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LAUREA SPECIALISTICA IN INGEGNERIA MATEMATICA

EFFECTIVENESS OF DESIGN OF EXPERIMENT

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Annotation

This diploma thesis is about design and analysis of experiments. It deals with the influence of number of central points in the plan of experiment for finding the significant factor of process. The method Monte Carlo is used to analyse this influence. The measure of finding the significant factors is quantified by this method. Simulation of experiment is created in MATLAB because of the fast random number generator which is important part of the simulation procedure. The last part of the thesis deals with results of the simulation and there is shown how the determination if the factor is significant depends on the number of factors in experiment and on the number of replication in the central point.

Anotace

Diplomová práce se zabývá plánováním a analýzou experimentu. Je zde zkoumán vliv počtu centrálních bodů v plánu experimentu na nalezení významných faktorů procesu. Pro určení tohoto vlivu je použita metoda Monte Carlo, pomocí které hledáme míru nalezení významných faktorů procesu. Simulace experimentu byla vytvořena v programu MATLAB, kde je především využíván Statistics toolbox pro generování náhodných čísel, což je důležitá část této metody. V závěru je zhodnoceno a graficky ukázáno, jak závisí určení, zda daný faktor procesu je významný, na počtu uvažovaných faktorů experimentu a na počtu měření v centrálním bodě.

Key words:

Regression analysis, Analysis of variance, Design of experiments, Model adequacy checking, Test of significance of effect

Klíčová slova:

Regresní analýza, Analýza rozptylu, Plánování experimentu, Test adekvátnosti, Test významnosti efektu

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I declare that I have elaborated this thesis under a guidance of Doc. RNDr. Maroš, CSc. exclusively on my own and that I have presented all sources and literature I used.

I would like to thank to my diploma thesis tutor, doc. RNDr. Bohumil Maroš, CSc. of Department of Mathematics for his kind supervision, expert guidance, valuable advices and observations to the given topic, to all my close people and, last but not least, to my family for the support during the whole study.

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Contents

1 Introduction

Design of Experiments (DOE) is a powerful technique used for exploring new processes, gaining increased knowledge of the existing processes and optimizing them for achieving world class performance.

Experiments are performed today in many manufacturing organizations to increase the understanding and the knowledge of various manufacturing processes. Experiments in manufacturing companies are often conducted in a series of trials or tests which produce quantifiable outcomes. For continuous improvement in product/process quality, it is fundamental to understand the process behaviour, the amount of variability and its impact on processes. Exploration refers to understanding the data from the process.

Statistical thinking and statistical methods play an important role in planning, conducting, analysing and interpreting data from engineering experiments. When several variables influence a certain characteristic of a product, the best strategy is then to design an experiment so that valid, reliable and sound conclusions can be drawn effectively, efficiently and economically.

In the thesis we will study DOE to obtain better knowledge how to design the best plan of the experiment to get the optimal ratio between the money that are spent for conducting the experiment and the reliability of conclusions.

We are going to investigate linear model of order one and we compare results from two different experiments. It will be used my own program written in MATLAB (I particularly take advantage of Statistics Toolbox for MATLAB) that simulates our experiments, computes their analysis, repeats them for different parameter σ and finally plots the graphs that illustrate dependence of determination if the factor is significant on the number of factors in experiment and on the number of replications in the central point. All simulations, analysis and graphs in the thesis will be created with significance level of the test $\alpha = 0.05$, graphs and tables for case $\alpha = 0.01$ are in Appendix.

2 Basic statistical concepts

2.1 Random variable and its characteristics

The nonempty set of all the possible outcomes ω of an experiment is known as the *sample space* Ω of the experiment.

$\mathcal{F}$ is a *σ-algebra* of subsets of Ω. It items are called *events*. Properties of σ-algebra are:

(i) If $A \in \mathcal{F}$, then $A^c \in \mathcal{F}$

(ii) If $A_1, A_2, \ldots \in \mathcal{F}$, then $\bigcup_{k=1}^{\infty} A_k \in \mathcal{F}, \bigcap_{k=1}^{\infty} A_k \in \mathcal{F}$

The *probability measure* P is a function from $\mathcal{F}$ to $\mathbb{R}$ that assigns to each event A a number $P(A)$ such that

(i) $P(A) \geq 0 \quad \forall A \subseteq \Omega$, where Ω is the sample space.

(ii) $P(\Omega) = 1$.

(iii) If $A_1, A_2, \ldots$ are disjoint sets in $\mathcal{F}$, then $P\left(\bigcup_{k=1}^{\infty} A_k\right) = \sum_{k=1}^{\infty} P(A_k)$.

A triple $(\Omega, \mathcal{F}, P)$ is called a *probability space* provided by arbitrary set Ω, $\mathcal{F}$ is a σ-algebra of subsets of Ω, and P is a probability measure on $\mathcal{F}$.

A mapping $X : \Omega \to \mathbb{R}^n$ is called an n-dimensional *random variable.*

Distribution function of random variable X is real function

$$F(X) = P(X < x) = P(X \in (-\infty; x)),$$

which is defined for $\forall x \in (-\infty; \infty)$. Distribution function has following properties:

(i) $0 \leq F(x) \leq 1$ for $\forall x \in (-\infty; \infty)$,

(ii) $F(x)$ is non-decreasing, continuous from the left, has finite number of discontinuities on $(-\infty; \infty)$,

(iii) $\lim_{x \to -\infty} F(x) = F(-\infty) = 0, \ \lim_{x \to \infty} F(x) = F(\infty) = 1,$

(iv) $P(a \leq X < b) = F(b) - F(a)$ for any real numbers $a < b$, specially $P(a \leq X) = 1 - F(a), \ P(X < b) = F(b), \ P(-\infty < X) = P(X < \infty) = 1,$

(v) $P(X = c) = \lim_{x \to c+} F(x) - F(c)$ for all $c \in \mathbb{R}$.

Random variable X is uniquely determined with its distribution function and its probability distribution is given.

If random variable X is *discrete*, we call the probability distribution of X, say $p(x)$, the *probability function* of X. Probability function is sequence

$$p(x) = P(X = x) > 0 \text{ for } x = x_1, x_2, ...$$

with following properties:

(i) $\sum_x p(x) = 1,$

(ii) $F(x) = \sum_{t<x} p(t)$ for $\forall x \in (-\infty; \infty)$,

(iii) $P(X \in M) = \sum_{x \in M} p(x)$ for any set of real number M.

If random variable X is continuous, the probability distribution of X, say $f(x)$, is often called the *probability density function* for X. Probability density function is a non-negative function $f(x)$, such that

$$F(x) = \int_{-\infty}^{x} f(t)\,\mathrm{d}t \text{ for } x \in (-\infty; \infty)$$

with following properties:

(i) $\int_{-\infty}^{\infty} f(x)\mathrm{d}x = 1,$

(ii) $f(x) = F'(x)$, if the derivative exists,

(iii) $P(a \le X \le b) = P(a < X < b) = P(a \le X < b) = P(a \le X < b) =$

$= \int_a^b f(x)\,\mathrm{d}x = F(b) - F(a)$ for any real numbers $a < b$,

(iv) $P(X = c) = 0$ for any $c \in \mathbb{R}$.

The location of the probability distribution of random variable is characterized by its *expected value* (or *mean value*). The expected value of a random variable X is denoted as $E(X)$ or μ. We define the expected value

$$E(X) = \sum_x xp(x) \quad \text{if the random variable } X \text{ is discrete,}$$

$$E(X) = \int_{-\infty}^{\infty} xf(x)\mathrm{d}x \quad \text{if the random variable } X \text{ is continuous.}$$

Expected value has properties:

(i) $E(aX + b) = aE(X) + b$ for any $a, b \in \mathbb{R}$,

(ii) $E\left(\sum_{i=1}^{n} X_i\right) = \sum_{i=1}^{n} E(X_i)$ for random variables $X_1, X_2, ..., X_n$.

The spread or dispersion of a probability distribution of random variable can be measured by the *variance*. Variance is symbolised as $D(X)$ or σ^2. We define the variance

$$D(X) = \sum_x (x - E(X))^2 p(x) \qquad \text{if the random variable } X \text{ is discrete,}$$

$$D(X) = \int_{-\infty}^{\infty} (x - E(X))^2 f(x) \mathrm{d}x \qquad \text{if the random variable } X \text{ is continuous.}$$

We can express the variance as $D(X) = E\left(\left[X - E(X)\right]^2\right)$. Variance has following properties:

(i) $D(X) \geq 0$,

(ii) $D(aX + b) = a^2 D(X)$ for any $a, b \in \mathbb{R}$,

(iii) $D\left(\sum_{i=1}^{n} X_i\right) = \sum_{i=1}^{n} D(X_i)$ for independent random variables $X_1, X_2, ..., X_n$.

Standard deviation of random variable X is defined as $\sigma(X) = \sqrt{D(X)}$. Standard deviation has properties:

(i) $\sigma(X) \geq 0$,

(ii) $\sigma(aX + b) = |a| \sigma(X)$ for any $a, b \in \mathbb{R}$,

If we have two random variables X and Y, the relationship between X and Y is expressed by *covariance*

$$\operatorname{cov}(X, Y) = E\left(\left[x - E(X)\right]\left[y - E(Y)\right]\right) = E(XY) - E(X)E(Y)$$

Properties of covariance are

(i) $\operatorname{cov}(X, Y) = \operatorname{cov}(Y, X)$,

(ii) $\operatorname{cov}(X, X) = D(X), \operatorname{cov}(Y, Y) = D(Y)$,

(iii) $D(X + Y) = D(X) + D(Y) + 2\operatorname{cov}(X, Y)$,

(iv) if X and Y are independent, then $\operatorname{cov}(X, Y) = 0$,

(v) $\operatorname{cov}(aX + b, cY + d) = ac \operatorname{cov}(X, Y)$ for any $a, b, c, d \in \mathbb{R}$.

Covariance forms the *covariance matrix*

$$\mathbf{cov}(X, Y) = \begin{bmatrix} D(X) & \operatorname{cov}(X, Y) \\ \operatorname{cov}(Y, X) & D(Y) \end{bmatrix},$$

which is symmetric and positive-definite.

Correlation coefficient indicates a linear relationship between two random variables X and Y

$$\rho(X,Y) = \operatorname{cov}\left(\frac{X-E(X)}{\sigma(X)}, \frac{Y-E(Y)}{\sigma(Y)}\right) = \frac{\operatorname{cov}(X,Y)}{\sigma(X)\sigma(Y)} = \frac{\operatorname{cov}(X,Y)}{\sqrt{D(X)D(Y)}}.$$

Properties of correlation coefficient are

(i) $\rho(X,Y) = \rho(Y,X)$,

(ii) $\rho(X,X) = \rho(Y,Y) = 1$,

(iii) $-1 \le \rho(X,Y) \le 1$,

(iv) $\rho(aX+b, cY+d) = \dfrac{ac}{|ac|}\rho(X,Y)$ for any $a,b,c,d \in \mathbb{R}, ac \ne 0$,

(v) $Y = aX + b \Leftrightarrow |\rho(X,Y)| = 1, \quad a,b \in \mathbb{R}, a \ne 0$,

(vi) if X and Y are independent, then $\rho(X,Y) = 0$.

If $\rho(X,Y) = 0$ (it means also $\operatorname{cov}(X,Y) = 0$), then we say that random variables X and Y are uncorrelated. However independent random variables are uncorrelated, uncorrelated random variables do not have to be independent. But uncorrelated normal distributed random variables are also independent. Correlation coefficient forms the correlation matrix

$$\boldsymbol{\rho}(X,Y) = \begin{bmatrix} 1 & \rho(X,Y) \\ \rho(Y,X) & 1 \end{bmatrix},$$

which is symmetric and positive-semidefinite.

2.2 Random sample and sampling characteristics

In statistical terms a *random sample* is a consequence of independent, identically distributed random variables $X_1, X_2, ..., X_n$. In practise the random sample is obtained if we repeat n-times the same experiment. The *sample mean* is

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i,$$

the *sample variance* is

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}\left(X_i - \bar{X}\right)^2,$$

and the *sample standard deviation* is

$$S = \sqrt{S^2}.$$

Basic characteristics of sample mean $\overline{X}$ and sample variance S^2 are:

(i) If the random variable X has expected value $E(X)$, then

$$E(\overline{X}) = E(X).$$

(ii) If the random variable X has variance $D(X)$, then

$$D(\overline{X}) = \frac{D(X)}{n}, \ \sigma(\overline{X}) = \frac{\sigma(X)}{\sqrt{n}}, \ E(S^2) = D(X).$$

2.3 Important types of probability distribution of continuous random variable

Before we show some examples of continuous probability remind some basic from mathematical analysis.

Gamma function $\Gamma(a)$ is defined as

$$\Gamma(a) = \int_0^\infty x^{a-1} \mathrm{e}^{-x} \mathrm{d}x, \qquad a > 0.$$

Beta function $B(a,b)$ is defined as

$$B(a,b) = \int_0^1 x^{a-1} (1-x)^{b-1} \mathrm{d}x, \quad a > 0, \ \ b > 0.$$

Most often we make use of these properties:

(i) $\Gamma(a+1) = a\Gamma(a)$

(ii) $B(a,b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$

(iii) $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$

Gamma function is generalisation of factorial because for $a \in \mathbb{N}$ is $\Gamma(a) = (a-1)!$.

One of the most important distributions is the *normal distribution*, also called Gaussian distribution. If X is a normal random variable, then the probability density function of X is

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \mathrm{e}^{\frac{-(x-\mu)^2}{2\sigma^2}}, \qquad x \in \mathbb{R},$$

where $\mu \in \mathbb{R}$ is mean of the distribution and $\sigma^2 > 0$ is the variance. If a real-valued random variable X is normally distributed with mean μ and variance $\sigma^2 \geq 0$, we write $X \sim N(\mu, \sigma^2)$. The *standard normal distribution* is the normal distribution with mean zero and variance one.

We see that if $X \sim N\left(\mu,\sigma^2\right)$, then the random variable

$$Y = \frac{X-\mu}{\sigma}$$

follows the standard normal distribution, denoted $Y \sim N\left(0,1\right)$. The operation is called standardizing the normal random variable. Examples of normal distributions for the same μ and various σ are shown in Figure 2-1.

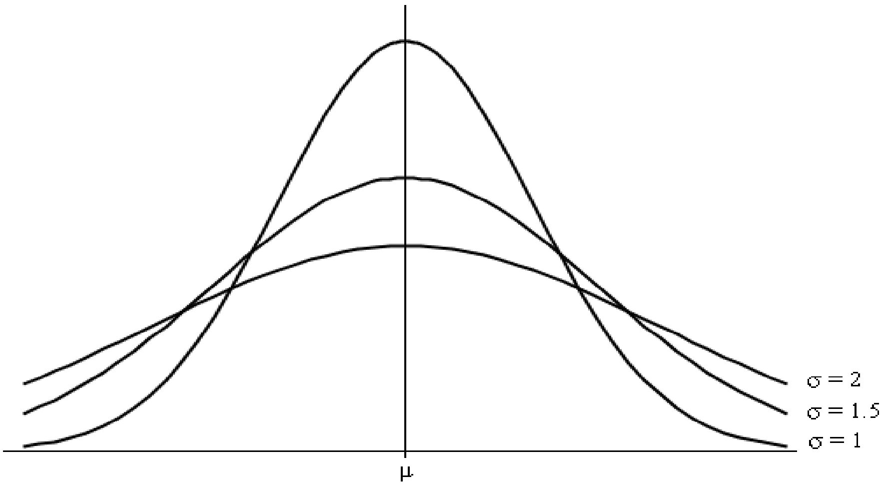

Figure 2-1 Examples of several normal distributions with the same mean.

Chi-square or χ^2 *distribution* with k degrees of freedom has probability density function

$$f\left(x\right) = \begin{cases} \dfrac{1}{2^{\frac{k}{2}}\Gamma\left(\dfrac{k}{2}\right)} \mathrm{e}^{-\frac{x}{2}} x^{\frac{k}{2}-1} & \text{for} \quad x \in \left\langle 0;\infty\right), \\ 0 & \text{for} \quad x \in \left(-\infty,0\right). \end{cases}$$

The distribution is asymmetric with mean $\mu = k$ and variance $\sigma^2 = 2k$. Examples of chi-square distribution are shown in Figure 2-2.

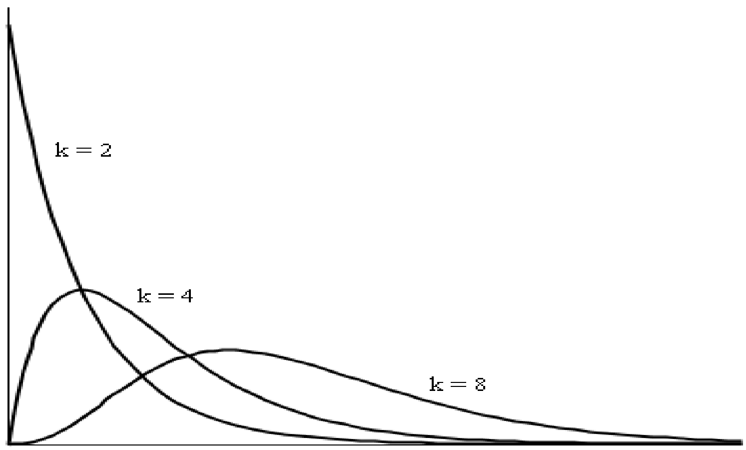

Figure 2-2 Examples of chi-square distribution.

If $X \sim N(0,1)$ and $Y \sim \chi_k^2$ are independent random variables, then the random variable

$$t_k = \frac{X}{\sqrt{\chi_k^2}}\sqrt{k}$$

follows the *t-distribution* with k degrees of freedom. The probability density function is

$$f(x) = \frac{\Gamma\left(\frac{k+1}{2}\right)}{\sqrt{\pi k}\,\Gamma\left(\frac{k}{2}\right)}\left(1+\frac{x^2}{k}\right)^{-\frac{k+1}{2}}, \quad x \in (-\infty;\infty).$$

The distribution is symmetric with mean $\mu = 0$ and variance $\sigma^2 = \frac{k}{k-2}$ for $k > 2$. If $k = \infty$, the *t*-distribution becomes the standard normal distribution. Several t-distributions are shown in Figure 2-3.

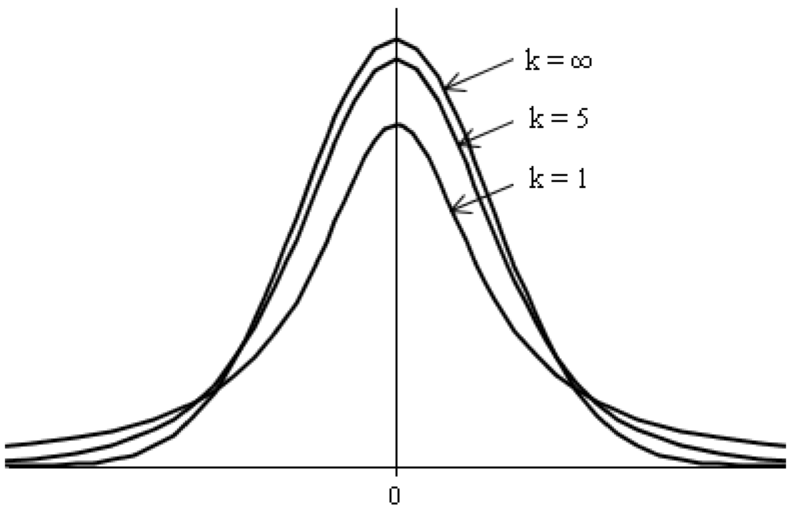

Figure 2-3 Examples of *t*-distributions.

If $X \sim N(\delta,1)$ and $Y \sim \chi_k^2$ are independent random variables, then the random variable

$$t_k = \frac{X}{\sqrt{\chi_k^2}}\sqrt{k}$$

is a *non-central t-distributed* random variable with k degrees of freedom and non-centrality parameter δ. The probability density function for the non-central *t*-distribution is

$$f(t) = \frac{k^{\frac{k}{2}} e^{\frac{-k\delta^2}{2(t^2+k)}}}{\sqrt{\pi}\,\Gamma\left(\frac{k}{2}\right) 2^{\frac{k-1}{2}} \left(t^2+k\right)^{\frac{k+1}{2}}} \int_0^\infty x^k e^{-\frac{1}{2}\left(x-\frac{\delta t}{\sqrt{t^2+k}}\right)^2} \mathrm{d}x$$

where $k > 0$. The mean and variance of the non-central *t*-distribution are $\mu = \delta \sqrt{\frac{k}{2}} \frac{\Gamma((k-1)/2)}{\Gamma(k/2)}$ for $k > 1$ and $\sigma^2 = \frac{k(1+\delta^2)}{k-2} - \frac{\delta^2 k}{2}\left(\frac{\Gamma((k-1)/2)}{\Gamma(k/2)}\right)^2$ for $k > 2$. Non-central *t*-distribution with two degrees of freedom ($k = 2$) and various non-centrality parameters are shown in Figure 2-4. In the $\delta = 0$ case, the non-central *t*-distribution becomes the *t*-distribution. The non-central *t*-distributions with δ and $-\delta$ non-centrality parameters are symmetrical with respect to vertical axis.

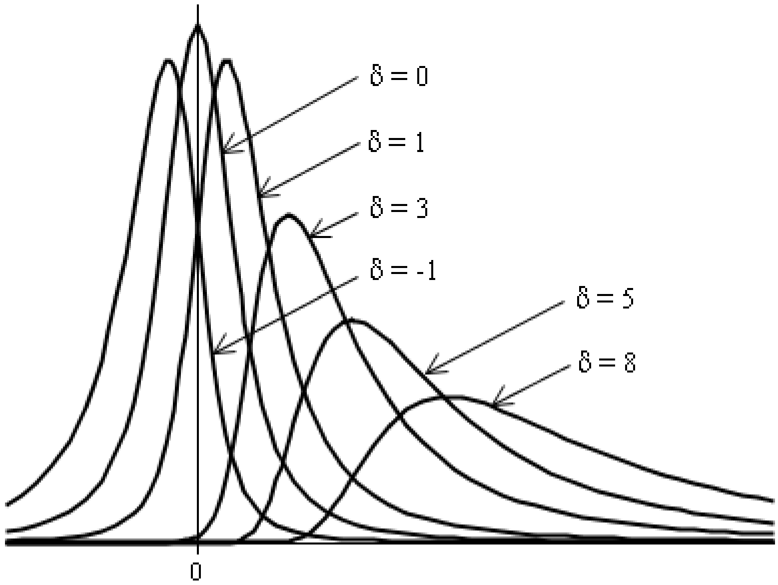

Figure 2-4 Examples of non-central *t*-distributions with 2 degrees of freedom and various non-centrality parameters.

