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# Models Nonlinear by Parameters

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**Abstract**

In this work we spoke about the method of construction of models nonlinear by parameters with solution of system of nonlinear algebraic equations by combination of methods. We observed that method of shortest downhill is though universal, but rough for obtaining amplified values, we can use more subtle Newton-Rafson's method but we must take into account initial meanings of parameters rather close to real, which we can obtain by preliminary use of method of shortest downhill. Numerical example is given and methods for overcoming of difficulties is shown.

Mathematical models which are constructed according to the results of analysis of experimental data often have the form [1]:

$$y = f(b_j; x_j), \tag{1}$$

where $y$ is a dependent variable, $x_j$ is a set of independent variables $j = \overline{0,p}$, where $p$ is any integer number, $b_j$ is a set of parameters of the right part of the model. If the model (1) is nonlinear according to independent variables, it is easy to linearize it by substitutional method.

It is constructed by method of least squares with solution of the system of normal equations which are linear in coordination with the parameters $b_j$.

If the model (1) is nonlinear by parameters $b_j$, this case is more difficult, and it is connected with solution of systems of nonlinear algebraic equations with all consequences followed (initial aproximations are known, convergence or divergence of solution, extremum etc.).

Which reflects the fenomenon in consideration may have local extremums besides the global one, that is why there is no confidence that in process of solution of system of nonlinear algebraic equations we get that particular result the researcher has been striving for. Also it should be born in mind that the choice of the number of parameters depends on researcher's intuitive conceptions and is a procedure to a considerable extent arbitrary. From the technical point of view during execution with exponents one more difficulty is met. Intermediate results often have very small value (for example $0.1 \times 100^{-200}$) such a situation is called "machine zero".

That's why the problem of construction of a model nonlinear by parameters is as a rule solved by computers many times, the number of parameters being varied in various ways with various initial approximations.

During non-linear parametrization appears a necessity of solving the system of non-linear algebraic equation

$$\begin{array}{c} f_1(b_1, b_2, \ldots, b_p) = 0 \\ f_2(b_1, b_2, \ldots, b_p) = 0 \\ \ldots\ldots\ldots\ldots\ldots \\ f_p(b_1, b_2, \ldots, b_p) = 0 \end{array} \tag{2}$$

It is clear that besides parameters $b_j$ in the system dependent variables $y_i$ and independent variables $x_{ij}$ are present. They are omitted for briefness, because differentiation of the expression

$$U = \sum_{i=1}^{n} W_i [y_i - \eta(\vec{\beta}, \vec{x})]^2 \tag{3}$$

was carried out with respect to the parameters $b_j$.

It is necessary to find value of $B$ that satisfies expression (2), where $B$ presents $p$ - dimensional vector of unknown parameters

$$B = \left\| \begin{array}{c} b_1 \\ b_2 \\ \vdots \\ b_p \end{array} \right\| \tag{4}$$

System (2) can be rewritten as $p$ - dimensional vectorial equation:

$$F(B) = 0 \tag{5}$$

Let's suppose that the difference between the initial approximation $B^o$ and the solution of system of nonlinear equations is a small vector $\Delta B$ if the function $F(B)$ is differentiable for sufficient number of times in $B^o$ Taylor's decomposition can be used

$$F(B) = F(B^o + \Delta B) = FB^o + J_o(B - B^o) + \ldots = 0 \tag{6}$$

where $J_o$ is Jakoby's array at the point $B^o$

$$J_o = \begin{Vmatrix} \frac{\partial f_1}{\partial b_1^o} & \frac{\partial f_1}{\partial b_2^o} & \cdots & \frac{\partial f_1}{\partial b_p^o} \\ \frac{\partial f_2}{\partial b_1^o} & \frac{\partial f_2}{\partial b_2^o} & \cdots & \frac{\partial f_2}{\partial b_p^o} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial f_p}{\partial b_1^o} & \frac{\partial f_p}{\partial b_2^o} & \cdots & \frac{\partial f_p}{\partial b_p^o} \end{Vmatrix} \tag{7}$$

If in decomposition we limit ourselves with only linear terms we'll obtain:

$$0 \approx F(B^o) + J_o(B - B^o) \tag{8}$$

$$\Rightarrow B = B^o - J_o^{-1} F(B^o) \tag{9}$$

This value of $B$ is approximative but it can be used as an initial value on the next step of iteration. In general case a recurrent formula is obtained

$$B^{k+1} = B^k - J_k^{-1} F(B^k) \tag{10}$$

The process has been repeated till we have obtained $\mid \Delta B \mid \leq \varepsilon$ for some $\varepsilon$ given beforehand which is changed according to the precision of calculations.

