, 2.0, and 2.8) and **two levels** of the **ratio** O/G (4 and 9).

They also ran a **center point** at $V/G = 2$ and $O/G = 6.5$.

Designs for mixtures

Example 6: Harvey Wallbangers

Their actual design included **incomplete blocks** (so that no evaluator consumed more than a small number of drinks). However, there were **no apparent evaluator differences**, so the average score was used as response for each mixture, and **blocks were ignored**.

Evaluators rated the drinks on a 1 to 7 scale. The data are given in Table 4, which also shows the actual proportions of the three components.

Designs for mixtures

Example 6: Harvey Wallbangers

O/G	V/G	G	V	O	Rating
4.0	1.2	.161	.194	.645	3.6
9.0	1.2	.089	.107	.804	5.1
4.0	2.8	.128	.359	.513	3.8
9.0	2.8	.078	.219	.703	3.8
6.5	2.0	.105	.211	.684	4.7
4.0	2.0	.143	.286	.571	2.4
9.0	2.0	.083	.167	.750	4.0

Table 4: Harvey Wallbanger mixture experiment.

Designs for mixtures

Complete mixtures through pseudo components

A **second class** of complete-mixture designs arises when we have **lower bounds** for **each component**: $x_k \geqslant d_k > 0$, where $\sum d_k = D < 1$. Here, we define ***pseudocomponents***

$$x'_k = \frac{x_k - d_k}{1 - D}$$

and do a **simplex lattice** or **simplex centroid** design in the **pseudocomponents.**

Designs for mixtures

Complete mixtures through pseudo components

The **pseudocomponents map back** to the **original components** via

$$x_k = d_k + (1 - D)x'_k.$$

Designs for mixtures

Dealing with more complex constraints

Many **realistic mixture problems** are **constrained** in some way so that the **available design space** is **not** the **full simplex or** even a **simplex of pseudocomponents**:

- a **regulatory constraint** might say that ice cream **must contain at least** a certain percent fat, so we are constrained to use mixtures that contain at least the required amount of fat;

- and an **economic constraint** requires that our recipe **cost less than a fixed amount.**

Mixture designs can be adapted to such situations, but we often **need special software** to determine a good design for a specific model over a constrained space.

Contents

Models for mixture designs

Polynomial models

Polynomial models for a **mixture response** have **fewer parameters** than the general polynomial model found in ordinary response surfaces for the same number of design variables.

This **reduction** in parameters arises **from** the **simplex constraints** on the mixture components –some terms disappear due to the linear restrictions among the mixture components.

Models for mixture designs

First-order model

For example, consider a **first-order model** for a **mixture** with **three components.** In such a mixture, we have $x_1 + x_2 + x_3 = 1$. Thus,

$$\begin{aligned} f(x_1, x_2, x_3) &= \bar{\beta}_0 + \bar{\beta}_1 x_1 + \bar{\beta}_2 x_2 + \bar{\beta}_3 x_3 \\ &= \bar{\beta}_0(x_1 + x_2 + x_3) + \bar{\beta}_1 x_1 + \bar{\beta}_2 x_2 + \bar{\beta}_3 x_3 \\ &= (\bar{\beta}_1 + \bar{\beta}_0)x_1 + (\bar{\beta}_2 + \bar{\beta}_0)x_2 + (\bar{\beta}_3 + \bar{\beta}_0)x_3 \\ &= \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 \end{aligned}$$

Models for mixture designs

Canonical Form of first-order Models

In this model, the **linear constraint** on the mixture components has allowed us to **eliminate the constant** from the model.

This **reducted model** is called the **canonical form** of the **mixture polynomial**.

Models for mixture designs

Canonical Form of second-order Models

Mixture constraints also permit **simplifications** in **second-order** models.

