5. Response Surface Methodology

So far, we have considered experiments where the aim is to study comparisons between treatments, e.g. comparative experiments, or the estimation of main effects and interactions in factorial experiments. A further type of experiment aims to study and *understand* the relationship between the controllable factors and the response:

- model (describe) the relationship between factors and response;
- predict the response at unobserved combinations of factor values;
- optimise the response: find factor values that produce a maximum or minimum response.

Typically, such experiments only consider a few factors, say 3 or 4. If there are more factors that may be important, a fractional factorial design should be used first in a *screening experiment* to identify the most important factors.

These aims are achieved via the use of *Response Surface Methodology* (RSM); a sequential strategy of experimentation, statistical modelling and optimisation.

Example 11: (Wu and Hamada, pg. 394)

An experiment to maximise the yield of a chemical reaction. There are two factors: reaction time (x_1) and temperature (x_2). The response is the yield (y) of the reaction.

Assume the following mathematical relationship between the response and the factors

$$Y = f(x_1, x_2) + \varepsilon\,,$$

with $\varepsilon \overset{\text{iid}}{\sim} N(0, \sigma^2)$ and $f(\cdot)$ an unknown function.

5.1. Sequential Process

Response surface methodology has broadly three phases:

1. **Phase 1:** Experiment to determine if the current operating conditions are near optimal.
2. **Phase 2:** Hill climb toward optimum
3. **Phase 3:** Fitting and interpreting a second-order model

Phase 1: Experimentation to determine if the current operating conditions are near optimal.

We could consider two models:

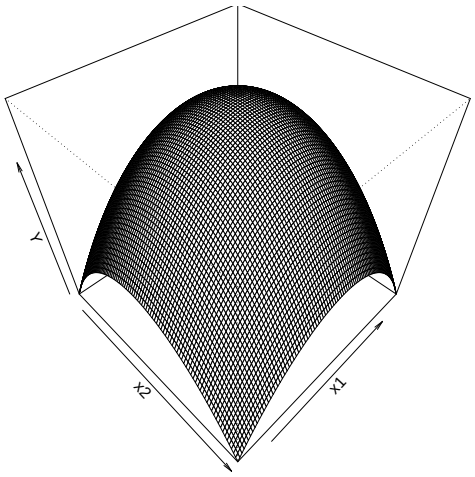
- A first order model

$$Y = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \varepsilon \,. \tag{5.1}$$

- A second order model

$$Y = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \sum_{i=1}^{m} \sum_{j>i}^{m} \beta_{ij} x_i x_j + \varepsilon \,. \tag{5.2}$$

At this stage, a first-order model is usually assumed for the response (i.e. we approximate $f(\cdot)$ with a linear function):



This model is most appropriate if the current conditions are far from optimal. At this stage of RSM, we want to test if this model is adequate for the response. A design capable of estimating model (5.2) is called a *first-order design*; typically a factorial or fractional factorial design *with repeated centre points* to check for curvature.

Example 11 cont.

Run	Time	Temp.	Yield
1	-1	-1	65.6
2	-1	1	45.6
3	1	-1	78.7
4	1	1	63.0
5	0	0	64.8
6	0	0	64.3

In fact, time $\in [75, 85]$ mins and temperature $\in [180, 190]^\circ$C but we scale so $x_1, x_2 \in [-1, 1]$; i.e.

$$x_1 = \frac{2(\text{time} - 75)}{85 - 75} - 1.$$

In general if we consider $x \in [x_{\min}, x_{\max}]$ we can renormalize it to $[-1, 1]$ by

$$2\frac{x - x_{\min}}{x_{\max} - x_{\min}} - 1 \tag{5.3}$$

So for time $x_{\min} = 75$, $x_{\max} = 85$ and we define $x_c = \frac{1}{2}(x_{\max} - x_{\min}) = 80$ as the midway-point and $|x_c - x_{\min}| = |x_c - x_{\max}|$ as the *half-range*. Once a variable is normalized in $[-1, 1]$, $x_c = 0$ and the half-range is equal to 1.