The particular example of construction of a model nonlinear by parameters is expediently to examine. There are the following independent variables in this model:

$t$ is the age of concrete on the moment of observation and $(t - \tau)$ — time of observation in the dryings. This example is significant also because of the fact that we didn't manage to solve the system of algebraic equations using Newton-Rafson's method so we had to use the method of shortest downhill for construction of model for calculation of extension of creep of concrete of age $28 \leq \tau \leq 360$ days (more frequent case in constructions). The form of the model is usually like that:

$$C_(t,\tau) = \theta_\tau f(t-\tau) = (C_o + Ae^{-\gamma\tau})[1 - De^{\gamma_1(t-\tau)}] \tag{11}$$

If we introduce the symbols which are usually used in the practice of constructing empirical formula by statistical method: $y = C(t,\tau)$; $x_1 = \tau$; $x_2 = (t-\tau)$; $b_o = D$; $b_1 = \gamma$; $b_2 = \gamma_1$, then formula (11) will look as follows

$$y = (C_o + Ae^{-b_1 x_1})(1 - b_o e^{-b_2 x_2}) \tag{12}$$

Expression (12) is nonlinear by parameters $b_o, b_1, b_2$. If we have vector-columns of observation for $y, C_o, x_1, x_2, A$ it is possible to find parameters $b_o, b_1, b_2$. Using the method of estimation nonlinear we should take into consideration the already known value of $C_o$ and $A$ which are obtained by the following way:

$$C_o = 0.5C_{(\infty,28)}; \qquad A = 0.7C_{(\infty,28)}, \tag{13}$$

where $C_{(\infty,28)}$ is the limit value of size of creep of concrete

$$C_{(\infty,28)} = 63.68 * 10^{-7} \prod_{j=1}^{j=11} k_j \tag{14}$$

Initial data for calculation are taken from publications of many specialists. Initial meanings of independent variable $\hat{y}$ are calculated with the help of formula (12) at generally accepted meanings for $b_o, b_1, b_2$

Using Lejandr's principle we can write down that the sum of squares of deviations of value calculated by formula (12) from experimental values, must be minimal

$$U = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2_{min} \tag{15}$$

where

$$\hat{y} = (C_{oi} + A_i e^{-b_1 x_{1i}})(1 - b_o e^{-b_2 x_{2i}}) \tag{16}$$

In other words we should choose such values of parameters $b_o, b_1, b_2$ which would minimize the sum of squares of deviations $U$. So the problem consists in finding the minimum of function $U_b$. Let us find partial derivates on all parameters and equate them with

$$\frac{\partial U(b)}{\partial b_o} = 0; \quad \frac{\partial U(b)}{\partial b_1} = 0; \quad \frac{\partial U(b)}{\partial b_2} = 0; \tag{17}$$

If we introduce the symbols

$$e_i(b) = y_i - \hat{y}_i(b) \tag{18}$$

formula (15) can be rewritten like this

$$U(b) = \sum_{i=1}^{n} e_i^2(b) \tag{19}$$

than we calculate

$$\begin{cases} \frac{\partial U(b)}{\partial b_o} = \sum\limits_{i=1}^{n} 2e_i(b)\frac{\partial e_i(b)}{\partial b_o}; \\ \\ \frac{\partial U(b)}{\partial b_1} = \sum\limits_{i=1}^{n} 2e_i(b)\frac{\partial e_i(b)}{\partial b_1}; \\ \\ \frac{\partial U(b)}{\partial b_2} = \sum\limits_{i=1}^{n} 2e_i(b)\frac{\partial e_i(b)}{\partial b_2}; \end{cases} \tag{20}$$

Taking into consideration (18) we obtain

$$\begin{aligned} \frac{\partial e_i(b)}{\partial b_o} &= \frac{\partial}{\partial b_o}\Big[y_i - \hat{y}_i(b)\Big] = -\frac{\partial \hat{y}_i(b)}{\partial b_o}; \\ \frac{\partial e_i(b)}{\partial b_1} &= \frac{\partial}{\partial b_1}\Big[y_i - \hat{y}_i(b)\Big] = -\frac{\partial \hat{y}_i(b)}{\partial b_1}; \\ \frac{\partial e_i(b)}{\partial b_2} &= \frac{\partial}{\partial b_2}\Big[y_i - \hat{y}_i(b)\Big] = -\frac{\partial \hat{y}_i(b)}{\partial b_2}; \end{aligned} \tag{21}$$

