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Selected illustrations of response surface method — Central composite design

Illustrations choisies de méthodologie à surface de réponse — Plans composites centrés

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Contents

Foreword

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The committee responsible for this document is ISO/TC 69, *Applications of statistical methods*, Subcommittee SC 7, *Applications of statistical and related techniques for the implementation of Six Sigma*.

Introduction

The present Technical Report takes one specific statistical tool (Central Composite Designs in Response Surface Methodology) and develops the topic somewhat generically (in the spirit of International Standards) but then illustrates it through the use of four detailed and distinct applications. The generic description focuses on the Central Composite Designs.

The annexes containing the four illustrations follow the basic framework but also identify the nuances and peculiarities in the specific applications. Each example offers at least one “wrinkle” to the problem, which is generally the case for real applications. It is hoped that practitioners can identify with at least one of the four examples, if only to remind them of the basic material on response surface method that was encountered during their training.

Each of the four examples is developed and analysed using statistical software of current vintage. The explanations throughout are devoid of mathematical detail—such material can be readily obtained from the many design and analysis of experiments textbooks (such as those given in References [1] to [7]).

Selected illustrations of response surface method — Central composite design

1 Scope

This Technical Report describes the steps necessary to understand the scope of Response Surface Methodology (RSM) and the method to analyse data collected using Central Composite Designs (CCD) through illustration with four distinct applications of this methodology.

Response surface methodology (RSM) is used in order to investigate a relation between the response and the set of quantitative predictor variables or factors. Especially after specifying the vital few controllable factors, RSM is used in order to find the factor setting which optimizes the response.

2 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

2.1
experiment
purposive investigation of a system through selective adjustment of controllable conditions and allocation of resources

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.1. (The notes are not reproduced here.)

2.2
response variable
variable representing the outcome of an *experiment* (2.1)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.3. (Except for NOTE 3 the notes are not reproduced here.)

Note 2 to entry: A common synonym is “output variable”.

Note 3 to entry: The response variable is likely to be influenced by one or more *predictor variables* (2.3), the nature of which can be useful in controlling or optimizing the response variable.

2.3
predictor variable
variable that can contribute to the explanation of the outcome of an *experiment* (2.1)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.4. (The notes are not reproduced here.)

Note 2 to entry: Natural predictor variables are expressed in natural units of measurement such as degrees Celcius (°C) or grams per liter, for example. In RSM work, it is convenient to transform the natural variables to coded variables which are dimensionless variables, symmetric around zero and all with the same spread.

2.4
model
<experiment> formalized representation of outcomes of an *experiment* (2.1)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.2. (The notes and examples are not reproduced here except for NOTE 2 which is NOTE 1 in ISO 3534-3.)

Note 2 to entry: The model consists of three parts. The first part is the *response variable* (2.2) that is being modelled. The second part is the deterministic or the systematic part of the model that includes *predictor variable(s)* (2.3). Finally, the third part is the *residual error* (2.12) that can involve *pure random error* (2.13) and *misspecification error* (2.14). The model applies for the experiment as a whole and for separate outcomes denoted with subscripts. The model is a mathematical description that relates the response variable to predictor variables and includes associated assumptions. Outcomes refer to recorded or measured observations of the response variable.

Note 3 to entry: In some areas the term transfer function is used for the systematic part of the model.

EXAMPLE In the models considered in response surface methodology the deterministic or systematic part are polynomials in the predictor variables. A second order model with two predictor variables is written as

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \varepsilon$$

where ε is the random error. The associated assumptions on the random error could be either that individual random errors are uncorrelated with constant variance or independent and normally distributed. The deterministic part of the model is the second degree polynomial in the predictor variables x_1 and x_2

$$\mathrm{E}y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2$$

which explains the mean (E*y*) of the response variable as a function of the predictor variables.

2.5
factor

<design of experiments> feature under examination as a potential cause of variation

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.5. (The notes are not reproduced here.)

Note 2 to entry: Generally the symbol *k* is used to indicate the number of factors in the experiment.

2.6
factor level

setting, value or assignment of a *factor* (2.5)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition (3.1.12). (The notes are not reproduced here.)

