RESTORATION OF SOME NONLINEAR FUNCTIONAL DEPENDENCIES BY MEANS OF THE GENERALIZED TECHNIQUE OF IDENTIFICATION

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Abstract

In the present work there are realized developed by the authors general methods for identification of nonlinear regressions for a certain class of functional dependencies, which are determined as the most frequently occurring in the investigations by expert estimations of the leading scientists from a number of institutes. The essence of the general methods consists in minimization of the modified method of the least squares, which is reduced to the solving of the nonlinear equations (in considered cases one or two) by means of an iterative algorithm, for which the initial range of definition of parameters is found by means of elaborated by the authors *modified method of tests* using algorithms of interpolation [1, 2, 3]. Besides, the properties of the considered nonlinear functions depending on the values of parameters included in them are investigated in the work and the appropriate diagrams are given. The latter are very important at identification of functional dependencies for a correct choice of an analytical kind of the function corresponding to experimental data.

Key words and phrases: Identification, Nonlinear Function, Algorithm, Interpolation, Iterative method.

AMS subject classification:

Introduction

The problem of restoration of functional dependencies is urgent at processing experimental data for the quantitative description of unknown dependencies between observable variables. The restoration of functional dependencies is widely used both in science and in practice at solving of different problems. For example, restoration of dependence between two measure values, establishment of transfer function of dynamic system or its separate units, restoration of law of chemical reaction course, etc. [4, 5, 6, 7].

The essence of general methods of identification of nonlinear functional dependencies, whose concrete realizations for the certain set of functions are given in this work, consists in the following [1]. It is supposed that between observed values x and y there exist an unknown functional dependence, which is approximated by a function of the given class $f(a_1, ..., a_m, x)$ on the basis of experimental data x_i, y_i, $i = 1, ..., N$, i.e. the verity of dependence is supposed

$$y_i = f(a_1, ..., a_m, x_i) + \varepsilon_i, \qquad i = 1, ..., N, \tag{1.1}$$

where a_1, ..., a_m are unknowns coefficients, whose values are estimated on the basis of observation results x_i, y_i, $i = 1, ..., N$; ε_i are random fluctuations with the characteristics $\mathrm{M}(\varepsilon_\mathrm{i}) = 0$, $\mathrm{D}(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$, $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{j}) = \mathrm{R_{ij}}$, $i \neq j$, $i, j = 1, ..., N$.

Values of parameters a_1, ..., a_m are sought so that the weighted sum of squares of disparities

$$S = \sum_{i=1}^{N} \lambda_i \cdot |f((a_1, ..., a_m, x_i) - y_i|^2 \tag{1.2}$$

be minimal; here λ_i are given weight coefficients. The solving of the given optimization problem determines statistical estimations $\hat{a}_1$, ..., $\hat{a}_m$ of the corresponding parameters (estimation of least squares method).

In the case, when the restoring dependence is linear with respect to the parameters, searching of their statistical estimations is not difficult: the problem is reduced to the solving of a system of m linear equations [8]. If the dependence of an approximating function on the parameters is not linear, for the solving of the considered problem are used different iteration methods, among them, when an approximating function $f(a_1, ..., a_m, x)$ is insufficiently smooth, and its derivatives receive large values in an area of definition of parameters a_1, ..., a_m, are used iteration algorithms without usage of derivatives, including algorithm of Hooke-Jeeves [4, 9]. At application of these algorithms there rise difficulties, connected with the necessity of correct selection of parameters search areas, as it essentially influence on the time of calculus and accuracy of received results.

The above-mentioned complexities of utilization of iteration algorithms at determination of minimum of the functional (1.2) appear the more important, the greater is a number of parameters on which f function depends non-linearly. Below we offer a method which frequently allows to reduce a number of parameters, relatively to which the approximating function is non-linear.

Let us allow, that the sequence of unknown parameters of function f can be divided into two groups

$$[a_1, ..., a_m] = [A_1, ..., A_r, C_1, ..., C_n]$$

$(m = r + n)$ so that the approximating function be linear relatively to the parameters A_1, ..., A_r, i.e. the following representation is possible:

$$f(a_1, ..., a_m,\, x) = \sum_{k=1}^{r} A_k \cdot \varphi_k(C_1, ..., C_n,\, x).$$

Then the minimum value of (1.2) – sum of squares of disparities at fixed values C_1, ..., C_n - is reached in the case when the parameters A_1, ..., A_r satisfy the system of linear equations

$$\sum_{k=1}^{r} \alpha_{jk}\, A_k = B_j \qquad (j = 1, ..., r)$$

and is equal

$$S_v(C_1, ..., C_n) = \sum_{l=1}^{N} \lambda_l \cdot y_l^2 - \sum_{k=1}^{r} A_k\, B_k,$$

here

$$\alpha_{jk} = \sum_{l=1}^{N} \lambda_l \cdot \varphi_j(C_1, ..., C_n,\, x_l) \cdot \varphi_k(C_1, ..., C_n,\, x_l);$$

$$B_j = \sum_{l=1}^{N} \lambda_l \cdot \varphi_j(C_1, ..., C_n,\, x_l) \cdot y_l$$

are the coefficients dependent from C_1, ..., C_n.

Estimations of the least squares method of parameters C_1, ..., C_n can be determined by different iteration methods, including the method of Hooke-Jeeves. In the latter method the function $S_v(C_1, ..., C_n)$ minimizes, and estimations of parameters A_1, ..., A_r can be found by solving of the system of linear equations, and it is necessary to solve this system for each next calculation of the function $S_v(C_1, ..., C_n)$. The iteration process stops when deviation between adjacent computed values S_v is less than the given value.

At sufficiently general conditions, the least squares criterion, where the functional (1.2) minimizes, can be replaced by the modified least squares criterion, where the following value minimizes

$$S' = \sum_{i=1}^{N} \lambda'_i \cdot \Big(g\big(a_1, ..., a_m,\, x_i\big)\big) - g(y_i)\Big)^2; \tag{1.3}$$

here $g(y)$ is some suitable twice differentiable function; $\lambda'_i = \lambda_i / \big(\dot{g}(y_i)\big)^2$; $\dot{g}(y) \equiv \frac{d}{dy} g(y)$ [1]. Here takes place

$$S' = S \cdot (1 + u/2)^2, \tag{1.4}$$

where u is the parameter which satisfies the condition $|u| \leq G$,

$$\left| \frac{\ddot{g}(y_i - v_i)}{\dot{g}(y_i)} \cdot \varepsilon_i \right| < G.$$

The value S' approximates S better when the value of G is smaller, which, on its side, depends on the nature of the function g and values of random components ε_i. At the given g and characteristics of ε_i it is always possible to evaluate the maximum error of the approximation (1.4) with the given probability. The condition $G \ll 1$ is executed, if the function $\dot{g}(y)$ is smooth enough, and if disparities ε_i are small enough. In many practical problems the last condition is executed.

In each certain case the function $g(.)$ is selected depending on the approximating function $f(.)$, so that it nonlinearly include as few as possible number of parameters, by which the functional S' is minimized.

Finding of estimations of the parameters included non-linearly in $g(.)$ is implemented by minimization of the functional S' by means of different iteration methods, for which it is necessary to find intervals from their definition domains, which include true values with probability one.

Let us denote the determined vector of non-linearly entering parameters through $c = (c_1, ..., c_n)$, and search area of the given parameters – through $[C_H,\, C_B]$. It is supposed, that the given area is the hyper parallelepiped, restricted by the coordinates of vectors C_H, C_B. For convergence of the algorithm, and also for minimization of the necessary time for search of estimations, the required area should be as small as possible, and in addition, the probability that it includes true value of c should be close to one.

One of the universal, independent from a concrete kind of a restored functional dependence, methods of definition of intervals of searching the estimations of approximating parameters is the method given in [1], which is called the *trial-and-error method.* This method is universal and is applicable even when all parameters of model are included in it non-linearly, i.e. when the estimations of parameters are searched by direct minimization of criterion (1.2).

The set of all points (x_j, y_j), $j = 1, ..., N$, of the plane (x, y), corresponding to the measured values, is divided on L groups, each of them containing n number of points; here L is integer part of the number N/n. For each of the given groups, if it is possible, the function $f(c_1, ..., c_n,\, x)$ is interpolated, i.e. such values of parameters $c_1, ..., c_n$ are determined, that the plot of function $f(c_1, ..., c_n,\, x)$ passes through all n points of the considered group. The sequence of c parameter values thus obtained $[c^{(1)},\, c^{(2)},\, ...,\, c^{(\nu)}]$ we call a sequence of *trial values* of this parameter; each trial value $c^{(k)}$ corresponds to one of groups of points (x_j, y_j), for which the interpolation of the function $f(c_1, ..., c_n,\, x)$ is possible, i.e. the corresponding set of equations has a solution. Length of this sequence, apparently, satisfies the relationship $0 \leq \nu \leq L$. As the borders of the search area C_H and C_B are taken the vectors, whose components are equal to minimum and maximum values of the corresponding components of vectors of the sequence $c^{(k)}$.