The centre points (0,0) allow us to test for curvature across the design region; evidence of substantial curvature suggests we may be in the region of an optimum.

Assume that there are n_f points in the factorial design, and n_c centre points. Let $\bar{Y}_f$ be the average of responses from the n_f factorial points and let $\bar{Y}_c$ be the average of responses from the n_c centre points.

Consider a second order model for $f(x_1, \ldots, x_m)$:

$$f(x_1, \ldots, x_m) = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \sum_{i=1}^{m} \sum_{j>i}^{m} \beta_{ij} x_i x_j \,. \tag{5.4}$$

Under model (5.4)

$$
\begin{aligned}
\mathrm{E}(\bar{Y}_c) &= \frac{1}{n_c}\left(\sum_{k=1}^{n_c}\left(\beta_0 + \sum_{i=1}^{m}\beta_i(0) + \sum_{i=1}^{m}\beta_{ii}(0) + \sum_{i=1}^{m}\sum_{j>i}^{m}\beta_{ij}(0)(0)\right)\right), \\
&= \beta_0, \\
\mathrm{E}(\bar{Y}_f) &= \frac{1}{n_f}[\\
&\quad \beta_0 + \beta_1(-1) + \ldots \beta_m(-1) + \beta_{11}(-1)^2 \cdots + \beta_{mm}(-1)^2 \\
&\qquad + \beta_{12}(-1)(-1) + \cdots + \beta_{mm}(-1)(-1) \\
&\quad +\beta_0 + \beta_1(+1) + \ldots \beta_m(-1) + \beta_{11}(+1)^2 \cdots + \beta_{mm}(-1)^2 \\
&\qquad + \beta_{12}(+1)(-1) + \cdots + \beta_{mm}(-1)(-1) \\
&\quad \ldots \\
&\quad +\beta_0 + \beta_1(+1) + \ldots \beta_m(+1) + \beta_{11}(+1)^2 \cdots + \beta_{mm}(+1)^2 \\
&\qquad + \beta_{12}(+1)(+1) + \cdots + \beta_{mm}(+1)(+1)]\,, \\
&= \frac{1}{n_f}\left[2^m\beta_0 + 2^m\beta_{11} + \ldots 2^m\beta_{mm}\right], \\
&= \beta_0 + \sum_{i=1}^{m}\beta_{ii} \qquad \text{since } n_f = 2^m.
\end{aligned}
$$

Therefore

$$\mathrm{E}(\bar{Y}_f - \bar{Y}_c) = \sum_{i=1}^{m} \beta_{ii}\,,$$

and we can use the sample difference $\bar{Y}_f - \bar{Y}_c$ to test if the overall curvature, measured by $\hat{\beta}_{11} + \hat{\beta}_{22} + \cdots + \hat{\beta}_{mm}$, is zero. Now

$$\mathrm{Var}(\bar{Y}_f - \bar{Y}_c) = \sigma^2 \left(\frac{1}{n_f} + \frac{1}{n_c}\right)\,,$$

and hence we can use the following t-test for the curvature: reject H_0: $\sum_{i=1}^{m} \beta_{ii} = 0$ if

$$\frac{|\bar{Y}_f - \bar{Y}_c|}{s\sqrt{(\frac{1}{n_f} + \frac{1}{n_c})}} > t_{n_{c-1}}(\alpha/2)\,. \tag{5.5}$$

Here, s^2 is the sample variance from the n_c centre points, and we are assuming β_{ii} have the same sign (otherwise they may cancel and lead to a deceptively small measure of curvature). This rarely occurs in practice unless experiment has been carried out near a saddle point (zero gradient but neither a minimum or maximum). To use t-test (5.5), we need a reasonable number of centre points on which to base s^2; a (very) rough rule of thumb: $n_c > 5$ to use (5.5).

Otherwise, you can compare $\sum \hat{\beta}_{ii}$ (i.e. $\left(\bar{Y}_f - \bar{Y}_c\right)$) to $\hat{\beta}_1, \ldots, \hat{\beta}_m$ (linear terms); if they are comparable in size, curvature may be present.