If we substitute $\hat{y}_i(b)$ in (21) we'll get the system

$$\begin{cases} \frac{\partial e_i(b)}{\partial b_o} = e^{-b_2 x_2}(C_{oi} + A_i e^{-b_1 x_{1i}}); \\ \frac{\partial e_i(b)}{\partial b_1} = x_{1i} A_i e^{-b_1 x_{1i}}(1 - b_o e^{-b_2 x_{2i}}); \\ \frac{\partial e_i(b)}{\partial b_2} = x_{2i} b_o e^{-b_2 x_{2i}}(C_{oi} + A_i e^{b_1 x_{1i}}). \end{cases} \tag{22}$$

If we substitute (20) in (17) and take into consideration (22) we'll get the system

$$\begin{cases} \sum\limits_{i=1}^{n} e_i(b) e^{-b_2 x_{2i}} C_{oi} + A_i e^{-b_1 x_{1i}}) = 0; \\ \sum\limits_{i=1}^{n} e_i(b) x_{1i} A_i e^{-b_1 x_{1i}}(1 - b_o e^{-b_2 x_{2i}}) = 0; \\ \sum\limits_{i=1}^{n} e_i(b) x_{2i} b_o e^{-b_2 x_{2i}}(C_{oi} + A_i e^{-b_1 x_{1i}}) = 0. \end{cases} \tag{23}$$

This we call the system of algebraic equations $b_o, b_1, b_2$ nonlinear $b_x$ parameters. Its solution isn't very simple because the convergence here depends on chosen method of solution of system and initial approximations of coefficients $b_o, b_1, b_2$. When trying to solve the problem at first attempt we take as initial approximations those values of parameters which can usually come across in research work or concrete creeping $b_o^o = D = 0.85; b_1^o = \gamma = 0.012; b_2^o = \gamma_1 = 0.006$. On the basis of initial approximations the meanings have been calculated $\hat{y}_i(b)$ and $\hat{e}_i(b)$. We have the set of initial data with number of experiments which equals 141.

Then $\sum_{i=1}^{n} \left[e_i^2(b)\right]_o = 23067.64$. Attempt to solve the system (23) using the Newton-Rafson's method with the above shown initial approximations failed because the results diverge from the true ones. Then the second attempt was made to solve the system using method of shortest downhill, and a stable result was obtained. Newly found values of parameteres $b_o, b_1, b_2$ were taken as initial approximations when we used repeatedly Newton-Rafson's method and quickly convergent solution was obtained and considered to be a final one. Let's analyze the case of using method of shortest downhill using the example of the given problem. To make the solution simple we'll introduce symbols

$$\begin{cases} f_o(b_o, b_1, b_2) = \sum\limits_{i=1}^{n} e_i(b) e^{-b_2 x_{2i}} (C_{oi} + A_i e^{-b_1 x_{1i}}); \\ \\ f_1(b_o, b_1, b_2) = \sum\limits_{i=1}^{n} e_i(b) x_{1i} A_i e^{-b_1 x_{1i}} (1 - b_o e^{-b_2 x_{2i}}); \\ \\ f_2(b_o, b_1, b_2) = \sum\limits_{i=1}^{n} e_i(b) x_{2i} b_o e^{-b_2 x_{2i}} (C_{oi} + A_i e^{-b_1 x_{1i}}). \end{cases} \tag{24}$$

and rewrite the system in the following (23) way

$$\begin{cases} f_o(b_o, b_1, b_2) = 0; \\ \\ f_1(b_o, b_1, b_2) = 0; \\ \\ f_2(b_o, b_1, b_2) = 0. \end{cases} \tag{25}$$

Let's introduce also a new function

$$\Phi(b_o, b_1, b_2) = f_o^2(b_o, b_1, b_2) + f_1^2(b_o, b_1, b_2) + f_2^2(b_o, b_1, b_2). \tag{26}$$