The described method of determination of area $[C_H, C_B]$, which should include the parameter of approximation c, gives the satisfactory result, if the number of tentative values of this parameter $[c^{(1)}, c^{(2)}, ..., c^{(\nu)}]$ is big enough; Otherwise, instead of this method is used the *modified trial-and-error method*, which consists in extension of the area $[C_H, C_B]$ so, that the authenticity of finding in it of sought values of the parameters is not beneath of the given level [1]. In particular the borders of sought for interval are introduced by the way

$$\begin{aligned} C_H &= C_{min} - h_\nu(\alpha) \cdot (C_{max} - C_{min}); \\ C_B &= C_{max} + H_\nu(\alpha) \cdot (C_{max} - C_{min}), \end{aligned} \tag{1.5}$$

where the parameters $h = h_\nu(\alpha)$ and $H = H_\nu(\alpha)$ are determined as the solution of equations

$$\begin{aligned} \int_0^\infty \nu \cdot p(u) \cdot \Big(\Phi(u) - \Phi\big(uh/(1+h)\big)\Big)^{\nu-1} du &= \alpha/2; \\ \int_0^\infty \nu \cdot p(u) \cdot \Big(\Phi\big(-uH/(1+H)\big) - \Phi(-u)\Big)^{\nu-1} du &= \alpha/2, \end{aligned} \tag{1.6}$$

$\Phi(c)$ and $p(c)$ are function and density of distributions corresponding to c normalized random variable $(c - \check{c})/\sigma$; $(1 - \alpha)$ is probability that in an interval $[C_H, C_B]$ the true value of parameter is contained.

Results of realization of this method for a set of functional dependencies are represented below. The latter is determined on the basis of estimations of the leading specialists from a number of institutes as most frequently occurring in researches. The developed algorithms are used by the authors in the created by them package of the applied programs of processing of the experimental information (SDpro), the long exploitation of which at restoration of functional dependencies on experimental data of the most different nature have confirmed their high qualities on reliability, authenticity, efficiency and profitability of the received results [10].

2. Geometrical regression

The regression model

$$y_i = a \cdot x_i^b + \varepsilon_i, \qquad x_i > 0, \quad a > 0,$$

where a and b are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

For determination of coefficients a and b, the modified criterion of the least squares is used [4]:

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \left(A + b \cdot \ln x_i - \ln y_i\right)^2 \Rightarrow \min_{\{a,b\}}, \tag{2.7}$$

where $\lambda_i' = \lambda_i \cdot y_i^2$; $\lambda_i = 1/\sigma_i^2$; $A = \ln a$. Solving the optimization task (2.7) for unknown coefficients, we receive

$$\begin{bmatrix} A \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i' \cdot \begin{bmatrix} 1 & z_i \\ z_i & z_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i' \cdot \begin{bmatrix} \ln y_i \\ z_i \cdot \ln y_i \end{bmatrix};$$

$$z_i = \ln x_i.$$

If σ_i^2 are not known, it is possible to use their estimations

$$S_i^2 = \frac{1}{n_i} \cdot \sum_{k=1}^{n_i} y_{ik},$$

where y_{ik}, $k = 1, ..., m_i$ are repeated supervisions above y_i at given x_i.

3. Exponential regression

The regression model

$$y_i = a \cdot e^{bx_i} + \varepsilon_i, \qquad x_i > 0, \quad a > 0,$$

where a and b are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

The modified criterion of the least squares is written as follows:

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \left(A + b \cdot x_i - \ln y_i\right)^2 \Rightarrow \min_{\{a,b\}}, \tag{3.8}$$

where $\lambda_i' = \lambda_i \cdot y_i^2$; $\lambda_i = 1/\sigma_i^2$; $A = \ln a$. Minimizing (3.8), we receive

$$\begin{bmatrix} A \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i' \cdot \begin{bmatrix} 1 & x_i \\ x_i & x_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i' \cdot \ln y_i \begin{bmatrix} 1 \\ x_i \end{bmatrix}.$$

4. Logarithmic regression

The regression model

$$y_i = a \cdot \ln(b\, x_i) + \varepsilon_i, \qquad x_i > 0,$$

where a and b are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

The minimum of the weighted sum of squares of disparities with weight factors $\lambda_i = 1/\sigma_i^2$ is achieved in the case, when the parameters a and b are determined by the relations: $b = e^{B/a}$;

$$\begin{bmatrix} B \\ a \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} 1 & z_i \\ z_i & z_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i\, y_i \cdot \begin{bmatrix} 1 \\ z_i \end{bmatrix};$$

$$z_i = \ln x_i; \qquad \lambda_i = 1/\sigma_i^2.$$

5. Geometric-exponential regression

The regression model

$$y_i = a \cdot x_i^b \cdot e^{cx_i} + \varepsilon_i,$$

where a, b, c are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

The modified criterion of the least squares is written as follows:

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \left(A + b \cdot \ln x_i + c \cdot x_i - \ln y_i\right)^2 \Rightarrow \min, \tag{5.9}$$

where $\lambda_i' = \lambda_i \cdot y_i^2$; $\lambda_i = 1/\sigma_i^2$; $A = \ln a$. Minimum in (5.9) is achieved at

$$\begin{bmatrix} A \\ b \\ c \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i' \cdot \begin{bmatrix} 1 & z_i & x_i \\ z_i & z_i^2 & x_i\, z_i \\ z_i & x_i\, z_i & x_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i' \cdot \ln y_i \cdot \begin{bmatrix} 1 \\ z_i \\ x_i \end{bmatrix};$$

$$z_i = \ln x_i; \qquad \lambda_i = 1/\sigma_i^2.$$

6. Exponential regression with a free term

The regression model

$$y_i = a + b \cdot e^{cx_i} + \varepsilon_i,$$

where a, b, c are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

The criterion of the least squares has the following form:

$$S = \sum_{i=1}^{N} \lambda_i \cdot \left(a + b \cdot e^{cx_i} - y_i\right)^2 \Rightarrow \min,$$

where $\lambda_i = 1/\sigma_i^2$. The minimal value of the quantity S at fixed value of c is achieved at

$$\begin{bmatrix} a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} 1 & E_i \\ E_i & E_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i \cdot y_i \cdot \begin{bmatrix} 1 \\ E_i \end{bmatrix};$$

$$E_i = e^{cx_i},$$

and is equal to

$$S(c) = \sum_{i=1}^{N} \lambda_i \cdot y_i^2 - a\,\eta_1 - b\,\eta_2.$$

The value of the parameter c, at which the function $S(c)$ is minimal, is determined by the iterative method of Hooke-Jeeves [4, 9]. Borders of search area of this parameter (hereinafter, where for minimization of the modified criterion of the least squares is used an iterative method) are determined by the relations (1.5), (1.6), i.e. by *modified method of trials* [1].

7. Geometrical regression with a free term

The regression model

$$y_i = a + b \cdot x_\mathrm{i}^c + \varepsilon_i,$$

where a, b, c are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

This task is equivalent to the restoration of dependence $a + b \cdot e^{cz}$ (considered in the previous item) at the designation $z = \ln x$.

8. Inverse exponential regression

The regression model

$$y_i = a \cdot \left(1 - e^{-b\,x_i}\right) + \varepsilon_i,$$

where a and b are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

Minimal value of the weighted sum of squares of disparities with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed value of b is achieved at

$$a = \frac{\sum\limits_{i=1}^{N} \lambda_i\,y_i \cdot \left(1 - e^{-b\,x_i}\right)}{\sum\limits_{i=1}^{N} \lambda_i \cdot \left(1 - e^{-b\,x_i}\right)^2}$$

and is equal to

$$S(b) = \sum_{i=1}^{N} \lambda_i\,y_i \cdot \Big(y_i - a \cdot \left(1 - e^{-b\,x_i}\right)\Big).$$

The value of parameter b, at which the function $S(b)$ is minimal, is determined by an iterative method of Hooke-Jeeves. The borders of search area of this parameter are defined similarly to borders for parameter $-c$ at restoration of dependence $f(a,b,c,x) = a + b \cdot e^{cx}$ (see the section **??**).

9. Linear-exponential regression

The regression model

$$y_i = (a + b\,x_i) \cdot e^{cx_i} + \varepsilon_i,$$

where a, b, c are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

Minimal value of the weighted sum of squares of disparities with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed value of c is achieved at

$$\begin{bmatrix} a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i\,E_i \cdot \begin{bmatrix} 1 & x_i \\ x_i & x_i^2 E_i \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i\,y_i\,E_i \cdot \begin{bmatrix} 1 \\ x_i \end{bmatrix};$$

$$E_i = e^{cx_i},$$

and is equal to

$$S(c) = \sum_{i=1}^{N} \lambda_i \, y_i^2 - a \, \eta_1 - b \, \eta_2.$$

Value of the parameter c, at which the function $S(c)$ is minimal, is determined by an iterative method of Hooke-Jeeves. The borders of search area of this parameter are determined by *the modified method of trials* (1.5), (1.6).

10. Linear-exponential dependence with a free term

The regression model

$$y_i = h + (a + b \, x_i) \cdot e^{c \, x_i} + \varepsilon_i,$$

where h, a, b, c are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

Minimal value of the weighted sum of squares of disparities with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed value of c is achieved at

$$\begin{bmatrix} h \\ a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} 1 & E_i & x_i E_i \\ E_i & E_i^2 & x_i E_i^2 \\ x_i E_i & x_i E_i^2 & x_i^2 E_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i \, y_i \cdot \begin{bmatrix} 1 \\ E_i \\ x_i \, E_i \end{bmatrix};$$

$$E_i = e^{cx_i},$$

and is equal to

$$S(c) = \sum_{i=1}^{N} \lambda_i \, y_i^2 - h \, \eta_1 - a \, \eta_2 - b \, \eta_3.$$

Value of the parameter c, at which the function $S(c)$ is minimal, is determined by an iterative method of Hooke-Jeeves. The borders of search of this parameter are determined by *the modified method of trials* (1.5), (1.6).

