

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.

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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**?

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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.

Visualizing the Response

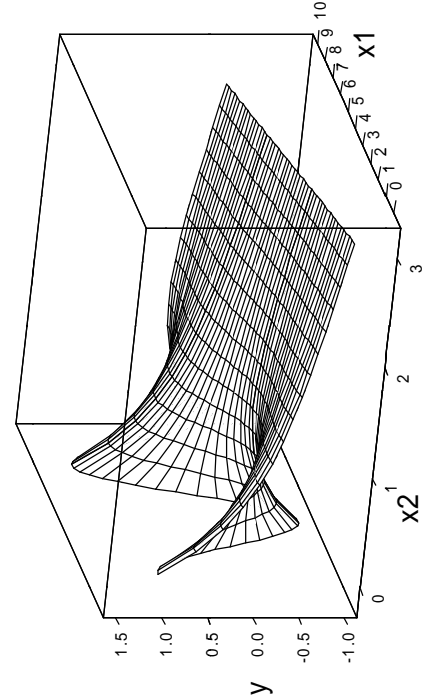


Figure 1: Sample perspective plot, using Minitab.

Visualizing the Response

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Contour Plot of y

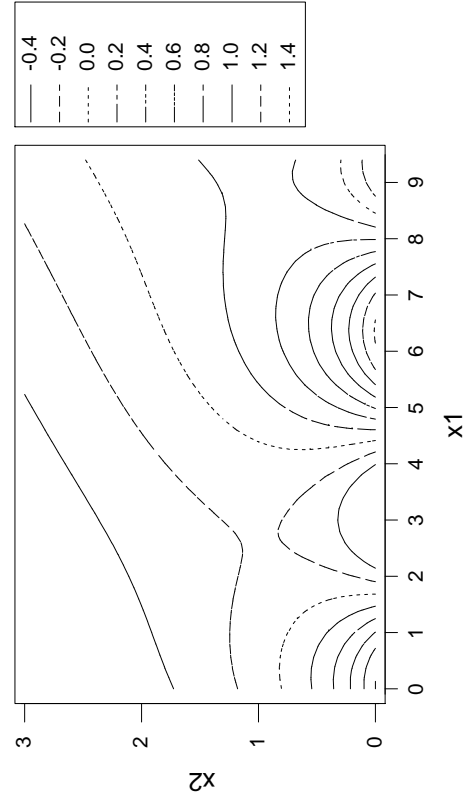


Figure 2: Sample contour plot, using Minitab.

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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 .**

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

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

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

where $\mathbf{x}_i = (x_{1i}, x_{2i}, \dots, x_{qi})'$ and $\boldsymbol{\beta} = (\beta_1, \beta_2, \dots, \beta_q)'$. 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

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

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

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

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 \mathbf{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

Introduction

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

For a **first-order surface**, design points \mathbf{x} and $\mathbf{x} + \delta$ 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**.



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 $\mathbf{x} + r\beta$, for some $r > 0$.

If we want the direction of **steepest descent**, then we **move to** $\mathbf{x} - r\beta$, 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**.



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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

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 ± 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 $(x_1 - 35)/2$, so that **33 minutes** is a **-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 2^q factorial with **center points**. The (coded) low and high values for each **variable** are ± 1 ; the **center points** are **m observations** taken with all variables at **0**.

This design has $2^q + m$ points. We may also use any $2^q - k$ 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

First-Order Designs

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 **2²** 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 $\mathbf{b} = \hat{\beta}$ 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

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 \mathbf{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**:

$$SS_{\text{Tot}} = SS_{\text{Model}} + SS_{\text{LoF}} + SS_{\text{PE}}$$

$$n - 1 = df_{\text{Model}} + df_{\text{LoF}} + df_{\text{PE}}$$

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 MS_{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 MS_{LoF} / MS_{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

Example 2: Cake baking, continued

Example 1 was a 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

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

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
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.

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

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 direction of **steepest ascent** in this model is proportional to **(.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**.

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.