If the overall curvature is not significant, we are probably not near the region of optimum response, and a direction in which to explore next is needed.

If the curvature is significant, we should consider augmenting the existing design to enable the fitting of a full second order model.

Example 11 cont.

$$\bar{Y}_f = 63.2 \qquad \bar{Y}_c = 64.5$$

$$|\bar{Y}_f - \bar{Y}_c| = 1.3$$

As there are only two centre points, we can't do a formal t-test but $\hat{\beta}_1 = 7.63$ and $\hat{\beta}_2 = -8.94$ (from $\hat{\boldsymbol{\beta}} = (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}\boldsymbol{Y}$). As the curvature is much smaller than linear effects, it is unlikely to be important.

Phase 2: Hill climbing towards an optimum

If an initial experiment did not identify a region around the optimum response (i.e. there was no evidence of curvature), we need to decide where to experiment next. If we assume we want to maximise the response, we need to identify the direction in which the response is increasing.

The fitted first order model is

$$\hat{Y} = \hat{\beta}_0 + \sum_{i=1}^{m} \hat{\beta}_i x_i \,,$$

and so

$$\begin{aligned} \frac{\partial \hat{Y}}{\partial x_i} &= \frac{\partial}{\partial x_i} \sum_{i=1}^{m} \hat{\beta}_i x_i, \\ &= \hat{\beta}_i, \end{aligned}$$

is the estimated gradient of the fitted surface in x_i-plane. If the first-order model is appropriate, then the line joining $(0, \ldots, 0)$ and $(\hat{\beta}_1, \ldots, \hat{\beta}_m)$ gives the path along which the response is increasing most quickly. This is called the path of steepest ascent.

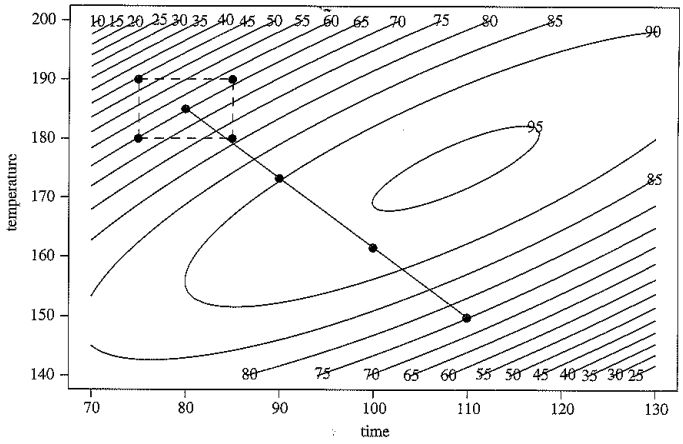
A strategy for finding the optimum response:

- choose a number of points along the path of steepest ascent, and measure the response at each;
- the point with the maximum observed response along this line should be used as centre point of the next design;
- use a first-order design once again, and check for curvature;
- if there is evidence of curvature, *augment* the design and fit the second-order model;
- otherwise, repeat the procedure and follow the new path.

If we want to minimise the response, the line joining $(0, \ldots, 0)$ and $(-\hat{\beta}_1, \ldots, -\hat{\beta}_m)$ is the path of *steepest descent*.

Example 11 cont.

Here $\hat{\beta}_1 = 7.62$ and $\hat{\beta}_2 = -8.94$ and so the path of steepest ascent is given by the line joining (0,0) and (7.62,-8.94). The pair of numbers (7.62,-8.94) can be renormalized as (7.62/7.62,-8.94/7.62)=(1,-1.173), that is, for one half-range increase in time there is a 1.173 half-range decrease in temperature. We consider increases in time by 2,4, and 6 half-ranges, which correspond to 90,100 and 110 minutes respectively. For temperature, -1.173*(2,4,6) corresponds to 173, 162 and 150° respectively. Thus three points were tested, (90 mins, 173°C), (100 mins, 162°C) [highest response, use as centre point in next experiment] and (110 mins, 150°C). The figure below shows a contour plot of true response surface (unknown to experimenters), the first design and path of steepest ascent.