If $X \sim \chi_u^2$ and $Y \sim \chi_v^2$ are two independent chi-square random variables with u and v degrees of freedom, then the random variable

$$F_{u,v} = \frac{\frac{X}{u}}{\frac{Y}{v}}$$

follows the *F distribution* with u and v degrees of freedom. The probability density function is

$$f(x) = \begin{cases} \frac{1}{B\left(\frac{u}{2}, \frac{v}{2}\right)} \left(\frac{u}{v}\right)^{\frac{u}{2}} x^{\frac{u}{2}-1} \left(1 + \frac{u}{v}x\right)^{-\frac{u+v}{2}} & \text{for } x \in \langle 0, \infty) \\ 0 & \text{for } x \in (-\infty, 0) \end{cases}$$

The distribution is asymmetric with mean $\mu = \frac{v}{v-2}$ for $v > 2$ and variance $\sigma^2 = \frac{2v^2(u+v-2)}{u(v-2)^2(v-4)}$ for $v > 4$. Several F distributions are shown in Figure 2-4.

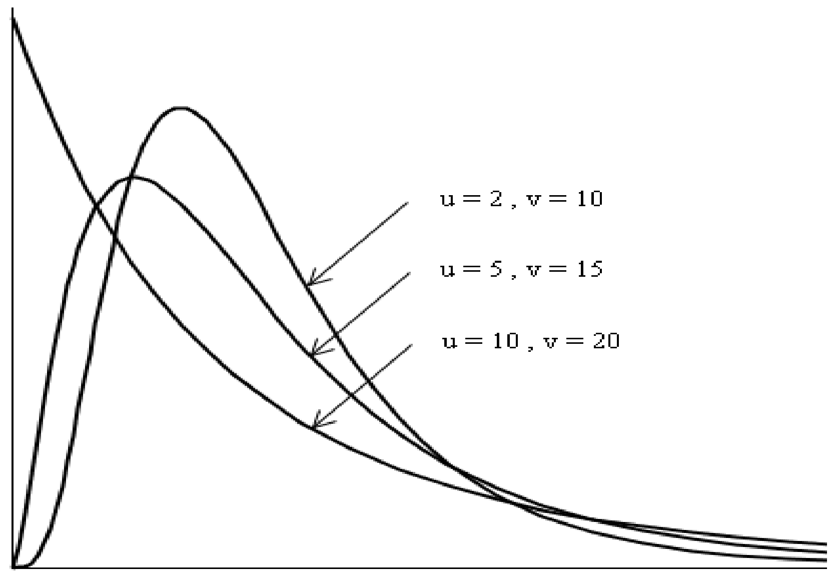

Figure 2-5 Examples of F distribution.

2.4 Graphical illustration of variability

We use graphical methods to analyse the data from an experiment. The *dot diagram*, displayed in Figure 2-5, is very useful device for displaying a small data volume (up to about 20 observations). The dot diagram helps to see central tendency of the observation and spread.

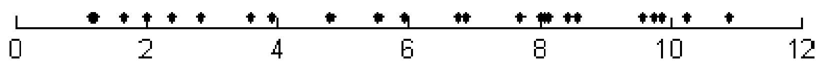

Figure 2-6 Example of dot plot.

If we have big quantity of data, analyse of dot diagram becomes difficult and it is useful to prefer a *histogram*. It is displayed in Figure 2-6.

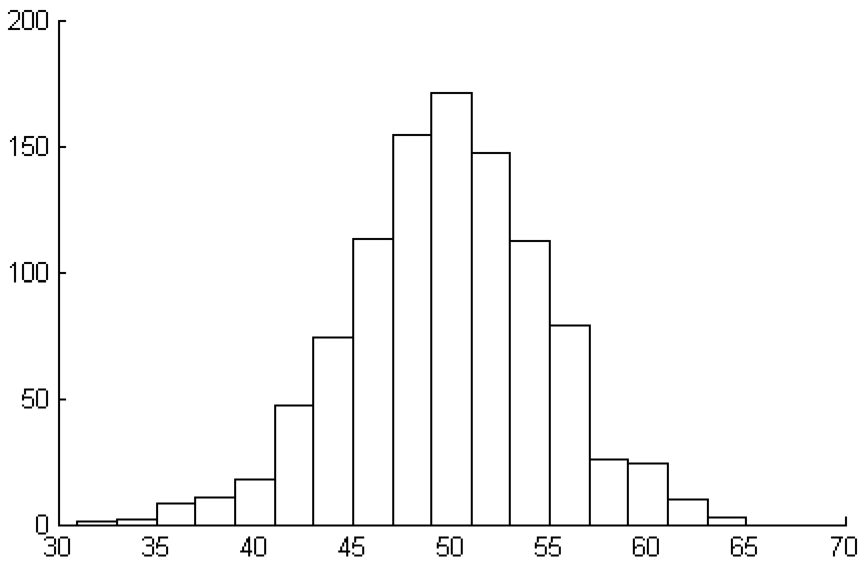

Figure 2-7 Example of histogram.

The histogram shows the central tendency, spread and general shape of the distribution of data. Histogram is constructed by dividing the horizontal the horizontal axis into intervals (usually of equal length) and drawing a rectangle over the *i*th interval with area of the rectangle proportional to n_i, the number of observations that fall in that interval.

The *box plot* is a useful way to display data. A rectangle contains middle part of organised set of observations, lower side of rectangle is 25th percentile and upper side is 75th percentile. Line inside the rectangle matches the median. Lower and upper quarters of set of observations are expressed dash lines above and below the rectangle. Values extra these sections are regarded as extremely deviated and they are called outliers. Examples of box plot are shown in Figure 2-6.

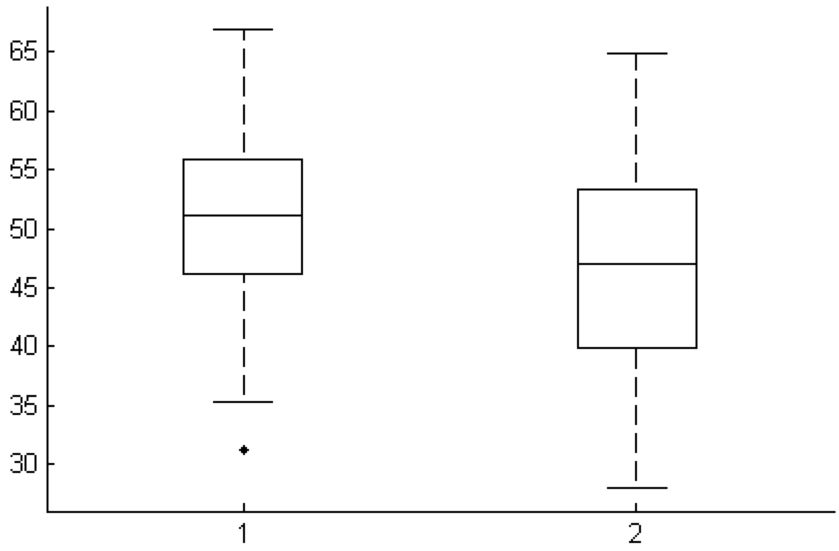

Figure 2-8 Examples of box plot.

2.5 Statistical hypothesis testing

A *statistical hypothesis* is a statement about the parameters of a probability distribution. A *statistical hypothesis test* is a method of verifying statistical hypothesis. A *null hypothesis*, usually denoted H_0, is a hypothesis set up to be refuted in order to support an *alternate hypothesis*, denoted H_1. If H_0 is hypothesis that parameter ϑ is of value ϑ_0, we write $H_0 : \vartheta = \vartheta_0$. If the alternate hypothesis is $H_1 : \vartheta \neq \vartheta_0$ it is called a *two-sided* alternate hypothesis since it would be true either if $\vartheta < \vartheta_0$ or $\vartheta > \vartheta_0$. If the alternate hypothesis is $H_1 : \vartheta < \vartheta_0$ or $H_1 : \vartheta > \vartheta_0$, it is called a *one-sided* alternate hypothesis.

To test a statistical hypothesis we devise a procedure for taking a random sample, computing an appropriate test statistic, and then rejecting or failing to reject the null hypothesis H_0. Part of this procedure is specifying the set of values for the test statistic that leads to rejection H_0. This set of values is called the *critical region* or *rejection region* for the test. We may commit two kinds of errors when testing hypotheses. If the null hypothesis is rejected when it is true, then a type I error has occurred. This error is also known as an "error of the first kind", an α error, or a "false positive". If the null hypothesis is not rejected when it is false, then a type II error has been made. It is also known as an "error of the second kind", a β error, or a "false negative". The probabilities of these two errors are

$$\alpha = P(\text{ type I error }) = P(\text{ rejected } H_0 \mid H_0 \text{ is true }),$$

$$\beta = P(\text{ type II error }) = P(\text{ fail to reject } H_0 \mid H_0 \text{ is false }).$$

The *power of a statistical test* is the probability that the test will reject a false null hypothesis (that it will not make a type II error). As power increases, the chances of a type II error decrease. Therefore power is

$$1-\beta = P(\text{ reject } H_0 \mid H_0 \text{ is false }).$$

The general procedure in hypothesis testing is to specify a value of the probability type I error α, called the significance level of the test, and then design the test procedure so that the probability of type II error β has a suitably small value.

An *F-test* is any statistical test in which the test statistic has an F-distribution if the null hypothesis is true. F-test which are frequently used are

- the test that the means of multiple normally distributed populations, having the same variance are equal,
- the test that the standard deviations of two normally distributed populations are equal, and thus that they are of comparable origin.

A *t-test* is any statistical test in which the test statistic has a Student's *t*-distribution if the null hypothesis is true. A t-test which are frequently used are

- the test of whether the mean of a normally distributed population has a value specified in a null hypothesis,
- the test of the null hypothesis that the means of two normally distributed populations having the same (but unknown) variance are equal.

3 Monte Carlo method

The expression Monte Carlo method is actually very general. A Monte Carlo method is a technique that involves using random numbers and probability statistics to solve problems. The term Monte Carlo is after the city in the Monaco principality, because of roulette, a simple random number generator.

By using computer models, computer simulation has to imitate real life or make predictions. When you create a model with a spreadsheet like Excel, you have a certain number of input parameters and a few equations that use those inputs to give you a set of outputs (or response variables). This type of model is usually deterministic, meaning that you get the same results no matter how many times you re-calculate.

Monte Carlo simulation is a method for iteratively evaluating a deterministic model using sets of random numbers as inputs. This method is often used when the model is complex, nonlinear, or involves more than just a couple uncertain parameters. A simulation can typically involve over 10,000 evaluations of the model, a task which in the past was only practical using super computers

By using random inputs, you are essentially turning the deterministic model into a stochastic model.

Monte Carlo simulation is categorized as a sampling method because the inputs are randomly generated from probability distributions to simulate the process of sampling from an actual population. So, we try to choose a distribution for the inputs that most closely matches data we already have, or best represents our current state of knowledge. The data generated from the simulation can be represented as probability distributions (or histograms) or converted to error bar, reliability predictions, tolerance zones, and confidence intervals.

All we need to do is follow the five simple steps listed below:

Step 1: Create a parametric model, $\mathrm{y} = f\left(\mathrm{x}_1, \mathrm{x}_2, \ ..., \ \mathrm{x}_q\right)$.

Step 2: Generate a set of random inputs, $\mathrm{x}_{i1}, \mathrm{x}_{i2}, \ ..., \ \mathrm{x}_{iq}$.

Step 3: Evaluate the model and store the results as y_i.

Step 4: Repeat steps 2 and 3 for $i = 1$ to n.

Step 5: Analyze the results using histograms, summary statistics, confidence intervals, etc.

4 Analysis of variance

The analysis of variance is a technique that consists of separating the total variation of data set into logical components associated with specific sources of variation in order to compare the mean of several populations. This analysis also helps us to test certain hypotheses concerning the parameters of the model, or to estimate the components of the variance.

Suppose there are a levels of factor A and b levels of factor B and each replicate contains all ab treatment combinations. In general, there are n replicates. The observations can be described by the linear statistical model

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \epsilon_{ijk} \begin{cases} i = 1, ..., a \\ j = 1, ..., b \\ k = 1, ..., n \end{cases} \quad (4.1)$$

where μ is a parameter common to all treatments called the *overall mean*, τ_i is the *treatment effect* of the ith level of the row factor A, β_i the treatment effect of the jth level of the column factor B, $(\tau\beta)_{ij}$ is the effect of the interaction between τ_i and β_i, and ϵ_{ijk} is a random error component. In general, the observed data will appear as in Table 4-1

		Factor B			
		1	2	...	b
	1	$y_{111}, y_{112}, ..., y_{11n}$	$y_{121}, y_{122}, ..., y_{12n}$		$y_{1b1}, y_{1b2}, ..., y_{1bn}$
	2	$y_{211}, y_{212}, ..., y_{21n}$	$y_{221}, y_{222}, ..., y_{22n}$		$y_{2b1}, y_{2b2}, ..., y_{2bn}$
Factor A	. . .				
	a	$y_{a11}, y_{a12}, ..., y_{a1n}$	$y_{a21}, y_{a22}, ..., y_{a2n}$		$y_{ab1}, y_{ab2}, ..., y_{abn}$

Table 4-1 Typical data for a two-factor experiment

We test appropriate hypotheses about the treatment effects and we want to estimate them. For hypothesis testing, the model errors are assumed to be normally and independently distributed random variables with mean zero and variance σ^2. The variance is assumed to be constant for all levels of the factors.

There are two different situations with respect to the treatment effects. First, the treatment is specifically chosen by the experimenter. In this situation we test hypotheses about the treatment means, and our conclusions apply only to the factor levels considered in the analysis. This is called the *fixed effect model*. Alternatively, the treatments could be a random sample from a larger population of treatments. Here the $\tau_i, \beta_j, (\tau\beta)_{ij}$ are random variables, and knowledge about the particular ones investigated is relatively useless. Instead, we test hypotheses about the variability of the $\tau_i, \beta_j, (\tau\beta)_{ij}$ and try to estimate them. This is called the *random effects model*.

4.1 Analysis of the two-factor fixed effects model

In the fixed effects model the treatments effects are defined as deviation from the overall mean, so $\sum_{i=1}^{a}\tau_i = 0$ and $\sum_{j=1}^{b}\beta_j = 0$. Similarly, the interaction effects are fixed and are defined such that $\sum_{i=1}^{a}(\tau\beta)_{ij} = 0$ and $\sum_{j=1}^{b}(\tau\beta)_{ij} = 0$. Since there are n replicates, there are abn total observations. We are interested in testing hypotheses about equality of row treatment effects, say

$$\begin{aligned} &H_0 : \tau_1 = \tau_2 = ... = \tau_a = 0 \\ &H_1 : \text{ at least one } \tau_i \neq 0 \end{aligned} \quad \text{(no main effect of factor } A\text{)}$$

and the equality of column treatment effects, say

$$\begin{aligned} &H_0 : \beta_1 = \beta_2 = ... = \beta_b = 0 \\ &H_1 : \text{ at least one } \beta_j \neq 0 \end{aligned} \quad \text{(no main effect of factor } B\text{)}$$

We are also interested in determining whether row and column treatments interact. Thus, we test

$$\begin{aligned} &H_0 : (\tau\beta)_{ij} = 0 \qquad \text{for all } i, j \\ &H_1 : \text{ at least one } (\tau\beta)_{ij} \neq 0 \end{aligned} \quad \text{(no interaction)}$$

The appropriate procedure for testing these hypotheses is a two-factor analysis of variance.

Let $y_{i..}$ denote the total of all observations under the ith level of factor A, $y_{.j.}$ denote the total of all observations under the jth level of factor B, $y_{ij.}$ denote the total of all observation in the ijth cell, and $y_{...}$ denote the grand total of all the observations. Define $\bar{y}_{i..}, \bar{y}_{.j.}, \bar{y}_{ij.}$ and $\bar{y}...$ as the corresponding row, column, cell and grand averages. Mathematical expression is

$$\begin{aligned} &y_{i..} = \sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk} && \bar{y}_{i..} = \frac{y_{i..}}{bn} && i = 1, 2, ..., a \\ &y_{.j.} = \sum_{i=1}^{a}\sum_{k=1}^{n} y_{ijk} && \bar{y}_{.j.} = \frac{y_{.j.}}{an} && j = 1, 2, ..., b \\ &y_{ij.} = \sum_{k=1}^{n} y_{ijk} && \bar{y}_{ij.} = \frac{y_{ij.}}{n} && i = 1, 2, ..., a \quad j = 1, 2, ..., b \\ &y_{...} = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk} && \bar{y}_{...} = \frac{y_{...}}{abn} && \end{aligned} \tag{4.2}$$

The total corrected sum of squares

$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}\left(y_{ijk} - \bar{y}_{...}\right)^2 \tag{4.3}$$

is used as a measure of overall variability in the data. If we divide SS_T by appropriate number of degrees of freedom (in this case, $abn-1$), we have the sample variance of y and the sample variance is a standard measure of variability. The total corrected sum of squares may be written as

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}\left(y_{ijk}-\overline{y}_{...}\right)^2=\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}\Big[\left(\overline{y}_{i..}-\overline{y}_{...}\right)+\left(\overline{y}_{.j.}-\overline{y}_{...}\right)+$$

$$+\left(\overline{y}_{ij.}-\overline{y}_{i..}-\overline{y}_{.j.}+\overline{y}_{...}\right)+\left(y_{ijk}-\overline{y}_{ij.}\right)\Big]^2=$$

$$=bn\sum_{i=1}^{a}\left(\overline{y}_{i..}-\overline{y}_{...}\right)^2+an\sum_{j=1}^{b}\left(\overline{y}_{.j.}-\overline{y}_{...}\right)^2+ \tag{4.4}$$

$$+n\sum_{i=1}^{a}\sum_{j=1}^{b}\left(\overline{y}_{ij.}-\overline{y}_{i..}-\overline{y}_{.j.}+\overline{y}_{...}\right)^2+\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}\left(y_{ijk}-\overline{y}_{...}\right)^2$$

since the six cross products on the right-hand side are zero. The total sum of squares has been partitioned into a sum of squares due to factor A, SS_A, a sum of squares due to factor B, SS_B, a sum of squares due to the interaction between A and B, SS_{AB}, and the sum of squares due to error, SS_E. From the last component on the right-hand side of Equation (4.4) we see that there must be at least two replicates to obtain an error sum of squares. We may write the Equation (4.4) as

$$SS_T=SS_A+SS_B+SS_{AB}+SS_E \tag{4.5}$$

The number of degrees of freedom associated with each sum of square is

Effect	**Degrees of freedom**
A	$a-1$
B	$b-1$
AB interaction	$(a-1)(b-1)$
Error	$ab(n-1)$
Total	$abn-1$

The quantities

$$MS_A=\frac{SS_A}{a-1},\qquad MS_B=\frac{SS_B}{b-1},\qquad MS_{AB}=\frac{SS_{AB}}{(a-1)(b-1)},\qquad MS_E=\frac{SS_E}{ab(n-1)}$$

are called *mean squares*. The expected values of the mean squares are

$$E\left(MS_A\right)=E\left(\frac{SS_A}{a-1}\right)=\sigma^2+\frac{bn\sum_{i=1}^{a}\tau_i^2}{a-1}$$

$$E(MS_B) = E\left(\frac{SS_B}{b-1}\right) = \sigma^2 + \frac{an\sum_{j=1}^{b}\beta_j^2}{b-1}$$

$$E(MS_{AB}) = E\left(\frac{SS_{AB}}{(a-1)(b-1)}\right) = \sigma^2 + \frac{n\sum_{i=1}^{a}\sum_{j=1}^{b}(\tau\beta)_{ij}^2}{(a-1)(b-1)}$$

and

$$E(MS_E) = E\left(\frac{SS_E}{ab(n-1)}\right) = \sigma^2 .$$

If the null hypotheses of no row treatment effects, no column treatment effects and no interaction are true, then MS_A, MS_B, MS_{AB} and MS_E all estimate σ^2. If we assume that the model, Equation (4.1), is adequate and that the error terms ϵ_{ijk} are normally and independently distributed with constant variance σ^2, then each of the ratios of means squares are distributed as F with $a-1$, $b-1$ and $(a-1)(b-1)$ numerator degrees of freedom, respectively, and $ab(n-1)$ denominator degrees of freedom. The critical region would be the upper tail of the F distribution. The test procedure is usually summarized in an analysis of variance table, Table 4-2.