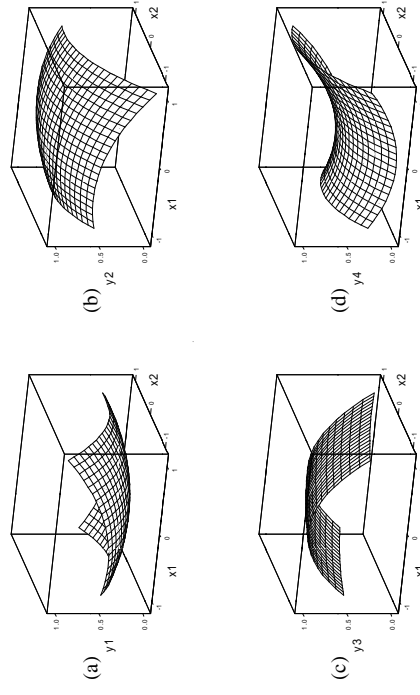


Figure 3: Sample second-order surfaces: (a) minimum, (b) maximum, (c) ridge, and (d) saddle, using Minitab.

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.

Canonical variables

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

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

where $\mathbf{v} = (v_1, v_2, \dots, v_q)'$ is the design variables expressed in canonical coordinates; $f_v(\mathbf{v})$ 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 \mathbf{x} value that maps to $\mathbf{0}$ in the canonical variables is called the **stationary point** and is denoted by \mathbf{x}_0 ; thus $f_v(\mathbf{0}) = f(\mathbf{x}_0)$.

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.

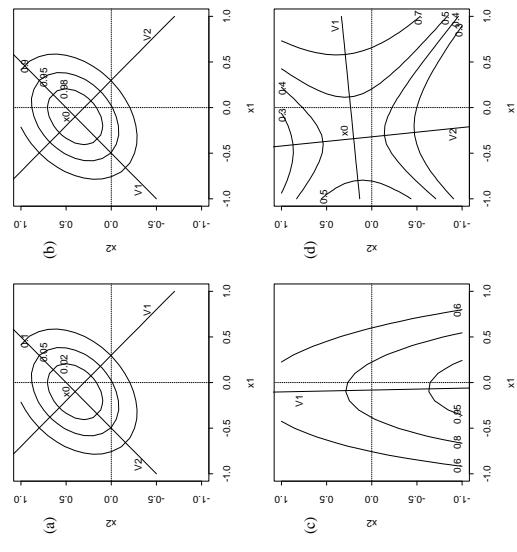


Figure 4: Contours, stationary points, and canonical axes for Figure 3.

Contours

As shown in this figure (a) and (b), **contours** for surfaces with **maxima** or **minima** are **ellipses**. The stationary point \mathbf{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

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

Second-Order Models

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**

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

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

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

Second-Order Models

Change of coordinates

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

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

where

$$f_v(\mathbf{0}) = f(\mathbf{x}_0) = \beta_0 + \frac{1}{2} \mathbf{x}_0' \boldsymbol{\beta}.$$

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

Change of coordinates

The numbers λ_k are the **eigenvalues** of \mathbf{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 $\mathbf{v}' = (v_1, v_2, \dots, v_q)$ **via**

$$\mathbf{v} = H'(\mathbf{x} - \mathbf{x}_0).$$

Subtracting \mathbf{x}_0 shifts the origin, and multiplying by H' rotates to the canonical axes.

Second-Order Models

Shape analysis

- 1) If all of the λ_k 's are positive, \mathbf{x}_0 is a minimum.
- 2) If all of the λ_k 's are negative, \mathbf{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, \mathbf{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**.

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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.

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

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

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

Orthogonal blocking

We can achieve this **orthogonality** by choosing

- α and
- 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	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

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

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 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.

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**.

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 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

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

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

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

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 $q \geq 3$, as they require **large numbers** of design points.

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 ± 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 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: $\beta_{11} = \beta_{12} = \dots = \beta_{1q} = 0$.

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

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.

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

Second-Order Analysis

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 \mathbf{b} and \mathbf{B}** computed in the multiple regression.

Second-Order Analysis

Estimates

We **estimate the stationary point** as

$$\hat{\mathbf{x}}_0 = -\mathbf{B}^{-1} \mathbf{b}/2,$$

and the **eigenvectors and eigenvalues of \mathbf{B}** are estimated by the **eigenvectors and eigenvalues of \mathbf{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.

Introduction	First-Order Response Surfaces	Second-Order Response Surfaces	Mixture Experiments	Appendix
oo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo
oo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo
oo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo

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

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.