2.7
coding of factor levels

<design of experiments> one-to-one relabelling of factor levels

Note 1 to entry: The coding of factor levels facilitates the identification of the design and the properties of the design.

Note 2 to entry: In response surface experiments the actual (or natural or operational) levels are relabelled such that the coded levels are numeric and symmetric around 0.

Note 3 to entry: A two-level factor is usually coded to have coded levels −1 and +1. A factorial design where all factors are two-level factors can be coded such that all runs are represented as *factorial runs* (2.9).

Note 4 to entry: In central composite designs numeric (or continuous) factors with five levels are considered, except for the face-centred central composite deigns, where only three levels are needed, see note 6 to 2.7. If the actual (or natural or operational) levels are $l_1 < l_2 < l_3 < l_4 < l_5$ then the middle level l_3 shall be the average of the lowest level l_1 and the highest level l_5, and, furthermore, l_3 shall be the average of the intermediate levels l_2 and l_4. The form of the coding operation can be expressed as

$$\text{coded value} = \frac{\text{actual value} - l_3}{C}$$

where C is half the distance from l_2 to l_4. With this coding of the factors each *run* (2.8) of a central composite design can be identified as either a *factorial point* (2.9), a *centre point* (2.10), or an *star point* (2.11). This is the coding used in textbooks for discussing central composite designs.

Note 5 to entry: An alternative coding is sometimes applied in the computations in software programs. The form of the coding operation can be expressed as

$$\text{coded value} = \frac{\text{actual value} - l_3}{M}$$

where M is half the distance from the lowest level l_1 to the highest level l_5. This coding will be referred to as *software coding* in this Technical Report.

Note 6 to entry: In the face-centred CCD, only three levels of each factor are needed, so $l_1 = l_2 < l_3 < l_4 = l_5$, and l_3 shall be the average of the lowest level l_1 and the highest level l_5. This design could be of interest if it is difficult to select five levels of the factors. For the face-centred CCD, the possible coded values of a factor are only −1, 0, 1.The face-centred CCD is not rotatable, see 2.18.

Note 7 to entry: A class of designs that can be used to fit second order models and only require three equidistant levels of each factor are Box-Behnken designs. Box-Behnken designs are not central composite designs and are therefore not treated in this Technical Report. But they may be a useful alternative, if only three equidistant levels of each factor can be used, see References [5], [2] and [7].

2.8
run
experimental treatment

<design of experiments> specific settings of every *factor* (2.5) used on a particular *experimental unit* (2.15)

Note 1 to entry: Ultimately, the impact of the factors will be captured through their representation in the *predictor variables* (2.3) and the extent to which the model matches the outcome of the *experiment* (2.1).

EXAMPLE Consider a chemical process *experiment* (2.1) in which a high yield is the objective and the predictor variables are temperature, duration, and concentration of a catalyst. A run could be a setting of temperature of 350 °C, 30 min duration and 10 % concentration of the catalyst, assuming that all of these settings are possible and permissible.

Note 2 to entry: Adapted from ISO 3534-3:2013, definition 3.1.13.

2.9
factorial point
factorial run
cube point
cube run

vector of factor level settings of the form (a_1, a_2, ..., a_k), where each a_i equals −1 or +1 as a notation for the coded levels of the factors

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.37. (The notes are not reproduced here.)

2.10
centre point
centre run

vector of factor level settings of the form (a_1, a_2, ..., a_k), where all a_i equal 0, as notation for the coded levels of the factors

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.38. (The notes are not reproduced here.)

2.11

star point

axial point

star run

axial run

vector of *factor level* (2.7) settings of the form (a_1, a_2, ..., a_k), where one a_i equals α or $-\alpha$ and the other a_i's equal 0, as notation for the coded levels of the *factors* (2.6)

Note 1 to entry: For a k factor experiment, this process yields $2k$-star points of the form: (±α, 0, ..., 0), (0, ±α, 0, ..., 0), ..., (0, 0, ..., ±α).

Note 2 to entry: Star points are added to the design in order to estimate a quadratic response surface.