Source of variation	**Sum of squares**	**Degrees of freedom**	**Mean square**	F_0
A treatments	SS_A	$a-1$	$MS_A = \frac{SS_A}{a-1}$	$F_0 = \frac{MS_A}{MS_E}$
B treatments	SS_B	$b-1$	$MS_B = \frac{SS_B}{b-1}$	$F_0 = \frac{MS_B}{MS_E}$
Interaction	SS_{AB}	$(a-1)(b-1)$	$MS_{AB} = \frac{SS_{AB}}{(a-1)(b-1)}$	$F_0 = \frac{MS_{AB}}{MS_E}$
Error	SS_E	$ab(n-1)$	$MS_E = \frac{SS_E}{ab(n-1)}$	
Total	SS_T	$abn-1$		

Table 4-2 The analysis of variance table, fixed effects model¨

Computational formulas for the sums of squares in Equation (4.5) may be obtained easily. The total sum of squares is computed as usual by

$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk}^2 - \frac{y_{\dots}^2}{abn} \tag{4.6}$$

The sums of squares for the main effects are

$$SS_A = \sum_{i=1}^{a} \frac{y_{i..}^2}{bn} - \frac{y_{...}^2}{abn} \tag{4.7}$$

and

$$SS_B = \sum_{j=1}^{b} \frac{y_{.j.}^2}{an} - \frac{y_{...}^2}{abn} \tag{4.8}$$

It is convenient to obtain the SS_{AB} in two stages. First we compute the sum of squares between the ab cells totals, which is called the sum of squares due to subtotals

$$SS_{\text{Subtotals}} = \sum_{i=1}^{a}\sum_{j=1}^{b} \frac{y_{ij.}^2}{n} - \frac{y_{...}^2}{abn}$$

This sum of squares also contains SS_A and SS_B. Therefore the SS_{AB} is

$$SS_{AB} = SS_{\text{Subtotals}} - SS_A - SS_B \tag{4.9}$$

We may compute SS_E by subtraction as

$$SS_E = SS_T - SS_{\text{Subtotals}}$$

or

$$SS_E = SS_T - SS_{AB} - SS_A - SS_B \tag{4.10}$$

4.2 Analysis of the general fixed effects model

The results from two-factor analysis may be extend to the general case where there are a levels of factor A, b levels of factor B, c levels of factor C and so on. In general there will be $abc...n$ total observations if there are n replicates of the complete experiment. If all factors are fixed, we may easily formulate and test hypotheses about the main effects and interactions. Test statistics for each main effect and interaction may be constructed by dividing the corresponding mean square for the effect or interaction by the mean square error. The number of freedom for any main effect is the number of levels of the factor minus one and the number of degrees of freedom for any interaction is the product of the number of degrees of freedom associated wit the individual components of the interaction.

For example consider the three-factor analysis with underlying model

$$y_{ijkl} = \mu + \tau_i + \beta_j + \gamma_k + (\tau\beta)_{ij} + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} + (\tau\beta\gamma)_{ijk} + \epsilon_{ijkl} \begin{cases} i = 1,...,a \\ j = 1,...,b \\ k = 1,...,c \\ l = 1,...,n \end{cases} \tag{4.11}$$

The analysis of variance table is shown in Table 4-3.

Source of variation	**Sum of squares**	**Degrees of freedom**	**Mean square**	F_0
A	SS_A	$a-1$	MS_A	$F_0 = \frac{MS_A}{MS_E}$
B	SS_B	$b-1$	MS_B	$F_0 = \frac{MS_B}{MS_E}$
C	SS_C	$c-1$	MS_C	$F_0 = \frac{MS_C}{MS_E}$
AB	SS_{AB}	$(a-1)(b-1)$	MS_{AB}	$F_0 = \frac{MS_{AB}}{MS_E}$
AC	SS_{AC}	$(a-1)(c-1)$	MS_{AC}	$F_0 = \frac{MS_{AC}}{MS_E}$
BC	SS_{BC}	$(b-1)(c-1)$	MS_{BC}	$F_0 = \frac{MS_{BC}}{MS_E}$
ABC	SS_{ABC}	$(a-1)(b-1)(c-1)$	MS_{ABC}	$F_0 = \frac{MS_{ABC}}{MS_E}$
Error	SS_E	$abc(n-1)$	MS_E	
Total	SS_T	$abcn-1$	MS_T	

Table 4-3 The analysis of variance table for three-factor fixed effects model

We give the computing formulas for the sums of squares in Table 4-3. The total sum of squares is found as

$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\sum_{l=1}^{n} y_{ijkl}^2 - \frac{y_{....}^2}{abcn} \tag{4.12}$$

The sums of squares for the main effects are found as

$$SS_A = \sum_{i=1}^{a} \frac{y_{i...}^2}{bcn} - \frac{y_{....}^2}{abcn} \tag{4.13}$$

$$SS_B = \sum_{j=1}^{b} \frac{y_{.j..}^2}{acn} - \frac{y_{....}^2}{abcn} \tag{4.14}$$

$$SS_C = \sum_{k=1}^{c} \frac{y_{i...}^2}{abn} - \frac{y_{....}^2}{abcn} \tag{4.15}$$

To compute the two-factor interaction sums of squares, the totals for the $A \times B$, $A \times C$, $B \times C$ cells are needed. The sums of squares are found from

$$SS_{AB} = \sum_{i=1}^{a}\sum_{j=1}^{b} \frac{y_{ij..}^2}{cn} - \frac{y_{....}^2}{abcn} - SS_A - SS_B = SS_{\text{Subtotals}(AB)} - SS_A - SS_B \tag{4.16}$$

$$SS_{AC} = \sum_{i=1}^{a}\sum_{k=1}^{c} \frac{y_{i.k.}^2}{bn} - \frac{y_{....}^2}{abcn} - SS_A - SS_C = SS_{\text{Subtotals}(AC)} - SS_A - SS_C \tag{4.17}$$

and

$$SS_{BC} = \sum_{j=1}^{b}\sum_{k=1}^{c}\frac{y_{.jk.}^2}{an} - \frac{y_{....}^2}{abcn} - SS_B - SS_C = SS_{\text{Subtotals}(BC)} - SS_B - SS_C \quad (4.18)$$

The sums of squares for the two-factor subtotals are found from the totals in each two-way table. The three-factor interaction sum of squares is computed from the three-way cell totals, $y_{ijk.}$, as

$$\begin{aligned} SS_{ABC} &= \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\frac{y_{ijk.}^2}{n} - \frac{y_{....}^2}{abcn} - SS_A - SS_B - SS_C - SS_{AB} - SS_{AC} - SS_{BC} = \\ &= SS_{\text{Subtotals}(ABC)} - SS_A - SS_B - SS_C - SS_{AB} - SS_{AC} - SS_{BC} \end{aligned} \quad (4.19)$$

The error sum of squares may be found by subtracting

$$SS_E = SS_T - SS_A - SS_B - SS_C - Ss_{AB} - SS_{AC} - SS_{BC} - SS_{ABC}$$

or by

$$SS_E = SS_T - SS_{\text{Subtotals}(ABC)} \quad (4.20)$$

5 Regression analysis

Regression analysis is a technique used for the modelling and analysis of numerical data consisting of values of a dependent variable Y and of independent variables which are represented by random vector $\boldsymbol{X} = (X_1, X_2, ..., X_k)$. The dependent variable is assumed to be a random variable, due to the presence of observational errors. The independent variable is assumed to be error-free. To describe the dependence Y on $\boldsymbol{X}$ the regression analysis is used. This dependence is expressed by regression equation

$$\eta = E(Y | \boldsymbol{X} = \boldsymbol{x}) = \varphi(\boldsymbol{x}, \boldsymbol{\beta}),$$

where $\boldsymbol{x} = (x_1, ..., x_k)$ is vector of independent variables (value of random vector $\boldsymbol{X}$), $\boldsymbol{\beta} = (\beta_1, ..., \beta_m)$ is vector of parameters, so-called regression coefficients β_j, $j = 1, ..., m$, and $\eta = E(Y | \boldsymbol{X} = \boldsymbol{x})$ is conditional expectation value. We may estimate regression coefficients β_j if the residual sum of squares is minimized

$$L = \sum_{i=1}^{n} \left[y_i - \varphi(\boldsymbol{x}_i, \boldsymbol{\beta}) \right]^2$$

and this method is called *the least squares method*.

5.1 Linear regression

Suppose the true relationship between y and $\boldsymbol{x}$ is linear. The general problem of fitting the model

$$y = \beta_0 + \beta_1 x_1 + ... + \beta_k x_k + \epsilon \tag{5.1}$$

is called the multiple linear regression problem.

y	x_1	x_2	$\cdots$	x_k
y_1	x_{11}	x_{21}	$\cdots$	x_{k1}
y_2	x_{12}	x_{22}	$\cdots$	x_{k1}
$\vdots$	$\vdots$	$\vdots$		$\vdots$
y_n	x_{1n}	x_{2n}	$\cdots$	x_{kn}

Table 5-5-1 Data for linear regression

The model describes a hyperplane in the *k*-dimensional space of the regressor variables x_i. The method of least squares is used to estimate the regression coefficients. Suppose that $n > k$ observations are available, and let x_{ij} denote the *j*th observation of variable x_i. The data appear as in Table 5-1. The estimation procedure requires that the random error components are normally distributed with $E(\epsilon) = 0$ and $D(\epsilon) = \sigma^2$ and that ϵ are uncorrelated.

We may write the model as

$$y_j = \beta_0 + \beta_1 x_{1j} + \beta_2 x_{2j} + \ldots + \beta_k x_{kj} + \epsilon_j = \beta_0 + \sum_{i=1}^{k} \beta_i x_{ij} + \epsilon_j \qquad j = 1, 2, \ldots, n \tag{5.2}$$

and the least square function is

$$L = \sum_{j=1}^{n} \epsilon_j^2 = \sum_{j=1}^{n} \left[y_j - \beta_0 - \sum_{i=1}^{k} \beta_i x_{ij} \right]^2 \tag{5.3}$$

We want to minimize L with respect to $\beta_0, \beta_1, \ldots, \beta_k$. The least squares estimators of $\beta_0, \beta_1, \ldots, \beta_k$, say $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_k$ must satisfy

$$\left.\frac{\partial L}{\partial \beta_0}\right|_{\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_k} = -2 \left[\sum_{j=1}^{n} y_j - \hat{\beta}_0 - \sum_{u=1}^{k} \hat{\beta}_u x_{uj} \right] = 0 \tag{5.4}$$

and

$$\left.\frac{\partial L}{\partial \beta_i}\right|_{\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_k} = -2 \left[\sum_{j=1}^{n} y_j - \hat{\beta}_0 - \sum_{i=1}^{k} \hat{\beta}_i x_{ij} \right] x_{ij} = 0 \qquad i = 1, 2, \ldots, k \tag{5.5}$$

Simplifying Equations (5.4) and (5.5) we obtain the least square normal equations

$$\begin{aligned}
n\hat{\beta}_0 + \hat{\beta}_1 \sum_{j=1}^{n} x_{i1} + \hat{\beta}_2 \sum_{j=1}^{n} x_{i2} + \ldots + \hat{\beta}_k \sum_{j=1}^{n} x_{ik} &= \sum_{j=1}^{n} y_j \\
\hat{\beta}_0 \sum_{j=1}^{n} x_{i1} + \hat{\beta}_1 \sum_{j=1}^{n} x_{i1}^2 + \hat{\beta}_2 \sum_{j=1}^{n} x_{i1} x_{i2} + \ldots + \hat{\beta}_k \sum_{j=1}^{n} x_{i1} x_{ik} &= \sum_{j=1}^{n} x_{i1} y_j \\
&\vdots \\
\hat{\beta}_0 \sum_{j=1}^{n} x_{ik} + \hat{\beta}_1 \sum_{j=1}^{n} x_{ik} x_{i1} + \hat{\beta}_2 \sum_{j=1}^{n} x_{ik} x_{i2} + \ldots + \hat{\beta}_k \sum_{j=1}^{n} x_{ik}^2 &= \sum_{j=1}^{n} x_{ik} y_j
\end{aligned} \tag{5.6}$$

There are $p = k + 1$ normal equations, one for each of the unknown regression coefficients. The solution to the normal equations is the least squares estimators, $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_k$. The matrix notation of the normal equations is

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{21} & \cdots & x_{k1} \\ 1 & x_{12} & x_{22} & \cdots & x_{k2} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{1n} & x_{2k} & \cdots & x_{kn} \end{bmatrix}, \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} \text{ and } \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

In general $\mathbf{y}$ is an $(n\times 1)$ vector of responses, $\mathbf{X}$ is an $(n\times p)$ matrix of the levels of the regressor variables, $\boldsymbol{\beta}$ is a $(p\times 1)$ vector of the regression coefficients, and $\boldsymbol{\epsilon}$ is an $(n\times 1)$ vector of random errors. We want to find the vector of least squares estimators $\hat{\boldsymbol{\beta}}$ that minimizes

$$L=\sum_{j=1}^{n}\boldsymbol{\epsilon}_j^2=\boldsymbol{\epsilon}'\boldsymbol{\epsilon}=(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})'(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})$$

L may be expressed as

$$L=\mathbf{y}'\mathbf{y}-\boldsymbol{\beta}'\mathbf{X}'\mathbf{y}-\mathbf{y}'\mathbf{X}\boldsymbol{\beta}+\boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta}=\mathbf{y}'\mathbf{y}-2\boldsymbol{\beta}'\mathbf{X}'\mathbf{y}+\boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta} \qquad (5.7)$$

since $\boldsymbol{\beta}'\mathbf{X}'\mathbf{y}$ is a (1×1) matrix, or a scalar, and its transpose $(\boldsymbol{\beta}'\mathbf{X}'\mathbf{y})'=\mathbf{y}'\mathbf{X}\boldsymbol{\beta}$ is the same scalar. The least squares estimators must satisfy

$$\left.\frac{\partial L}{\partial\boldsymbol{\beta}}\right|_{\hat{\boldsymbol{\beta}}}=-2\mathbf{X}'\mathbf{y}+2\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}}=\mathbf{0}$$

which simplifies to

$$\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}}=\mathbf{X}'\mathbf{y} \qquad (5.8)$$

Equations (5.8) are the least square normal equations and they are identical to Equations (5.6). To solve the normal equations, multiply both sides of Equations (5.8) by inverse of $\mathbf{X}'\mathbf{X}$. Thus, the least squares estimator of $\boldsymbol{\beta}$ is

$$\hat{\boldsymbol{\beta}}=(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \qquad (5.9)$$

The fitted regression model is

$$\hat{y}_j=\hat{\beta}_0+\sum_{i=1}^{k}\hat{\beta}_i x_{ij} \qquad (5.10)$$

The difference between the observation y_j and the fitted value $\hat{y}_j$ is a residual $\mathrm{e}_j=y_j-\hat{y}_j$. The $(n\times 1)$ vector of residuals is denoted by

$$\mathbf{e}=\mathbf{y}-\hat{\mathbf{y}}.$$

Expectation value of the least squares estimator $\hat{\boldsymbol{\beta}}$ is

$$E(\hat{\boldsymbol{\beta}})=E\left[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}\right]=E\left[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'(\mathbf{X}\boldsymbol{\beta}+\boldsymbol{\epsilon})\right]=E\left[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\boldsymbol{\beta}+(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\epsilon}\right]=\boldsymbol{\beta}$$

since $E(\boldsymbol{\epsilon})=0$ and $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}=\mathbf{I}$. Thus, $\hat{\boldsymbol{\beta}}$ is unbiased estimator of $\boldsymbol{\beta}$.

Variance property of $\hat{\boldsymbol{\beta}}$ is expressed in the covariance matrix:

$$\operatorname{cov}\left(\hat{\boldsymbol{\beta}}\right) = E\left(\left[\hat{\boldsymbol{\beta}} - E\left(\hat{\boldsymbol{\beta}}\right)\right]\left[\hat{\boldsymbol{\beta}} - E\left(\hat{\boldsymbol{\beta}}\right)\right]'\right),$$

which is symmetric matrix and ith main diagonal element is the variance of $\hat{\beta}_i$ and (ij)th element is the covariance between $\hat{\beta}_i$ and $\hat{\beta}_j$. The covariance matrix of $\hat{\boldsymbol{\beta}}$ is

$$\operatorname{cov}\left(\hat{\boldsymbol{\beta}}\right) = \sigma^2 \left(\mathbf{X}'\mathbf{X}\right)^{-1}.$$

The inverse matrix $\left(\mathbf{X}'\mathbf{X}\right)^{-1}$ is easy to obtain if $\mathbf{X}'\mathbf{X}$ is diagonal. This seems to be advantageous, not only because of the computational simplicity but also because the estimators of all regression coefficients are uncorrelated, that is, $\operatorname{cov}\left(\hat{\beta}_i, \hat{\beta}_j\right) = 0$. If we can choose the levels of x_{ij} before the data are collected, we may design the experiment so that $\mathbf{X}'\mathbf{X}$ will be diagonal. We know that the off diagonal elements in $\mathbf{X}'\mathbf{X}$ are the sums of cross-products of $\mathbf{X}$. Therefore we must make the scalar product of the columns of $\mathbf{X}$ equal to zero; that is, these columns must be orthogonal. Experimental designs that have this property for fitting a regression model are called *orthogonal design*.

In linear regression we test hypotheses about the model parameters. We assume that the errors are normally, independently distributed random variables with mean 0 and variance σ^2. A direct consequence of this assumption is that the observations y_j are normally, independently distributed random variables with mean $\beta_0 + \sum_{i=1}^{k} \beta_i x_{ij}$ and variance σ^2. The significance of regression is obtained by testing

$$\begin{aligned} &H_0 : \beta_1 = \beta_2 = \ldots = \beta_k = 0 \\ &H_1 : \beta_i \neq 0 \quad \text{at least one } i. \end{aligned} \tag{5.11}$$

Rejection of H_0 implies that at least one variable in the model contributes significantly to the model. The *total sum of squares* for y is

$$S_{yy} = \sum_{j=1}^{n} \left(y_j - \bar{y}\right)^2 = \sum_{j=1}^{n} y_j^2 - \frac{1}{n}\left(\sum_{j=1}^{n} y_j\right)^2 = \mathbf{y}'\mathbf{y} - \frac{1}{n}\left(\sum_{j=1}^{n} y_j\right)^2 \tag{5.12}$$

The total sum of squares S_{yy} may be written as

$$S_{yy} = SS_R + SS_E\,, \tag{5.13}$$

where SS_E is *error* or *residual sum of squares*

$$SS_E = \sum_{j=1}^{n} \mathrm{e}_j^2 = \sum_{j=1}^{n} \left(y_j - \hat{y}_j\right)^2 \tag{5.14}$$

and SS_R is *regression sum of squares*. We can obtain computational formula for SS_R as follows:

$$SS_E = \sum_{j=1}^{n}\left(y_j - \hat{y}_j\right)^2 = \left(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}\right)'\left(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}\right) = \mathbf{y}'\mathbf{y} - \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} = \mathbf{y}'\mathbf{y} - \frac{1}{n}\left(\sum_{j=1}^{n} y_j\right)^2 - \left[\hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} - \frac{1}{n}\left(\sum_{j=1}^{n} y_j\right)^2\right]$$

Since $S_{yy} = SS_R + SS_E$, the regression sum of squares is

$$SS_R = \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} - \frac{1}{n}\left(\sum_{j=1}^{n} y_j\right)^2 \tag{5.15}$$

If $H_0 : \beta_i = 0$ is true, then $\frac{SS_R}{\sigma^2} \sim \chi_k^2$, where the number of degrees of freedom are equal to the regressor variables in model, $\frac{SS_E}{\sigma^2} \sim \chi_{n-k-1}^2$ and SS_E and SS_R are independent. Therefore, we compute

$$F_0 = \frac{\dfrac{SS_R}{k}}{\dfrac{SS_E}{n-k-1}} = \frac{MS_R}{MS_E} \tag{5.16}$$

and reject H_0 if $F_0 > F_{\alpha,k,n-k-1}$. Note that $MS_R = \frac{SS_R}{k}$ is regression mean square and $MS_E = \frac{SS_E}{n-k-1}$ is error mean square. The procedure is summarized in an analysis of variance table, Table 5-2.

Source of variation	Sum of squares	Degrees of freedom	Mean squares	F_0
Regression	SS_R	k	MS_R	$F_0 = \frac{MS_R}{MS_E}$
Error	SS_E	$n-k-1$	MS_E	
Total	S_{yy}	$n-1$		

Table 5-2 Analysis of variance for significance of regression

We frequently test hypotheses on the individual regression coefficients to determine the value of each of the regressor variables in the model.

The least square estimator $\hat{\boldsymbol{\beta}}$ is a random variable. Since $\hat{\boldsymbol{\beta}}$ is a linear combination of the observations y_j, the distribution of $\hat{\boldsymbol{\beta}}$ is

$$\hat{\boldsymbol{\beta}} \sim N\left(\boldsymbol{\beta}, \sigma^2\left(\mathbf{X}'\mathbf{X}\right)^{-1}\right).$$

The variance of the regression coefficients $\hat{\beta}_i$ is σ^2 times the $(i+1)$st diagonal element of $(\mathbf{X'X})^{-1}$, say V_{ii}. Therefore, each coefficient has the following distribution

$$\hat{\beta}_i \sim N\left(\beta_i, \sigma^2 V_{ii}\right).$$

The hypotheses for testing the significance of any individual coefficient are

$$\begin{aligned} H_0 &: \beta_i = 0 \\ H_1 &: \beta_i \neq 0 \end{aligned} \tag{5.17}$$

The appropriate test statistic is

$$t_0 = \frac{\hat{\beta}_i}{\sqrt{MS_E V_{ii}}} \tag{5.18}$$

and $H_0 : \beta_i = 0$ is rejected if $|t_0| > t_{\alpha/2, n-k-1}$.

6 Design of experiments

The *experiment* is a set of observations performed to discover something about a particular process of systems. A *designed experiment* is a test in which we make changes of the input variables of the process so that we may observe and identify the reasons for changes in the output response. We can visualize the process as a combination of machines, methods, people and other sources that transform some input to output. Some of the process variables $x_1, x_2, ..., x_p$ are controllable and other process variables $z_1, z_2, ..., z_q$ are uncontrollable. The objectives of the experiments are

- determining whether specific factor or factors have the influence on the response, y,
- determining the levels of factors to obtain the desired value of y.

Experimental design methods have found broad application in many disciplines. The experimental design is an important tool for improving the performance of a manufacturing process or for development of new processes. The objective in many cases may be develop a robust process, that is a process affected minimally by external sources of variability (the z's).

By the *statistical design of experiments*, we refer to the process of planning the experiment so that appropriate data will be collected, resulting in valid and objective conclusions. The statistical approach to experimental design is necessary if we wish to make meaningful conclusion from the data. When the problem involves data that are subject to experimental errors, statistical methodology is the only objective approach to analysis. Thus, there are two aspects to any experimental problem: the design of the experiment and the statistical analysis of the data.