Phase 3: Fitting and interpreting a second-order model

If there is evidence of significant curvature in the surface, the second-order model should be fitted:

$$Y = \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \sum_{i=1}^{m} \sum_{j>i}^{m} \beta_{ij} x_i x_j + \varepsilon \, .$$

This requires a *second-order design* capable of estimating this more detailed model; such a design is often obtained by augmenting a first-order design (see later).

Example 11 cont.

A first-order design in the region identified using steepest ascent (see above) was augmented to allow estimation of the second-order model:

Run	Time	Temp.	Yield
1	-1	-1	91.2
2	-1	1	94.2
3	1	-1	87.5
4	1	1	94.4
5	0	0	93.0
6	0	0	93.1
7	-1.41	0	93.6
8	1.41	0	91.2
9	0	-1.41	88.7
10	0	1.41	95.1

Here the coded units refer to new updated ranges for the factors: time is in $[93, 107]$mins and $[154, 170]^{\circ}$C.

The second-order model is fitted using least-squares

$$\hat{\boldsymbol{\beta}} = (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}\boldsymbol{Y}$$

to obtain $\hat{\beta}_0 = 93.05$, $\hat{\beta}_1 = -0.87$, $\hat{\beta}_2 = 2.36$, $\hat{\beta}_{12} = 0.99$, $\hat{\beta}_{11} = -0.43$ and $\hat{\beta}_{22} = -0.65$. This model fits well, with $R^2 = 0.995$ and adjusted $R^2 = 0.990$.

Predictions are given by

$$\hat{Y} = \hat{\beta}_0 + \sum_{i=1}^{m} \hat{\beta}_i x_i + \sum_{i=1}^{m} \hat{\beta}_{ii} x_i^2 + \sum_{i=1}^{m} \sum_{j>i}^{m} \hat{\beta}_{ij} x_i x_j \,,$$

which can be written as

$$\hat{Y} = \hat{\beta}_0 + \boldsymbol{x}^{\mathrm{T}}\boldsymbol{b} + \boldsymbol{x}^{\mathrm{T}}B\boldsymbol{x} \,,$$

where

$$\boldsymbol{x}^{\mathrm{T}} = (x_1, \ldots, x_m) \,, \qquad \boldsymbol{b}^{\mathrm{T}} = (\hat{\beta}_1, \ldots, \hat{\beta}_m) \,,$$

and

$$B = \begin{bmatrix} \hat{\beta}_{11} & \frac{1}{2}\hat{\beta}_{12} & \dots & \frac{1}{2}\hat{\beta}_{1m} \\ \frac{1}{2}\hat{\beta}_{12} & \hat{\beta}_{22} & & \vdots \\ \vdots & & \ddots & \vdots \\ \frac{1}{2}\hat{\beta}_{1m} & \dots & \dots & \hat{\beta}_{mm} \end{bmatrix}$$

(an $m \times m$ symmetric matrix).

This equation can be used to find the location of the optimum. First, we differentiate $\hat{Y}$ with respect to $\boldsymbol{x}$ and set equal to 0:

$$\frac{\partial \hat{Y}}{\partial \boldsymbol{x}} = \boldsymbol{b} + 2B\boldsymbol{x} = 0\,.$$

This is a vector of the form

$$\begin{bmatrix} \frac{\partial \hat{Y}}{\partial x_1} \\ \frac{\partial \hat{Y}}{\partial x_2} \\ \vdots \end{bmatrix}.$$

Therefore,

$$\boldsymbol{x}_s = -\frac{1}{2}B^{-1}\boldsymbol{b}$$

is a *stationary point* of quadratic surface. The response at this stationary point is

$$\begin{aligned} \hat{Y}_s &= \hat{\beta}_0 - \frac{1}{2}\boldsymbol{b}^{\mathrm{T}}B^{-1}\boldsymbol{b} + \frac{1}{4}\boldsymbol{b}^{\mathrm{T}}B^{-1}\boldsymbol{b} \\ &= \hat{\beta}_0 - \frac{1}{4}\boldsymbol{b}^{\mathrm{T}}B^{-1}\boldsymbol{b}\,. \end{aligned}$$

Note that the stationary point may be outside the experimental region (see example below). If this is the case, be careful as this is *extrapolation* and we do not know if the model is still a good description of the response. It may be better to explore the model graphically.