11. Product of geometrical dependencies

The regression model

$$y_i = a \cdot x_i^c \cdot (1 - b\,x_i)^d + \varepsilon_i,$$

where a, b, c, d are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

The modified criterion of the least squares can be written as follows

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \big(A + c \cdot \ln x_i + d \cdot \ln(1 - b\,x_i) - \ln y_i\big)^2 \Rightarrow \min,$$

where $\lambda_i' = \lambda_i \cdot y_i^2$; $\lambda_i = 1/\sigma_i^2$; $A = \ln a$. Minimal value of the quantity S' at fixed value of b is achieved at

$$\begin{bmatrix} A \\ c \\ d \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i' \cdot \begin{bmatrix} 1 & P_i & Q_i \\ P_i & P_i^2 & P_i Q_i \\ Q_i & P_i Q_i & Q_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i' \cdot \ln y_i \cdot \begin{bmatrix} 1 \\ P_i \\ Q_i \end{bmatrix};$$

$$P_i = \ln x_i; \qquad Q_i = \ln\big(1 - b\,x_i\big),$$

and is equal to

$$S'(b) = \sum_{i=1}^{N} \lambda_i' \cdot \big(\ln y_i\big)^2 - A\,\eta_1 - c\,\eta_2 - d\,\eta_3.$$

Value of the parameter b, at which the function $S'(b)$ is minimal, is determined by an iterative method of Hooke-Jeeves. The borders of search area of this parameter are determined by *the modified method of trials* (1.5), (1.6).

12. Sum of exponential dependencies

The regression model

$$y_i = a \cdot e^{c\,x_i} + b \cdot e^{d\,x_i} + \varepsilon_i,$$

where a, b, c, d are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

Minimal value of the weighted sum of squares of disparities $S(c, d)$ with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed values of c and d is achieved at

$$\begin{bmatrix} a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} P_i^2 & P_i Q_i \\ P_i Q_i & Q_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i \, y_i \cdot \begin{bmatrix} P_i \\ Q_i \end{bmatrix};$$

$$P_i = e^{c\,x_i}; \qquad Q_i = e^{d\,x_i},$$

and is equal to

$$S(c, d) = \sum_{i=1}^{N} \lambda_i \, y_i^2 - a\,\eta_1 - b\,\eta_2.$$

Values of the parameters c and d, at which the function $S(c, d)$ is minimal, are determined by an iterative method of Hooke-Jeeves. The borders of search area of these parameters are determined by *the modified method of trials* (1.5), (1.6).

13. Sum of geometrical dependencies

The regression model

$$y_i = a \cdot x_i^c + b \cdot x_i^d + \varepsilon_i,$$

where a, b, c, d are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

This problem is equivalent to the restoration of dependence $a\,e^{cz} + b\,e^{dz}$ (considered in the previous section) at denotation $z = \ln x$.

14. Sum of exponential dependencies with a free term

The regression model

$$y_i = h + a \cdot e^{c\,x_i} + b \cdot e^{d\,x_i} + \varepsilon_i,$$

where h, a, b, c, d are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

Minimal value of the weighted sum of squares of disparities $S(c,d)$ with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed values of c and d is achieved at

$$\begin{bmatrix} h \\ a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} 1 & P_i & Q_i \\ P_i & P_i^2 & P_i Q_i \\ Q_i & P_i Q_i & Q_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i\, y_i \cdot \begin{bmatrix} 1 \\ P_i \\ Q_i \end{bmatrix};$$

$$P_i = e^{c\,x_i}; \qquad Q_i = e^{d\,x_i},$$

and is equal to

$$S(c,d) = \sum_{i=1}^{N} \lambda_i\, y_i^2 - h\,\eta_1 - a\,\eta_2 - b\,\eta_3.$$

Values of the parameters c and d, at which the function $S(c,d)$ is minimal, are determined by an iterative method of Hooke-Jeeves. The borders of search area of these parameters are determined by *the modified method of trials* (1.5), (1.6).

15. Sum of geometrical dependencies with a free term

The regression model

$$y_i = h + a \cdot x_i^c + b \cdot x_i^d + \varepsilon_i,$$

where h, a, b, c, d are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

This problem is equivalent to the restoration of the dependence $h + a\,e^{cz} + b\,e^{dz}$ (considered in the previous section) at the denotation $z = \ln x$.

16. Exponential-sine wave regression

The regression model

$$y_i = e^{cx_i} \cdot \big(a\,\cos(\omega x_i) + b\,\sin(\omega x_i)\big) + \varepsilon_i,$$

where a, b, c, ω are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

Minimal value of the weighted sum of squares of disparities $S(c, \omega)$ with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed values of c and ω is achieved at

$$\begin{bmatrix} a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} P_i^2 & P_i Q_i \\ P_i Q_i & Q_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i \, y_i \cdot \begin{bmatrix} P_i \\ Q_i \end{bmatrix};$$

$$P_i = e^{c x_i} \cdot \cos(\omega x_i); \qquad Q_i = e^{c x_i} \cdot \sin(\omega x_i),$$

and is equal to

$$S(c, \omega) = \sum_{i=1}^{N} \lambda_i \, y_i^2 - a\,\eta_1 - b\,\eta_2.$$

Values of parameters c and ω, at which the function $S(c, \omega)$ is minimal, is determined by the iterative method of Hooke-Jeeves. The borders of search area of these parameters are determined by *the modified method of trials* (1.5), (1.6).

At definition of borders for parameter ω, it is also taken into account, that the difference between neighboring zero points of the function $f(a, b, c, \omega, x)$ is equal to $\Delta x = \pi/\omega$.

17. Exponential-sine wave regression with a free term

The regression model

$$y_i = h + e^{c x_i} \cdot \big(a\,\cos(\omega x_i) + b\,\sin(\omega x_i)\big) + \varepsilon_i,$$

where h, a, b, c, ω are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

Minimal value of the weighted sum of squares of disparities $S(c, \omega)$ with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed values of c and ω is achieved at

$$\begin{bmatrix} h \\ a \\ b \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix},$$

where

$$\xi = \sum_{i=1}^{N} \lambda_i \cdot \begin{bmatrix} 1 & P_i & Q_i \\ P_i & P_i^2 & P_i Q_i \\ Q_i & P_i Q_i & Q_i^2 \end{bmatrix}; \quad \eta = \sum_{i=1}^{N} \lambda_i \, y_i \cdot \begin{bmatrix} 1 \\ P_i \\ Q_i \end{bmatrix};$$

$$P_i = e^{cx_i} \cdot \cos(\omega x_i); \quad Q_i = e^{cx_i} \cdot \sin(\omega x_i),$$

and is equal to

$$S(c, \omega) = \sum_{i=1}^{N} \lambda_i \, y_i^2 - h\,\eta_1 - a\,\eta_2 - b\,\eta_3.$$

Values of parameters c and ω, at which the function $S(c, \omega)$ is minimal, is determined by an iterative method of Hooke-Jeeves. The borders of search area of these parameters are determined by *the modified method of trials* (1.5), (1.6).

At definition of borders for parameter ω, it is also taken into account, that the difference between neighboring maximum points (and minimum points) of the function $f(h, a, b, c, \omega, x)$ is equal $\Delta x = 2\pi/\omega$.

18. Polynomial regression

The regression model

$$y_i = \sum_{k=0}^{m} p_k \, x_i^k + \varepsilon_i,$$

where p_0, ..., p_m are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

Minimum of the weighted sum of squares of disparities with weight factors $\lambda_i = 1/\sigma_i^2$ is achieved at

$$\begin{bmatrix} p_0 \\ p_1 \\ ... \\ p_m \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ ... \\ \eta_M \end{bmatrix},$$

where $M = m + 1$; ξ is $M \times M$ matrix with elements

$$\xi_{jk} = \sum_{L=1}^{N} \lambda_L \cdot x_L^{j+k-2};$$

$$\eta_k = \sum_{L=1}^{N} \lambda_L \cdot y_L \, x_L^{k-1};$$

$\lambda_L = 1/\sigma_L^2$.

The possibility of automatic choice of degree of the model, i.e. identification not only of coefficients, but also of degree of the polynomial, is realized in the program by the following algorithm.

Let the minimal dispersion correspond to the model with degree m_0; $1 \le m_0 \le n$, where n is the greatest possible order of model. Let us denote this dispersion through $S^2(m_0)$. Let us construct a confidence interval

$$\frac{(N-m_0-1)\cdot S^2(m_0)}{\chi_{1-\alpha/2}} \le \sigma^2(m_0) \le \frac{(N-m_0-1)\cdot S^2(m_0)}{\chi_{\alpha/2}},$$

where $\sigma(m_0)$ is unknown true value of dispersion; $\chi_{\alpha/2}$ and $\chi_{1-\alpha/2}$ are quantiles of the orders $\alpha/2$ and $1-\alpha/2$, accordingly, of distribution of the χ-square with $N-m_0-1$ degrees of freedom; $1-\alpha$ is confidence probability.

As restored dependence we shall accept the model with the minimal order from a set of restored models, whose dispersions occurred in the constructed confidence interval.

The choice of degree of the model is similarly carried out at restoration of other dependencies for which it is necessary.

19. Geometrical-polynomial regression

The regression model

$$y_i = x_i^c \cdot \sum_{k=0}^{m} p_k\, x_i^k + \varepsilon_i,$$

where c, p_0, ..., p_m are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \ne k$.

