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Design of simulation experiments using Central Composite Design

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Abstract: In the context of research and development, it is key to achieve accurate and reliable results. However, often to obtain these results, a large number of experiments must be performed, which can significantly extend the research time and increase computational requirements. The solution to these problems may be efficient experimental planning, which allows for a reduction in the number of trials and optimization of the process. This article provides an insight into Central Composite Design (CCD) and its use in simulation experiments. We introduce various types of CCD designs, such as CCC (Central Composite Circumscribed), CCF (Central Composite Face centered), and CCI (Central Composite Inscribed), and analyze their use in creating second-order regression models. We also discuss the specific advantages and disadvantages of these approaches, as well as their possible alternatives, such as the Draper-Lin CCD design.

1 Introduction

Simulation experiments are today an integral part of research and development in various fields of science and technology. Their effectiveness and accuracy, however, largely depend on proper planning and design of these experiments or significant computational power to carry out all the experiments [1,2]. Since a large number of experiments often need to be carried out, especially in simulations, it is necessary to approach experimental design [3]. When creating models based on Response Surface Methodology (RSM), we often need to calculate both linear and nonlinear (quadratic) terms and two-factor interactions. To do this, all factors must be set at least on 3 levels. For this reason, the use of Full Factorial Design (FFD) method is inefficient as it would require a large number of trials [4].

One of the popular alternatives to FFD, used by many researchers, is Central Composite Design (CCD) [5]. These designs are suitable for creating nonlinear descriptive models. The structure of a CCD design consists of a cube, star, and central point, providing a comprehensive framework for evaluating interactions between multiple factors at different levels.

The core of the article is to address various aspects of CCD designs, including its various types such as CCC (Central Composite Circumscribed), CCF (Central Composite Face centered), and CCI (Central Composite Inscribed). We will also deal with the process of creating these designs, as well as their use in research. Various types of CCD designs are proposed and used, depending on the needs and possibilities within experimentation. The article analyzes the advantages and disadvantages of these different approaches with a description of how CCD designs are used to create second-order regression models and how these models help scientists better understand and interpret their data.

2 Methodology

Before we define the details and technical aspects of using Central Composite Design (CCD), it is important to emphasize that the basic philosophy of this approach is efficiency and accuracy in evaluating experimental data. Since our models often require the calculation of both linear and nonlinear (quadratic) terms and two-factor interactions, it is necessary to set all factors to at least three levels. This puts us in a situation where the use of Full Factorial Design (FFD) or Unifactorial Experiments (UFE) may seem inefficient due to the number of trials needed. At this point, CCD becomes an attractive alternative. CCD provides us with a structure that includes a cube, a star, and a central point, thus allowing a comprehensive evaluation of interactions between multiple factors at different levels. The principle of creation is shown in Figure. 1.

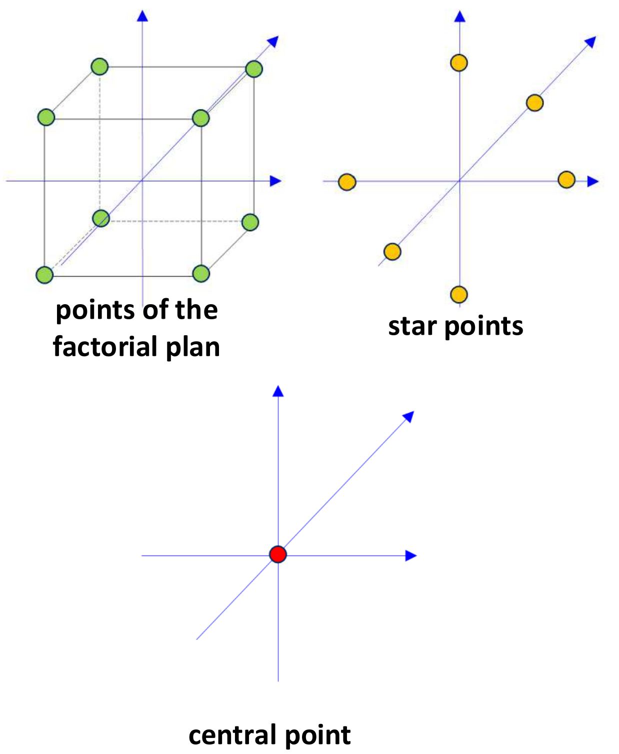

Figure 1 Principle of CCD design creation [6]

Now let's look more closely at how this design is created and what specific benefits its use brings within research experiments. For practical experimentation purposes, several types of CCD designs were proposed. The most famous are plans of type [7]:

- CCC (Central Composite Circumscribed) – rotatable plan, α = 1.4142, which uses 5 factor levels.
- CCF (Central Composite Face centered) – plan centered on the face, α = 1, which uses 3 factor levels, is used if it is not possible to set the factors to 5 levels.
- CCI (Central Composite Inscribed) – inscribed plan, which we get if we replace the coded values (+1) and (-1) with numbers (+1/α) and (-1/α) and the axial values (+α) and (-α) replace the numbers (+1) and (-1). This type of plan is used if it is not possible to set the factor levels within the range (-α) to (+α).