Formula (26) takes minimal values at those values of parameters $b_o, b_1, b_2$ which answers to equations of the system, the calculations are made by the following formula

$$\begin{aligned} b_{o1,k+1} &= b_{o,k} - \Lambda_k \tfrac{\partial \Phi(b_{o,k}; b_{1,k}; b_{2,k})}{\partial b_o}; \\ \\ b_{1,k+1} &= b_{1,k} - \Lambda_k \tfrac{\partial \Phi(b_{o,k}; b_{1,k}; b_{2,k})}{\partial b_1}; \\ \\ b_{2,k+1} &= b_{2,k} - \Lambda_k \tfrac{\partial \Phi(b_{o,k}; b_{1,k}; b_{2,k})}{\partial b_2}; \end{aligned} \tag{27}$$

$$\Lambda_k = \frac{\Phi(b_{o,k}; b_{1,k}; b_{2,k})}{A + B + C} \tag{28}$$

$$A = \Big[\frac{\partial\Phi(b_{o,k}; b_{1,k}; b_{2,k})}{\partial b_o}\Big]^2; \tag{29}$$

$$B = \Big[\frac{\partial\Phi(b_{o,k}; b_{1,k}; b_{2,k})}{\partial b_1}\Big]^2; \tag{30}$$

$$C = \Big[\frac{\partial\Phi(b_{o,k}; b_{1,k}; b_{2,k})}{\partial b_2}\Big]^2; \tag{31}$$

From formula (26) we can see that:

$$\begin{aligned} \frac{\partial\Phi(b_o, b_1, b_2)}{\partial b_o} &= \frac{\partial}{\partial b_o}\Big[f_o^2(b_o, b_1, b_2) + f_1^2(b_o, b_1, b_2) + f_2^2(b_o, b_1, b_2)\Big] \\ &= 2\Big[f_o(b_o, b_1, b_2)\frac{\partial f_o(b_o, b_1, b_2)}{\partial b_o} \\ &\quad + f_1(b_o, b_1, b_2)\frac{\partial f_1(b_o, b_1, b_2)}{\partial b_o} \\ &\quad + f_2(b_o, b_1, b_2)\frac{\partial f_o(b_o, b_1, b_2)}{\partial b_o}\Big]; \end{aligned} \tag{32}$$

$$\begin{aligned} \frac{\partial\Phi(b_o, b_1, b_2)}{\partial b_1} &= \frac{\partial}{\partial b_1}\Big[f_o^2(b_o, b_1, b_2) + f_1^2(b_o, b_1, b_2) + f_2^2(b_o, b_1, b_2)\Big] \\ &= 2\Big[f_o(b_o, b_1, b_2)\frac{\partial f_o(b_o, b_1, b_2)}{\partial b_1} \\ &\quad + f_1(b_o, b_1, b_2)\frac{\partial f_1(b_o, b_1, b_2)}{\partial b_1} \\ &\quad + f_2(b_o, b_1, b_2)\frac{\partial f_o(b_o, b_1, b_2)}{\partial b_1}\Big]; \end{aligned} \tag{33}$$

$$\frac{\partial\Phi(b_o, b_1, b_2)}{\partial b_2} = \frac{\partial}{\partial b_2}\Big[f_o^2(b_o, b_1, b_2) + f_1^2(b_o, b_1, b_2) + f_2^2(b_o, b_1, b_2)\Big]$$

$$= 2\Big[f_o(b_o,b_1,b_2)\frac{\partial f_o(b_o,b_1,b_2)}{\partial b_2} + f_1(b_o,b_1,b_2)\frac{\partial f_1(b_o,b_1,b_2)}{\partial b_2} + f_2(b_o,b_1,b_2)\frac{\partial f_o(b_o,b_1,b_2)}{\partial b_2}\Big]. \quad (34)$$

in the formula (30)–(32)

$$\frac{\partial f_o(b_o,b_1,b_2)}{\partial b_o} = \sum_{i=1}^{n} e^{-2b_2x_{2i}}(C_{oi} + A_i e_{-b_1x_{1i}})^2; \quad (35)$$

$$\frac{\partial f_o(b_o,b_1,b_2)}{\partial b_1} = \sum_{i=1}^{n} x_{1i}A_i e^{-(b_1x_{1i}+b_2x_{2i})} \times\Big[(1-b_oe^{-b_2x_{2i}})(C_{oi}+A_ie^{-b_1x_{1i}}) - e_i(b)\Big]; \quad (36)$$

$$\frac{\partial f_o(b_o,b_1,b_2)}{\partial b_2} = -\sum_{i=1}^{n} x_{2i}e^{-b_2x_{2i}}(C_{oi}+A_ie^{-b_1x_{1i}}) \times\Big[e_i(b) + b_oe^{-b_2x_{2i}}(C_{oi}+A_ie^{-b_1x_{1i}})\Big]; \quad (37)$$