Minimal value of the weighted sum of squares of disparities with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed value of c is achieved at

$$\begin{bmatrix} p_0 \\ p_1 \\ \dots \\ p_m \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \dots \\ \eta_M \end{bmatrix},$$

where $M = m+1$; ξ is the $M \times M$ matrix with elements

$$\xi_{jk} = \sum_{L=1}^{N} \lambda_L \cdot x_L^{j+k+2c-2};$$

$$\eta_k = \sum_{L=1}^{N} \lambda_L \cdot y_L \, x_L^{k+c-1},$$

and is equal

$$S(c) = \sum_{L=1}^{N} \lambda_L \, y_L^2 - \sum_{k=1}^{M} p_{k-1} \, \eta_k.$$

Value of the parameter c, at which the function $S(c)$ is minimal, is determined by an iterative method of Hooke-Jeeves. The borders of search area of this parameter are determined by *the modified method of trials* (1.5), (1.6).

20. Exponential-polynomial regression

The regression model looks like

$$y_i = e^{cx_i} \cdot \sum_{k=0}^{m} p_k \, x_i^k + \varepsilon_i,$$

where c, p_0, ..., p_m are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

Minimal value of the weighted sum of squares of disparities with weight factors $\lambda_i = 1/\sigma_i^2$, at fixed value of c is achieved at

$$\begin{bmatrix} p_0 \\ p_1 \\ \cdots \\ p_m \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \cdots \\ \eta_M \end{bmatrix},$$

where $M = m + 1$; ξ is the $M \times M$ matrix with elements

$$\xi_{jk} = \sum_{L=1}^{N} \lambda_L \cdot \exp(2c\, x_L) \cdot x_L^{j+k-2};$$

$$\eta_k = \sum_{L=1}^{N} \lambda_L \cdot \exp(2c\, x_L) \cdot y_L \, x_L^{k-1},$$

and is equal to

$$S(c) = \sum_{L=1}^{N} \lambda_L \, y_L^2 - \sum_{k=1}^{M} p_{k-1} \, \eta_k.$$

Value of the parameter c, at which the function $S(c)$ is minimal, is determined by an iterative method of Hooke-Jeeves. The borders of search area of this parameter are determined by *the modified method of trials* (1.5), (1.6).

21. Logarithmic-polynomial regression

The regression model looks like

$$y_i = c \cdot \ln\left(\sum_{k=0}^{m} p_k\, x_i^k\right) + \varepsilon_i,$$

where c, p_0, ..., p_m are unknown coefficients determined by experimental data: x_i, y_i, $i = 1, ..., N$; $\mathrm{M}\,(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}\,(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

The modified criterion of the least squares can be written as follows

$$S' = \sum_{i=1}^{N} \lambda_i' \cdot \left(\sum_{k=0}^{m} p_k\, x_i^k - \exp\bigl(y_i/c\bigr)\right)^2 \Rightarrow \min,$$

where $\lambda_i' = \lambda_i \cdot \exp\bigl(-2y_i/c\bigr)$. Minimal value of the quantity S' at fixed value of c is achieved at

$$\begin{bmatrix} p_0 \\ p_1 \\ \cdots \\ p_m \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \cdots \\ \eta_M \end{bmatrix},$$

where $M = m + 1$; ξ is the $M \times M$ matrix with elements

$$\xi_{jk} = \sum_{L=1}^{N} \lambda_L' \cdot x_L^{j+k-2};$$

$$\eta_k = \sum_{L=1}^{N} \lambda_L' \cdot \exp\bigl(y_L/c\bigr) \cdot x_L^{k-1},$$

and is equal to

$$S'(c) = \sum_{L=1}^{N} \lambda_L' \cdot \exp\bigl(2y_L/c\bigr) - \sum_{k=1}^{M} p_{k-1}\, \eta_k.$$

Value of the parameter c, at which the function $S'(c)$ is minimal, is determined by an iterative method of Hooke-Jeeves. The borders of search area of this parameter are determined by *the modified method of trials* (1.5), (1.6).

22. Periodic regression

Let us consider a model

$$y_j = f(t_j) + \varepsilon_j, \qquad j = 1, ..., N,$$

where $\mathrm{M}(\varepsilon_\mathrm{j}) = 0$; $\mathrm{D}(\varepsilon_\mathrm{j}) = \sigma_\mathrm{j}^2$; $\mathrm{cov}(\varepsilon_\mathrm{j}, \varepsilon_\mathrm{k}) = 0$, $j \neq k$; $f(t)$ is a periodic function with the period $T = 2\pi/\omega$ [4, 11].

The consecutive values t_j of independent variable should be equidistant from each other with a step T/r, where r – *a number of the measured values in one period* – is integer, greater than or equal to 3; the general number of the measured values N should be more than or equal to $2r$; besides, the number N should be divided entirely on r. If the last condition is broken, at definition of unknown parameters first are considered only rp values of t_j and y_j, and others are not taken into account; here p is integer part of number N/r.

The considered dependence satisfies the condition $f(t_{j+r}) = f(t_j)$. Hence, the following representation is possible

$$f(t_j) = A_0 + \sum_{k=1}^{(r-1)/2} \Big(A_k \cdot \cos(2\pi kj/r) + B_k \cdot \sin(2\pi kj/r) \Big),$$

if r is odd number and

$$f(t_j) = A_0 + \sum_{k=1}^{r/2-1} \Big(A_k \cdot \cos(2\pi kj/r) + B_k \cdot \sin(2\pi kj/r) \Big) + A_{r/2} \cdot (-1)^j,$$

if r is even number.

Thus, the restored dependence looks like

$$f\big(A_0, ..., A_{m+1}, B_1, ..., B_m, t\big) = A_0 + \sum_{k=1}^{m+1} A_k \cos(k\omega t) + \sum_{k=1}^{m} B_k \sin(k\omega t),$$

where m is whole part of the number $(r-1)/2$; A_0, ..., A_{m+1}, B_1, ..., B_m are parameters of approximation, and in case of odd r $A_{m+1} = 0$, and in case of even r $A_{m+1} = A_{r/2}$.

The estimations on the method of the least squares of parameters of approximation are calculated so:

$$\hat{A}_0 = \frac{1}{N} \sum_{j=1}^{N} y_j;$$

$$\hat{A}_k = \frac{2}{N} \sum_{j=1}^{N} y_j \cdot \cos(2\pi kj/r); \quad \hat{B}_k = \frac{2}{N} \sum_{j=1}^{N} y_j \cdot \sin(2\pi kj/r)$$

$(k = 1, ..., m)$ and

$$A_{r/2} = \frac{1}{N} \sum_{j=1}^{N} y_j \cdot (-1)^j$$

at even r.

Dispersions of A_0 and $A_{r/2}$ are equal to σ^2/N, and dispersions of A_k and B_k – $2\sigma^2/N$ $(k = 1, ..., m)$. The unbiased estimation of the dispersion σ^2 is calculated under the formula

$$S^2 = \frac{1}{N-r} \cdot \left(\sum_{j=1}^{N} y_j^2 - N \cdot \left(A_0^2 + A_{m+1}^2\right) - \frac{1}{2} \sum_{k=1}^{m} \left(A_k^2 + B_k^2\right) \right)^2 . \quad (22.10)$$

After calculation of coefficients A_k and B_k for every $k = 1, ..., m$ the zero hypothesis H_0: $A_k = B_k = 0$ is checked. If this hypothesis is correct, the statistics

$$v^2 = \frac{N \cdot R^2(k)}{4\,S^2},$$

where $R^2(k) = A_k^2 + B_k^2$, and S^2 calculated on (22.10), is subordinated to F – the Fisher's distribution with 2 and $N - r$ degrees of freedom. Thus, the zero hypothesis is accepted if

$$v^2 \le v_{1-\alpha}^2(2, N - r),$$

where α is the given significance value, $v_{1-\alpha}^2(2, N-r)$ is quantile with order $1 - \alpha$ of the Fisher's distribution with $(2, N - r)$ degrees of freedom.

The automatic choice of model's order is carried out similarly to the item **??**.

23. The regression analysis

At identification of the above-stated functional dependencies in the developed package SDpro there is an opportunity of inclusion of the mode of check of regression model on adequacy. In the given mode is checked the hypothesis about conformity of restored dependence to experimental data by the following algorithm. The interval of giving of independent variable (x_{min}, x_{max}) is divided on K groups and the following value is calculated

$$v^2 = \frac{\frac{1}{K-m} \cdot \sum\limits_{i=1}^{K} m_i \, |\bar{y}_i - f(\hat{a}, x_i^o)|^2}{\frac{1}{N-K} \cdot \sum\limits_{i=1}^{K} \sum\limits_{k=1}^{m_i} |y_{ik} - \bar{y}_i|^2},$$

where N is the sample size; m – quantity of estimated parameters in restored functional dependence $f(a,x)$; m_i – the number of measurements which have got in the i-th interval; x_i^o – average point of i-th interval of the grouping data; $\bar{y}_i$ is an arithmetic mean values of the dependent variable, got in i-th interval; $f(\hat{a}, x_i^o)$ is value of restored regress in the point x_i^o, $\hat{a}$ is estimations of unknown parameters; y_{ik} is k-th under the account value of the dependent variable, got in the i-th interval.

If the following takes place

$$v_{\alpha/2}^2 < v^2 < v_{1-\alpha/2}^2,$$

where $v_{\alpha/2}$ and $v_{1-\alpha/2}$ are the quantiles of the orders $\alpha/2$ and $1-\alpha/2$, accordingly, of the Fisher's distribution with $(K-m, N-K)$ degrees of freedom, the decision about no contradiction of restored regression to experimental data with probability $1-\alpha$ is made. Here $1-\alpha$ is confidence probability.