The three basic principles of experimental design are replication, randomization and blocking. These principles are an important part of every experiment. By *replication* we mean a repetition of basic experiment. Replication has two important properties. It allows the experimenter to obtain an estimate of the experimental error and if the sample mean $\bar{y}$ is used to estimate the effect of the factor in experiment, then replication permits to obtain a more precise estimate of this effect.

By *randomization* we mean that the order in which the individual runs of the experiment are to be performed are randomly determined. Statistical methods require that the observations (or errors) are independently distributed random variables. Randomization usually makes this assumption valid.

Blocking is the arrangement of experimental units into groups (blocks) that are similar to one another. Blocking reduces known but irrelevant sources of variation between units and thus allows greater precision in the estimation of the source of variation under study.

6.1 Two-level factorial design

Many experiments involve the study of the effects of two or more factors. In general, *factorial designs* are most efficient for this type of experiment. By a factorial design we mean that in each complete trial or replication of the experiment all possible combinations of the levels of the factors are investigated. When the factors are arranged in a factorial design, they are often said to be *crossed*. The effect of a factor is defined as the change in response produced by the change in level of the factor. This is frequently called a *main effect* because it refers to the primary factors of interest in the experiment.

The most important case is that of k factors, each at only two levels. These levels may be quantitative, such as two values of pressures or temperature, or they may be qualitative, such as two operators or two machines. A complete replicate of such a design requires $2\times2\times...\times2=2^k$ observations and is called a 2^k factorial design. The 2^k design is particularly useful in the early stages of experimental work, when there are likely to be many factors to be investigated. Because there are only two levels for each factor, we must assume that the response is approximately linear over the range of the factor levels.

6.1.1 The 2^3 design

Design with three factors, e.g. A,B,C, each at two levels, is called 2^3 factorial design. The levels of the factors may be arbitrary called *low* and *high*. If every factor has exactly two levels we can make a linear transformation such that the low and high level is -1 and +1, respectively. These transformed variable are called coded variables and we denote coded variables x_1,x_2,x_3.

We denote the effect of a factor by a capital letter. Thus, A refers to the effect of a factor A, B refers to the effect of a factor B, C refers to the effect of a factor C, AB refers to the AB interaction, AC refers to the AC interaction, BC refers to the BC interaction and ABC refers to the ABC interaction.

The plan of the experiment can be tabulated as follows

Run	A	B	C	Average Response
1	-1	-1	-1	$\bar{y}_{(1)}$
2	+1	-1	-1	$\bar{y}_A$
3	-1	+1	-1	$\bar{y}_B$
4	+1	+1	-1	$\bar{y}_{AB}$
5	-1	-1	+1	$\bar{y}_C$
6	+1	-1	+1	$\bar{y}_{AC}$
7	-1	+1	+1	$\bar{y}_{BC}$
8	+1	+1	+1	$\bar{y}_{ABC}$

Table 6-1 Plan of experiment with coded levels

The average response is average of the total of all n observations taken at corresponding treatment combination point of plan. The index of average response denotes which factors are at the high level, (1) denotes that all factors are at low level.

Effects of factors can be obtained using Table 6-1. Simply multiply the average response by the appropriate column, row by row, and add and this grand total multiply by $\frac{1}{2^{k-1}}$, where k is a number of factors in experiment.

Thus, the effects of factors A, B, C are

$$A = \frac{1}{4}\left[-\overline{y}_{(1)} + \overline{y}_A - \overline{y}_B + \overline{y}_{AB} - \overline{y}_C + \overline{y}_{AC} - \overline{y}_{BC} + \overline{y}_{ABC}\right],$$

$$B = \frac{1}{4}\left[-\overline{y}_{(1)} - \overline{y}_A + \overline{y}_B + \overline{y}_{AB} - \overline{y}_C - \overline{y}_{AC} + \overline{y}_{BC} + \overline{y}_{ABC}\right],$$

and

$$C = \frac{1}{4}\left[-\overline{y}_{(1)} - \overline{y}_A - \overline{y}_B - \overline{y}_{AB} + \overline{y}_C - \overline{y}_{AC} + \overline{y}_{BC} + \overline{y}_{ABC}\right].$$

To obtain interaction of factors simply add columns to Table 6-1 and fill in appropriate values -1 or +1. For example, to fill in column of interaction AB just multiply columns A and B, row by row.

Run	A	B	C	AB	AC	BC	ABC	Average Response
1	-1	-1	-1	+1	+1	+1	-1	$\overline{y}_{(1)}$
2	+1	-1	-1	-1	-1	+1	+1	$\overline{y}_A$
3	-1	+1	-1	-1	+1	-1	+1	$\overline{y}_B$
4	+1	+1	-1	+1	-1	-1	-1	$\overline{y}_{AB}$
5	-1	-1	+1	+1	-1	-1	+1	$\overline{y}_C$
6	+1	-1	+1	-1	+1	-1	-1	$\overline{y}_{AC}$
7	-1	+1	+1	-1	-1	+1	-1	$\overline{y}_{BC}$
8	+1	+1	+1	+1	+1	+1	+1	$\overline{y}_{ABC}$

Table 6-2 Plan of experiment with coded levels, including interactions

Using Table 6-2 we can compute interactions AB, AC, BC, ABC, or

$$AB = \frac{1}{4}\left[\overline{y}_{(1)} - \overline{y}_A - \overline{y}_B + \overline{y}_{AB} + \overline{y}_C - \overline{y}_{AC} - \overline{y}_{BC} + \overline{y}_{ABC}\right],$$

$$AC = \frac{1}{4}\left[\overline{y}_{(1)} - \overline{y}_A + \overline{y}_B - \overline{y}_{AB} - \overline{y}_C + \overline{y}_{AC} - \overline{y}_{BC} + \overline{y}_{ABC}\right],$$

$$BC = \frac{1}{4}\left[\overline{y}_{(1)} + \overline{y}_A - \overline{y}_B - \overline{y}_{AB} - \overline{y}_C - \overline{y}_{AC} + \overline{y}_{BC} + \overline{y}_{ABC}\right],$$

and

$$ABC = \frac{1}{4}\left[-\overline{y}_{(1)} + \overline{y}_A + \overline{y}_B - \overline{y}_{AB} + \overline{y}_C - \overline{y}_{AC} - \overline{y}_{BC} + \overline{y}_{ABC}\right].$$

The average of the entire experiments is

$$\overline{y} = \frac{1}{8}\left[\overline{y}_{(1)} + \overline{y}_A + \overline{y}_B + \overline{y}_{AB} + \overline{y}_C + \overline{y}_{AC} + \overline{y}_{BC} + \overline{y}_{ABC}\right].$$

We use a regression model to predict the response for different combinations of process parameters at their best levels. The first step is to determine the regression coefficients. For factors at 2-levels, the estimators of regression coefficients are obtained by dividing the effects by 2. A regression model for factors at 2-levels is usually of the form

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \hat{\beta}_{12} x_1 x_2 + \hat{\beta}_{13} x_1 x_3 + \hat{\beta}_{23} x_2 x_3 + \hat{\beta}_{123} x_1 x_2 x_3 \qquad (6.1)$$

where $\hat{\beta}_1, ..., \hat{\beta}_{123}$ are the estimators of regression coefficients corresponding to appropriate effects and $\hat{\beta}_0$ is the average of the entire experiments. Model (6.1) is fitted regression model of

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3 + \epsilon, \qquad (6.2)$$

where ϵ are the errors which are normally, independently distributed random variables with mean 0 and variance σ^2. Further we denote estimators $\hat{\beta}_0, ..., \hat{\beta}_{123}$ as $b_0, ..., b_{123}$.

We can obtain these coefficients in easier way. The first step is rewrite plan of experiment into a matrix, this matrix is denoted $\mathbf{X}$ and also called plan of experiment, and add first column which contains only +1. In this case matrix $\mathbf{X}$ is

$$\mathbf{X} = \begin{bmatrix} +1 & -1 & -1 & -1 & +1 & +1 & +1 & -1 \\ +1 & +1 & -1 & -1 & -1 & -1 & +1 & +1 \\ +1 & -1 & +1 & -1 & -1 & +1 & -1 & +1 \\ +1 & +1 & +1 & -1 & +1 & -1 & -1 & -1 \\ +1 & -1 & -1 & +1 & +1 & -1 & -1 & +1 \\ +1 & +1 & -1 & +1 & -1 & +1 & -1 & -1 \\ +1 & -1 & +1 & +1 & -1 & -1 & +1 & -1 \\ +1 & +1 & +1 & +1 & +1 & +1 & +1 & +1 \end{bmatrix}$$

This plan of experiment $\mathbf{X}$ is orthogonal plan because every column is orthogonal to each other column, it means that the scalar product of the columns of $\mathbf{X}$ equals to zero. If we have the same number of replications for all treatment combinations we can obtain estimators of regression coefficients as

$$\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\, \mathbf{X}'\mathbf{y} \qquad (6.3)$$

where the vector $\mathbf{y} = \begin{bmatrix} \bar{y}_{(1)} \\ \bar{y}_A \\ \bar{y}_B \\ \bar{y}_{AB} \\ \bar{y}_C \\ \bar{y}_{AC} \\ \bar{y}_{BC} \\ \bar{y}_{ABC} \end{bmatrix}$ and the vector $b = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_{12} \\ b_3 \\ b_{13} \\ b_{23} \\ b_{123} \end{bmatrix}$.

Then a regression model for predict the response for different combinations of process parameters can be written as

$$\hat{\mathbf{y}} = \mathbf{Xb} \tag{6.4}$$

If the number of replications is not the same for all treatment combinations we can obtain the estimators of regression coefficients as

$$\mathbf{b} = \left(\mathbf{X}'\mathbf{P}\mathbf{X}\right)^{-1} \mathbf{X}'\mathbf{P}\mathbf{y} \tag{6.5}$$

where $\mathbf{P} = \begin{bmatrix} p_1 & 0 & \cdots & 0 \\ 0 & p_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & p_n \end{bmatrix}$, p_i is number of replications for ith treatment combination and n is number of treatment combinations.

6.1.2 Test of model adequacy

We have obtained a regression model. To know if the model is adequate to measured values it is necessary to perform the test of model adequacy. We may implement this test only if there are at least two replications of at least one treatment combination.

Suppose that we have n treatment combinations and p_i replications of ith treatment combination, $i = 1, 2, \ldots, n$. Total number of observation is $N = \sum_{i=1}^{n} p_i$, we denote each observation y_{ij}, $i = 1, 2, \ldots, n$, $j = 1, \ldots, p_i$. If there is at least one $p_i > 1$ then we can estimate the inaccuracy of measurement in terms of sample variance

$$s_e^2 = \frac{1}{N-n} \sum_{i=1}^{n} \sum_{j=1}^{p_i} \left(y_{ij} - \bar{y}_i\right)^2, \tag{6.6}$$

where $\bar{y}_i = \frac{1}{p_i} \sum_{j=1}^{p_i} y_{ij}$ is the average of observations at ith treatment combination. The sample variance

$$s_r^2 = \frac{1}{n-k-1} \sum_{i=1}^{n} \left(\bar{y}_i - \hat{y}_i\right)^2 \tag{6.7}$$

is the measure of difference between model and average values, where $\hat{y}_i$ is predict response for ith treatment combination and k is the number of factors of process. The test quantity is

$$F = \frac{s_r^2}{s_e^2} \tag{6.8}$$

and if $F \geq F\left(1-\alpha, n-k-1, N-n\right)$ then we reject the null hypothesis that the model is adequate. $F\left(1-\alpha, n-k-1, N-n\right)$ is quantile F-distribution with significance level of test α

and $u = n - k - 1$ and $v = N - n$ degrees of freedom. Quantities s_r^2 and s_e^2 are estimators of variance σ^2, thus we can consider these two variances to be two sample variances of one population. If we do not reject the null hypothesis, it means that there is no statistically significant difference between s_r^2 and s_e^2, then we can compute the weighted mean of variances

$$s^2 = \frac{(n-k-1)s_r^2 + (N-n)s_e^2}{(N-n)+(n-k-1)} = \frac{\sum_{i=1}^{n}\sum_{j=1}^{p_i}\left(y_{ij} - \bar{y}_i\right)^2 + \sum_{i=1}^{n} p_i\left(\bar{y}_i - \hat{y}_i\right)^2}{N-k-1} = \frac{\sum_{i=1}^{n}\sum_{j=1}^{p_i}\left(y_{ij} - \hat{y}_i\right)^2}{N-k-1} \tag{6.9}$$

6.1.3 Significance of coefficients

We have obtained coefficient b_i from the Equation (6.3) or Equation (6.5). Although coefficients b_i do not have to be equal to zero it does not mean that the coefficients b_i are statistically different from zero. It is possible to determine the significance of each coefficient by using the estimator of variance of coefficient. The estimator of variance of coefficient b_i is

$$D(b_i) = s^2 V_{jj}, \tag{6.10}$$

where V_{jj} is term of *j*th row and *j*th column of matrix $\mathbf{V} = \left(\mathbf{X'PX}\right)^{-1}$, where $j = i + 1$, and $s^2 = \frac{(n-k-1)s_r^2 + (N-n)s_e^2}{(N-n)+(n-k-1)}$ .The test quantity is

$$t = \frac{b_i}{\sqrt{D(b_i)}} \tag{6.11}$$

and if $|t| \geq t(1-\alpha/2, N-k-1)$ then we reject the null hypothesis that there is insignificant difference between the coefficient b_i and zero. $t(1-\alpha/2, N-k-1)$ is quantile *t*-distribution with significance level of test α and $N-k-1$ degrees of freedom. If the coefficient b_i is statistically different from zero then there is the significant influence of corresponding factor in opposite case the influence of factor has not been proven.

6.1.4 Centre points

If we want to repeat observations and keep the orthogonality of plan of experiment we can either repeat observation at all treatment combinations or make observations in centre point. The centre point is point in plan where all factors are set at their midpoint, $x_i = 0,\ i = 1, \ldots, k$. Such runs are called centre-point runs (or centre points), since they are, in a sense, in the centre of the design. In plan of experiment $\mathbf{X}$ will be next row with 1 at the first position and with zero at remaining positions.

7 Effectiveness of DOE

In this chapter we deal with question of influence of number of central points in the plan of experiment for finding the significant factor of the process. Also there is investigated the influence of number of factors in experiment.

We work with linear model of process and we assume no interaction between factors. There are investigated 5 models; linear model with 2, 3, 4, 5 and 6 factors

$$\eta = \beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k,\; k = 2,3,4,5,6. \tag{7.1}$$

These models are given and we want to simulate "real" observations by using Monte Carlo Method and then analyze the outcomes. We have two cases of experiment and in both cases we consider factors at two levels. In first case we have no centre points and we make two replications for every treatment combination, in second case we have only one replication for every treatment combination and the same number of replications in the centre point. It means that we have the same number of observations but we obtained them in different ways. Every experiment is repeated 5000-times for given parameter σ and we have approximately 60 values of this parameter, results and meaning of these simulations is described further.

7.1 Experiment with two replications for every treatment combination

7.1.1 Test of significance of coefficients without the test of model adequacy

We have five designs, design with 2, 3, 4, 5 and 6 factors. Thus we have design with k factors, each at two levels, it is 2^k factorial design, $k = 2,3,4,5,6$. We want to simulate experiment. Plan of experiment is the matrix $\mathbf{X}$ which contains all treatment combinations, these plans are orthogonal, e.g.

$$\mathbf{X} = \begin{bmatrix} +1 & -1 & -1 \\ +1 & +1 & -1 \\ +1 & -1 & +1 \\ +1 & +1 & +1 \end{bmatrix} \text{ if } k=2,\quad \mathbf{X} = \begin{bmatrix} +1 & -1 & -1 & -1 \\ +1 & +1 & -1 & -1 \\ +1 & -1 & +1 & -1 \\ +1 & +1 & +1 & -1 \\ +1 & -1 & -1 & +1 \\ +1 & +1 & -1 & +1 \\ +1 & -1 & +1 & +1 \\ +1 & +1 & +1 & +1 \end{bmatrix} \text{ if } k=3 \text{ and so on.}$$

There is written program in Matlab which presents the experiment and analysis of experiment. It is called `lmk_sc.m`, where $k = 2,3,4,5,6$. The procedure in these m-files is the same up to different number of factors, it means that there is different plan of experiment $\mathbf{X}$.

The input is the vector $\boldsymbol{\beta}$ of coefficients of $E\left(y|\mathbf{x}\right) = \eta = \beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k,\; k = 2,3,4,5,6$, where

$$y = \beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k + \epsilon,\; k = 2,3,4,5,6 \tag{7.2}$$

The $\boldsymbol{\epsilon}$ is the random error of process and random error components are normally distributed with $E(\boldsymbol{\epsilon})=0$ and $D(\boldsymbol{\epsilon})=\sigma^2$ and $\boldsymbol{\epsilon}$ are uncorrelated. Another input is standard deviation σ of this error. Thus we know expected value of response y and know the standard deviation of random error $\boldsymbol{\epsilon}$.

The procedure is that we compute the expected values for every treatment combination $\eta = \mathbf{Yv} = \mathbf{X} * \boldsymbol{\beta}$ and add the error component $\boldsymbol{\epsilon} \sim N(0,\sigma^2)$ which is generated by random generator in Matlab. By this adding we obtain random values of response y with $E(y|x)=\eta$ and $D(y)=\sigma^2$. We do this two times for every treatment combination then compute the average $\mathbf{Ypr}$ of observations for every treatment combination. The matrix $\mathbf{P}$, the $2^k \times 2^k$ matrix with number of replications for treatment combination on diagonal, is $\mathbf{P} = 2*\mathbf{I}$, where $\mathbf{I}$ is $2^k \times 2^k$ identity matrix. The estimators of coefficients $\boldsymbol{\beta}$ are

$$\mathbf{b} = (\mathbf{X'PX})^{-1} \mathbf{X'PYpr}. \tag{7.3}$$

We have to check if the coefficients b_i are statistically different from zero so we perform the test of significance of coefficients. To find the estimators of variance σ^2 we have to compute s_e^2 and s_r^2 by using Equation (6.6) and (6.7). In this case we suppose that the computed model is adequate, it means that there is no statistically significant difference between s_r^2 and s_e^2. Thus we can compute the weighted mean of variance

$$s^2 = \frac{(n-k-1)s_r^2 + (N-n)s_e^2}{N-k-1}, \tag{7.4}$$

where N is total number of observations, k is number of factors and n is number of points of plan. For this test it is necessary to compute matrix $\mathbf{V} = (\mathbf{X'PX})^{-1}$ which is used for calculation of estimator of variance of coefficients b_i, $D(b_i) = s^2 V_{jj}$, where $j = i+1$. The test quantity is

$$t = \frac{b_i}{\sqrt{D(b_i)}} \tag{7.5}$$

and if $|t| \geq t(1-\alpha/2, N-k-1)$, where $t(1-\alpha/2, N-k-1)$ is quantile *t*-distribution with significance level of test α and $N-k-1$ degrees of freedom, then we say that the coefficient b_i is statistically different from zero and we put $\mathbf{sc}(j)=1$, $j=1,...,k+1$. $\mathbf{sc}(j)$ is *j*th component of output vector $\mathbf{sc}$ and the size of $\mathbf{sc}$ is the same as the size of $\boldsymbol{\beta}$. If the coefficient b_i is not statistically different from zero we put $\mathbf{sc}(j)=0$. If the coefficient b_i is statistically different from zero then there is the significant influence of corresponding factor, in opposite case the influence of factor has not been proven.But in fact all coefficients are different from zero because we have input vector of coefficients of model (7.1) and this output vector $\mathbf{sc}$ just gives the information if the appropriate estimator of coefficient was marked as statistically different from zero or was not (the *i*th component corresponds to *i*th coefficient).

There are written another m-files `sign`*k*`_sc.m`, where $k = 2, 3, 4, 5, 6$ to get know how many times these coefficients was marked as statistically different from zero for given fixed σ. The output of this file is vector **significance**, its components are percentage expressions of events when the appropriate coefficient was marked as statistically different from zero. It means that this is a percentage expression of events when we say that there is the significant influence of corresponding factor.

M-file `graphs_sc.m` is written to determine the dependence of percentage expression of positive events on σ of random error ϵ. In fact we investigate the dependence on β_i/σ, where $i = 0, 1, ..., k$, and $k = 2, 3, 4, 5, 6$. The percentage expression of positive events for given β_i/σ is the quantity $P(|T| \geq t) \cdot 100\%$. T is a non-central t-distributed random variable with degrees of freedom $\mathrm{df} = N - k - 1$ (N is total number of observation and k is the number of factors of model) and non-centrality parameter $\delta = \beta_i / \left(\sigma\sqrt{V_{jj}}\right)$, where $j = i + 1$ (V_{jj} is the (j, j) element of matrix $\mathbf{V} = (\mathbf{X}'\mathbf{P}\mathbf{X})^{-1}$). The quantity $t = t(1 - \alpha/2, N - k - 1)$ is quantile *t*-distribution with significance level of test α and $N - k - 1$ degrees of freedom. The probability $P(|T| \geq t)$ is computed in Matlab as

$$P(|T| \geq t) = \mathrm{cdf}\left(\text{'Nct'}, -t, \mathrm{df}, \delta\right) + 1 - \mathrm{cdf}\left(\text{'Nct'}, t, \mathrm{df}, \delta\right), \tag{7.6}$$

where $\mathrm{cdf}(\text{'Nct'}, -t, \mathrm{df}, \delta)$ is a cumulative density function from $(-\infty)$ to $(-t)$ of non-central *t*-distribution with $\mathrm{df} = N - k - 1$ degrees of freedom and non-centrality parameter δ, similar for $\mathrm{cdf}(\text{'Nct'}, t, \mathrm{df}, \delta)$. Because of symmetry the non-central *t*-distributions with non-centrality parameters δ and $-\delta$ with respect to vertical axis we can transform the Equation (7.6) to

$$P(|T| \geq t) = 1 - \mathrm{cdf}\left(\text{'Nct'}, t, \mathrm{df}, -\delta\right) + 1 - \mathrm{cdf}\left(\text{'Nct'}, t, \mathrm{df}, \delta\right). \tag{7.7}$$

In this case we have same number of replications for all treatment combinations, it means that there is preserved the orthogonality of the plan of experiment, and there are no centre points therefore all elements on diagonal of the matrix $\mathbf{V}$ are the same, e.g.

$$\mathbf{V} = \begin{bmatrix} 0.1250 & 0 & 0 \\ 0 & 0.1250 & 0 \\ 0 & 0 & 0.1250 \end{bmatrix} \text{for } k = 2, \mathbf{V} = \begin{bmatrix} 0.0625 & 0 & 0 & 0 \\ 0 & 0.0625 & 0 & 0 \\ 0 & 0 & 0.0625 & 0 \\ 0 & 0 & 0 & 0.0625 \end{bmatrix} \text{for } k = 3.$$

Hence it is not necessary to investigate the dependence of percentage expression for each coefficient of model. It is enough to investigate just the first one.