Example 11 cont.

For the chemical reaction experiment, $\hat{\beta}_0 = 93.05$, $\boldsymbol{b}^{\mathrm{T}} = (-0.87, 2.36)$ and

$$B = \begin{bmatrix} -0.43 & 0.50 \\ 0.50 & -0.65 \end{bmatrix}.$$

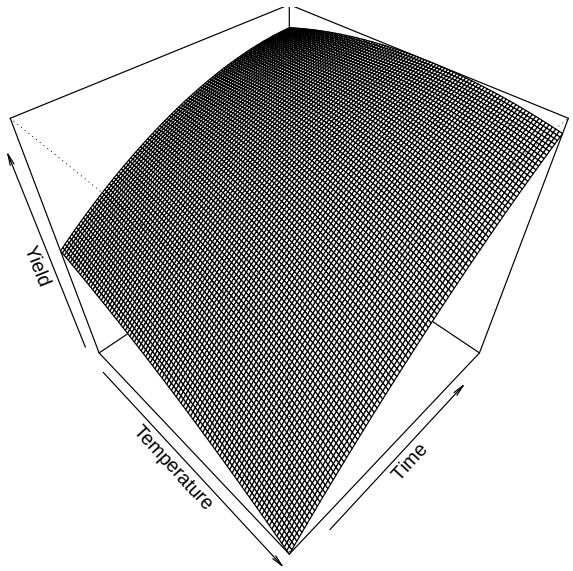
Therefore, the stationary point is

$$\boldsymbol{x}_s = -\frac{1}{2} \begin{bmatrix} -0.43 & 0.5 \\ 0.5 & -0.65 \end{bmatrix}^{-1} \begin{bmatrix} -0.87 \\ 2.36 \end{bmatrix} = \begin{bmatrix} 8.74 \\ 8.47 \end{bmatrix}.$$

This is well outside the experimental region.

$$\begin{aligned} \hat{Y}_s &= 93.05 - \frac{1}{4} \begin{pmatrix} -0.87 & 2.36 \end{pmatrix} \begin{pmatrix} -0.43 & 0.5 \\ 0.5 & -0.65 \end{pmatrix}^{-1} \begin{pmatrix} -0.87 \\ 2.36 \end{pmatrix} \\ &= 99.24\,. \end{aligned}$$

As the stationary point lies outside the experimental region, it may be best to explore the model graphically (see figure below).



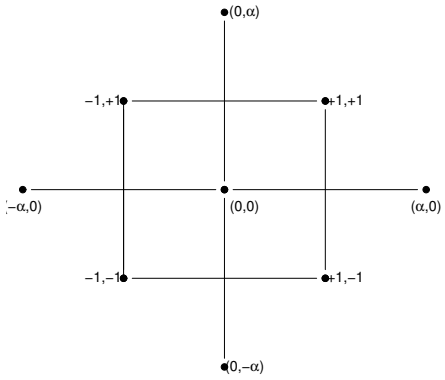
5.2. Central Composite Designs

Desirable properties for a good response surface design include:

- allowing accurate estimators of model parameters and predictions;
- allowing lack of fit to be tested;
- not having too many runs.

These properties are often in conflict, so a compromise must be made.

A popular choice of response surface design is the *Central Composite Design* (CCD), which is built up sequentially from a first-order design. Below is an example for two factors.



Components of a central composite design

1. Factorial component or cube points: the n_f points of a standard two-level factorial or fractional factorial design.
2. Centre points: n_c points at the centre of the design region.
3. Axial component or star points: $n_a = 2m$ points of the form $(0, \ldots, 0, \pm\alpha, 0, \ldots, 0)$.

Example 12: CCD for 3 factors with $n_f = 2^3 = 8$, $n_a = 2 \times 3 = 6$ and n_c centre points.