Note 3 to entry: Special values of α give a nice geometric structure. For a k factor experiment, if $\alpha = \sqrt{k}$ then the factorial points and the star points are all on the sphere with radius $\sqrt{k}$. This design is therefore called a spherical CCD. If $\alpha = 1$, the star points are on the faces of the unit cube and the design is a face-centred CCD.

2.12

residual error

error term

random variable representing the difference between the *response variable* (2.3) and its prediction based on an assumed *model* (2.4)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.6. (The notes are not reproduced here.)

2.13

pure random error

pure error

part of the residual error (2.12) associated with replicated observations

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.9. (The notes are not reproduced here.)

2.14

misspecification error

part of the *residual error* (2.12) not accounted for by *pure random error* (2.13)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.9. (The notes are not reproduced here.)

2.15

experimental unit

<design of experiments> basic unit of the experimental material

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.24. (The notes are not reproduced here.)

2.16

designed experiment

experiment (2.1) with an explicit objective and structure of implementation

Note 1 to entry: The purpose of a properly designed experiment is to provide the most efficient and economical method of reaching valid and relevant conclusions from the experiment.

Note 2 to entry: Associated with a designed experiment is an *experimental design* (2.17) that includes the *response variable* (2.2) or variables and the *experimental treatments* (2.8) with prescribed *factor levels* (2.6). A class of models that relates the response variable to the predictor variables could also be envisaged.

Note 3 to entry: Adapted from ISO 3534-3:2013, definition 3.1.27.

2.17

experimental design

assignment of *experimental treatments* (2.7) to each *experimental unit* (2.15)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.28. (The notes are not reproduced here.)

2.18
rotatability
characteristic of a *designed experiment* (2.16) for which the *response variable* (2.2) that is predicted from a fitted *model* (2.4) has the same variance at all equal distances from the centre of the design

Note 1 to entry: A design is rotatable if the variance of the predicted response at any point $\boldsymbol{x}$ depends only on the distance of $\boldsymbol{x}$ from the *centre point* (2.10). A design with this property can be rotated around its centre point without changing the prediction variance at $\boldsymbol{x}$.

Note 2 to entry: Rotatability is a desirable property for *response surface designs* (2.25).

Note 3 to entry: Rotatability of a central composite design is obtained setting α equal to the fourth root of the number of factorial points, i.e

$$\alpha = (n_\mathrm{F})^{1/4}$$

where n_F denotes the number of factorial points in a CCD.

Note 4 to entry: The definition and notes 1 and 2 are adapted from ISO 3534-3:2013, definition 3.1.40.

2.19
interaction
influence of one *factor* (2.6) on one or more other factors' impact on the *response variable* (2.2)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.17. (The notes are not reproduced here.)

2.20
factorial experiment
designed experiment (2.16) with one or more *factors* (2.5) and with at least two levels applied for one of the factors

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.2.1. (The notes are not reproduced here.)

2.21
full factorial experiment
factorial experiment (2.12) consisting of all possible combinations of the levels of the *factors* (2.6)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.2.2. (The notes are not reproduced here.)

2.22
fractional factorial experiment
factorial experiment (2.12) consisting of a subset of the *full factorial experiment* (2.21)

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.2.3. (The notes are not reproduced here.)

2.23
randomization
process used to assign treatments to experimental units so that each experimental unit has an equal chance of being assigned a particular treatment

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.26. (The notes are not reproduced here.)

2.24
replication
performance of an experiment more than once for a given set of predictor variables

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.1.35. (The notes are not reproduced here.)

2.25

response surface design

designed experiment (2.16) that identifies a subset of *factors* (2.5) to be optimized

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.2.19. (The notes are not reproduced here.)

2.26

analysis of variance

ANOVA

technique which subdivides the total variation of a *response variable* (2.2) into components associated with defined sources of variation

Note 1 to entry: Adapted from ISO 3534-3:2013, definition 3.3.8. (The notes are not reproduced here.)