In Figure 7-1 there is the dependence of percentage expression of positive events on β_i/σ, where $i = 0, 1, ..., k$, and $k = 2, 3, 4, 5, 6$. The values of curves are from Equation (7.7) (we change the σ and df, quantil t is the same for given number of factors k) and corresponding points are the output values of `sign`*k*`_sc.m`, where $k = 2, 3, 4, 5, 6$. It is possible to see that the empirical results of experiments which is simulated in `lm`*k*`_sc.m` and repeated in `sign`*k*`_sc.m`, where $k = 2, 3, 4, 5, 6$, fit the appropriate curve. In Figure 7-1 the red represents the experiment with $k=2$ factors, the green represents the experiment with $k=3$ factors, the blue represents the experiment with $k=4$ factors, the magenta represents the experiment with $k=5$ factors and the cyan represents the experiment with $k=6$ factors.

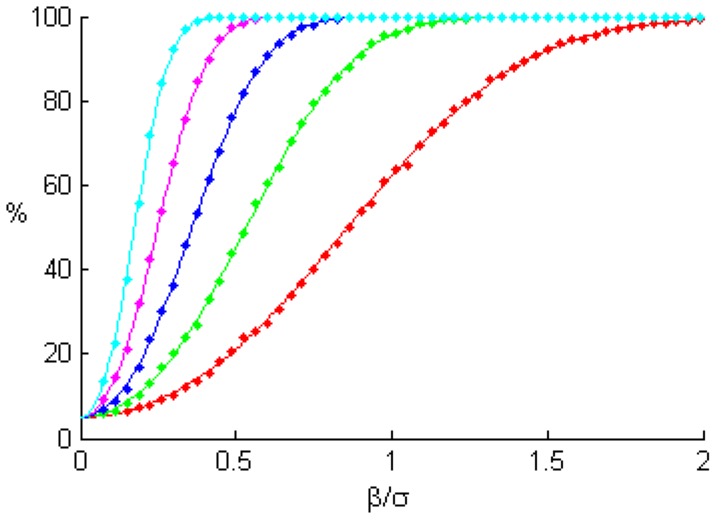

Figure 7-1 Graphic representation of positive determination of significance of factor, experiments with two replications for every treatment combination, test of significance of coefficients without test of model adequacy, $\alpha = 0.05$

In Table 7-1 there are values of percentage expression of positive events for some ratios β_i/σ, where $i = 0,1,\ldots,k$. We see that there are considerable differences between experiments with different number of factors. It is produced by different total number of observations, e.g. we have $N=16$ if $k=2$ and $N=64$ if $k=5$. Therefore our conclusions are more reliable if we have larger number of observations (it means that we have more information about process).

$\frac{\beta_i}{\sigma}$	Number of factors				
	2	3	4	5	6
0.1	5.63%	6.57%	8.48%	12.34%	20.22%
0.2	7.52%	11.43%	19.37%	34.98%	61.21%
0.3	10.73%	19.75%	37.34%	65.55%	92.03%
0.5	21.14%	45.22%	77.84%	97.58%	99.99%
0.8	44.85%	83.54%	99.18%	100%	100%
1.0	62.28%	95.58%	99.98%	100%	100%
1.5	91.86%	99.98%	100%	100%	100%
2.0	99.29%	100%	100%	100%	100%

Table 7-1 Chosen information from Figure 7-1

Figure 7-1 and therefore also Table 7-1 are for case $\alpha=0.05$. Results for case $\alpha=0.01$ are in Appendix I.

7.1.2 Test of significance of coefficients with the test of model adequacy

The experiments are the same as in Chapter 7.1.1 but the analysis is little bit different. The experiments and their analysis are in m-files `lmk_ta_sc.m`, where $k = 2,3,4,5,6$. We simulate the experiment, two replications for every treatment combination, and then compute the estimators of coefficients $\boldsymbol{\beta}$, i.e. $\mathbf{b}$ by using Equation (7.3).

Before we start to test the significance of estimators **b** we make the test of adequacy of model

$$\hat{y} = b_0 + b_1 x_1 + ... + b_k x_k, k = 2,3,4,5,6. \quad (7.8)$$

We have to compute two estimators of variance σ^2,

$$s_e^2 = \frac{1}{N-n} \sum_{i=1}^{n} \sum_{j=1}^{p_i} \left(y_{ij} - \bar{y}_j \right)^2 \quad (7.9)$$

and

$$s_r^2 = \frac{1}{n-k-1} \sum_{i=1}^{n} \left(\bar{y}_i - \hat{y}_i \right)^2 \quad (7.10)$$

The test quantity is the ratio

$$F = \frac{s_r^2}{s_e^2} \quad (7.11)$$

and if $F \geq F\left(1-\alpha, n-k-1, N-n\right)$, where N is total number of observations, k is number of factors and n is number of points of plan, then we reject the null hypothesis that the model is adequate. $F\left(1-\alpha, n-k-1, N-n\right)$ is quantile F-distribution with significance level of test α and $u = n-k-1$ and $v = N-n$ degrees of freedom. If we say that the model is adequate then we test the significance of coefficients in the same way as in the previous Chapter 7.1.1. But if we say that the model is not adequate then we put the output vector **significance** directly equal to the zero vector. We repeat this experiment in m-files `signk_ma_sc.m`, where $k = 2,3,4,5,6$. To know how the percentage expression of positive events depends on ratio β_i/σ there is written m-file `graphs_sc.m`. In Figure 7-2 there are curves which predict the values if we suppose that the model is always adequate (it is the case of Chapter 7.1.1) and the points are computed values if we make the test of model adequacy.

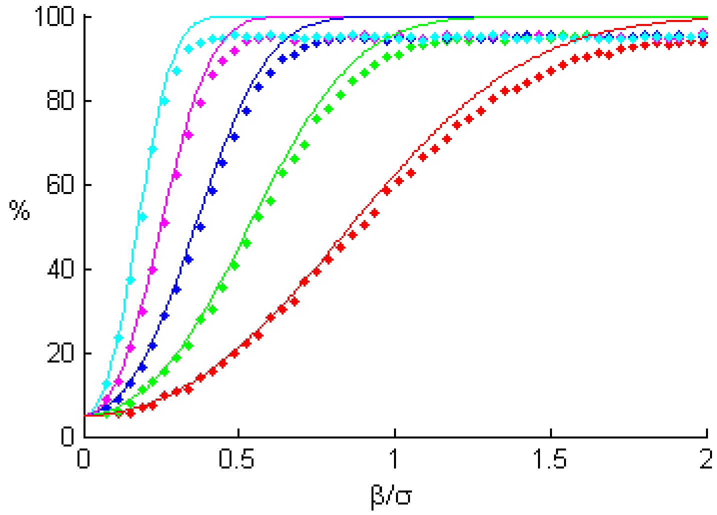

Figure 7-2 Graphic representation of positive determination of significance of factor, experiments with two replications for every treatment combination, test of significance of coefficients with the test of model adequacy, $\alpha = 0.05$

Colour representation is the same as in Figure 7-1. We see that the computed values are slightly lower than the values of the curve. In this case the values do not go to 100% as before but just to 95%. It is caused by the F-test and the chosen $\alpha = 0.05$. If we choose the $\alpha = 0.01$ the values would go to 99%.

Following Table 7-2 shows approximate values from Figure 7-2 for some ratios β_i/σ.

$\frac{\beta_i}{\sigma}$	Number of factors				
	2	3	4	5	6
0.1	5.34%	6.15%	8.17%	11.37%	19.23%
0.2	7.29%	10.32%	18.62%	33.17%	58.51%
0.3	10.27%	18.53%	34.74%	62.26%	88.03%
0.5	19.73%	42.55%	74.07%	92.58%	95.00%
0.8	42.53%	79.51%	94.10%	95%	95%
1.0	59.26%	90.48%	94.91%	95%	95%
1.5	87.19%	94.86%	95%	95%	95%
2.0	94.35%	95%	95%	95%	95%

Table 7-2 Approximated value of percentage expression if we make the test of model adequacy

Figure 7-2 and therefore also Table 7-2 are for case $\alpha = 0.05$. Results for case $\alpha = 0.01$ are in Appendix II.

7.2 Experiment with just one replication for every treatment combination and same number of replications in centre point

7.2.1 Test of significance of coefficients without the test of the model adequacy

We have again five designs, design with 2, 3, 4, 5 and 6 factors. We want to simulate experiment with just one replication at every treatment combination and the same number of replications in centre point, thus we have the same number of observation for experiments with the same numbers of factors. Plan of experiment is the matrix $\mathbf{X}$ which contains all treatment combinations and centre point, these plans are orthogonal too, e.g.

$$\mathbf{X} = \begin{bmatrix} +1 & -1 & -1 \\ +1 & -1 & +1 \\ +1 & +1 & -1 \\ +1 & +1 & +1 \\ +1 & 0 & 0 \end{bmatrix} \text{ if } k = 2, \quad \mathbf{X} = \begin{bmatrix} +1 & -1 & -1 & -1 \\ +1 & +1 & -1 & -1 \\ +1 & -1 & +1 & -1 \\ +1 & +1 & +1 & -1 \\ +1 & -1 & -1 & +1 \\ +1 & +1 & -1 & +1 \\ +1 & -1 & +1 & +1 \\ +1 & +1 & +1 & +1 \\ +1 & 0 & 0 & 0 \end{bmatrix} \text{ if } k = 3 \text{ and so on.}$$

In this case the number of points of plan is $n = 2^k + 1$. There is written program in Matlab which presents the experiment and analysis of this experiment. It is called `lm`*k*`_cp_sc.m`, where $k = 2,3,4,5,6$.

One of the inputs is the vector $\boldsymbol{\beta}$ which contains the coefficients of model (7.2) and the second output is the standard deviation σ of normal distributed random error of process ϵ. As before random error components are normally distributed with $E(\epsilon)=0$ and $D(\epsilon)=\sigma^2$ and ϵ are uncorrelated.

We compute the expected values for every treatment combination $\eta = \mathbf{Yv} = \mathbf{X}*\boldsymbol{\beta}$ and add the random error component $\epsilon \sim N\left(0,\sigma^2\right)$ which is generated by random generator in Matlab. We do this just once for every treatment combination and 2^k for the centre point, where $k = 2,3,4,5,6$. We put these quantities into a matrix with 2^k+1 rows and $p = \max\limits_{i=1,..,n} p_i$ columns, in our case $p = 2^k$. It means that no all components in the matrix have to represent the observations, e.g. for *i*th row just *1*st till p_ith components represent the observations and remaining components of the row are quantities which we do not care about, it can be $0,1$ or whatever else.

Then compute the average $\mathbf{Ypr}$ of observations for every treatment combination. The matrix $\mathbf{P}$, the $\left(2^k+1\right)\times\left(2^k+1\right)$ matrix with number of replications for treatment combination on diagonal, has all components on diagonal equal to 1 except the last one, $\mathbf{P}\left(2^k+1,2^k+1\right)=2^k$. Then we compute the estimators of coefficients $\boldsymbol{\beta}$ using the Equation (7.3) and then we check if the coefficients b_i are statistically significant.

In this case we again suppose that the computed model is adequate, it means that there is no statistically significant difference between s_r^2 and s_e^2. Thus we can compute the weighted mean of variance s^2 using equation (7.4), We have to also compute matrix $\mathbf{V} = \left(\mathbf{X'PX}\right)^{-1}$ for calculation of estimator of variance of coefficients b_i, $D\left(b_i\right) = s^2 V_{jj}$, where $j = i+1$.

The test quantity is

$$t = \frac{b_i}{\sqrt{D\left(b_i\right)}} \tag{7.12}$$

and if $|t| \geq t\left(1-\alpha/2, N-k-1\right)$, where $t\left(1-\alpha/2, N-k-1\right)$ is quantile *t*-distribution with significance level of test α and $N-k-1$ degrees of freedom, then we say that the coefficient b_i is statistically significant and we put $\mathbf{sc}(j)=1$, $j=1,...,k+1$ it is *i*th component of output vector $\mathbf{sc}$.

As before we have all coefficients different from zero because we have input vector of coefficients of model (7.1) and this output vector $\mathbf{sc}$ just gives the information if the appropriate estimator of coefficient was marked as statistically different from zero or was not (the *i*th component corresponds to *i*th coefficient).

M-files `signk_cp_sc.m`, where $k = 2,3,4,5,6$, are written to get know how many times these coefficients was marked as statistically different from zero for given fixed σ. Components of output vector **significance** are percentage expression of events when the appropriate coefficient was marked as statistically different from zero, i.e. percentage expression of events when we say that the corresponding factor has significant influence.

For determination the dependence of percentage expression of positive events on the ratio β_i/σ there is written m-file `graphs_cp_sc.m`. The percentage expression of positive events for given β_i/σ is the quantity $P(|T| \geq t) \cdot 100\%$, where $P(|T| \geq t)$ is the probability that a non-central t-distributed random variable T that can get the values which absolute value is greater or equal than quantil $t = t(1-\alpha/2, N-k-1)$ of *t*-distribution. The quantity $P(|T| \geq t)$ is computed in Matlab using the Equation (7.7).

In this case we do not have the same number of replications for all treatment combinations but the orthogonality of the plan of experiments is still preserved because the difference is in the centre point, therefore matrix $\mathbf{V}$ is still diagonal. But the components are not all the same, e.g.

$$\mathbf{V} = \begin{bmatrix} 0.1250 & 0 & 0 \\ 0 & 0.2500 & 0 \\ 0 & 0 & 0.2500 \end{bmatrix} \text{for } k=2, \mathbf{V} = \begin{bmatrix} 0.0625 & 0 & 0 & 0 \\ 0 & 0.1250 & 0 & 0 \\ 0 & 0 & 0.1250 & 0 \\ 0 & 0 & 0 & 0.1250 \end{bmatrix} \text{for } k=3.$$

It is not necessary to investigate the dependence of percentage expression for each coefficient of model because components of $\mathbf{V}$ is same for coefficients b_i, $i = 1,\ldots,k$, and only one difference is in b_0. Thus it is enough to investigate the dependence just for two coefficients. In Figure 7-3 there is the dependence of percentage expression of positive events on β_0/σ and in Figure 7-4 is the dependence of percentage expression of positive events on β_i/σ, where $i = 1,\ldots,k$, and $k = 2,3,4,5,6$.

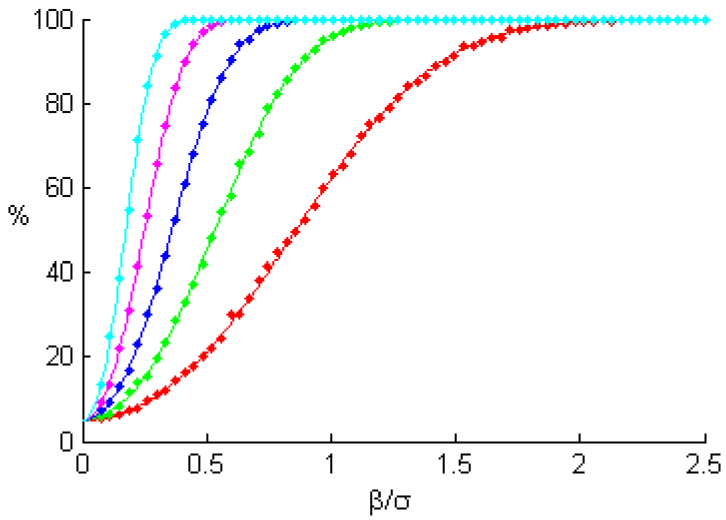

Figure 7-3 Graphic representation of positive determination of significance of factor for coefficient b_0, experiments with one replication for every treatment combination and same number of replications in centre point, test of significance of coefficients without test of model adequacy, $\alpha = 0.05$

The values of curves are from Equation (7.7) (we change the σ and df, quantil t is the same for given number of factors k) and corresponding points are the output values of `signk_cp_sc.m`, where $k = 2,3,4,5,6$. The representations of colours in figure 7-3 and Figure 7-4 there are the same as in Figure 7-1.

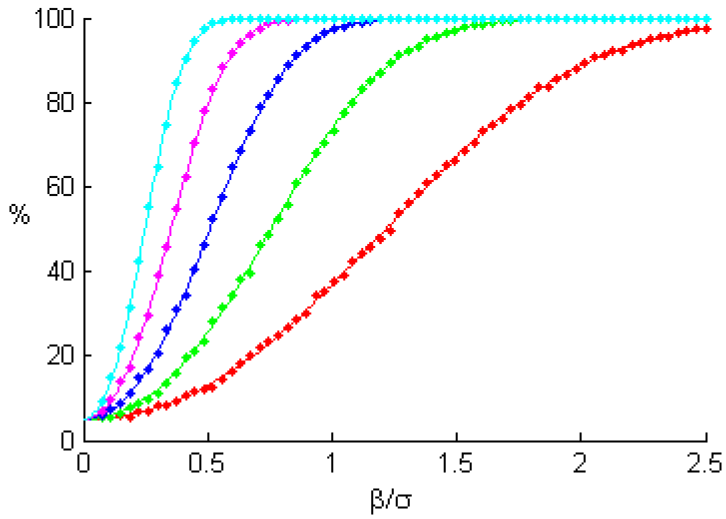

Figure 7-4 Graphic representation of positive determination of significance of factor for coefficient b_i, where $i = 1,...,k$, experiments with one replication for every treatment combination and same number of replications in centre point, test of significance of coefficients without test of model adequacy, $\alpha = 0.05$

Table for β_0/σ would be the same as the Table 7-1 because of the same first element on diagonal of matrix $\mathbf{V}$ and the same number of degrees of freedom $N-k-1$.

In Table 7-3 there are values of percentage expression of positive events for some ratios β_i/σ, where $i = 1,...,k$.

$\frac{\beta_i}{\sigma}$	Number of factors				
	2	3	4	5	6
0.1	5.31%	5,78%	6.72%	8.61%	12.47%
0.2	6.25%	8.17%	12.05%	19.95%	35.49%
0.3	7.84%	12.25%	21.21%	38.57%	66.31%
0.5	13.00%	25.60%	48.76%	79.43%	97.77%
0.8	25.66%	54.79%	86.96%	99.36%	100%
1.0	2682%	73.80%	97.09%	99.98%	100%
1.5	67.22%	97.28%	99.99%	100%	100%
2.0	88.73%	99.93%	100%	100%	100%

Table 7-3 Chosen information from Figure 7-4

Figure 7-3, Figure 7-4 and also Table 7-3 are for case $\alpha = 0.05$. Results for case $\alpha = 0.01$ are in Appendix III.

7.2.2 Test of significance of coefficients with test of model adequacy

The experiments are the same as in Chapter 7.2.1 but the analysis is different. The experiments and their analysis are in m-files `lmk_cp_ta_sc.m`, where $k = 2,3,4,5,6$. We simulate the experiment, one replication for every treatment combination and the same number of replication in centre point, and then compute the estimators of coefficients $\boldsymbol{\beta}$, i.e. $\mathbf{b}$ by using Equation (7.3). Before we start to test the significance of these estimators $\mathbf{b}$ we make the test of adequacy of model (7.8). We again compute the estimators of variance σ^2 of error ϵ, s_e^2 and s_r^2 by using Equations (7.9) and (7.10) respectively.

The test quantity is the ratio

$$F = \frac{s_r^2}{s_e^2} \tag{7.13}$$

and if $F \geq F\left(1-\alpha, n-k-1, N-n\right)$, where N is total number of observations, k is number of factors and n is number of points of plan, then we reject the null hypothesis that the model is adequate. $F\left(1-\alpha, n-k-1, N-n\right)$ is quantile F-distribution.

If the model is adequate then we test the significance of coefficients as in the previous Chapter 7.2.1. But if the model is not adequate then we put the output vector **significance** directly equal the zero vector. We repeat this experiment in m-files `signk_cp_ma_sc.m`, where $k = 2,3,4,5,6$. To know how the percentage expression of positive events depends on ratio β_i/σ there is written m-file `graphs_cp_sc.m`. Matrix $\mathbf{V}$ is the same as in Chapter 7.2.1 because the plan is the same the only thing which is different is the analysis. Thus we investigate the dependence for two cases, for b_0/σ and for b_i/σ, where $i = 1,\ldots,k$, k is the number of factors. In Figure 7-5 and Figure 7-6 are curves which predict the values if we suppose that the model is always adequate (it is the case of Chapter 7.2.1) and points are computed values if we make the test of model adequacy.