The design is

x_1	x_2	x_3
-1	-1	-1
-1	-1	1
-1	1	-1
-1	1	1
1	-1	-1
1	-1	1
1	1	-1
1	1	1
-α	0	0
α	0	0
0	-α	0
0	α	0
0	0	-α
0	0	α
0	0	0
$\vdots$	$\vdots$	$\vdots$
0	0	0

Choice of Factorial Component is influenced by number of factors and number of runs available. Large number of factors and small number of runs means a fractional factorial must be used. Often, a CCD will be constructed sequentially and the factorial component will be the first-order design that was initially run.

An ideal choice is a resolution V or higher fractional factorial design

- all main effects and two-factor interactions can be independently estimated
- and can be chosen to allow rotatability (see later)

If a resolution V fraction is not possible (too many factors or too few runs available), then resolution III is actually better than resolution IV. A resolution III design aliases main effects with two-factor interactions but the axial points can help "break" this aliasing, as they provide extra information about the main effects. A resolution IV design aliases two-factor

interactions together. Axial points do not provide any information about interactions (think back to a one factor at a time design), and so cannot break this aliasing.

A good design would be resolution III*. This is a resolution III design with no words of length four in the defining relation, and hence no aliasing between two-factor interactions.

For example, consider two different fractional factorial designs for six factors:

Design 1: $I = 123456 = 123 = 456$,

Design 2: $I = 12345 = 1236 = 456$.

Both designs are resolution III but design 1 has no words of length four in the defining relation. Hence it is resolution III* and would be preferred as the factorial component of a CCD.

Choice of α is usually between $1 \leq \alpha \leq \sqrt{m}$.

- A *cuboid design* has $\alpha = 1$. The axial points lie on the faces of the (hyper-) cube and each factor only takes three values. Such a design is useful if it is not possible to set factors to more values (e.g. if you have qualitative factors with three levels).
- A *spherical design* has $\alpha = \sqrt{m}$, and the axial points lie on the same sphere as the factorial points.

Alternatively, the value of α may be chosen to give the design particular properties.

1. **Rotatability**: the accuracy of the predicted response is the same on spheres around the centre of the design. That is, $\text{Var}\{\hat{Y}(\boldsymbol{x})\}$ depends only on $||\boldsymbol{x}|| = (x_1^2 + x_2^2 + \ldots + x_m^2)^{1/2}$ (Euclidean distance from the origin), where $\hat{Y}(\boldsymbol{x})$ is the predicted response at $\boldsymbol{x} = (x_1, x_2, \ldots, x_m)$.

   A design with this property is *rotatable*. A CCD with a resolution V or higher fractional factorial component is rotatable if

   $$\alpha =^4 \sqrt{n_f}\,.$$

   In Example 11, $\alpha = 1.41 =^4 \sqrt{4}$, and so the design was rotatable.

2. **Orthogonality**: the parameters $\boldsymbol{\beta}$ are estimated independently of each other. That is, the variance-covariance matrix of $\hat{\boldsymbol{\beta}}$ is diagonal, and the sums of squares in the ANOVA table will not depend on the order in the models are compared. This allows decisions to be made on which model terms (linear, interaction and quadratic) are important.

   For a CCD to be orthogonal, we choose

$$\alpha = \left(\frac{\sqrt{n_f \times N} - n_f}{2} \right)^{1/2} . \tag{5.6}$$

   Note that we can rearrange (5.6) to obtain

$$\begin{aligned} N &= \frac{(n_f + 2\alpha^2)^2}{n_f} \\ \Rightarrow \quad n_c &= \frac{4\alpha^2(\alpha^2 + n_f)}{n_f} - n_\alpha \, . \end{aligned}$$

   Hence, for given α (e.g chosen for rotatability), we can choose n_c to ensure orthogonality. However, n_c may not always be integer from this equation, and therefore this condition may not always give realisable designs.

Choice of n_c: The centre points provide an independent estimate of σ^2 and allow lack of fit testing. The number of centre points can sometimes be chosen to help ensure orthogonality (see above). In practice, the number of centre points is usually determined by the number of runs it is possible to do. Most experiments have somewhere between two and six centre points.