Not only can we eliminate the constant, but we can also **eliminate** the **pure quadratic** terms! For example:

$$\begin{aligned} x_1^2 &= x_1 x_1 \\ &= x_1(1 - x_2 - x_3 - \cdots - x_q) \\ &= x_1 - x_1 x_2 - x_1 x_3 - \cdots - x_1 x_q. \end{aligned}$$

Models for mixture designs

Canonical Form of second-order Models

By making **similar substitutions** for all **pure quadratic terms**, we get the **canonical form**:

$$f(x_1, x_2, \cdots, x_q) = \sum_{k=1}^{q} \beta_k x_k + \sum_{k<l}^{q} \beta_{kl} x_k x_l.$$

Models for mixture designs

Canonical Form of third-order Models

Third-order models are sometimes fit for mixtures; the canonical form for the full third-order model is:

$$\begin{aligned} f(x_1, x_2, \ldots, x_q) &= \sum_{k=1}^{q} \beta_k x_k + \sum_{k<l}^{q} \beta_{kl} x_k x_l \\ &+ \sum_{k<l}^{q} \delta_{kl} x_k x_l (x_k - x_l) + \sum_{k<l<n}^{q} \beta_{klm} x_k x_l x_n. \end{aligned}$$

Models for mixture designs

Special Cubic Models

A **subset** of the full cubic model called the **special cubic model** sometimes appears:

$$f(x_1, x_2, \ldots, x_q) = \sum_{k=1}^{q} \beta_k x_k + \sum_{k<l}^{q} \beta_{kl} x_k x_l + \sum_{k<l<n}^{q} \beta_{kln} x_k x_l x_n.$$

Models for mixture designs

Interpreting polynomial coefficients

Coefficients in mixture canonical polynomials have **interpretations** that are **somewhat different from standard polynomials**.

If the mixture is pure (that is, contains only a single component, say component k), then x_k is 1 and the other components are 0. The predicted response is β_k. Thus the **"linear" coefficients** give the **predicted response** when the **mixture** is simply a **single component.**

Models for mixture designs

Interpreting polynomial coefficients

If the **mixture** is **pure** (that is, contains only a single component, say component k), then x_k is 1 and the other components are 0.

The predicted response is

$$\beta_k .$$

Thus the **“linear” coefficients** give the **predicted response** when the **mixture** is simply a **single component.**

Models for mixture designs

Interpreting polynomial coefficients

If the **mixture** is a **50** $-$ **50 mix** of components k and l, then the predicted response is

$$\beta_k/2 + \beta_l/2 + \beta_{kl}/4.$$

Thus the **bivariate interaction** terms correspond to **deviations from** a simple **additive fit**, and in particular show how the response for pairwise blends varies from additive.

Models for mixture designs

Interpreting polynomial coefficients

The **three-way interaction** term β_{klm} has a **similar interpretation** for triples.

The **cubic interaction** term δ_{kl} provides some **asymmetry** in the **response** to **two-way blends**.

Models for mixture designs

Fewer factors as an alternative to reduced models

We may use **ordinary polynomial** models in $q - 1$ **factors instead** of **reduced polynomial** models in q **factors.**

For example, the canonical quadratic as model in $q = 3$ factors is

$$y = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3.$$

We can instead use the model

$$y = \tilde{\beta}_0 + \tilde{\beta}_1 x_1 + \tilde{\beta}_2 x_2 + \tilde{\beta}_{12} x_1 x_2 + \tilde{\beta}_{11} x_1^2 + \tilde{\beta}_{22} x_2^2,$$

which is the usual quadratic model for $q = 2$ factors.

Models for mixture designs

Fewer factors as an alternative to reduced models

The **models** are **equivalent mathematically**, and which model you **choose** is **personal preference**.

There are **linear relations between the models** that allow you to transfer between the representations.

