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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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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*.

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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]).

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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.)

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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 (Ey) 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.

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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.)

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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.)

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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

$$\alpha = (n_F)^{1/4}$$

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.)

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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
$\hat{y}_S$	Predicted response variable at the stationary point
$\boldsymbol{x}_S$	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

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