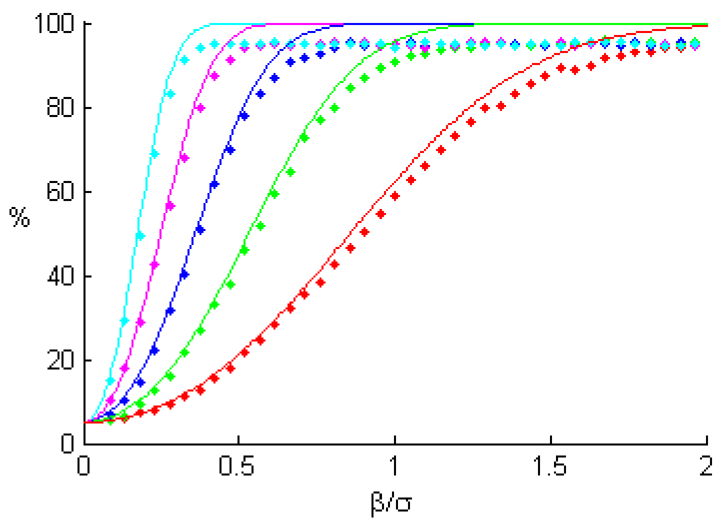

Figure 7-5 Graphic representation of positive determination of significance of factor for coefficient b_0, experiments with one replication for every treatment combination and same number of replications in centre point, test of significance of coefficients with test of model adequacy, $\alpha = 0.05$

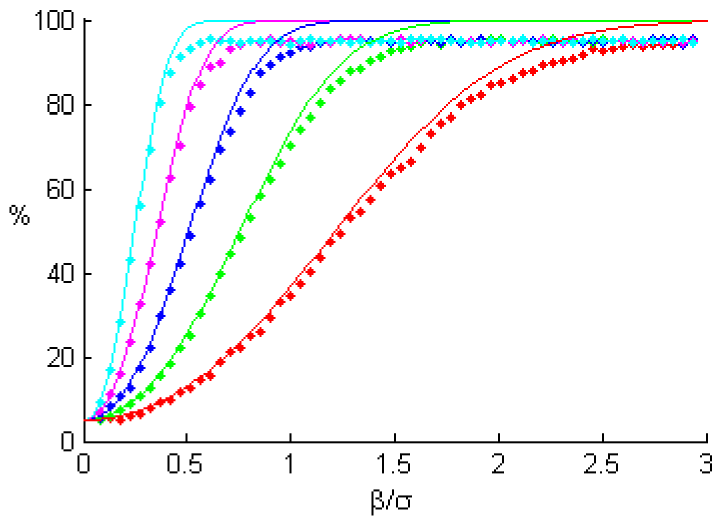

Figure 7-6 Graphic representation of positive determination of significance of factor for coefficient b_i, where $i = 1,...,k$, experiments with one replication for every treatment combination and same number of replications in centre point, test of significance of coefficients with test of model adequacy, $\alpha = 0.05$

The representations of colours in figure 7-5 and Figure 7-6 are the same as in Figure 7-1. Table for β_0/σ would be the same as the Table 7-2 because of the same first element on diagonal of matrix $\mathbf{V}$ and the same number of degrees of freedom $N-k-1$.

Table 7-4 shows approximate values from Figure 7-2 of percentage expression of positive events for some ratios β_i/σ, where $i = 1,...,k$.

$\frac{\beta_i}{\sigma}$	Number of factors 2	3	4	5	6
0.1	5.30%	5.74%	6.53%	8.17%	11.96%
0.2	6.03%	7.51%	11.27%	19.45%	33.48%
0.3	7.69%	11.47%	20.21%	35.91%	62.34%
0.5	12.01%	24.34%	46.32%	75.67%	92.81%
0.8	24.17%	51.70%	82.80%	94.47%	94.93%
1.0	34.67%	70.27%	92.32%	94.83%	95%
1.5	63.78%	92.33%	95%	95%	95%
2.0	84.05%	94.98%	95%	95%	95%

Table 7-4 Approximated value of percentage expression if we make the test of model adequacy

Figure 7-5, Figure 7-6 and also Table 7-4 are for case $\alpha = 0.05$. Results for case $\alpha = 0.01$ are in Appendix IV.

7.3 Comparison of experiments

7.3.1 Test of significance of coefficients without the test of the model adequacy

We conducted two types of experiments which had for given number of factors k the same number of observations but they were obtained in different way. First case is experiment with two replications for every treatment combination with no centre point, Experiment A, and the second case is experiment with just one replication for every treatment combination and the same number of replications in centre point, Experiment B.

Now we want to compare the dependence of percentage expression of positive events on ratio β_i/σ, where $i = 0,1,...,k$, and $k = 2,3,4,5,6$ if we suppose that the model is adequate and make no test of model adequacy. We have to distinguish two cases of ratios, β_0/σ and β_i/σ, where $i = 1,...,k$, because for the first ratio there is not the same dependence as for the others ratios for both cases of experiments.

In Figure 7-7 is comparison of dependence of percentage expression of positive events on ratio β_0/σ. The corresponding curves coincide. It is caused by the same first component on diagonal of matrix $\mathbf{V}$, the same number of degrees of freedom $\mathrm{df} = N-k-1$ and the same quantity $t = t(1-\alpha/2, N-k-1)$ for both experiments for given number of factors k. Therefore computed values of dependence of percentage expression approximately fit the same curve.

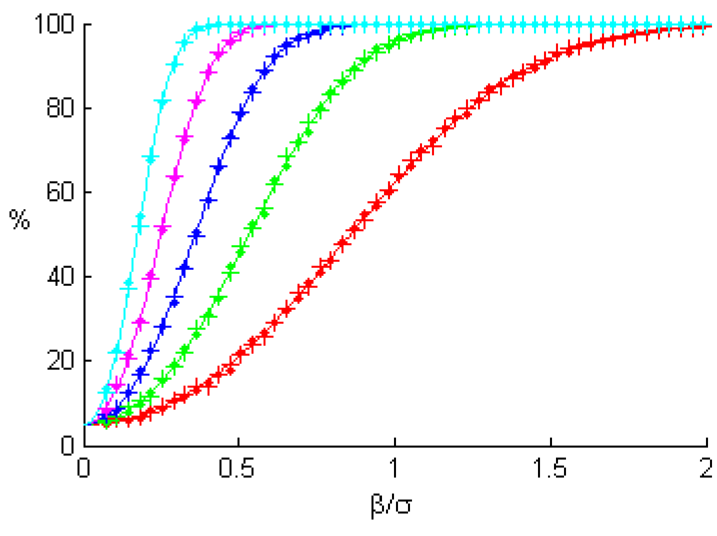

Figure 7-7 Comparison of graphic representation of positive determination of significance of factor for coefficient b_0 of Experiment A and Experiment B, test of significance of coefficients without the test of model adequacy, $\alpha = 0.05$

Table of values from Figure 7-7 is same as the Table 7-1 in Chapter 7.1.1. Representations of colours in figure 7-7 and Figure 7-8 are the same as in Figure 7-1.

In Figure 7-8 there is comparison of dependence of percentage expression of positive events on ratio β_i/σ, where $i = 1,...,k$. Now there are differences between corresponding curves. It is caused by the different components on diagonal of matrix $\mathbf{V}$, although there is the same number of degrees of freedom $\text{df} = N - k - 1$ and the same quantity $t = t(1-\alpha/2, N-k-1)$ for both experiments for given number of factors k. Points and their curves represent the results for Experiment A and crosses and their curves represent the results for Experiment B for given number of factors.

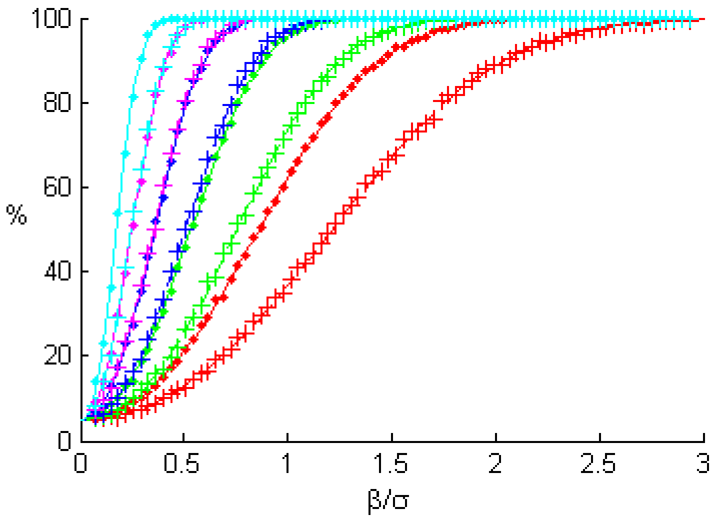

Figure 7-8 Comparison of graphic representation of positive determination of significance of factor for coefficients b_i, where $i = 1, \dots, k$, of Experiment A and Experiment B, test of significance of coefficients without the test of model adequacy, $\alpha = 0.05$

In Table 7-5 there are compared values of percentage expression of positive events for some β_i/σ, where $i = 1, \dots, k$ for Experiment A and experiment B from Figure 7-8.

$\frac{\beta_i}{\sigma}$	Number of factors									
	2		3		4		5		6	
	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B
0.1	5.63%	5.31%	6.57%	5.78%	8.48%	6.72%	12.34%	8.61%	20.22%	12.47%
0.2	7.52%	6.25%	11.43%	8.17%	19.37%	12.05%	34.98%	19.95%	61.21%	35.49%
0.3	10.73%	7.84%	19.75%	12.25%	37.34%	21.21%	65.55%	38.57%	92.03%	66.31%
0.5	21.14%	13.00%	45.22%	25.60%	77.84%	48.76%	97.58%	79.43%	99.99%	97.77%
0.8	44.85%	25.66%	83.54%	54.79%	99.18%	86.96%	100%	99.36%	100%	100%
1.0	62.28%	26.82%	95.58%	73.80%	99.98%	97.09%	100%	99.98%	100%	100%
1.5	91.86%	67.22%	99.98%	97.28%	100%	99.99%	100%	100%	100%	100%
2.0	99.29%	88.73%	100%	99.93%	100%	100%	100%	100%	100%	100%

Table 7-5 Comparison of values of percentage expression of positive events for some value of ratios β_i/σ, where $i = 1, \dots, k$, for Experiment A and Experiment B

Figure 7-7, Figure 7-8 and also Table 7-5 are for case $\alpha = 0.05$. Results for case $\alpha = 0.01$ are in Appendix V.

7.3.2 Test of significance of coefficients with the test of the model adequacy

We again conducted two types of experiments which had for given number of factors k the same number of observations but they were obtained in different way, Experiment A and Experiment B.

Now we want to compare the dependence of percentage expression of positive events on ratio β_i/σ, where $i = 0,1,...,k$, and $k = 2,3,4,5,6$ if we make the test of model adequacy. We again have to distinguish two cases of ratios, β_0/σ and β_i/σ, where $i = 1,...,k$.

In Figure 7-9 there is comparison of dependence of percentage expression of positive events on ratio β_0/σ. The corresponding curves again coincide and therefore computed values of dependence of percentage expression approximately have the same behaviour. Computed values are a bit lower than the predicted curves, it is caused by the test of model adequacy. Curves describe the behaviour if we suppose that the model is adequate and make no test of model adequacy.

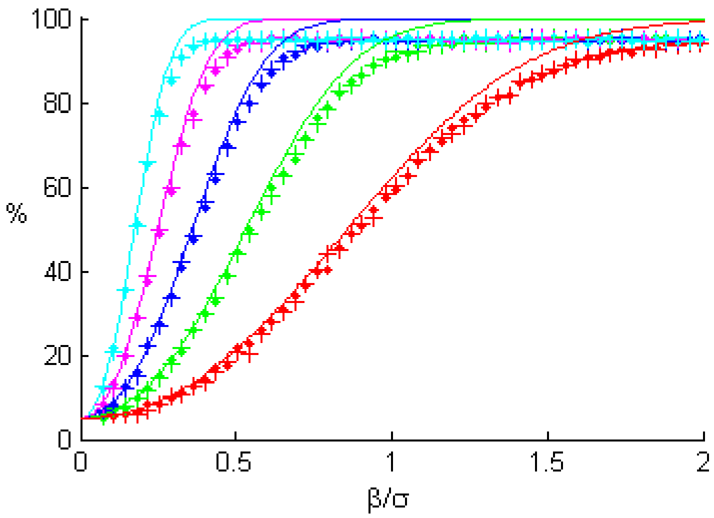

Figure 7-9 Comparison of graphic representation of positive determination of significance of factor for coefficient b_0 of Experiment A and Experiment B, test of significance of coefficients with test of model adequacy, $\alpha = 0.05$

Table of values from Figure 7-9 is same as Table 7-2 in Chapter 7.1.2. Representations of colours in Figure 7-9 and Figure 7-10 are the same as in Figure 7-1.

In Figure 7-10 there is comparison of dependence of percentage expression of positive events on ratio β_i/σ, where $i = 1,...,k$. There are again differences between corresponding curves. Points and their curves represent the results for Experiment A and crosses and their curves represent the results for Experiment B for given number of factors.

It is possible to see, that the experiment A gives better values of percentage expression of positive events than Experiment B, it means that for given number of factors and given number of observation it is better if we choose the Experiment A.

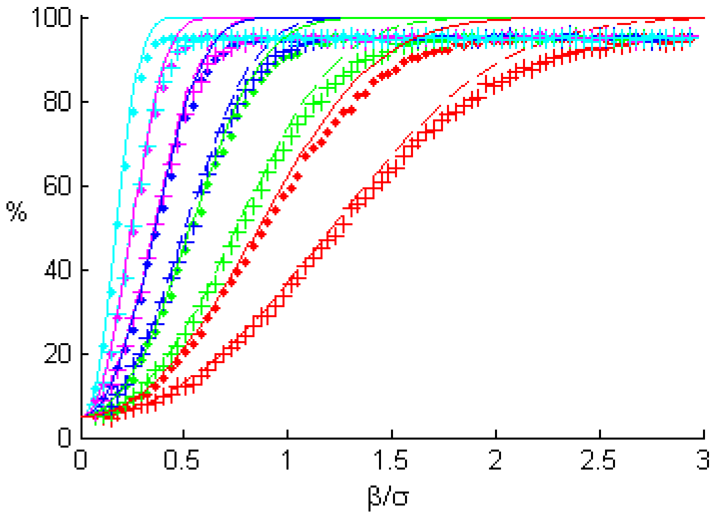

Figure 7-10 Comparison of graphic representation of positive determination of significance of factor for coefficients b_i, where $i = 1,...,k$, of Experiment A and Experiment B, test of significance of coefficients without the test of model adequacy, $\alpha = 0.05$

In Table 7-6 there are compared approximated values of percentage expression of positive events for some β_i/σ, where $i = 1,...,k$ for Experiment A and experiment B from Figure 7-10.

$\frac{\beta_i}{\sigma}$	Number of factors									
	2		3		4		5		6	
	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B
0.1	5.34%	5.30%	6.15%	5.74%	8.17%	6.53%	11.37%	8.17%	19.23%	11.96%
0.2	7.29%	6.03%	10.32%	7.51%	18.62%	11.27%	33.17%	19.45%	58.51%	33.48%
0.3	10.27%	7.69%	18.53%	11.47%	34.74%	20.21%	62.26%	35.91%	88.03%	62.34%
0.5	19.73%	12.01%	42.55%	24.34%	74.07%	46.32%	92.58%	75.67%	95%	92.81%
0.8	42.53%	24.17%	79.51%	51.70%	94.10%	82.80%	95%	94.47%	95%	94.93%
1.0	59.26%	34.67%	90.48%	70.27%	94.91%	92.32%	95%	94.83%	95%	95%
1.5	87.19%	63.78%	94.86%	92.33%	95%	95%	95%	95%	95%	95%
2.0	94.35%	84.05%	95%	94.98%	95%	95%	95%	95%	95%	95%

Table 7-6 Comparison of approximated values of percentage expression of positive events for some value of ratios β_i/σ, where $i = 1,...,k$, for Experiment A and Experiment B

Figure 7-9, Figure 7-10 and also Table 7-6 are for case $\alpha = 0.05$. Results for case $\alpha = 0.01$ are in Appendix VI.

7.4 Change of number of centre points

7.4.1 Test of significance of coefficients without the test of the model adequacy

Now we want to see if there are significance differences if we change the number of centre points in Experiment B. We choose only one number of factors $k=5$ and investigate differences for this one. If we have 5 factors it means that we make $2^5 = 32$ observations in centre point. We make replications to determine the model adequacy, because we can compute the estimator of variance σ^2 of random error ϵ, s_e^2, only if we have duplicate observations. To preserve the orthogonality of plan of experiment we can duplicate observations for all treatment combinations, it is Experiment A, or we can make some observations in centre point. In Experiment B the number of replications in centre point is such that the total number of observations is the same as in Experiment A for given number of factors.

The question is how many observations in centre point we actually need?

Therefore we make the Experiment B and decrease the number of replications in the centre point. There are written m-files `lm5_jcp_sc.m`, where $j = 4,8,12,16,20,24,28,32$ denotes the number of replications in centre point. The procedure is the same as in Chapter $7.2.1$, the difference is in the total number of observations and therefore degrees of freedom $N-k-1$ are different. The first element on the diagonal of matrix $\mathbf{V} = (\mathbf{X'PX})^{-1}$ is also different because matrix $\mathbf{P}$ is little bit transformed with every change of replications in centre point. In this case we suppose again that the computed model is adequate.

Experiments are repeated in `sign5_jcp_sc.m`, where $j = 4,8,12,16,20,24,28,32$ and the dependence of the percentage expression of positive events on β_i/σ is investigate in m-file `graphs_cp_sc.m`.

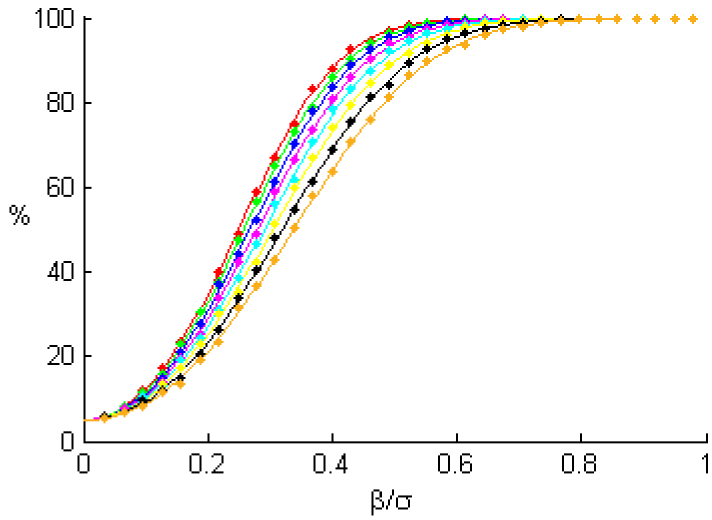

Figure 7-11 Comparison of graphic representation of positive determination of significance of factor for coefficients b_0 for experiment with 5 factors with different number of replications in the centre point, test of significance of coefficients without the test of model adequacy, $\alpha = 0.05$

In Figure 7-11 there are shown the differences for β_0/σ of percentage expression of positive events for experiment with 5 factors and the red represents the experiment with nomber of replications in centre point $j=32$, the green is for $j=28$, the blue for $j=24$, the magenta for $j=20$, the cyan for $j=16$, the yellow for $j=12$, the black for $j=8$ and the orange is for $j=4$.

In following Table 7-7 there are value of percentage expression of positive events for some β_0/σ.

$\frac{\beta_0}{\sigma}$	Number of centre points							
	4	8	12	16	20	24	28	32
0.1	8.95%	9.43%	9.91%	10.40%	10.88%	11.36%	11.85%	12.34%
0.2	21.33%	23.32%	25.30%	27.27%	29.23%	31.17%	33.08%	34.98%
0.3	41.40%	45.38%	49.19%	52.83%	56.28%	59.55%	62.64%	65.55%
0.4	64.16%	69.07%	73.43%	77.26%	80.61%	83.53%	86.06%	88.23%
0.5	82.71%	86.69%	89.83%	92.28%	94.17%	95.63%	96.74%	97.58%
0.6	93.61%	95,78%	97.24%	98.21%	98.85%	99.27%	99.54%	99.71%
0.8	99.63%	99.84%	99.93%	99.97%	99.99%	100%	100%	100%
1.0	99.99%	100%	100%	100%	100%	100%	100%	100%

Table 7-7 Comparison of approximated values of percentage expression of positive events for some value of ratios β_0/σ for experiment with 5 factors with different number of replications in the centre point

In Figure 7-12 there are shown the differences for β_i/σ, $i=1,\ldots,5$ of percentage expression of positive events for experiment with 5 factors. Representations of colours are the same as in Figure 7-11.

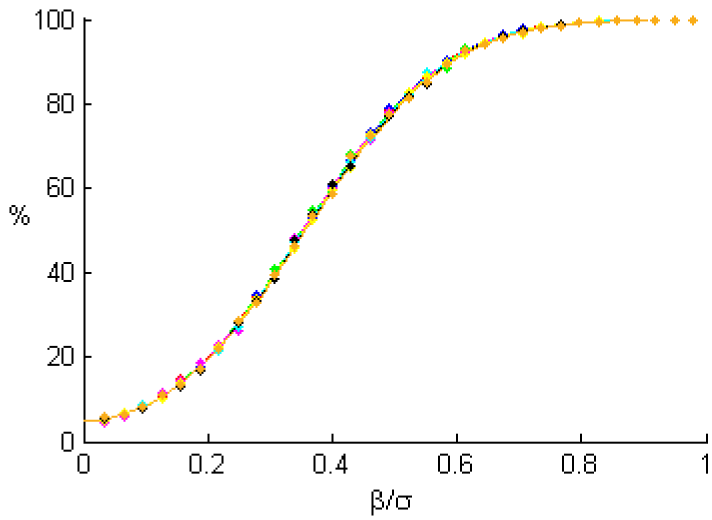

Figure 7-12 Comparison of graphic representation of positive determination of significance of factor for coefficients b_i, where $i=1,\ldots,5$,for experiment with 5 factors with different number of replications in the centre point, test of significance of coefficients without the test of model adequacy, $\alpha=0.05$

It is possible to see that the curve which predict the computed values are almost coincident but there are differences beetween them and in following four pictures are details of

Figure 7-12 which show that the curves are not identical. The details are without the computed values for better differentiation of the curves.