For example,

$$\tilde{\beta}_0 = \beta_3 \quad (x_3 = 1, x_1 = x_2 = 0),$$

and

$$\tilde{\beta}_0 + \tilde{\beta}_1 + \tilde{\beta}_{11} = \beta_1 \quad (x_1 = 1, x_2 = x_3 = 0).$$

Models for mixture designs

Factorial ratios, model choice

Factorial ratios experiments also have the option of using **polynomials** in the **components**, polynomials in the **ratios**, or a **combination of the two.**

The **choice of model** can **sometimes** be determined **a priori** but will **frequently** be determined by **choosing** the **model** that **best fits** the data.

Models for mixture designs

Example 7: Harvey Wallbangers, continued

Listing 4 shows the results from **fitting** the **canonical second-order** model to Harvey Wallbanger data (Example 6).

```
       Coef    StdErr         t
g   -518.14   41.143   -12.594
o   -12.625   1.1111   -11.363
v    100.56   5.8373    17.226
og   812.73   55.472    14.651
vg   126.64   56.449    2.2435
ov  -101.53   5.8706   -17.294

N: 7, MSE: 0.0042851, DF: 1, R^2: 0.99996
Regression F(6,1): 4344.4, Durbin-Watson: 2.1195
```

Listing 4: MacAnova output for second-order model of Harvey Wallbanger data.

Models for mixture designs

Example 7: Harvey Wallbangers, continued

All terms are **significant** with the **exception** of the **vodka by Galliano interaction** (**though there is only 1 degree of freedom for error, so significance testing is rather dubious**).

It is **difficult** to **interpret** the **coefficients directly**.

Models for mixture designs

Example 7: Harvey Wallbangers, continued

The **usual interpretations** for **coefficients** are for **pure** mixtures and **two-component mixtures**, but this experiment was conducted on a **small region** in the **interior** of the **design space**.

Thus using the model for pure mixtures or two-component mixtures would be an unwarranted extrapolation.

The **best approach** is to **plot** the **contours** of the **fitted response surface**, as shown in Figure 8.

Models for mixture designs

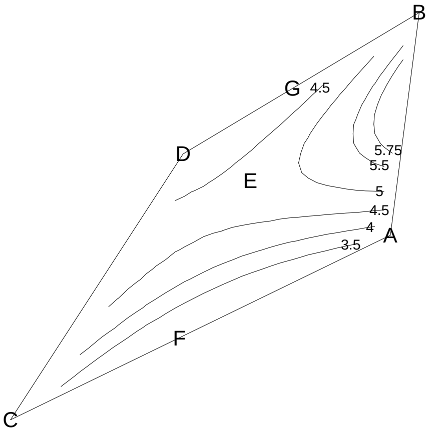

Figure 8: Contour plot for Harvey Wallbanger data, using S-Plus. Letters indicate the points of Table 4 in the table order.

Models for mixture designs

Example 7: Harvey Wallbangers, continued

We see that

- there is a **saddle point** near the **fifth design point** (the center point denoted by E on Figure 8), and

- the **highest estimated responses** are on the **boundary between the first two design points** (denoted by A and B). This has the V/G ratio at 1.2 and the O/G ratio between 4.0 and 9.0, but somewhat closer to 9.0.

Appendix

Further Reading and Extensions: RSM and Mixtures

As might be expected, there is much more to the subjects we discussed.

Box and Draper (1987) and Cornell (1990) provide excellent booklength coverage of response surfaces and mixture experiments respectively.

Appendix

Further Reading and Extensions: Constraints

Earlier we alluded to the issue of constraints on the design space. These constraints can make it difficult to run standard response surface or mixture designs.

Special-purpose computer software (for example, Design-Expert) can construct good designs for constrained situations.

These designs are generally chosen to be optimal in the sense of minimizing the estimation variance. See Cook and Nachtsheim (1980) or Cook and Nachtsheim (1989).

Appendix

Further Reading and Extensions: Multiresponse

A second interesting area is trying to optimize when there is more than one response. Multiple responses are common in the real world, and methods have been proposed to compromise among the competing criteria. See Myers, Khuri, and Carter (1989) and the references cited there.