An example of the principle of creating CCC and CCF plans is shown in Figure 2.

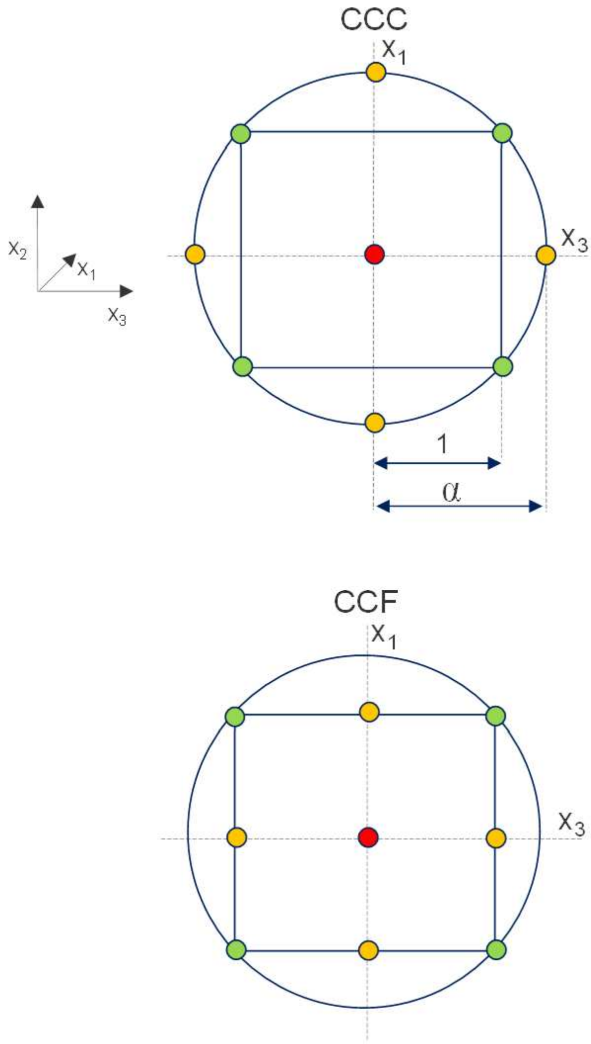

Figure 2 Principle of creating CCC and CCF plans

CCD designs use two-stage experiment designs (Table 1). In the first stage, a regular two-level experiment design is used. In the second stage, additional missing trials are added to the first stage design.

Table 1 Principle of creating CCD experiment designs

Trial	x1	x2	x3
1	**- 1**	**-1**	**-1**
2	**- 1**	**-1**	**1**
3	**- 1**	**1**	**-1**
4	**- 1**	**1**	**1**
5	**1**	**-1**	**-1**
6	**1**	**-1**	**1**
7	**1**	**1**	**-1**
8	**1**	**1**	**1**
9	**- α**	**0**	**0**
10	**+ α**	**0**	**0**
11	**0**	**- α**	**0**
12	**0**	**+ α**	**0**

13	**0**	**0**	**- α**
14	**0**	**0**	**+ α**
15	**0**	**0**	**0**
16	**0**	**0**	**0**
17	**0**	**0**	**0**
18	**0**	**0**	**0**
19	**0**	**0**	**0**
20	**0**	**0**	**0**
21	**0**	**0**	**0**
22	**0**	**0**	**0**
23	**0**	**0**	**0**

As can be seen from Table 1, the first stage of the CCD design is formed by a two-level design of type 23 (marked in yellow in Table 1). To this design, we add central and axial points (trials) in the second stage. Orange is depicted 6 axial points and blue 9 central points. The number α is determined based on the plan requirements, according to the relationship:

$$\alpha = \sqrt[4]{2^k} \qquad (1)$$

where the symbol *k* denotes the number of factors. The meaning of α is evident from Figure 3.