$$\frac{\partial f_1(b_o,b_1,b_2)}{\partial b_o} = \frac{\partial f_o(b_o,b_1,b_2)}{\partial b_1} \quad (38)$$

$$\frac{\partial f_1(b_o,b_1,b_2)}{\partial b_1} = \sum_{i=1}^{n} x_{1i}^2 A_i e^{-b_1x_{1i}}(1-b_oe^{-b_2x_{2i}}$$

$$\times\Big[A_i e^{-b_1x_{1i}}(1-b_oe^{-b_2x_{2i}})-e_i(b)\Big]; \qquad (39)$$

$$\frac{\partial f_1(b_o,b_1,b_2)}{\partial b_2} = \sum_{i=1}^{n} x_{1i}x_{2i}b_oe^{-(b_1x_{1i}+b_2x_{2i})} \times\Big[(1-b_oe^{-b_2x_{2i}})(C_{oi}+A_ie^{-b_1x_{1i}})-e_i(b)\Big].(40)$$

$$\frac{\partial f_2(b_o,b_1,b_2)}{\partial b_o} = \frac{\partial f_2(b_o,b_1,b_2)}{\partial b_2} \qquad (41)$$

$$\frac{\partial f_2(b_o,b_1,b_2)}{\partial b_1} = \frac{\partial f_1(b_o,b_1,b_2)}{\partial b_2} \qquad (42)$$

$$\frac{\partial f_2(b_o,b_1,b_2)}{\partial b_2} = \sum_{i=1}^{n} x_{2i}^2b_oe^{-b_2x_{2i}}(C_o+A_ie^{-b_1x_{1i}}) \times\Big[(b_oe^{-b_2x_{2i}}(C_{oi}+A_ie^{-b_1x_{1i}})-e_i(b)\Big]. \qquad (43)$$

Algorithm of solution of system of nonlinear equations using the Newton-Rafsons method is given above. As has already been noted above the attempt to use the Newton-Rafson's method at once for the solutions of system (25) at initial approximations $b_0^0 = 0.85; b_1^0 = 0.012; b_2^0 = 0.006$ failed. Probably these approximations were too far from true values of parameters and vector $\Delta B$ wasn't a small value. During the second step an attempt was made to solve the system using the method of shortest downhill at the same initial approximations. Calculations were being carried out with the help of computer at the number of observations n=141. The results happened to be rather encouraging and showed good convergence of method of shortest downhill while solving such problems. Already on the 8th iteration the error $\varepsilon_j = b_{j,k+1} - b_{j,k}$ was for $b_0 - 4.25 \times 10^{-5}\%$, for

$b_1 - 0.0493\%$, for $b_2 - 0,905\%$ and following values of parameters are obtained $b_0^8 = 0,85; b_1^8 = 0,0143; b_2^8 = 0,0047$. These values of parameters are taken as initial at repeated use of the method of Newton-Rafson, at the third step of solution of problem. On the 7th iteration the error took place: for $b_0 - 8,76 \times 10^{-6}\%$, for $b_1 - 0\%$,for $b_2 - 1.35 \times 10^{-5}\%$. And the following value of parameters $b_o = 0.683, b_1 = 0.0134, b_2 = 0.00344$ please compare with initial values: $b_0 = 0.85; b_1 = 0.012; b_2 = 0.006$. These values can be considered final for the taken array of experimental data and in this way the model becomes to look like:

$$C_{(t,\tau)} = \left(C_0 + A \times e^{-0.0134\tau}\right) \times \left[1 - 0.683e^{-0.00344(t-\tau)}\right] \qquad (44)$$

As we have already noted out at initial values of parameters the sum of square of deviation of calculated results from the experimental ones was:

$$\sum_{i=1}^{n} e_i^2 = 28067.64.$$

Calculation by method of shortest downhill made it possible to decrease this value up to value

$$\sum_{i=1}^{n} e_i^2 = 25391.61.$$

After amplificating parameter values using the Newton-Rafson's method finally obtained

$$\sum_{i=1}^{n} e_i^2 = 23887.52,$$

that is the sum of squares of deviation which has been decreased about 15%. The author hopes that above told method will allow many specialists to use the method of estimation nonlinear by parameters effectively for solution of practical problems.

## References

[1] E.Livovsky, Statistical Methods for Construction of Empirical Formulae, Moscow, "High Shcool", 1988, 240 p.

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