Appendix

Rotatability and moment matrices

Derived power and Schlaifflian matrix

It is convenient in expressing the polynomial model to make use of *derived power vectors* and *Schlaifflian matrices*.

Definition

If $\boldsymbol{z}' = (z_1, \ldots, z_k)$, then $\boldsymbol{z}'^{[p]}$, the derived power of degree p, is defined such that

$$\boldsymbol{z}'^{[p]} \boldsymbol{z}^{[p]} = (\boldsymbol{z}'\boldsymbol{z})^p.$$

Appendix

Rotatability and moment matrices

Derived power

For example if $\boldsymbol{z}' = (z_1, \ldots, z_3)$, then

$$\boldsymbol{z}'^{[2]} = (z_1^2, z_2^2, z_3^2, \sqrt{2}z_1 z_2, \sqrt{2}z_1 z_3, \sqrt{2}z_2 z_3)$$

and

$$\boldsymbol{z}'^{[1]} = \boldsymbol{z}' = (z_1, \ldots, z_3).$$

Appendix

Rotatability and moment matrices

Definition

If a vector $\boldsymbol{x}$ is formed from a vector $\boldsymbol{z}$ containing k elements through the transformation

$$\boldsymbol{x} = \boldsymbol{H}\boldsymbol{z}$$

then the Schlaifflian matrix $\boldsymbol{H}^{[p]}$ is defined such that

$$\boldsymbol{x}^{[p]} = \boldsymbol{H}^{[p]}\boldsymbol{z}^{[p]}.$$

Appendix

Rotatability and moment matrices

Remark 1

It is readily seen that if the transformation $\boldsymbol{H}$ is orthogonal, then $\boldsymbol{H}^{[p]}$ is also orthogonal. One can write

$$\boldsymbol{x}'^{[p]}\boldsymbol{x}^{[p]} = \boldsymbol{z}'^{[p]}\boldsymbol{H}'^{[p]}\boldsymbol{H}^{[p]}\boldsymbol{z}^{[p]}. \qquad (1)$$

The left-hand side of Equation 1 is, by definition, $(\boldsymbol{z}'\boldsymbol{z})^p$. Because $\boldsymbol{H}$ is orthogonal,

$$(\boldsymbol{x}'\boldsymbol{x})^p = (\boldsymbol{z}'\boldsymbol{z})^p = \boldsymbol{z}'^{[p]}\boldsymbol{z}^{[p]}$$

and thus the Schlaifflian matrix $\boldsymbol{H}^{[p]}$ is orthogonal.

Appendix

Rotatability and moment matrices

Remark

Another result which is quite useful in what follows is that, given two vectors x and z, each having k elements, then

$$(\boldsymbol{x}'\boldsymbol{z})^p = \boldsymbol{x}'^{[p]}\boldsymbol{z}^{[p]}$$

and thus the Schlaifflian matrix $\boldsymbol{H}^{[p]}$ is orthogonal.

Appendix

Rotatability and moment matrices

Response function

For a response function of order d, the estimated response $\hat{y}$ can be written in the form

$$\hat{y} = \boldsymbol{x}'^{[d]}\boldsymbol{b} \tag{2}$$

where for a point $(x_1, x_2, \ldots, x_k)$ we have

$$\boldsymbol{x}' = (1, x_1, x_2, \ldots, x_k)$$

and the vector $\boldsymbol{b}$ contains the least squares estimators b_0, b_1, $\ldots$, and so on, with suitable multipliers.