If $v^2 < v_{\alpha/2}^2$, the message "simplify regression" is displayed, i.e. for restoration of functional dependence it is necessary to choose more simple dependence from among offered in the menu. If $v^2 > v_{1-\alpha/2}^2$, the message "complicate regress" is displayed.

In the program of realization of this algorithm there is an opportunity to set any allowable value of K – quantity of groups (interval of allowable values is underlined in the bottom line of the display) and α – the significance value of criterion.

24. Linear multiple regression

In this task, as against all the considered above, a dependent variable is represented as a function from m independent variables X_1, ..., X_m. The regression model looks like [12]

$$y_i = \sum_{k=1}^{m} A_k \, X_{ki} + \varepsilon_i,$$

where the unknown coefficients A_1, ..., A_m are necessary to determine on the basis of experimental data: y_i, x_{ki}, $k = 1, ..., m$; $i = 1, ..., N$; $\mathrm{M}(\varepsilon_\mathrm{i}) = 0$; $\mathrm{D}(\varepsilon_\mathrm{i}) = \sigma_\mathrm{i}^2$; $\mathrm{cov}(\varepsilon_\mathrm{i}, \varepsilon_\mathrm{k}) = 0$, $i \neq k$.

The criterion of the least squares is written as follows:

$$S = \sum_{i=1}^{N} \lambda_i \cdot \left(\sum_{k=1}^{m} A_k \, X_{ki} - y_i \right)^2 \Rightarrow \min,$$

where $\lambda_i = 1/\sigma_i^2$. The minimum is achieved at

$$\begin{bmatrix} A_1 \\ A_2 \\ \cdots \\ A_m \end{bmatrix} = \xi^{-1} \cdot \begin{bmatrix} \eta_1 \\ \eta_2 \\ \cdots \\ \eta_m \end{bmatrix},$$

where ξ is the $m \times m$ matrix with elements

$$\xi_{jk} = \sum_{L=1}^{N} \lambda_L \cdot X_{jL}\, X_{kL};$$

$$\eta_k = \sum_{L=1}^{N} \lambda_L \cdot y_L\, X_{kL}.$$

25. The basic properties of restored dependencies

Geometrical dependence

$$f(x) = a \cdot x^b.$$

The plots of the function $f(x)$ at $a > 0$ and different, accordingly, positive and negative values of parameter b are given on the figure 1 a) and b). At $a < 0$ the appropriate plots can be received from the given on the figure by mirror display concerning the axis x. At $b < 0$ the axes of coordinates serve as asymptotes of the plots.

Exponential dependence

$$f(x) = a \cdot e^{bx}.$$

The plots of the function $f(x)$ at $a = 1$ and different values of the parameter b are given in figure 2. The plots pass through the point $\{0, 1\}$ and have the common asymptote, coincide with the axis x.

Logarithmic dependence The plots of the function $f(x)$ at $b = 1$ and different values of the parameter a are given in the figure 3. The plots pass through the point $\{1, 0\}$ and have common asymptote, coincide with the axis y. At $b \neq 1$ the plots of the function $f(x)$ turn out from the given on the figure at shift last along the axis of ordinates on distance $a \cdot \ln b$.

Geometric-Exponential dependence

$$f(x) = a \cdot x^b \cdot e^{cx}$$

at $x > 0$.

If the number $x_0 = -b/c$ belongs to the domain of the function $f(x)$ (i.e. if $bc < 0$), then the considered function has unique extreme in the point $x = x_0$, otherwise it has no extreme. If the plot of this function has an inflection point, an abscess of this point is equal

$$x_1 = \frac{-b + \sqrt{b}}{c} \quad \text{or} \quad x_2 = \frac{-b - \sqrt{b}}{c}.$$

The plots of the function $f(x)$ at $a > 0$ are represented in the fig. 4; at $a < 0$ corresponding plots can be received from the given on the figure by mirror display concerning the axis x. Depending on values of the parameters b and c there are eight possible cases:

a) at $c > 0$ and $b > 1$ the function increases monotonously; the plot is tangent to the axis x in the point $\{0, 0\}$;

b) at $c > 0$ and $b = 1$ the function increases monotonously; the plot passes through the point $\{0, 0\}$ and is tangent in this point by the straight line $y = x$;

c) at $c > 0$ and $0 < b < 1$ the function increases monotonously; the plot is tangent to the axis y in the point $\{0, 0\}$ and has one inflection point with abscess x_1;

d) at $c > 0$ and $b < 0$ the function has a minimum in the point x_0; the axis y is the asymptote of the plot;

e) at $c < 0$ and $b > 1$ the function has a maximum in the point x_0; the plot is tangent to the axis x in the point $\{0, 0\}$ and has two inflection points; the axis x is the asymptote;

f) at $c < 0$ and $b = 1$ the function has a maximum in the point $x_0 = -1/c$; the plot passes through the point $\{0, 0\}$ and is tangent in this point to the straight line $y = ax$; has one inflection point with the abscess $x_2 = -2/c$;

g) at $c < 0$ and $0 < b < 1$ the function has a maximum in the point x_0; the plot is tangent to the axis y in the point $\{0, 0\}$ and has one inflection point with the abscess x_2;

h) at $c < 0$ and $b < 0$ the function monotonously decreases; the axes of ordinates are the asymptotes of the plot.

Inverse-Exponential dependence

$$f(x) = a \cdot \left(1 - e^{-bx}\right).$$

The plots of the function $f(x)$ at $a > 0$ and various positive values of the parameter b are represented in the fig. 5. The plots pass through the origin of coordinates and have common horizontal asymptote, represented by the equation $y = a$. At $a < 0$ the corresponding plots can be received from the given on the figure by mirror display concerning the axis x.

Geometrical dependence with a free term

$$f(x) = a + b \cdot x^c.$$

The plots of this function turn out from the considered above plots of geometrical dependence $F(x) = b \cdot x^c$ at shift the latter along the axis of ordinates on the distance a.

Exponential dependence with a free term

$$f(x) = a + b \cdot e^{cx}.$$

The plots of this function turn out from the considered above plots of exponential dependence $F(x) = b \cdot e^{cx}$ at shift the latter along the axis of ordinates on the distance a.

Linear-Exponential dependence

$$f(x) = (a + b\,x) \cdot e^{cx}$$

at $bc \neq 0$.

This function has an unique point of extreme

$$x_0 = -1/c - a/b,$$

being a point of the minimum at $b > 0$ and point of the maximum at $b < 0$.

The plot of this function has a unique inflection point with abscess

$$x_{inf} = -2/c - a/b.$$

The function $f(x)$ becomes zero at $x = x_z = -a/b$.

At $x \to -\infty \cdot \mathrm{sing\,c} \quad f(x) \to 0$; at $x \to +\infty \cdot \mathrm{sing\,c} \quad f(x) \to +\infty \cdot \mathrm{sing\,(bc)}$. Here

$$\mathrm{sing\,x} = \begin{cases} -1 & \text{at } x < 0, \\ 1 & \text{at } x > 0. \end{cases}$$

The plots of the dependence $f(x)$ from $x + a/b$ at different signs of b and c are represented in the fig. 6.

Linear-Exponential dependence with a free term

$$f(x) = h + (a + b\,x) \cdot e^{cx}.$$

The plots of this function turn out from the considered above plots of the linear-exponential dependencies

$$F(x) = (a + b\,x) \cdot e^{cx}.$$

at shift of the latter along the axis of ordinates on the distance h.

Product of geometrical dependencies

$$f(x) = a\,x^c \cdot (1 - b\,x)^d.$$

The conditions are assumed executed: $a, b, c, d \neq 0$; $0 < x < 1/b$ at $b > 0$ or $0 < x < +\infty$ at $b < 0$. Let us denote

$$x_0 = \frac{c}{b\,(c + d)};$$

then $1 - bx_0 = d/(c + d)$.

If the number x_0 belongs to domain of the function $f(x)$ then the considered function has unique extreme in the point $x = x_0$; otherwise it has no extremes. If the plot of this function has an inflection point then the abscess of this point is equal to x_1 or x_2, where bx_1 and bx_2 are roots of the square equation

$$(c + d)(c + d - 1) \cdot x^2 - 2c\,(c + d - 1) \cdot x + c\,(c - 1) = 0.$$

The plots of the function $f(x)$ at $a > 0$ are represented in the fig. 7; at $a < 0$ the corresponding plots can be received from the given on the figure by mirror display concerning the axis x. Depending on signs of the parameters b, c and d the different cases are possible.

a) $b > 0$, $c > 0$ and $d > 0$. The function $f(x)$ has the maximum in the point x_0; at $x \to 0$ and at $x \to 1/b$ $f(x) \to 0$;

b) $b > 0$, $c > 0$ and $d < 0$. The function increases everywhere; at $x \to 0$ $f(x) \to 0$; at $x \to 1/b$ $f(x) \to +\infty$; the straight line $x = 1/b$ is the asymptote of the plot of the considered function.

c) $b > 0$, $c < 0$ and $d > 0$. The function everywhere decreases; at $x \to 0$ $f(x) \to +\infty$; at $x \to 1/b$ $f(x) \to 0$; the axis y is the asymptote of the plot of the considered function.

d) $b > 0$, $c < 0$ and $d < 0$. The function has a minimum in the point x_0; at $x \to 0$ and at $x \to 1/b$ $f(x) \to +\infty$; the plot of the function has two vertical asymptote: $x = 0$ and $x = 1/b$.

e) $b < 0$, $c > 0$ and $c + d > 0$. The function increases monotonously; at $x \to 0$ $f(x) \to 0$; at $x \to +\infty$ $f(x) \to +\infty$.