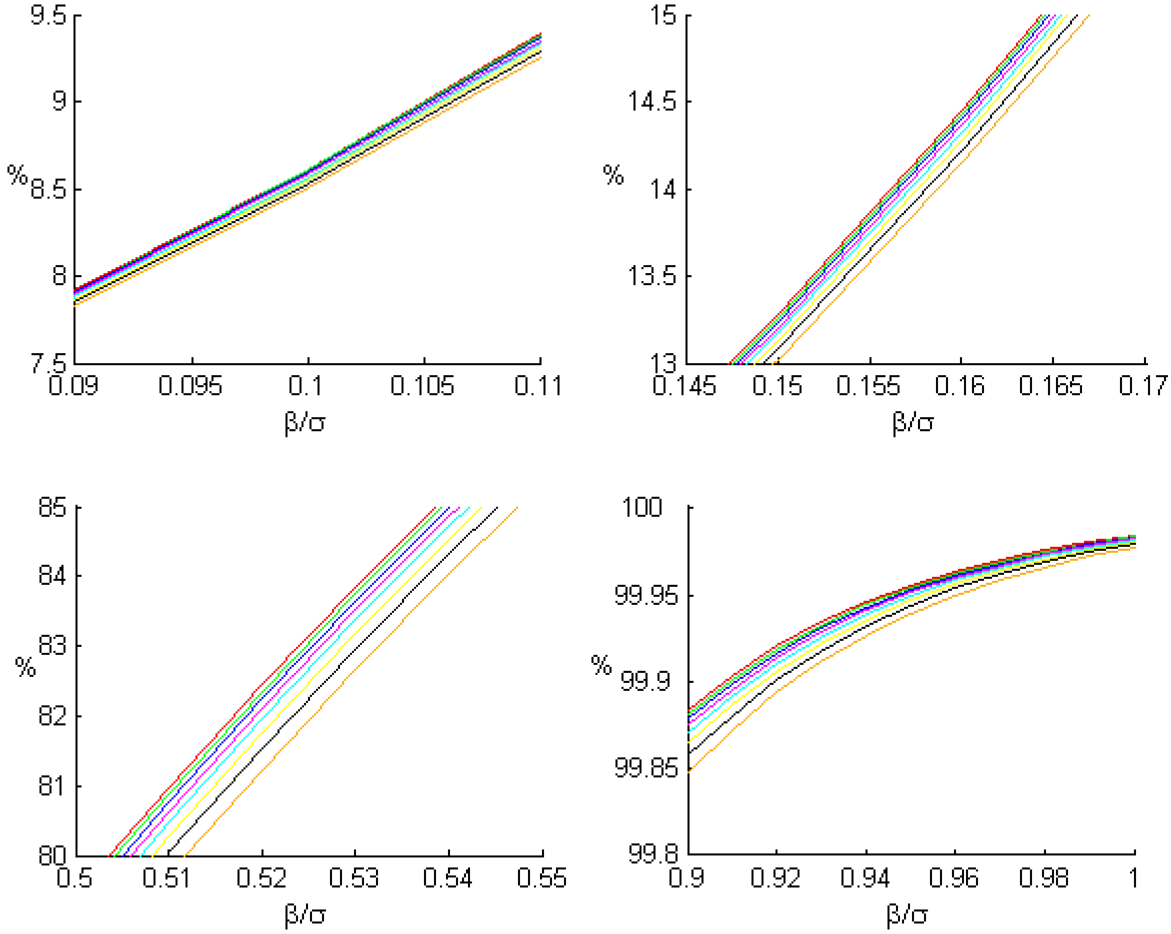

Figure 7-13 Details of Figure 7-12

In following Table 7-8 there are value of percentage expression of positive events for some β_i/σ, where $i=1,\ldots,5$.

$\frac{\beta_i}{\sigma}$	Number of centre points 4	8	12	16	20	24	28	32
0.1	8.50%	8.53%	8.55%	8.57%	8.58%	8.60%	8.61%	8.61%
0.2	19.48%	19.59%	19.68%	19.75%	19.82%	19.87%	19.91%	19.95%
0.3	37.57%	37.81%	38.00%	38.16%	38.29%	38.40%	38.49%	38.57%
0.4	59.10%	59.43%	59.69%	59.90%	60.08%	60.23%	60.35%	60.46%
0.5	78.14%	78.46%	78.71%	78.91%	79.07%	79.21%	79.33%	79.43%
0.6	90.72%	90.94%	91.10%	91.24%	91.35%	91.44%	91.52%	91.58%
0.8	99.22%	99.25%	99.28%	99.31%	99.32%	99.34%	99.35%	99.36%
1.0	99.98%	99.98%	99.98%	99.98%	99.98%	99.98%	99.98%	99.98%

Table 7-8 Comparison of approximated values of percentage expression of positive events for some value of ratios β_i/σ, where $i=1,\ldots,5$, for experiment with 5 factors with different number of replications in the centre point

Figure 7-11, Figure 7-12 and also Table 7-7 and Table 7-8 are for case $\alpha=0.05$. Results for case $\alpha=0.01$ are in Appendix VII.

7.4.2 Test of significance of coefficients with the test of the model adequacy

In Chapter 7.4.1 we see the differences if we change the number of centre points in Experiment B for 5 factors and suppose that the model is adequate.

We see that in Chapter 7.4.1 significant changes only in the coefficient b_0 and in the other coefficients the changes are very small. Therefore we do not have to do all observations. It is necessary to make just few observations in centre point to be able to determine the model adequacy.

There are written m-files `lm5_jcp_sc.m`, where $j = 4, 8, 12, 16, 20, 24, 28, 32$ denote the number of duplicate measurements. The procedure is almost the same as in Chapter 7.4.1, there are the same total number of observations N and therefore degrees of freedom $N-k-1$ are same. The matrix $\mathbf{V} = (\mathbf{X'PX})^{-1}$ is also same because matrixes $\mathbf{P}$ and $\mathbf{X}$ are same. The difference is that before we start to test the significance of coefficients b_i, where $i = 0, 1, \dots, 5$. We make the test of model adequacy and if the model is adequate then we test the significance of coefficients and if the model is not adequate we put the output vector **significance** identically equal to zero.

Experiments are repeated in `sign5_jcp_ma_sc.m`, where $j = 4, 8, 12, 16, 20, 24, 28, 32$ and the dependence of the percentage expression of positive events on β_i/σ is investigate in m-file `graphs_cp_ma_sc.m`.

In Figure 7-11 there are shown the differences for β_0/σ of percentage expression of positive events for experiment with 5 factors. Representations of colours in Figure 7-14 and Figure 7-15 are the same as in Figure 7-11.

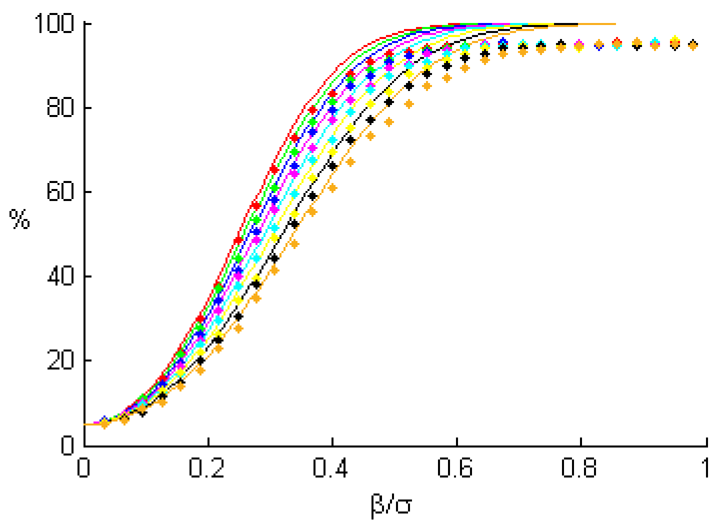

Figure 7-14 Comparison of graphic representation of positive determination of significance of factor for coefficients b_0 for experiment with 5 factors with different number of replications in the centre point, test of significance of coefficients with the test of model adequacy, $\alpha = 0.05$

In Figure 7-15 there are shown the differences for β_i/σ, $i=1,...,5$ of percentage expression of positive events for experiment with 5 factors.

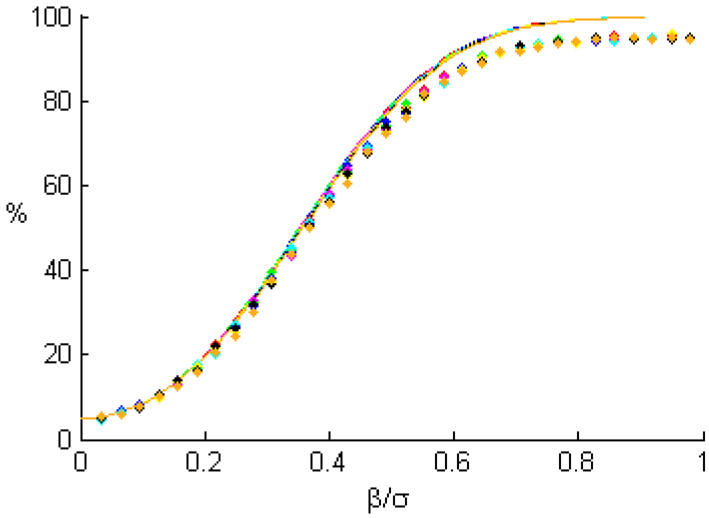

Figure 7-15 Comparison of graphic representation of positive determination of significance of factor for coefficients b_i, where $i=1,...,5$,for experiment with 5 factors with different number of replications in the centre point, test of significance of coefficients with the test of model adequacy, $\alpha = 0.05$

From Figure 7-14 and Figure 7-15 we see that computed values follow the trend of appropriate curves, they are just a bit lower then the case if we suppose that the model is always adequate. The computed values are very close and tables from these values would be inaccurate. The differences between percentage expressions are similar as in Tables 7-7 and Tables 7-8, only if the ratio β_i/σ increases the values go to 95% not to 100% as before.

Figure 7-14, Figure 7-15 are for case $\alpha=0.05$. Results for case $\alpha=0.01$ are in Appendix VIII.

In both cases, if we suppose that the model is adequate or is not, we see that the decreasing of number of centre points has influence only on percentage expression of coefficient b_0, for other coefficients the percentage expression is almost the same. But the determination of significance is much more important for other coefficients, because if the coefficient b_i, $i=1,..,5$, is statistically different from zero then there is the significant influence of corresponding factor and this is what we want to know.

Therefore we reduce the total number of observations in Experiment B almost at one half and the results about significance of factors stay the same.

8 Conclusion

The main goal of this thesis was to determine the influence of number of central points in the plan of experiment for finding the significant factors of process.

As first there were investigated the differences between experiments with different numbers of factors. There were two types of experiments, Experiment A and Experiment B, and in both cases the results were the same. If we consider greater number of factors we have to make more observations and therefore we obtain more information about process and our conclusions are more reliable.

If we compare Experiment A and Experiment B for given number of factors we find out that Experiment A gives better results than Experiment B. If we suppose that there is same total number of observation it is always better to choose Experiment A. But further there were investigated the changes of outcomes of Experiment B when we decrease the number of replications in the centre point. The conclusions about significance of factors stayed almost unchanged. Therefore we find out that it is not necessary to make many replications in the centre point.

We decreased the total number of observations almost up to one half. Values of percentage expressions are almost the same as before but now we do not have to make so many observations. That is the question for one who tries to improve his process if he wants to make Experiment A and obtain more reliable results but pay for it more money or make Experiment B with decreased total number of observations and obtain, in comparison with Experiment A, not so good results but pay less money for it.

References

[1] ANDĚL, J. *Statistické metody*. 3rd edition. Praha : MatfyzPress, 2003.

[2] ANDĚL, J. *Základy matematické statistiky*. 1st edition. Praha : MatfyzPress, 2005.

[3] GENTLE, J. E. *Random number generation and Monte Carlo methods*. 2nd edition. New York : Springer, 2003.

[4] GIESBRECHT, F. G., GUMPERTZ, M. L. *Planning, contruction and statictical analysis of comparative experiment*. New Jersey : John Wiley & Sons, Inc., 2004.

[5] KARPÍŠEK, Z. *Matematika IV - Statistika a pravděpodobnost : Učební text*. Brno : CERM Brno, 2003.

[6] MASON, R. L., GUNST, R. F, HESS, L. H. *Statistical design and analysis of experiments : With applications to engineering and science*. 2nd edition. New York : John Wiley & Sons, Inc., 2003.

[7] MAROŠ, B. *Empirické modely I*. 2. ed. Brno : CERM Brno, 2001.

[8] MONTGOMERY, D. C. *Design and analysis of experiments*. 3rd edition. New York : John Wiley & Sons, Inc., 1991.

[9] MONTGOMERY, D. C. *Introducing to statistical quality control*. 5th edition. New York : John Wiley & Sons, Inc., 2005.

[10] MONTGOMERY, D. C., RUNGER, C. R. *Applied statictics and probability for engineers* . 3rd edition. New York : John Wiley & Sons, Inc., 2003.

[11] RYAN, T. P. *Modern engineering statistics*. New Jersey : John Wiley & Sons, Inc., 2007.

[12] TOŠENOVSKÝ, J., NOSKIEVIČOVÁ, D. *Statistické metody pro zlepšování jakosti*. Ostrava : MOTANEX, 2000.

[13] WOOLFSON, M. M., PERT, G. J. *An introduction to computer simulation*. 1st edition. New York : Oxford University Press, Inc., 1999.

[14] *MATEMATIKA online* [online]. 2005 [cited April 2005]. Available from www: <http://mathonline.fme.vutbr.cz/>.

[15] *Wikipedie* [online]. 2008, [cited April 2008]. Available from www: <http://en.wikipedia.org/wiki/Wikipedia>.

[16] *Wikipedie* [online]. 2008, [cited April 2008]. Available from www: <http://cs.wikipedia.org/wiki/Wikipedie>.

[17] *Wolfram MathWorld* [online]. 2008 [cited April 2008]. Available from www: <http://mathworld.wolfram.com/>.

List of shortcuts

$E(X)$ or μ	expected value (or mean value)
$D(X)$ or σ^2	variance
$\sigma(X)=\sqrt{D(X)}$	standard deviation
$\operatorname{cov}(X,Y)$	covariance
$\rho(X,Y)$	correlation coefficient
$\bar{X}$	sample mean
S^2	sample variance
$S=\sqrt{S^2}$	sample standard deviation
$N(\mu,\sigma^2)$	normal distribution with mean μ and variance $\sigma^2>0$
$B(a,b)$	beta function
H_1	alternate hypothesis
α	error of the first kind
β	error of the second kind
ϵ	random error
β	coefficients of regression model
$\hat{\beta},b$	estimators of coefficients of regression model
s_e^2	variance which express the inaccuracy of measurement
s_r^2	the measure of difference between model and average values
$\mathbf{P}$	matrix of replications
$\mathbf{V}=(\mathbf{X}'\mathbf{P}\mathbf{X})^{-1}$	matrix used to computation of variance of coefficients of model
Experiment A	experiment with two replications for every treatment combination
Experiment B	experiment with just one replication for every treatment combination and same number of replications in centre point

Appendix

I. Experiment A - Test of significance of coefficients without the test of model adequacy

II. Experiment A - Test of significance of coefficients with the test of model adequacy

III. Experiment B - Test of significance of coefficients without the test of model adequacy

IV. Experiment B - Test of significance of coefficients with the test of model adequacy

V. Comparison of Experiment A and Experiment B - Test of significance of coefficients without the test of model adequacy

VI. Comparison of Experiment A and Experiment B - Test of significance of coefficients with the test of model adequacy

VII. Change of number of centre points - Test of significance of coefficients without the test of the model adequacy

VIII. Change of number of centre points - Test of significance of coefficients with the test of model adequacy

I. Experiment A - Test of significance of coefficients without the test of model adequacy

In Appendix 1-6 the representation of colours in figures is as follows: the red represents the experiment with $k = 2$ factors, the green represents the experiment with $k = 3$ factors, the blue represents the experiment with $k = 4$ factors, the magenta represents the experiment with $k = 5$ factors and the cyan represents the experiment with $k = 6$ factors.

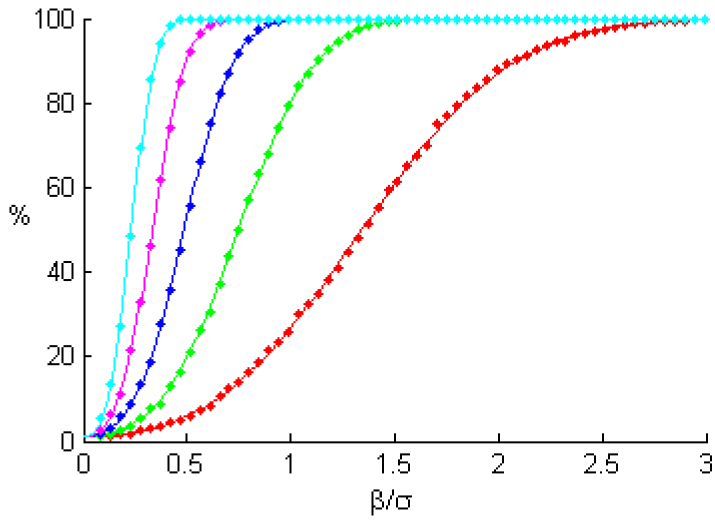

Figure A1-1 Graphic representation of positive determination of significance of factor, experiments with two replications for every treatment combination, test of significance of coefficients without test of model adequacy, $\alpha = 0.01$

$\frac{\beta_i}{\sigma}$	Number of factors				
	2	3	4	5	6
0.1	1.16%	1.47%	2.14%	3.65%	7.23%
0.2	1.66%	3.07%	6.54%	15.36%	36.54%
0.3	2.56%	6.29%	16.33%	40.35%	77.98%
0.5	5.92%	19.98%	53.15%	90.47%	99.87%
0.8	16.20%	57.24%	95.20%	99.99%	100%
1.0	26.96%	80.50%	99.67%	100%	100%
2.0	87.14%	100%	100%	100%	100%
3.0	99.70%	100%	100%	100%	100%

Table A1-1 Chosen information from Figure A1-1

II. Experiment A - Test of significance of coefficients with the test of model adequacy

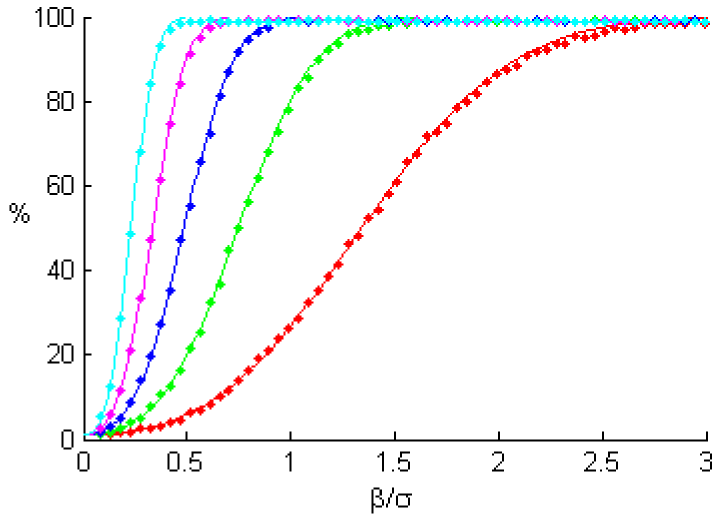

Figure A2-1 Graphic representation of positive determination of significance of factor, experiments with two replications for every treatment combination, test of significance of coefficients with the test of model adequacy, $\alpha = 0.01$

$\frac{\beta_i}{\sigma}$	Number of factors				
	2	3	4	5	6
0.1	1.17%	1.45%	2.08%	3.49%	7.21%
0.2	1.63%	2.98%	6.10%	14.92%	35.82%
0.3	2.53%	6.26%	16.12%	39.36%	76.73%
0.5	5.72%	19.51%	52.64%	89.91%	98.89%
0.8	16.03%	56.59%	94.53%	98.80%	98.96%
1.0	26.66%	79.74%	98.83%	98.93%	99%
2.0	86.45%	98.77%	99%	99%	99%
3.0	98.76%	99%	99%	99%	99%

Table A2-1 Approximated value of percentage expression if we make the test of model adequacy

III. Experiment B - Test of significance of coefficients without the test of model adequacy

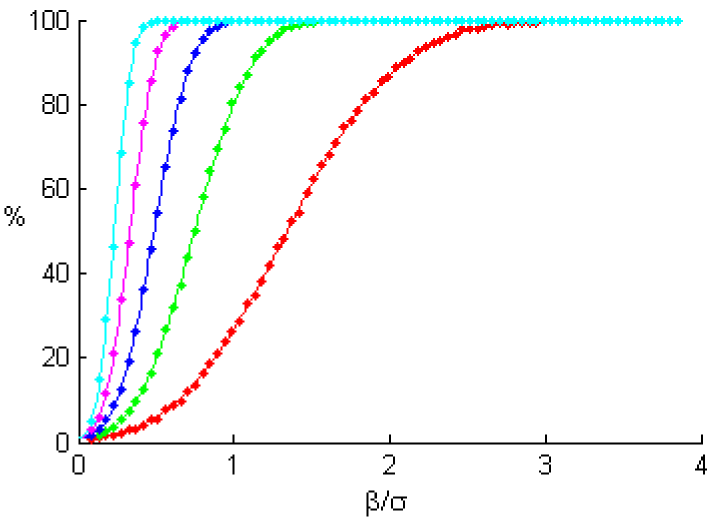

Figure A3-1 Graphic representation of positive determination of significance of factor for coefficient b_0, experiments with one replication for every treatment combination and same number of replications in centre point, test of significance of coefficients without test of model adequacy, $\alpha = 0.01$