Appendix

Rotatability and moment matrices

Response function (1/2)

For example, for $k = 2$, $d = 2$, then $\boldsymbol{x}' = (1, x_1, x_2)$, and $\boldsymbol{b}'$ and $\boldsymbol{x}'^{[2]}$ are given by

$$\begin{aligned} \boldsymbol{b}' &= (b_0, b_1/\sqrt{2}, b_2/\sqrt{2}, b_{11}, b_{22}, b_{12}/\sqrt{2}) \\ \boldsymbol{x}'^{[2]} &= (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1 x_2) \end{aligned} \qquad (3)$$

Appendix

Rotatability and moment matrices

Response function (2/2)

Thus, from Equation 2 we obtain

$$\begin{aligned} \text{Var}[\hat{y}(\boldsymbol{x})] &= \boldsymbol{x}'^{[d]}\text{Var}[\boldsymbol{b}]\boldsymbol{x}^{[d]} \\ &= \sigma^2 \boldsymbol{x}'^{[d]}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}^{[d]} \end{aligned} \tag{4}$$

where $\sigma^2(\boldsymbol{X}'\boldsymbol{X})^{-1}$ is the variance-covariance matrix of vector $\boldsymbol{b}$.

Appendix

Rotatability and moment matrices

Introducing a second point

Consider now a second point $(z_1, z_2, \ldots, z_k)$ which is at the same distance from the origin as the point described by $(x_1, x_2, \ldots, x_k)$. Denote by $\boldsymbol{z}'$ the vector $(1, z_1, z_2, \ldots, z_k)$. There is, then, an orthogonal matrix $\boldsymbol{R}$ for which

$$\boldsymbol{z} = \boldsymbol{R}\boldsymbol{x} \tag{5}$$

where $\boldsymbol{R}$ is of the form

$$\boldsymbol{R} = \begin{pmatrix} 1 & \boldsymbol{0}_k \\ \boldsymbol{0}'_k & \boldsymbol{H}_{k\times k} \end{pmatrix}. \tag{6}$$

and $\boldsymbol{H}$ is an orthogonal matrix of order k.

Appendix

Rotatability and moment matrices

Variance of a prediction

The variance pf the estimated response at the second point is then

$$\mathrm{Var}[\hat{y}(\boldsymbol{z})] = \sigma^2 \boldsymbol{z}'^{[d]} (\boldsymbol{X}'\boldsymbol{X})^{-1} \boldsymbol{z}^{[d]}.$$

Let $\boldsymbol{R}^{[d]}$ be the Schlaifflian matrix of the transformation in Equation 5.

$$\begin{aligned} \mathrm{Var}[\hat{y}(\boldsymbol{z})] &= \sigma^2 \boldsymbol{x}'^{[d]} \boldsymbol{R}'^{[d]} (\boldsymbol{X}'\boldsymbol{X})^{-1} \boldsymbol{R}^{[d]} \boldsymbol{x}^{[d]} \\ &= \sigma^2 \boldsymbol{x}'^{[d]} (\boldsymbol{R}'^{[d]} \boldsymbol{X}'\boldsymbol{X} \boldsymbol{R}^{[d]})^{-1} \boldsymbol{x}^{[d]} \end{aligned}$$

because $\boldsymbol{R}^{[d]}$ is orthogonal.

Appendix

Rotatability and moment matrices

Rotatability condition

For the design to be rotatable, $\mathrm{Var}[\hat{y}]$ is constant on spheres, which implies that for any orthogonal matrix $\boldsymbol{H}$ we have

$$\boldsymbol{X}'\boldsymbol{X} = \boldsymbol{R}'^{[d]}\boldsymbol{X}'\boldsymbol{X}\boldsymbol{R}^{[d]} \tag{7}$$

where $\boldsymbol{R}$ is of the form indicated in Equation 6. The requirement in Equation 7 essentially means that the moment matrix remains the same if the design is *rotated*.