3 Symbols and abbreviated terms

3.1 Symbols

y	Response variable
$\hat{y}$	Predicted response variable
$\hat{y}_{\mathrm{S}}$	Predicted response variable at the stationary point
$\boldsymbol{x}_{\mathrm{S}}$	Stationary point of fitted response surface
D_{S}	Distance of stationary point to the design centre
A, B, C, D	Factors
k	Number of factors
2^k	Number of runs in a full factorial experiment with k factors all having two levels
2^{k-p}	Number of runs in a fractional factorial experiment with k factors and fraction 2^{-p}
n_{F}	Number of factorial points in a CCD
n_{S}	Number of star points in a CCD
n_0	Number of centre points in a CCD
a_i, b_i, l_i	Levels of factors
+1, −1	High and low coded factorial levels
$-\alpha$, α	Axial levels of coded factors
σ	Standard deviation

3.2 Abbreviated terms

ANOVA	analysis of variance
CCD	central composite design
DOE	design of experiments

RSM	response surface methodology
R&R	repeatability and reproducibility

4 Generic descriptions of central composite designs

4.1 Overview of the structure of the examples in Annexes A to D

This Technical Report provides general guidelines on the design, conduct and analysis of central composite designs consisting of a specified number of two-level factors, and illustrates the steps with four distinct applications given in the annexes. Each of the four examples in Annexes A through D follows the basic structure as given in Table 1.

Table 1 — Basic steps in CCD design

1	Overall objective(s) of experiment
2	Description of the response variable(s)
3	Identification of factors affecting the response(s)
4	Selection of levels for each factor
5	Identification of measurement systems
6	Layout plan of the CCD (depending upon which main effects and two factor interactions are to be studied) with 'randomization' principle (if these are physical runs)
7	Analyse the results – numerical summaries and graphical displays
8	Present the results
9	Perform confirmation run

4.2 Overall objective(s) of a response surface experiment

Experiments may be conducted for a variety of reasons. Therefore, the primary objective(s) for the experiment should be clearly stated and agreed to by all parties involved in the design, conduct, analysis and implications of the experimental effort.

The main goal of response surface experiments is to create a model of the relationship between the factors and the response in order to explore optimum operating conditions. This involves choosing a design which allows the fitting of a quadratic function as the systematic part of the model. The Central Composite Design (CCD) can achieve this and this design has been popular since its introduction in the first paper on response surface methods in 1951.[1]

Although the fundamental method for fitting first order (linear) or second order (quadratic) function of the predictor variables to the response is regression, the focus is not on the individual regression coefficients but on the regression function, the response surface, as a whole. This emphasis is reflected in the name Response Surface Methodology. Strong arguments in favour of this approach are given on pages 508-509 of Reference [2].

Typically, the primary goal for the experiment is to find optimal operating conditions based on the estimated response surface, this could involve doing several experiments, using the results of one experiment to provide direction for what to do next. This next action could be to focus the experiment around a different set of conditions, or to collect more data in the current experimental region in order to fit a higher-order model or confirm what seemed to be the conclusion.

The CCD is an appropriate name because three types of design points can be identified after a coding of the factor levels: centre points (2.10), factorial points (2.9) and star points (2.11), and those design points are indeed centred at the origin of the design space after the coding of the factor levels (2.7).

Response surface experiments traditionally involve a small number of continuous factors. Some software packages have an upper limit of 8 factors. Response surface experiments are typically used when the investigators already know which factors are important. One way to obtain this knowledge is to apply a screening experiment, for example a fractional factorial experiment as explained in ISO/TR 12845.[11]

4.3 Description of the response variable(s)

Associated with the objective of an experiment is a continuous outcome or performance measure. A response of interest could involve maximization (larger is better), minimization (smaller is better) or meet a target value (be close to a specified value), but, in all cases, that task is one of optimization.

The response variable (denoted by the variable y) should be closely related to the objective of the experiment. For some situations, there are more than one variable of interest to be considered, although, typically, only a primary response variable will be associated with the experiment. In other cases, multiple responses should be considered. In case of multiple responses, the approach taken in response surface methodology is to analyse and optimize each response separately. The fitted response surfaces will then be studied to find settings that meet the requirements of all the responses. The example in Annex C has three responses.