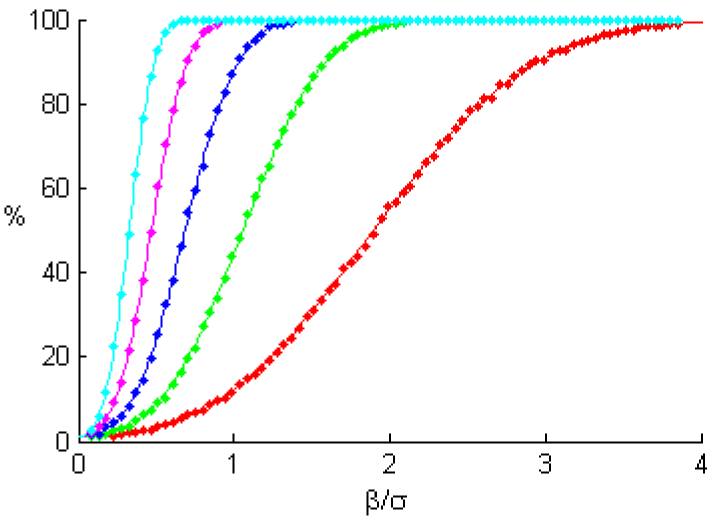

Figure A3-2 Graphic representation of positive determination of significance of factor for coefficient b_i, where $i = 1, ..., k$, experiments with one replication for every treatment combination and same number of replications in centre point, test of significance of coefficients without test of model adequacy, $\alpha = 0.01$

$\frac{\beta_i}{\sigma}$	Number of factors				
	2	3	4	5	6
0.1	1.08%	1.23%	1.55%	2.23%	3.74%
0.2	1.33%	1.97%	3.45%	7.00%	15.92%
0.3	1.75%	3.36%	7.39%	17.70%	41.73%
0.5	3.24%	8.91%	24.29%	56.81%	91.45%
0.8	7.58%	26.86%	66.52%	96.55%	99.99%
1.0	12.25%	44.68%	87.99%	99.82%	100%
2.0	55.18%	98.77%	100%	100%	100%
3.0	90.90%	100%	100%	100%	100%

Table A3-1 Chosen information from Figure A3-2

IV. Experiment B - Test of significance of coefficients with the test of model adequacy

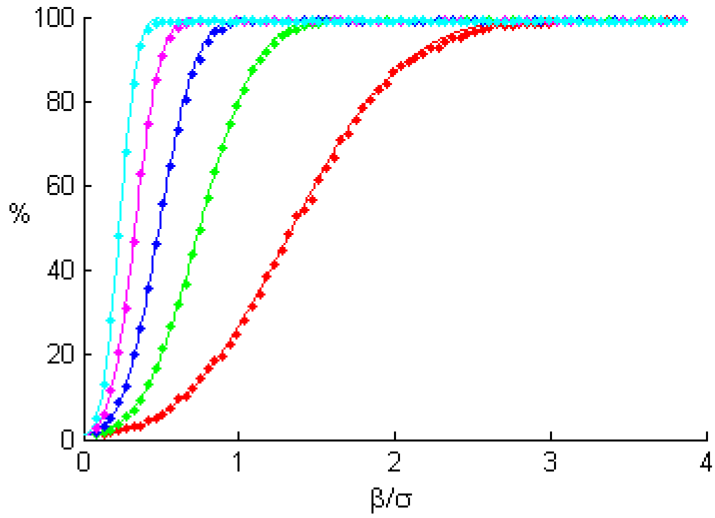

Figure A4-1 Graphic representation of positive determination of significance of factor for coefficient b_0 , experiments with one replication for every treatment combination and same number of replications in centre point, test of significance of coefficients with test of model adequacy, $\alpha = 0.01$

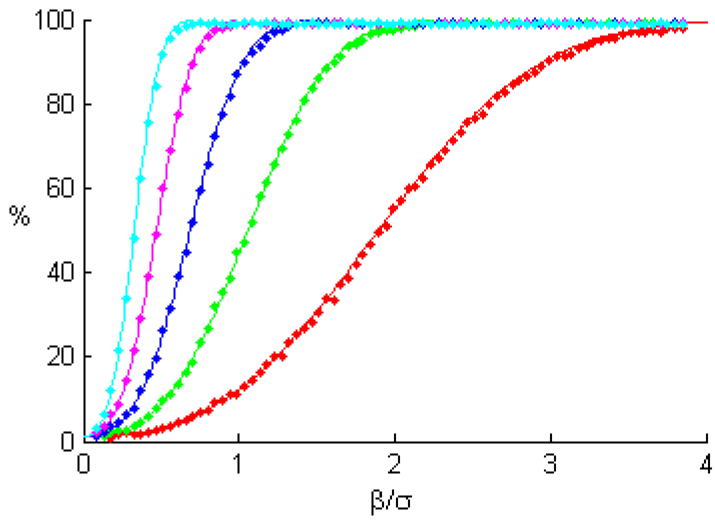

Figure A4-2 Graphic representation of positive determination of significance of factor for coefficient b_i , where $i = 1,...,k$, experiments with one replication for every treatment combination and same number of replications in centre point, test of significance of coefficients with test of model adequacy, $\alpha = 0.01$

$\frac{\beta_i}{\sigma}$	Number of factors				
	2	3	4	5	6
0.1	1.07%	1.16%	1.53%	2.19%	3.68%
0.2	1.29%	1.88%	3.42%	6.97%	15.73%
0.3	1.70%	3.47%	7.16%	17.37%	41.45%
0.5	2.88%	8.95%	23.98%	56.28%	90.56%
0.8	7.43%	26.54%	66.14%	95.94%	98.92%
1.0	11.76%	43.97%	87.34%	98.90%	99%
2.0	55.06%	97.71%	98.97%	99%	99%
3.0	98.63%	98.96%	99%	99%	99%

Table A4-1 Approximated value of percentage expression if we make the test of model adequacy

V. Comparison of Experiment A and Experiment B - Test of significance of coefficients without the test of model adequacy

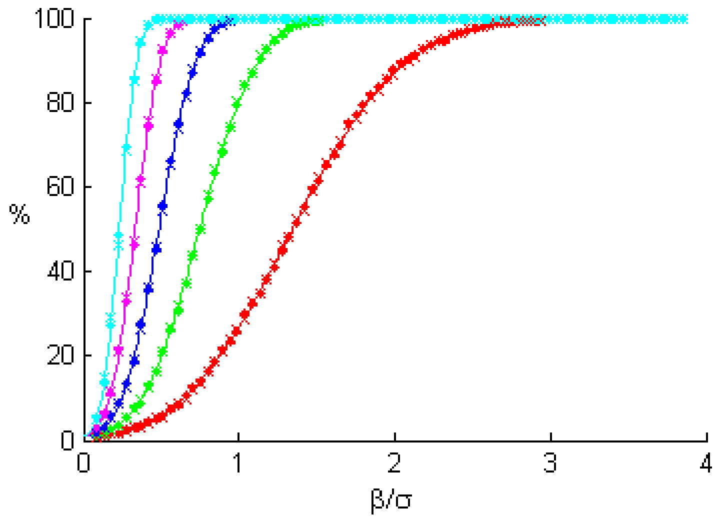

Figure A5-1 Comparison of graphic representation of positive determination of significance of factor for coefficient b_0 of Experiment A and Experiment B, test of significance of coefficients without the test of model adequacy, $\alpha = 0.01$

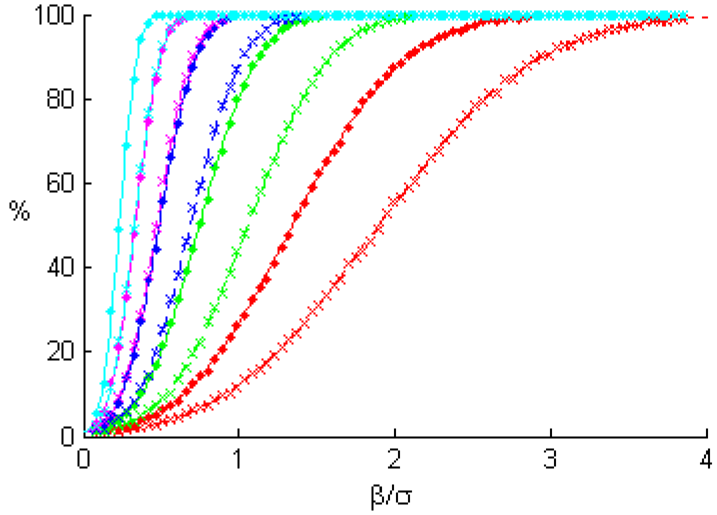

Figure A5-2 Comparison of graphic representation of positive determination of significance of factor for coefficients b_i, where $i = 1,...,k$, of Experiment A and Experiment B, test of significance of coefficients without the test of model adequacy, $\alpha = 0.01$

$\frac{\beta_i}{\sigma}$	Number of factors									
	2		3		4		5		6	
	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B
0.1	1.16%	1.08%	1.47%	1.23%	2.14%	1.55%	3.65%	2.23%	7.23%	3.74%
0.2	1.66%	1.33%	3.07%	1.97%	6.54%	3.45%	15.36%	7.00%	36.54%	15.92%
0.3	2.56%	1.75%	6.29%	3.36%	16.33%	7.39%	40.35%	17.70%	77.98%	41.73%
0.5	5.92%	3.24%	19.98%	8.91%	53.15%	24.29%	90.47%	56.81%	99.87%	91.45%
0.8	16.20%	7.58%	57.24%	26.86%	95.20%	66.52%	99.99%	96.55%	100%	99.99%
1.0	26.96%	12.25%	80.50%	44.68%	99.67%	87.99%	100%	99.82%	100%	100%
2.0	87.14%	55.18%	100%	98.77%	100%	100%	100%	100%	100%	100%
3.0	99.70%	90.90%	100%	100%	100%	100%	100%	100%	100%	100%

Table A5-1 Comparison of values of percentage expression of positive events for some value of ratios β_i / σ , where $i = 1, \ldots, k$ for Experiment A and Experiment B

VI. Comparison of Experiment A and Experiment B - Test of significance of coefficients with the test of model adequacy

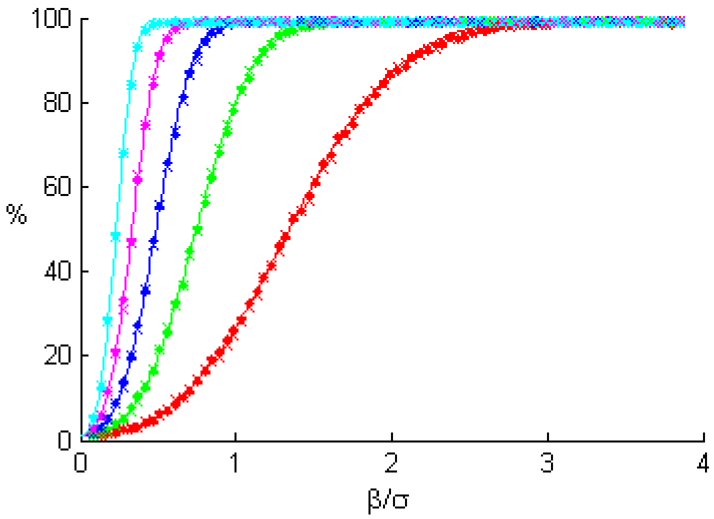

Figure A6-1 Comparison of graphic representation of positive determination of significance of factor for coefficient b_0 of Experiment A and Experiment B, test of significance of coefficients with test of model adequacy, $\alpha = 0.01$

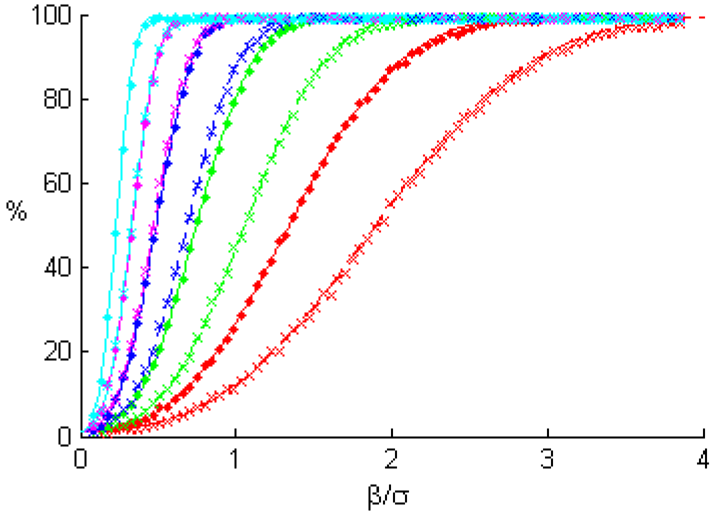

Figure A6-2 Comparison of graphic representation of positive determination of significance of factor for coefficients b_i, where $i = 1, ..., k$, of Experiment A and Experiment B, test of significance of coefficients with the test of model adequacy, $\alpha = 0.01$

$\frac{\beta_i}{\sigma}$	Number of factors									
	2		3		4		5		6	
	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B	Ex. A	Ex. B
0.1	1,17%	1.07%	1.45%	1.16%	2.08%	1.53%	3.49%	2.19%	7.21%	3.68%
0.2	1.63%	1.29%	2.98%	1.88%	6.10%	3.42%	14.92%	6.97%	35.82%	15.73%
0.3	2.53%	1.70%	6.26%	3.47%	16.12%	7.16%	39.36%	17.37%	76.73%	41.45%
0.5	5.72%	2.88%	19.51%	8.95%	52.64%	23.98%	89.91%	56.28%	98.89%	90.56%
0.8	16.03%	7.43%	56.59%	26.54%	94.53%	66.14%	98.80%	95.94%	98.96%	98.92%
1.0	26.66%	11.76%	79.74%	43.97%	98.83%	87.34%	98.93%	98.90%	99%	99%
2.0	86.45%	55.06%	98.77%	97.71%	99%	98.97%	99%	99%	99%	99%
3.0	98.76%	98.63%	99%	98.96%	99%	99%	99%	99%	99%	99%

Table 0-2 Comparison of approximated values of percentage expression of positive events for some value of ratios β_i / σ, where $i = 1, \ldots, k$, for Experiment A and Experiment B

VII. Change of number of centre points - Test of significance of coefficients without the test of the model adequacy

In Appendix 7 and Appendix 8 the representation of colours is as follows: the red represents the experiment with number of replications in centre point $j = 32$, the green is for $j = 28$, the blue for $j = 24$, the magenta for $j = 20$, the cyan for $j = 16$, the yellow for $j = 12$, black for $j = 8$ and the orange is for $j = 4$.

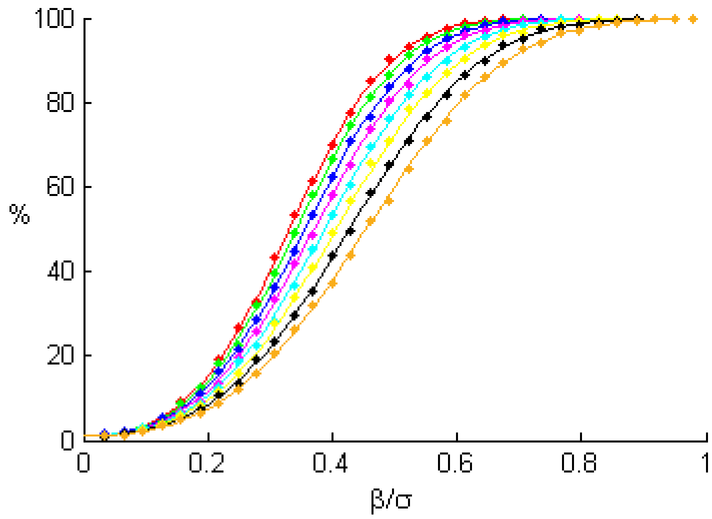

Figure A7-1 Comparison of graphic representation of positive determination of significance of factor for coefficients b_0 for experiment with 5 factors with different number of replications in the centre point, test of significance of coefficients without the test of model adequacy, $\alpha = 0.01$

β_0/σ	Number of centre points							
	4	8	12	16	20	24	28	32
0.1	2.32%	2.50%	2.68%	2.87%	3.06%	3.25%	3.45%	3.65%
0.2	7.47%	8.52%	9.58%	10.68%	11.80%	12.96%	14.15%	15.36%
0.3	19.11%	22.07%	25.08%	28.13%	31.20%	34.27%	37.33%	40.35%
0.4	37.91%	43.29%	48.48%	53.43%	58.10%	62.48%	66.54%	70.28%
0.5	60.18%	66.70%	72.42%	77.35%	81.56%	85.10%	88.04%	90.47%
0.6	79.48%	84.89%	89.03%	92.14%	94.44%	96.11%	97.30%	98.15%
0.8	97.45%	98.71%	99.37%	99.69%	99.86%	99.93%	99.97%	99.99%
1.0	99.90%	99.97%	99.99%	100%	100%	100%	100%	100%

Table A0-1 Comparison of approximated values of percentage expression of positive events for some value of ratios β_0/σ for experiment with 5 factors with different number of replications in the centre point

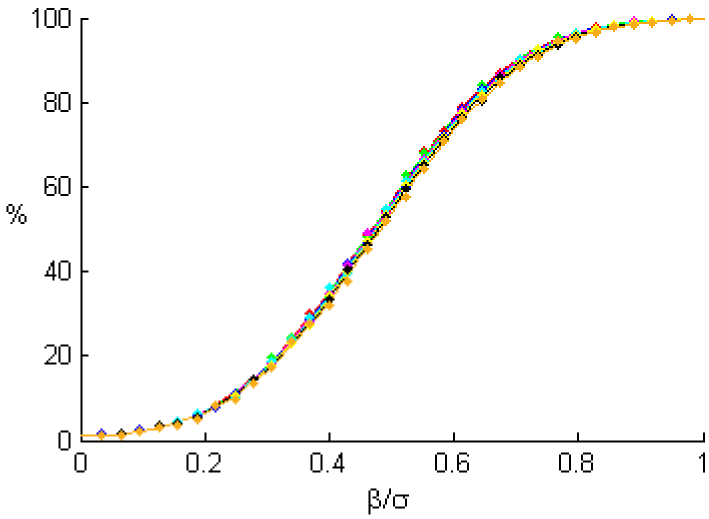

Figure A7-2 Comparison of graphic representation of positive determination of significance of factor for coefficients b_i, where $i=1,...,5$, for experiment with 5 factors with different number of replications in the centre point, test of significance of coefficients without the test of model adequacy, $\alpha = 0.01$

$\frac{\beta_i}{\sigma}$	Number of centre points 4	8	12	16	20	24	28	32
0.1	2.16%	2.17%	2.19%	2.20%	2.21%	2.21%	2.22%	2.23%
0.2	6.62%	6.71%	6.78%	6.84%	6.89%	6.94%	6.97%	7.00%
0.3	16.57%	16.84%	17.06%	17.23%	17.38%	17.50%	17.61%	17.70%
0.4	33.10%	33.62%	34.04%	34.38%	34.67%	34.91%	35.11%	35.29%
0.5	53.83%	54.56%	55.14%	55.60%	55.98%	56.31%	56.58%	56.81%
0.6	73.54%	74.27%	74.83%	75.28%	75.65%	75.96%	76.22%	76.45%
0.8	95.49%	95.77%	95.98%	96.15%	96.28%	96.39%	96.48%	96.55%
1.0	99.71%	99.74%	99.76%	99.78%	99.80%	99.81%	99.82%	99.82%

Table A7-2 Comparison of approximated values of percentage expression of positive events for some value of ratios β_i/σ, where $i=1,...,5$, for experiment with 5 factors with different number of replications in the centre point

VIII. Change of number of centre points - Test of significance of coefficients with the test of model adequacy

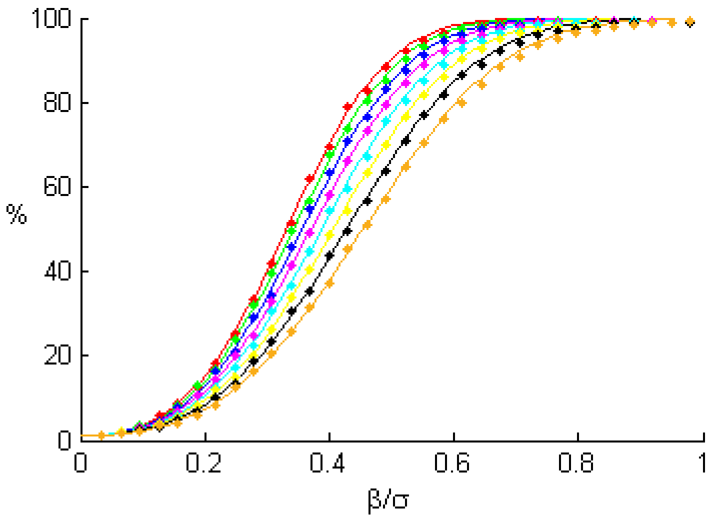

Figure A8-2 Comparison of graphic representation of positive determination of significance of factor for coefficients b_0 for experiment with 5 factors with different number of replications in the centre point, test of significance of coefficients with the test of model adequacy, $\alpha = 0.01$

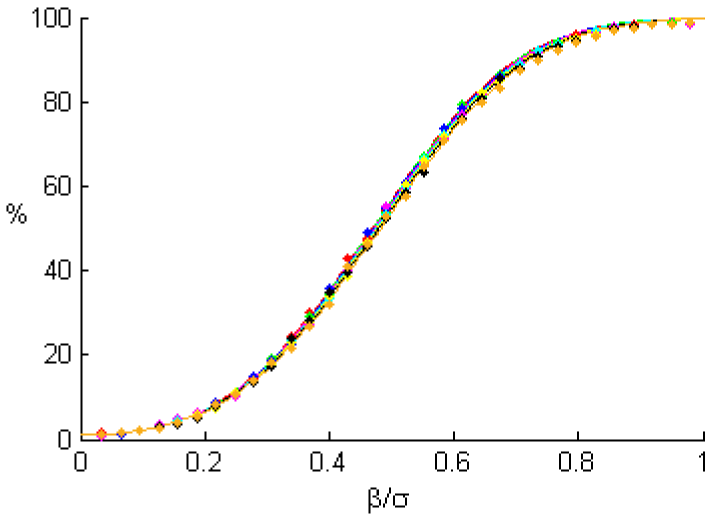

Figure A8-2 Comparison of graphic representation of positive determination of significance of factor for coefficients b_i, where $i = 1,...,5$,for experiment with 5 factors with different number of replications in the centre point, test of significance of coefficients with the test of model adequacy, $\alpha = 0.01$