The problem of the initial approximation for a special nonlinear least squares problem*

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Abstract. *In [6] the existence theorem for the best least squares approximation of parameters for the exponential function is proved. In this paper we consider the problem of choosing a good initial approximation of these parameters.*

Key words: *least squares, existence problem, exponential function*

Sažetak.**Problem početne aproksimacije u jednom specijalnom nelinearnom problemu najmanjih kvadrata**. *U radu [6] dokazan je teorem o egzistenciji najbolje diskretne L_2 aproksimacije za eksponencijalnu funkciju. U ovom radu razmatra se problem izbora kvalitetne početne aproksimacije tih parametara.*

Ključne riječi: *problem najmanjih kvadrata, problem egzistencije, eksponencijalna funkcija*

1. The least squares problem for the exponential function

A mathematical model described by an exponential function

$$f(t; b, c) = b\, e^{ct}, \quad b, c \in R \tag{1}$$

or a linear combination of such functions is very often used in different areas of applied research, e.g. biology (see [7]), chemistry (see [2]), electrical engineering (see [8], [11]), economy (see [12]), astronomy (see [4]), nuclear physics (see [13]), etc. The unknown parameters b and c have to be determined on the basis of experimental data (p_i, t_i, f_i), $i = 1, \ldots, m$, where t_i denote the values of

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independent variable, f_i are the measured values of the corresponding dependent variable and $p_i > 0$ are the data weights.

In the sense of least squares, one obtains optimal parameters $b^\star$ and $c^\star$ of the exponential function (1) by minimizing the functional:

$$F(b,c) = \frac{1}{2}\sum_{i=1}^{m} p_i (b\, e^{ct_i} - f_i)^2. \tag{2}$$

In [6] the existence theorem of the optimal parameters $b^\star$ and $c^\star$ is proved, i.e. it was shown that there exists a point $(b^\star, c^\star)$ at which the functional F attains the global minimum. In this paper we consider the problem of choosing a good initial approximation needed for the iterative process by which one can obtain a good approximation of the optimal parameters $b^\star$ and $c^\star$ (e.g. the Gauss - Newton method or the Levenberg-Marquardt method — see [3]). Finally, we give results of some numerical experiments, where we test some possibilities for the choice of the initial approximation.

2. The problem of the initial approximation

In [6] the existence of the best least squares approximation of parameters in the exponential model (1) was shown, provided the data satisfy either the condition of preponderant increase or preponderant decrease. First, let us give a definition (see [10]).

Definition 1. *The data (p_i, t_i, f_i), $i = 1, \ldots, m$, are said to have the* preponderant increase *(resp.* preponderant decrease*) property, if the slope of the associated linear regression is positive (resp. negative). If this coefficient is equal to zero, then the data are said to be* preponderantly stationary*.*

Remark 1. *Let (p_i, t_i, f_i), $i = 1, \ldots, m$, be the data. Denote:*

$$Q := \sum_{i=1}^{m} p_i t_i f_i \sum_{i=1}^{m} p_i - \sum_{i=1}^{m} p_i t_i \sum_{i=1}^{m} p_i f_i. \tag{3}$$

In [10] it was shown that the data have the preponderant increase (resp. preponderant decrease) property if and only if $Q > 0$ (resp. $Q < 0$).

The proof of the next theorem can be found in [6]).

Theorem 1. *Let the data (p_i, t_i, f_i), $i = 1, \ldots, m$, be given and suppose that $f_i > 0$, $i = 1, \ldots, m$. Then*

(i) If the data have the preponderant increase property, then there exists a point $(b^\star, c^\star) \in \operatorname{Int}\mathcal{U}$,

$$\mathcal{U} = \left\{ (b,c) \in R^2 \,:\, b \geq 0, c \geq 0 \right\},$$

which minimizes the functional F defined by (2) on the set $\mathcal{U}$.

(ii) If the data have the preponderant decrease property, then there exists a point $(b^\star, c^\star) \in \operatorname{Int}\mathcal{V}$,

$$\mathcal{V} = \left\{ (b,c) \in R^2 \,:\, b \geq 0, c \leq 0 \right\},$$

which minimizes the functional F defined by (2) on the set $\mathcal{V}$.