Appendix

Rotatability and moment matrices

Rotating model matrices

The requirement in Equation 7 essentially means that the moment matrix remains the same if the design is *rotated* –that is, if the rows of the *design* matrix, denoted by $\boldsymbol{D}$ in the equation

$$\begin{pmatrix} 1 & \\ 1 & \\ \vdots & \boldsymbol{D} \\ 1 & \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & x_{21} & \cdots & x_{k1} \\ 1 & x_{12} & x_{22} & \cdots & x_{k2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{1N} & x_{2N} & \cdots & x_{kN} \end{pmatrix} = \begin{pmatrix} \boldsymbol{x}'_1 \\ \boldsymbol{x}'_2 \\ \vdots \\ \boldsymbol{x}'_N \end{pmatrix} \tag{8}$$

are rotated via the transformation

$$\boldsymbol{z}_i = \boldsymbol{R}' \boldsymbol{x}_i.$$

Appendix

Rotatability and moment matrices

Moment generating function (1/3)

It is easily seen that the rotated design will have moment matrix (apart from the constant N^{-1}) equal to the right-hand side of Equation 7.

Consider now a vector $\boldsymbol{t}' = (1, t_1, t_2, \ldots, t_k)$ of dummy variables. The utility of these variables is in the construction of a generating function for the design moments. Consider the quantity

$$M.F. = N^{-1}\boldsymbol{t}'^{[d]}\boldsymbol{X}'\boldsymbol{X}\boldsymbol{t}^{[d]}.$$

Appendix

Rotatability and moment matrices

Moment generating function (2/3)

The matrix $\boldsymbol{X}'\boldsymbol{X}$ is alternatively given by

$$\boldsymbol{X}'\boldsymbol{X} = \sum_{u=1}^{N} \boldsymbol{x}_u^{[d]} \boldsymbol{x}_u'^{[d]}$$

where the vector $\boldsymbol{x}'_u = (1, x_{1u}, x_{2u}, \ldots, x_{Nu})$ refers to the u$^{\text{th}}$ row of the design matrix, augmented by 1–that is, the u$^{\text{th}}$ of the matrix in the Equation 8.

Appendix

Rotatability and moment matrices

Moment generating function (3/3)

Then

$$\begin{aligned} M.F. &= N^{-1}\sum_{u=1}^{N}(\boldsymbol{t}'^{[d]}\boldsymbol{x}_u^{[d]}\boldsymbol{x}'^{[d]}_u\boldsymbol{t}^{[d]}) \\ &= N^{-1}\sum_{u=1}^{N}(\boldsymbol{t}'\boldsymbol{x}_u)^{2d}. \end{aligned} \quad (9)$$

From Equation 9, it is seen that upon expanding $\boldsymbol{t}'\boldsymbol{x}_u$ we have

$$M.F. = N^{-1}\sum_{u=1}^{N}(1 + t_1x_{1u} + t_2x_{2u} + \cdots + t_kx_{ku})^{2d} \quad (10)$$

Appendix

Rotatability and moment matrices

Coefficients of M.F.

When Equation 10 is expanded, the terms involve moments of the design through order $2d$. In fact, the coefficient of $t_1^{\delta_1} t_2^{\delta_2} \cdots t_k^{\delta_k}$ is

$$\frac{(2d)!}{(2d-\delta)! \prod_{i=1}^{k} (\delta_i)!} [1^{\delta_1} 2^{\delta_2} \cdots k^{\delta_k}] \qquad (11)$$

where $\sum_{i=1}^{k} \delta_i = \delta \leqslant 2d$.

Appendix

Rotatability and moment matrices

Rotating M.F.

For a rotatable design,

$$\begin{aligned} M.F. &= N^{-1}\boldsymbol{t'}^{[d]}(\boldsymbol{X'X})\boldsymbol{t}^{[d]} = N^{-1}\boldsymbol{t'}^{[d]}(\boldsymbol{R'}^{[d]}\boldsymbol{X'XR}^{[d]})\boldsymbol{t}^{[d]} \\ &= N^{-1}(\boldsymbol{t'R'})^{[d]}\boldsymbol{X'X}(\boldsymbol{Rt})^{[d]} \end{aligned}$$

where $\boldsymbol{R}$ is a $(k+1) \times (k+1)$ orthogonal matrix introduced in Equation 6.