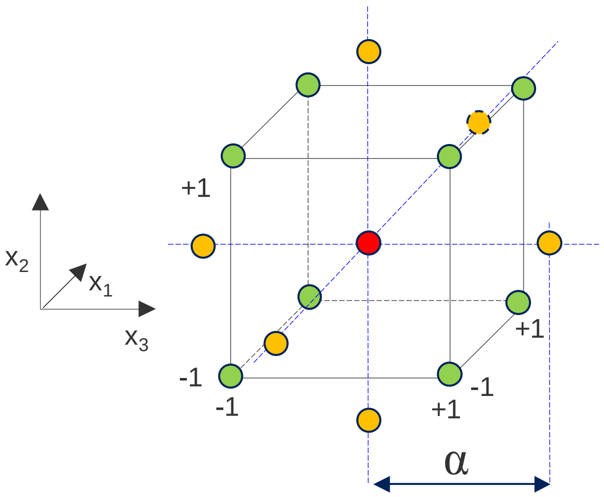

Figure 3 Meaning of the symbol α

The cube of the CCD design is always a two-level experiment design, usually with a resolution of IV or V. The star arises by varying individual factors such that we start from the middle point (so-called central point). The distance of the factor levels of this variation exceeds the distance of the cube levels in such a way that each factor is examined at 5 levels. A graphical representation of the experimental space for the CCD plan with three factors is shown in Figure 4.

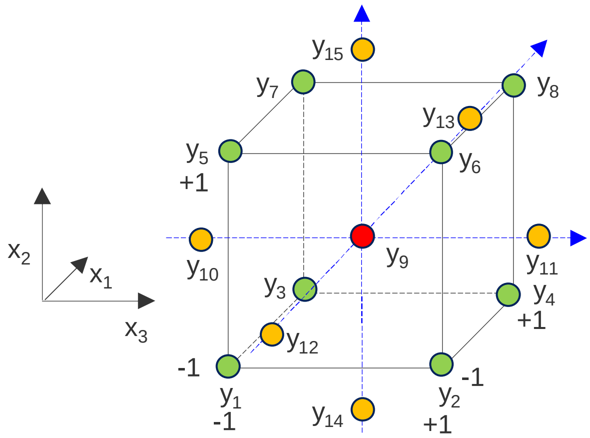

Figure 4 CCD design with three factors and two levels

As seen from Figure 4, in the first stage, a two-level design (cube) is created, to which additional trials (stars) are added in the second stage. This arrangement of the plan allows for the investigation of non-linear dependencies as well.

According to [8], we can create a CCD plan based on Figure 7-7, which is shown in Table 2.

Table 2 CCD design for 3 factors and 2 levels

Trial	x1	x2	x3	Response y
1	**- 1**	**-1**	**-1**	**y1**
2	**- 1**	**-1**	**1**	**y2**
3	**- 1**	**1**	**-1**	**y3**
4	**- 1**	**1**	**1**	**y4**
5	**1**	**-1**	**-1**	**y5**
6	**1**	**-1**	**1**	**y6**
7	**1**	**1**	**-1**	**y7**
8	**1**	**1**	**1**	**y8**
9	**0**	**0**	**0**	**y9**
10	**- -**	**0**	**0**	**y10**
11	**++**	**0**	**0**	**y11**
12	**0**	**- -**	**0**	**y12**
13	**0**	**++**	**0**	**y13**
14	**0**	**0**	**- -**	**y14**
15	**0**	**0**	**++**	**y15**

This design is initially created from a 2^3 design, so we carry out 8 trials. The ninth trial tests the central point (y9). The following trials test the variations, each for one factor, that exceed the cube's boundaries of the design. Therefore, when using a CCD design, 13 trials are sufficient to study 3 factors (see Table 3).

Various approaches are used to reduce the number of CCD design trials. The most well-known is the so-called Draper-Lin CCD design (also sometimes referred to as Face-Centered CCD), which differs from the classical CCD design in that none of its trials exceed the cube's dimensions. This allows for the reduction of trials to a theoretical minimum. An example of this type of experimental design is shown in Figure 5.

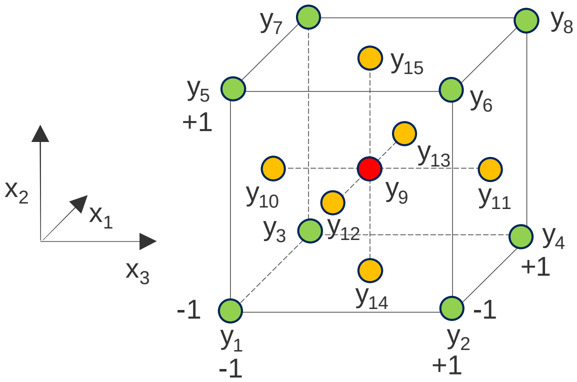

Figure 5 Draper-Lin CCD design

In Table 3, the number of necessary settings depending on the number of factors for CCD and Draper–Lin CCD is listed. As can be seen in Figure 5, the Draper-Lin CCD plan uses a cube, more densely populated with points (trials), in addition to the corner points, the center points of each surface have also been added.