f) $b < 0$, $c > 0$ and $c+d < 0$. The function has a maximum in the point x_0; at $x \to 0$ and at $x \to +\infty$ $f(x) \to 0$.

g) $b < 0$, $c < 0$ and $c+d > 0$. The function has a minimum in the point x_0; at $x \to 0$ and at $x \to +\infty$ $f(x) \to +\infty$.

h) $b < 0$, $c < 0$ and $c + d < 0$. The function monotonously decreases; at $x \to 0$ $f(x) \to +\infty$; at $x \to +\infty$ $f(x) \to 0$; the axes of ordinates are the asymptotes of the plot of the considered function.

i) At $x \to 0$ $f(x) \sim a \cdot x^c$. From here follows, that at $c > 0$ and anyone a, b, d the plot of the function $f(x)$ is tangent to the axis of abscess (at $c > 1$), or straight line $y = ax$ (at $c = 1$), or axis of ordinates (at $0 < c < 1$) in the point $\{0, 0\}$. At $b < 0$ plots of the function $f(x)$ behave similarly to the appropriate plots of the function $\varphi(x) = a \cdot x^c \cdot e^{(c+d)x}$ (see fig. 4).

j) At $b > 0$, $d > 0$ and anyone a and c the plot of the function $f(x)$ is tangent to the axis of abscess (at $d > 1$), or straight line $y = a\,b^{-c} - ad\,b^{1-c} \cdot x$ (at $d = 1$), or axis of ordinates (at $0 < d < 1$) in the point $\{0, 1/b\}$.

The sum of exponential dependencies

$$f(x) = a\,e^{cx} + b\,e^{dx}.$$

Let $c < d$. Then

a) at $abcd < 0$ the point

$$x_0 = (d - c)^{-1} \cdot \ln\left(-\frac{ac}{bd}\right)$$

is a unique point of extreme of the function $f(x)$, otherwise the considered function has no extremes;

b) at $ac > 0$ and $bd > 0$ the function $f(x)$ everywhere increases;

c) at $ac < 0$ and $bd < 0$ the function $f(x)$ everywhere decreases;

d) at $ac > 0$ and $bd < 0$ the function $f(x)$ has a maximum at $x = x_0$;

e) at $ac < 0$ and $bd > 0$ the function $f(x)$ has a minimum at $x = x_0$;

f) at $ab < 0$ the point

$$x_{inf} = (d - c)^{-1} \cdot \ln\left(-\frac{a\,c^2}{b\,d^2}\right)$$

is an unique inflection point of the plot of the function $f(x)$, otherwise the plot of considered function has no inflection points.

The plots of the function $f(x)$ at $|c| < |d|$ and different signs of the parameters a, b, c, d are represented in the fig. 8.

Depending on signs of the parameters a, b, c, d it is possible to allocate four types.

a) $ab > 0$ and $cd > 0$ (the squares A-1, C-1, A-4, C-4 in the fig. 8): the function everywhere is monotonous; the extremes and the zero points are absent; the plot has no inflection points; the axis x is the asymptote.

b) $ab > 0$ and $cd < 0$ (the squares B-1 and B-4 in the fig. 8): the function has one extreme (minimum at $a > 0$ and maximum at $a < 0$); zero points are absent; the plot has no inflection points and asymptotes;

c) $ab < 0$ and $cd > 0$ (the squares A-2, C-2, A-3, C-3 in the fig. 8): the function has one extreme (maximum at $a \cdot (d-c) > 0$ both minimum at $a \cdot (d-c) < 0$ and one zero point; the plot has one inflection point; the axis x is the asymptote;

d) $ab < 0$ and $cd < 0$ (the squares B-2 and B-3 in the fig. 8): the function has no extremes, everywhere is monotonous; has one zero point; the plot has one inflection point; asymptotes are absent.

The sum of geometrical dependencies

$$f(x) = a \cdot x^c + b \cdot x^d.$$

The function $f(x)$ will be transformed to the considered above function

$$F(t) = a \cdot e^{ct} + b \cdot e^{dt}.$$

at replacement of the independent variable $t = \ln x$. The plots of the function $f(x)$ at $|c| < |d|$ and different signs of the parameters a, b, c, d are represented in the fig. 9.

The sum of exponential dependencies with a free term

$$f(x) = h + a \cdot e^{cx} + b \cdot e^{dx}.$$

Plots of this function turn out from the considered above plots of the sum of exponential dependencies

$$F(x) = a \cdot e^{cx} + b \cdot e^{dx}.$$

at shift of the latter along the axis of ordinates on the distance h.

The sum of geometrical dependencies with a free term

$$f(x) = h + a \cdot x^c + b \cdot x^d.$$

Plots of this function turn out from the considered above plots of the sum of geometrical dependencies

$$F(x) = a \cdot x^c + b \cdot x^d.$$

at shift of the latter along the axis of ordinates on the distance h.

Exponential-sine wave dependence

$$f(t) = e^{ct} \cdot \big(A \cos(\omega t) + B \sin(\omega t)\big), \qquad t > 0,\ c\omega \neq 0.$$

This function can also be represented as

$$f(t) = a \cdot e^{ct} \cdot \cos(\omega t + \varphi) = a \cdot e^{ct} \cdot \sin(\omega t + \psi),$$

where

$$a^2 = A^2 + B^2; \quad \tan\varphi = -B/A; \quad \tan\psi = A/B; \quad \psi = \varphi + 2\pi/4.$$

Let us assign also auxiliary parameters

$$T \equiv 2\pi/\omega; \qquad \Omega \equiv |\omega - ic|; \qquad h \equiv \arg(\omega - ic),$$

where i is the imaginary unit.

The function $f(t)$ everywhere is continuous; becomes zero in the points $t_k = Tk/2 - \psi/\omega$, has maxima in the points $p'_k = Tk - (\varphi + h)/\omega$ and minima in the points $p''_k = T \cdot (k + 1/2) - (\varphi + h)/\omega$;

$$f(p'_k) = (a\omega/\Omega)\cdot\exp(-sp'_k); \quad f(p''_k) = -(a\omega/\Omega)\cdot\exp(-sp''_k) \quad (k = 0, \pm1, ...).$$

The function $f(t)$ is not periodic, however it becomes zero, and also achieves of the maximal and minimal values through intervals of identical length equal to T.

Plot of the function $f(t)$ (see fig. 10) is located in the area limited by the plots of the functions $y = a \cdot e^{ct}$ and $y = -a \cdot e^{ct}$ and has an asymptote, coincides with the axis of abscess. The abscess of points of tangency of the considered curve with plot of the function $y = a \cdot e^{ct}$ are equal to $q'_k = Tk - \varphi/\omega$; the abscess of points of tangency of this curve with plot of the function $y = -a \cdot e^{ct}$ are equal to $q''_k = T \cdot (k + 1/2) - \varphi/\omega$. The abscess of inflection points are $H_k = Tk/2 - (\psi + 2h)/\omega$.

Exponential-sine wave dependence with a free term

$$f(t) = h + e^{ct} \cdot \big(A \cos(\omega t) + B \sin(\omega t)\big), \qquad t > 0,\ c\omega \neq 0.$$

Plots of this function turn out from the considered above plots of the exponential-sine wave dependence

$$F(t) = e^{ct} \cdot \big(A \cos(\omega t) + B \sin(\omega t)\big)$$

at shift of the latter along the axis of ordinates on the distance h.

Polynomial dependence

$$f(x) = \sum_{k=0}^{m} p_k \, x^k.$$

If there is not imposed restrictions on the number m, the function $f(x)$ can have any number of maxima and minima in any points and accept any values in these points. Therefore it is not obviously possible to specify any general laws for this function.

The same is possible to say about all following functional dependencies:

Geometrical-Polynomial dependence

$$f(x) = x^c \cdot \sum_{k=0}^{m} p_k \, x^k;$$

Exponential-Polynomial dependence

$$f(x) = e^{cx} \cdot \sum_{k=0}^{m} p_k \, x^k;$$

Logarithmic-Polynomial dependence

$$f(x) = c \cdot \ln \left(\sum_{k=0}^{m} p_k \, x^k \right);$$

Periodic dependence

$$f(t) = \sum_{k=0}^{m} \bigl(A_k \cdot \cos(k\omega t) + B_k \cdot \sin(k\omega t) \bigr).$$

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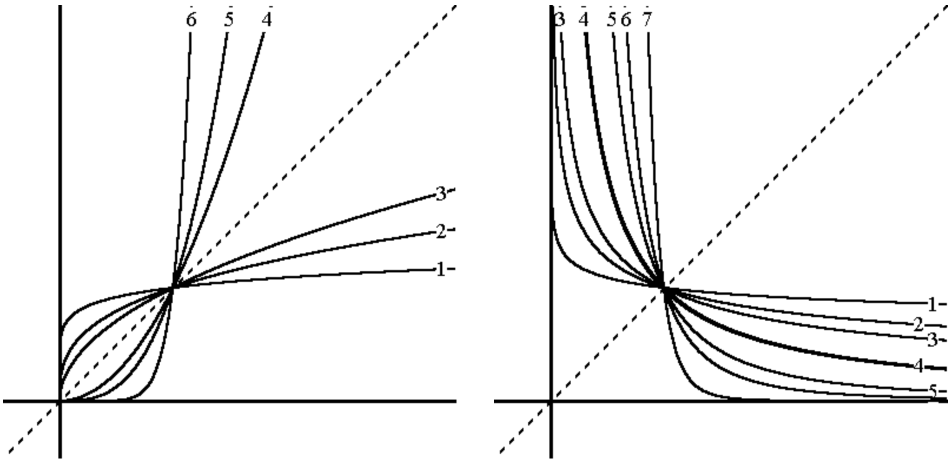