The numerical methods (see [1], [3], [14]) for the minimization of the functional (2) require an initial approximation which should be as good as possible. We will show how to determine a sufficiently small range for the initial approximation, which guarantees that the iterative process converges to the solution quickly. We are going to prove the next theorem, using the results of *Theorem 1*

Theorem 2. *Suppose the given data (p_i, t_i, f_i), $i = 1, \ldots, m$, satisfy $(0 < t_1 < \ldots < t_m)$ & $(f_i > 0,\ i = 1, \ldots, m)$, and let the functional F be defined by (2). Denote:*

$$f_p := \frac{\sum_{i=1}^m p_i f_i}{\sum_{i=1}^m p_i}, \quad \overline{f}_p := \frac{\sum_{i=1}^m p_i t_i f_i}{\sum_{i=1}^m p_i t_i}. \tag{4}$$

(i) If the data have the preponderant increase property, then the point $(b^\star, c^\star) \in \operatorname{Int}\mathcal{U}$ of the global minimum of the functional F on the set $\mathcal{U}$ belongs to the set

$$\mathcal{R} = \left\{ (b,c) \in \mathcal{U} : \overline{f}_p e^{-c(2t_m - t_1)} \leq b \leq f_p e^{-c(2t_1 - t_m)} \right\}.$$

(ii) If the data have the preponderant decrease property, then the point $(b^\star, c^\star) \in \operatorname{Int}\mathcal{V}$ of the global minimum of the functional F on the set $\mathcal{V}$ belongs to the set

$$\mathcal{S} = \left\{ (b,c) \in \mathcal{V} : f_p e^{-c(2t_1 - t_m)} \leq b \leq \overline{f}_p e^{-c(2t_m - t_1)} \right\}.$$

Proof. Let us first show *(i)*. By *Theorem 1* there is a point $(b^\star, c^\star) \in \operatorname{Int}\mathcal{U}$ which minimizes the functional F defined by (2) on the set $\mathcal{U}$. Since the gradient of the functional F vanishes at the point $(b^\star, c^\star)$, we have

$$\sum_{i=1}^m p_i (b^\star e^{c^\star t_i} - f_i) e^{c^\star t_i} = 0, \tag{5}$$

$$\sum_{i=1}^m p_i t_i (b^\star e^{c^\star t_i} - f_i) e^{c^\star t_i} = 0. \tag{6}$$

In order to show *(i)*, let us first prove the inequalities

$$f_p e^{-c^\star (2t_m - t_1)} \leq b^\star \leq f_p e^{-c^\star (2t_1 - t_m)}. \tag{7}$$

Since $c^\star > 0$, from (5) we have

$$b^\star = \frac{\sum_{i=1}^m p_i f_i e^{c^\star t_i}}{\sum_{i=1}^m p_i e^{2c^\star t_i}} \le \frac{e^{c^\star t_m} \sum_{i=1}^m p_i f_i}{e^{2c^\star t_1} \sum_{i=1}^m p_i} = f_p e^{-c^\star(2t_1 - t_m)}.$$

$$b^\star = \frac{\sum_{i=1}^m p_i f_i e^{c^\star t_i}}{\sum_{i=1}^m p_i e^{2c^\star t_i}} \ge \frac{e^{c^\star t_1} \sum_{i=1}^m p_i f_i}{e^{2c^\star t_m} \sum_{i=1}^m p_i} = f_p e^{-c^\star(2t_m - t_1)}.$$

Similarly, using (6) one can show

$$\overline{f}_p e^{-c^\star(2t_m - t_1)} \le b^\star \le \overline{f}_p e^{-c^\star(2t_1 - t_m)}. \tag{8}$$

Since $0 < t_1 < \ldots < t_m$, and $Q > 0$, we have $f_p < \overline{f}_p$. From this and the inequalities (7) and (8) we conclude that the point $(b^\star, c^\star)$ belongs to the set

$$\mathcal{R} = \left\{(b,c) \in \mathcal{U} : \overline{f}_p e^{-c(2t_m - t_1)} \le b \le f_p e^{-c(2t_1 - t_m)}\right\}$$

(see *Figure 1.a*). This proves (i).