Table 3 Number of necessary settings depending on the number of factors

Factor	Trial count	CCD	Draper-Lin plan
3	**10**	**13**	
4	**15**	**25**	**17**
5	**21**	**41**	**23**
6	**28**	**49**	**29**
7	**36**	**57**	**39**
8	**45**	**81**	**53**

It is typically necessary to use designs with three levels of factors when using second-order models that contain terms with higher powers (ax2). The disadvantage of designs that use 3 factors (3k) is the rapidly increasing number of necessary trials and at the same time it is necessary to determine a whole series of insignificant interactions. Therefore, in such a case, the CCD design is usually used. When using the CCD design, we use a 2k design and add the so-called central points and points called stars to it. By adding the necessary number of central points, the experimental design approximates an orthogonal design.

An example can be a simple experimental design with two factors that can take 2 levels of the type 2k, where k = 2.

Number of trials n = 22 = 4

To this design, a central point and star points are added:

- 1 central point
- star points

Then the total number of trials will be equal to 4+1+4 = 9.

Such a CCD experimental design, according to [9], is shown in Table 4.

Table 4 CCD plán experimentov

Trial	Factors	
	A	B
1	**-1**	**-1**
2	**+1**	**-1**
3	**-1**	**+1**
4	**+1**	**+1**
5	**0**	**0**
6	**- α**	**0**
7	**+ α**	**0**
8	**0**	**- α**
9	**0**	**+ α**

In Table 4, some rows contain the symbol α which, as Miller, I. (2010) states, has a value higher than 1 and its value is most often the square root of two, so it equals 1.41.

Krausova [7] provides the relationship and method of calculating the values of α (equation 1) and determining the number of zero points (their number approximates the design to the orthogonal design). Examples of such calculated values of α and the number of zero points are given in Table 5.

Table 5 Values α

Number of factors	α	Number of zero points
2	**1.414**	**8**
3	**1.682**	**9**
4	**2.000**	**12**
5	**2.378**	**16**

Based on the results of the CCD design, it is possible to create a second-order regression model, which will include interactions as well as the second powers of factors. An example of such type of models is the model:

$$y = b_0 + b_1 x_1 + b_2 x_2 + b_{11} x_1^2 + b_{22} x_2^2 + b_{12} x_1 x_2 \quad (2)$$

Appropriate software for statistical analysis is used to solve more complex models of this type. An example of experiment results processed in the statistical software Minitab is shown in Figure 6.

Term	Effect	Coef	SE Coef
Constant	31,8928	0,0909	351,03
Čas	1,7815	0,8907	0,0909
Počet pracovníkov	3,7339	1,8670	0,0909
Počet AGV	3,8813	1,9407	0,0909
Čas*Počet pracovníkov	-0,0963	-0,0481	0,0909
Čas*Počet AGV	0,5740	0,2870	0,0909
Počet pracovníkov*Počet AGV	0,6943	0,3471	0,0909
Čas*Počet pracovníkov*Počet AGV	-0,0342	-0,0171	0,0909

Term	T-Value	P-Value	VIF
Constant	0,000		
Čas	9,80	0,000	1,00
Počet pracovníkov	20,55	0,000	1,00
Počet AGV	21,36	0,000	1,00
Čas*Počet pracovníkov	-0,53	0,613	1,00
Čas*Počet AGV	3,16	0,016	1,00
Počet pracovníkov*Počet AGV	3,82	0,007	1,00
Čas*Počet pracovníkov*Počet AGV	-0,19	0,856	1,00

Figure 6 Experiment results from the Minitab system

Using coefficients calculated with the least squares method in the Minitab system, it is possible to construct the desired regression model. The p-value determines the significance of the linear terms of the model and also their potential substitution in the model with quadratic terms.

The evaluation of how well the model explains the obtained variability is done using the adjusted coefficient of determination, RADJ. With the responses obtained, we can then graphically display the response surface in the form of a contour or isopleth diagram.

3 Conclusions

Central Composite Design (CCD) represents a comprehensive and flexible tool for planning simulation experiments. This approach has proven advantageous for research in a wide range of areas where it is necessary to solve complex problems with multiple factors. Thanks to its ability to effectively and reliably create second-order regression models, CCD allows researchers to better understand and interpret their data. Various types of CCD plans, including CCC (Central Composite Circumscribed), CCF (Central Composite Face centered) and CCI (Central Composite Inscribed), provide different options for tailoring the experimental planning process to the specific needs and constraints of individual research projects.

It is important to emphasize that CCD is not always the most suitable solution. There are situations when it might be better to use alternative methods, such as the Draper-Lin CCD plan. Regardless of which method is used, it is crucial to carefully and thoughtfully plan experiments to ensure accurate and reliable results.

Despite this article providing a detailed view of the theory and application of CCD, it is important to continue exploring and improving these methods. Success in research and development often depends on our ability to effectively and innovatively use available tools like CCD. In the future, with the ongoing development of technologies and computational capacities, new possibilities are expected to emerge for the refinement and expansion of CCD use in the field of simulation experiment design.

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