Figure 1: The graph of the function $y = x^b$ at different values of b:

a) (positive values of b)

$b = 1/8$ (1), $b = 2$ (4),
$b = 1/3$ (2), $b = 3$ (5),
$b = 1/2$ (3), $b = 8$ (6).

b) (negative values of b)

$b = -1/8$ (1), $b = -2$ (5),
$b = -1/3$ (2), $b = -3$ (6),
$b = -1/2$ (3), $b = -8$ (7).
$b = -1$ (4),

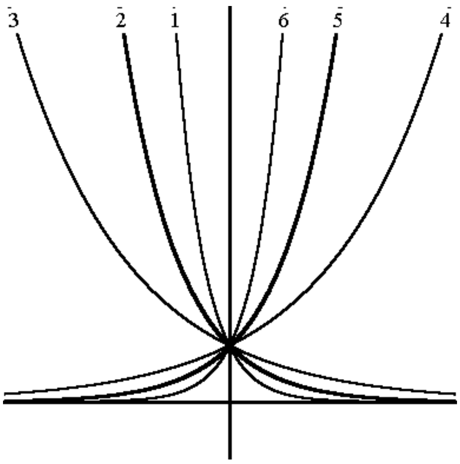


Figure 2: The graph of the function $y = e^{bx}$ at different values of b:

$a = -2$ (1), $a = 1/2$ (4),
$a = -1$ (2), $a = 1$ (5),
$a = -1/2$ (3), $a = 2$ (6).

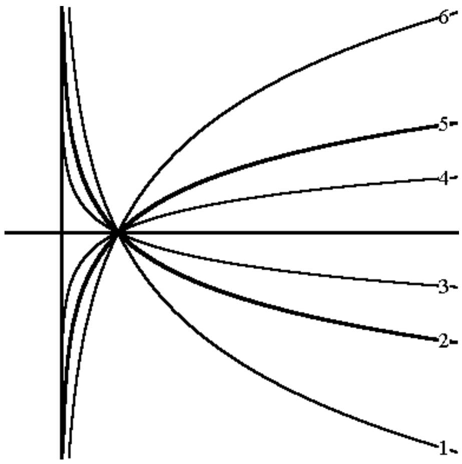


Figure 3: The graph of the function $y = a \cdot \ln x$ at different values of a:

$b = -2$ (1), $b = 1/2$ (4),
$b = -1$ (2), $b = 1$ (5),
$b = -1/2$ (3), $b = 2$ (6).

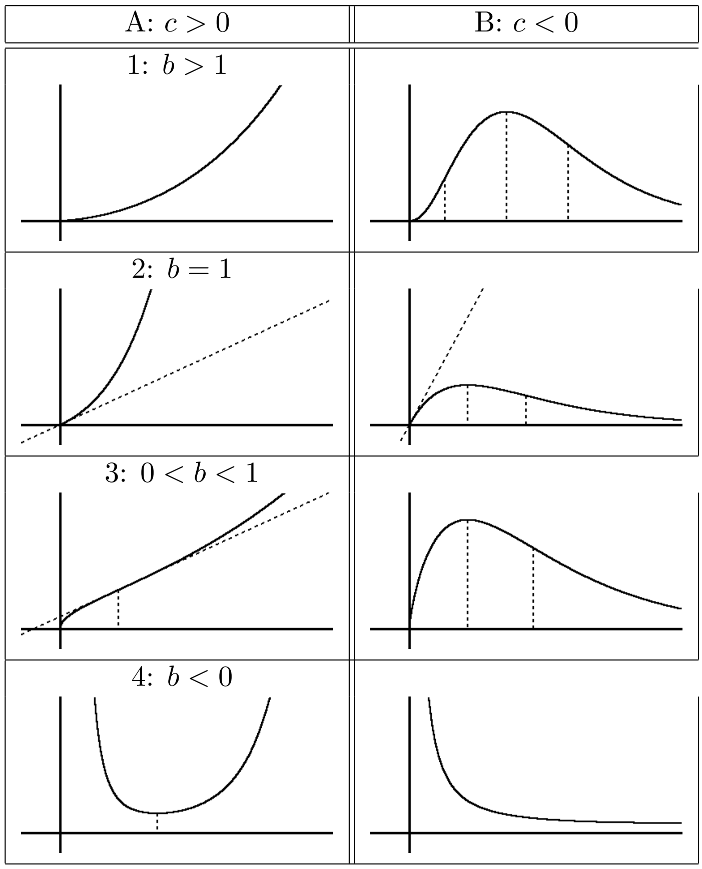


Figure 4: The graph of the function $y = a \cdot x^b \cdot e^{cx}$ at $a > 0$ and different areas of change of the parameters b and c.

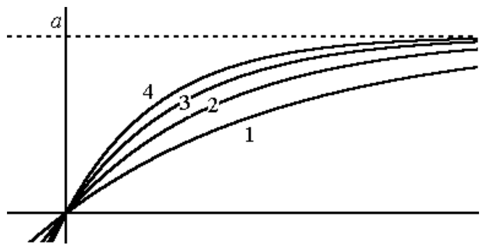


Figure 5: The graph of the function $y = a \cdot (1 - e^{-bx})$ at different values of b:

$$b = 0.5 \text{ (1)},\ b = 0.75 \text{ (2)},\ b = 1 \text{ (3)},\ b = 1.25 \text{ (4)}.$$

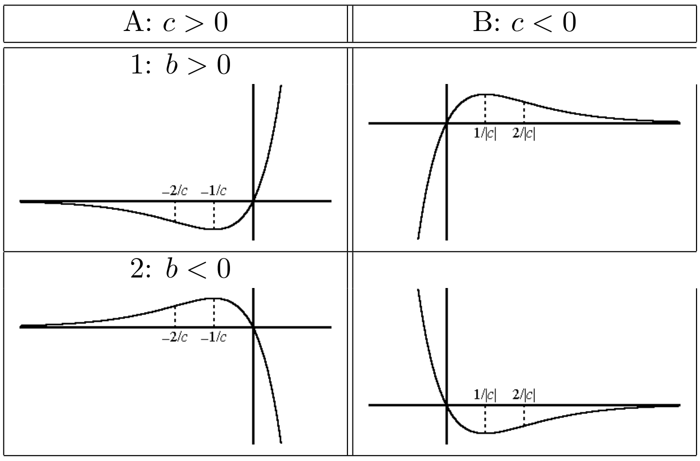
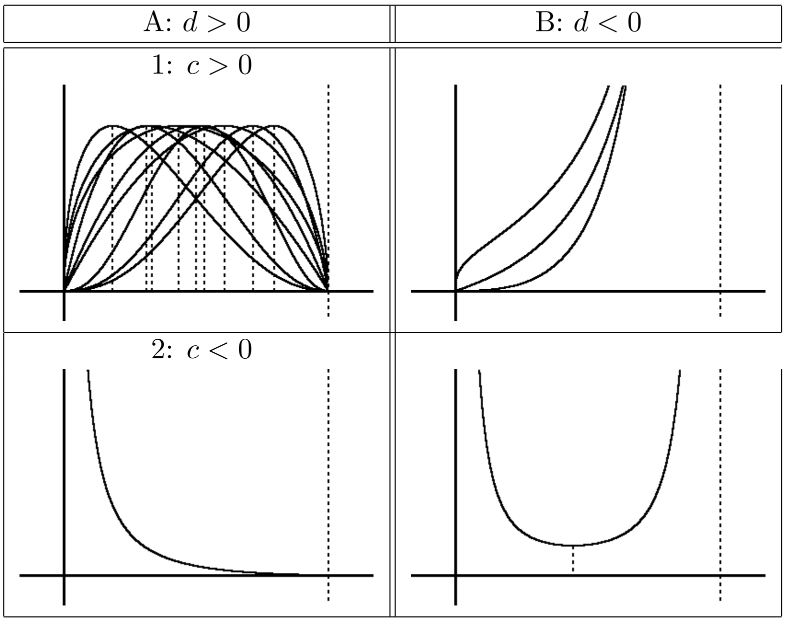


Figure 6: The graph of the function $y = (a + b\,x) \cdot e^{cx}$ from $t = x + a/b$ at different signs of the parameters b and c.

I: $b > 0$



II: $b < 0$

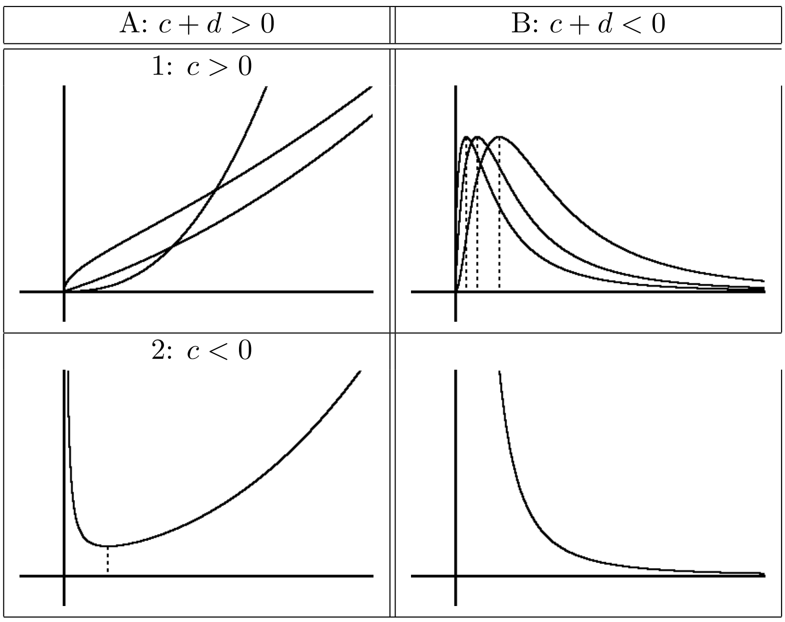


Figure 7: The graph of the function $y = a \cdot x^c \cdot (1 - b\,x)^d$ at $a > 0$ and different areas of change of the parameters b, c, d.