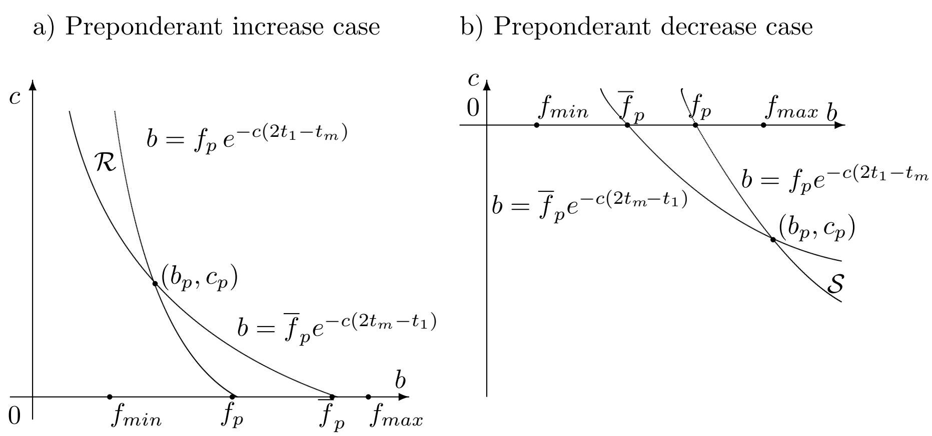

Figure 1.: The range for the choice of an initial approximation of optimal parameters

In order to show *(ii)*, suppose the data have the preponderant decrease property. By *Theorem 1* there is a point $(b^\star, c^\star) \in \operatorname{Int}\mathcal{V}$ which minimizes the functional F defined by (2) on the set $\mathcal{V}$. In the same way as proving *(i)*, one can prove the following inequalities

$$f_p e^{-c^\star(2t_1 - t_m)} \le b^\star \le f_p e^{-c^\star(2t_m - t_1)} \tag{9}$$

$$\overline{f}_p e^{-c^\star(2t_1 - t_m)} \le b^\star \le \overline{f}_p e^{-c^\star(2t_m - t_1)}. \tag{10}$$

Because $0 < t_1 < \ldots < t_m$ and $Q < 0$, we get $f_p > \overline{f}_p$. Using this and the inequalities (9) and (10), we conclude that the point $(b^\star, c^\star)$ belongs to the set

$$\mathcal{S} = \left\{(b,c) \in \mathcal{V} : f_p e^{-c(2t_1 - t_m)} \leq b \leq \overline{f}_p e^{-c(2t_m - t_1)}\right\}$$

(see *Figure 1.b*). □

According to *Theorem 2*, the initial approximation should be chosen either inside the set $\mathcal{R}$, or inside the set $\mathcal{S}$ (see *Figure 1*).

A possible good choice for the initial approximation is the point (b_p, c_p), the intersection point of the graphs of functions $c \mapsto b(c) = \overline{f}_p e^{-c(2t_m - t_1)}$ and $c \mapsto b(c) = f_p e^{-c(2t_1 - t_m)}$, i.e. the point

$$b_p = f_p \left(\frac{f_p}{\overline{f}_p}\right)^{(2t_1 - t_m)/(3t_m - 3t_1)}, \quad c_p = \frac{1}{3(t_m - t_1)} \ln\left(\frac{\overline{f}_p}{f_p}\right). \tag{11}$$

Another choice for a good initial approximation of the parameters for the model (1), is obtained by the known linearization method by taking logarithms (see e.g. [12], [13]). Namely, instead of minimizing the functional (2), we consider the minimization problem for the functional

$$\tilde{F}(b,c) = \frac{1}{2}\sum_{i=1}^{m} \omega_i \left[g(f(t_i; b, c)) - g(f_i)\right]^2, \tag{12}$$

where $g(x) = \ln(x)$, and ω_i are the new data weights. Note that because of the assumptions on the data in *Theorem 1*, the functional $\tilde{F}$ is well defined, and because of the properties of the logarithmic function, the minimization problem for the functional $\tilde{F}$ is a linear least squares problem, which always has a solution and is easily solved.