Introduction	First-Order Response Surfaces	Second-Order Response Surfaces	Mixture Experiments	Appendix
oo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo
oo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo
oo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo	oooooooooooooooooooooooooooo

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

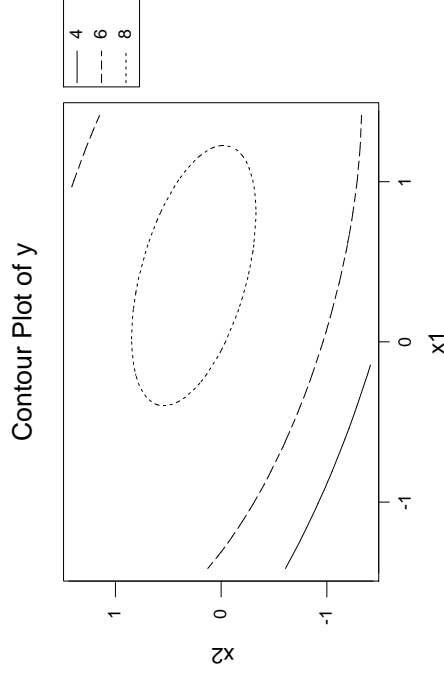


Figure 6: Contour plot of fitted second-order model for cake baking data, using Minitab.

Second-Order Analysis

Example 4: Cake baking, continued

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

Listing 3 shows a canonical analysis for this surface.

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

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

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



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.



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Mixture Experiments

Simplex

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

$$x_k \geq 0, \quad k = 1, 2, \dots, q$$

and

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

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

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
0	1	0	6.2	6.5
.5	.5	0	6.3	6.1
0	0	1	7.0	6.9
.5	0	.5	6.1	6.5
0	.5	.5	6.2	6.1

Table 3: Blends of fruit punch.

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

Model

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

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

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**.

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 $r = 0, 1, 2, \dots, m$.

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 $(0, 1/2, 1/2)$.

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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.

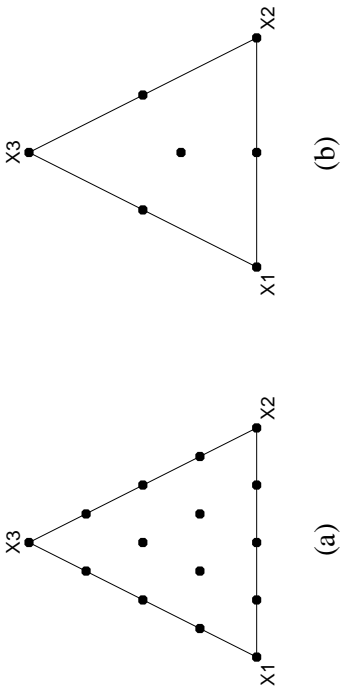


Figure 7: (a) $\{3,4\}$ simplex lattice and (b) three variable simplex centroid designs.

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 $1/2 - 1/3$ 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.

Simplex centroid designs

Alternatively, we may describe this design as

- all the **permutations** of $(1, 0, \dots, 0)$,
- all the **permutations** of $(1/2, 1/2, \dots, 0)$,
- all the **permutations** of $(1/3, 1/3, 1/3, \dots, 0)$, and
- so on
- to the **point** $(1/q, 1/q, \dots, 1/q)$.

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 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

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

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 $O/G = 6.5$.

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: $x_k \geq d_k > 0$, 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.

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Models for mixture designs

Canonical Form of second-order Models

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

$$f(X_1, X_2, \dots, X_q) = \sum_{k=1}^q \beta_k X_k + \sum_{k < l} \beta_{kl} X_k X_l.$$

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:

$$f(X_1, X_2, \dots, X_q) = \sum_{k=1}^q \beta_k X_k + \sum_{k < l} \beta_{kl} X_k X_l + \sum_{k < l < n} \beta_{klm} X_k X_l X_n.$$

Models for mixture designs

Special Cubic Models

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

$$f(X_1, X_2, \dots, X_q) = \sum_{k=1}^q \beta_k X_k + \sum_{k < l} \beta_{kl} X_k X_l + \sum_{k < l < n} \beta_{klm} X_k X_l X_n.$$

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

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	1.111	-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, R²: 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.

Appendix

Rotatability and moment matrices

Coefficients of a radial function

It is easily seen that the coefficient of $t_1^{\delta_1} t_2^{\delta_2} \dots t_k^{\delta_k}$ in Equation 12 is zero if any of the δ_j are odd.

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

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

Appendix

Rotatability and moment matrices

Moments of a rotatable design

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

for all δ_j even and

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

for any δ_j 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

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_j odd.

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

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

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