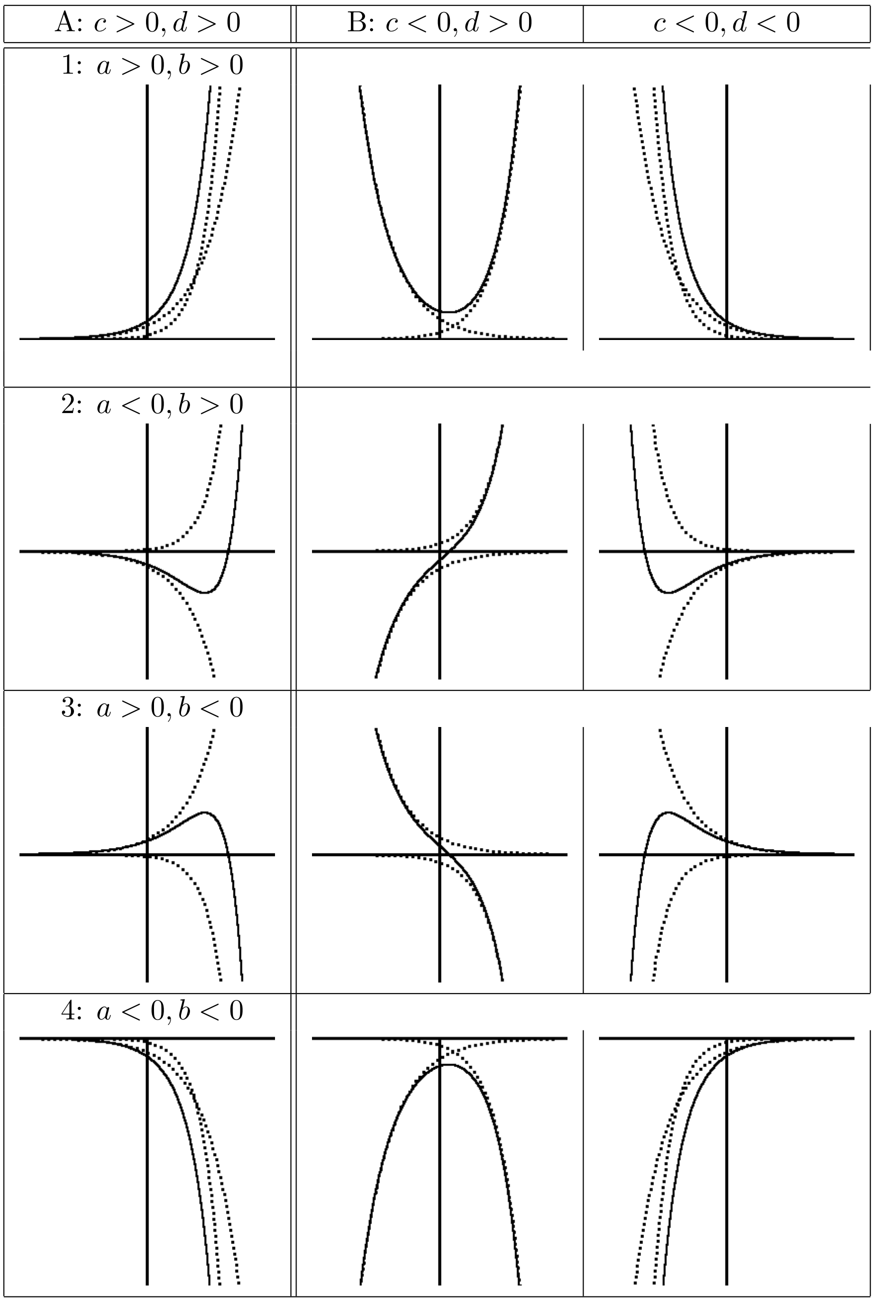


Figure 8: The graph of the function $y = a \cdot e^{cx} + b \cdot e^{dx}$ at different signs of the parameters a, b, c, d. Curves of dots in everyone cell of the table are plots of the exponential dependencies $y = a \cdot e^{cx}$ and $y = b \cdot e^{dx}$.

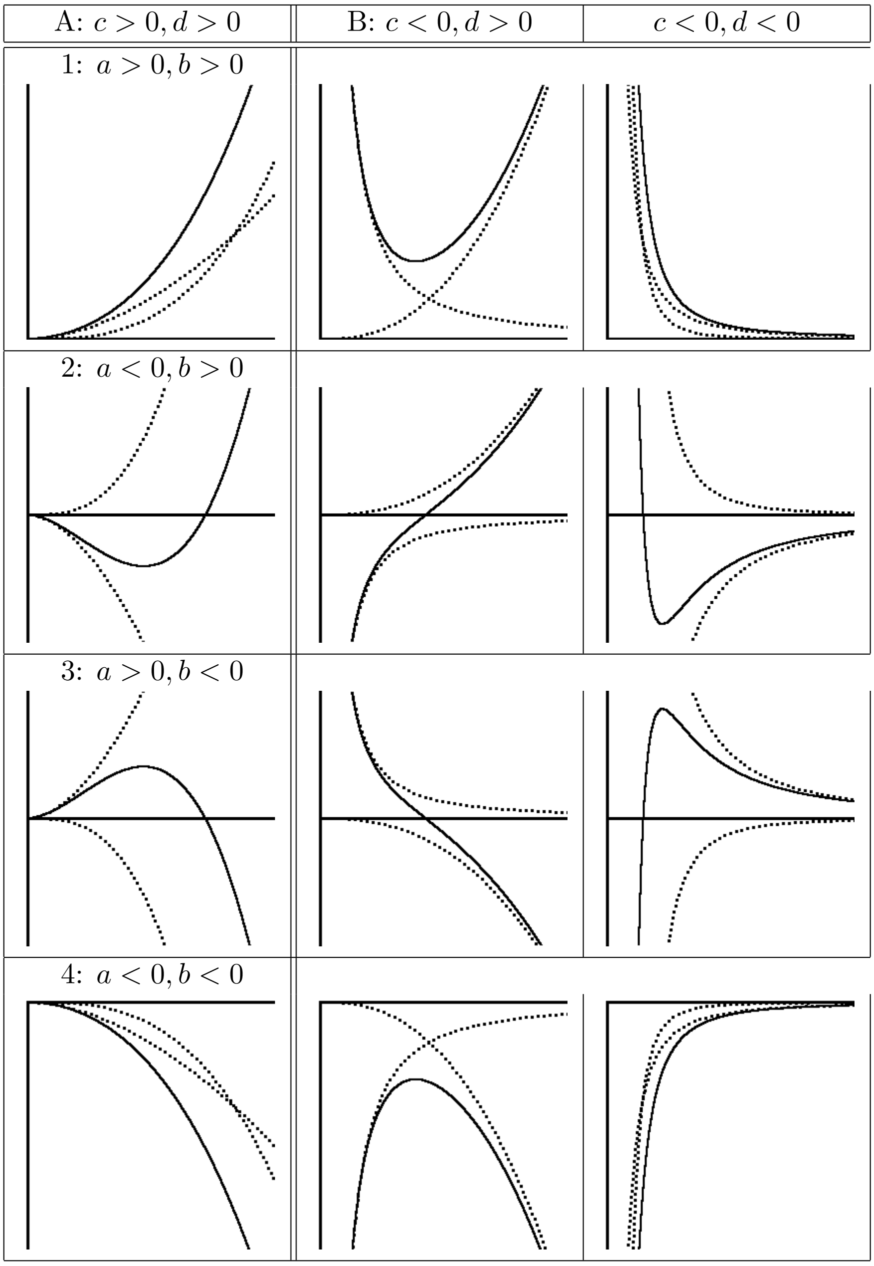


Figure 9: The graph of the function $y = a \cdot x^c + b \cdot x^d$ at different signs of the parameters a, b, c, d. Curves of dots in everyone cell of the table are plots of the geometrical dependencies $y = a \cdot x^c$ and $y = b \cdot x^d$.

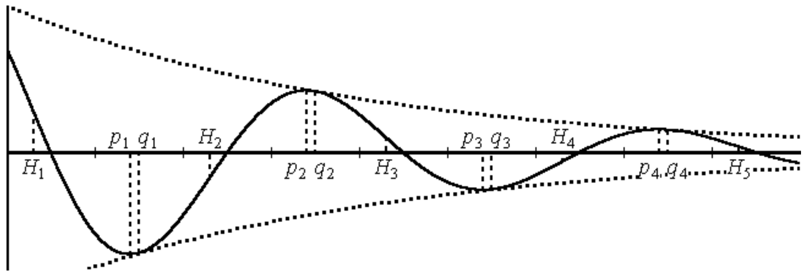


Figure 10: The graph of the function $y = e^{-ct}\left(a \cdot \cos(\omega\, t) + b \cdot \sin(\omega\, t)\right)$ (unbroken curve), $y = a \cdot e^{-ct}$ and $y = -a \cdot e^{-ct}$ (curves of dots).