We shall define the new data weights ω_i so that the functional $\tilde{F}$ attains its minimum in a neighborhood of the point $(b^\star, c^\star)$.

Using the Lagrange's mean value theorem, we have

$$\tilde{F}(b,c) \approx \frac{1}{2}\sum_{i=1}^{m} \omega_i \left[g'(f(t_i; b, c))(f(t_i; b, c) - f_i)\right]^2, \tag{13}$$

Then $F \approx \tilde{F}$, provided

$$\frac{\omega_i}{f^2(t_i; b, c)} = p_i, \quad i = 1, \ldots, m. \tag{14}$$

Replacing $f(t_i; b, c)$ by the approximative value f_i in (14), we can expect that the functional $\tilde{F}$ with the new data weights ω_i defined by

$$\omega_i = p_i\, f_i^{-2}, \quad i = 1, \ldots, m, \tag{15}$$

will attain its minimum in a neighborhood of the point $(b^\star, c^\star)$. It can easily be checked that the functional $\tilde{F}$ attains its minimum at the point (b_l, c_l), with

$$c_l = \frac{\sum_{i=1}^m \omega_i (t_i - \tilde{t}_p)(\tilde{\varphi}_i - \tilde{\varphi}_p)}{\sum_{i=1}^m \omega_i (t_i - \tilde{t}_p)^2}, \qquad \ln b_l = \tilde{\varphi}_p - c_l \tilde{t}_p, \tag{16}$$

where $\tilde{t}_p = \frac{1}{\omega}\sum_{i=1}^m \omega_i t_i$, $\tilde{\varphi}_p = \frac{1}{\omega}\sum_{i=1}^m \omega_i \tilde{\varphi}_i$, $\tilde{\varphi}_i = \ln f_i$, $\omega = \sum_{i=1}^m \omega_i$.

Example 1. *Finally, we give an example illustrating the importance of the choice of a good initial approximation. We choose the data* (p_i, t_i, f_i), $i = 1, \dots, m$, *so that*

$$m = 50, \quad p_i = 1, \quad t_i = i + 10, \quad i = 1, \dots, m,$$

$$f_i = f(t_i) + \epsilon_i, \qquad \epsilon_i \sim N(0, 1),$$
$$f(t) = 1 \cdot e^{0.05t}$$

In Fig. 2 *we show the graph of the function* f *and the data* (t_i, f_i), $i = 1, \dots, m$ *contaminated with errors* ϵ_i.

Figure 2. The function f and the data (t_i, f_i)

Figure 3. Choice of the initial approximation

We search for the point of the global minimum $(b^\star, c^\star)$ *of the functional* F *defined by (2) using the Gauss-Newton method with regulated step (see [3]). The initial approximation in the process is chosen either by (11), or by (16), or outside the set* $\mathcal{R}$ *(see Fig. 3).*

With precision $EPS = \frac{1}{2} \cdot 10^{-4}$ *we obtain*

$$b^\star = 1.03757, \quad c^\star = 0.0492524, \quad F(b^\star, c^\star) = 25.4221.$$

In Table 1. *we show the number of iterations and the computer time on a PC* 486 *needed for various choices of the initial approximation.*

Initial approx. (b_0, c_0)	$b_0 := b_p = 8.0748$ $c_0 := c_p = 0.0016$	$b_0 := b_l = 1.3094$ $c_0 := c_l = 0.0447$	$b_0 := f_{max} = 21.04$ $c_0 := c_p = 0.20$	$b_0 = 0.0001$ $c_0 = 0.0001$
$F(b_0, c_0)$	655.19	29.29	$1.8\,10^{13}$	2 126.26
number of iterations	21	5	491	5004
time in seconds	7.36	1.76	166	1692

Table 1.

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