4.4 Identification of measurement systems

Assessment of repeatability and reproducibility of the measurement systems for factors and responses should be done prior to designing the experiment.

4.5 Identification of factors affecting the response(s)

Response surface experiments are usually not done in isolation. They rely on prior knowledge concerning important influential variables on the selected response. If this knowledge is not available, it is necessary to conduct a different type of experiment to identify the factors affecting the response.

During the final selection of factors, attention shall be paid to the ability to set the levels of each individual factor independently of the other factors.

4.6 Selection of levels for each factor

There are two aspects to the selection of factors. One is selecting the *experimental region* which is the multidimensional range of interest for the factors selected. The other is the exact selection of the factor levels in such a way that the design has desirable properties. The first one requires subject matter knowledge as to the impact of factors on the response. The second one is more straightforward once the factors and the type of design to be used are known. The second one is further discussed in this Clause.

The response surface methods considered in this Technical Report are about the second order centre models using the CCD. The CCD is an augmentation of 2^k factorial experiments (or 2^{k-p} fractional factorial experiments). In addition to the two factorial levels that are used in the (fractional) factorial experiments, the user selects three additional levels, one centre level which is the average of the two factorial levels, and two extreme levels which are chosen symmetrically around the centre level and typically outside the range of the two factorial levels.

When the experimenter selects the levels of each factor he will be thinking in terms of the operational levels of a factor, the exact setting of a temperature, for example. But when studying the properties of the design and also when analysing the data from the design coded levels of the design are used.

If the actual (or operational) levels are $l_1 < l_2 < l_3 < l_4 < l_5$ then the middle level l_3 shall be the average of the lowest level l_1 and the highest level l_5, and, furthermore, l_3 shall be the average of the intermediate levels l_2 and l_4. The form of the coding operation can be expressed as Formula (1):

$$\text{coded value} = \frac{\text{actual value} - l_3}{C} \tag{1}$$

where C is half the distance from l_2 to l_4. The coded value of the upper extreme level, l_5, will be denoted by α, and the coded value of the lower extreme level, l_1, will be denoted by $-\alpha$. It is very important to note that the value of α is the same for all the factors of the design. Thus, the coded levels of all the factors are ($-\alpha$, −1, 0, 1, + α).

An alternative coding is sometimes applied in the computations in software programs. The form of the coding operation can be expressed as Formula (2):

$$\text{coded value} = \frac{\text{original value} - l_3}{M} \tag{2}$$

where M is half the distance from the lowest level l_1 to the highest level l_5.or, equivalently, the distance from l_3 to l_5. This coding will be referred to as *software coding* in this Technical Report.

When the levels of the factors have been chosen, the levels of the individual factors have to be combined to define the runs of the experiment. A CCD has three types of experimental runs: factorial, centre and axial ones.

4.6.1 Factorial runs

A factorial run is a setting of all k factors to coded levels either −1 or +1. The factorial runs are the runs used in 2^{k-p} fractional factorial experiments or 2^k factorial experiments.

Written as a k-dimensional vector in coded levels, the factorial run has the form (±1, ±1,..., ±1,..., ±1). Considered as points in k-dimensional space, the factorial runs are the vertices of a cube and the factorial runs are for this reason also called cube points.

There are 2^k different factorial runs with k factors.

4.6.2 Star runs

The star runs are those where one of the factors has its coded levels either $-\alpha$ or α and the remaining factors are at their coded level 0.

Written as a k-dimensional vector in coded levels, the star run has the form (0, 0,..., $\pm\alpha$,..., 0), having $-\alpha$ or α on the i^{th} position and 0 on all other positions.

Viewed as points in k-dimensional space, the star runs are located on the coordinate axes, and for this reason, the star runs are also called axial runs.

There are 2^k different star runs with k factors.

4.6.3 Centre run

The centre run is the one where all the factors are on their coded level 0. Written as a k-dimensional vector, it is the point (0, 0,..., 0).

There is only one centre run but the centre run may be replicated in a CCD. One reason for replicating the centre point is to get an estimate of pure error which can be used to check the fit of the model.