Appendix

Rotatability and moment matrices

M.F. is radial if rotatable design

This implies that for a rotatable design, an orthogonal transformation on $\boldsymbol{t}$ does not affect the M.F.

Because M.F. is a polynomial in the $\boldsymbol{t}$'s (also involving the design moments), for a rotatable design, M.F. must be a function of $\sum_{i=1}^{k} t_i^2$. That is a radial function of the form

$$M.F. = \sum_{j=0}^{d} a_{2j} \left(\sum_{i=1}^{k} t_i^2 \right)^j . \qquad (12)$$

Appendix

Rotatability and moment matrices

Coefficients of a radial function

It is easily seen that the coefficient of $t_1^{\delta_1} t_2^{\delta_2} \cdots t_k^{\delta_k}$ in Equation 12

is zero *if any of the* δ_i *are odd*.

For the case where all δ_i are even, the coefficient from the multinomial expansion of $(\sum_{i=1}^{k} t_i^2)^j$ is given by

$$\frac{a_\delta (\delta/2)!}{\prod_{i=1}^{k} (\delta_i/2)!} . \tag{13}$$

Appendix

Rotatability and moment matrices

Coefficients of a radial M.F.

We now consider Equation 13 with Equation 11, the former pertaining to the generating function for the moments *in general*, and the latter pertaining to the case of rotatable design, with the value being zero with any δ_i odd.

Upon equating the two and solving or the moment, the result is as given on the next slide.

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Appendix

Rotatability and moment matrices

Moments of a rotatable design

$$N^{-1}\sum_{u=1}^{N} x_{1u}^{\delta_1}x_{2u}^{\delta_2}\cdots x_{ku}^{\delta_k} = \frac{\lambda_\delta \prod_{i=1}^{k}(\delta_i)!}{2^{\delta/2}\prod_{i=1}^{k}(\delta_i/2)!} \tag{14}$$

for all δ_i even and

$$N^{-1}\sum_{u=1}^{N} x_{1u}^{\delta_1}x_{2u}^{\delta_2}\cdots x_{ku}^{\delta_k} = 0 \tag{15}$$

for any δ_i odd. Here λ_δ is given by

$$\lambda_\delta = \frac{a_\delta 2^{\delta/2}(\delta/2)!(2d-\delta)!}{(2d)!}\,. \tag{16}$$

Appendix

Rotatability and moment matrices

Moments of a first or second order rotatable design

If we consider Equations 14 and 16.

For the **first order** case, we have $d = 1$ and thus

- $[i] = [ij] = 0$, for $i \neq j$,
- $[ii] = \lambda_1$ (fixed by scaling).

For the **second order** case, we have $d = 2$ and thus

- $[i] = [ij] = [ijk] = [iij] = [iii] = 0$, for $i \neq j \neq k$,
- $[ii] = \lambda_2$ (fixed by scaling) and
- $[iiii]/[iijj] = 3$.

Appendix

Downloading the Datasets

Individual data sets can be accessed over the web as plain text files with labelled columns using a URL like
http://www.stat.umn.edu/~gary/book/fcdae.data/xxxx
The xxx takes the form of exmpl19.1 for example 1 from chapter 19, ex2.5 for exercise 5 from chapter 2, and pr13.14 for problem 14 from chapter 13.

Appendix

Downloading the Datasets

You can access these directly from R via, for example,

```
baseurl="http://users.stat.umn.edu/~gary/book/"
exmpl19.1url=paste(baseurl,"fcdae.data/exmpl19.1"
                   ,sep="")
str(read.table(exmpl19.1url,header=TRUE,
               encoding="latin1"))

## 'data.frame': 7 obs. of  3 variables:
##  $ time       : int  -1 1 -1 1 0 0 0
##  $ temperature: int  -1 -1 1 1 0 0 0
##  $ appeal     : num  3.89 6.36 7.65 6.79 8.36 7.
```