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A special nonlinear least-squares problem

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Abstract

In this paper we consider the existence of the solution of a special nonlinear least-squares problem. We find the necessary conditions on the data, which insure the existence of the optimal parameters for the asymmetric S-function in the sense of the least squares.

Keywords: Nonlinear least squares; Parameter estimation

1. Introduction

Applied research in biology, agriculture, economics, electrical engineering, medical sciences etc. often uses the so-called S-function model. By an S-function we mean a differentiable increasing function defined on the whole real line $\mathbb{R}$ such that its graph lies between two horizontal asymptotes. The most common S-function is the so-called *logistic function* (see [4,6,7,10])

$$f(t) = \frac{A}{1 + be^{-ct}}, \quad c > 0, \tag{1.1}$$

satisfying the well-known Verhulst differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}t} = cy\left(1 - \frac{y}{A}\right). \tag{1.2}$$

This equation describes the biological principle that the growth rate of the number of living organisms in a restricted environment is proportional to the number of living organisms itself and the amount of as yet unused resources at the given moment. The constant A denotes the saturation level. The logistic function is centrally symmetric with respect to the inflection point $I = \left((\ln b)/c, \frac{1}{2}A\right)$. Namely, we have

$$f(t_I) = \tfrac{1}{2}[f(t_I + t) + f(t_I - t)], \quad \forall t \in \mathbb{R}, \tag{1.3}$$

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where t_I is the first coordinate of the inflection point.

When using this model function in economics research, it becomes clear that this symmetry does not correspond to the real-life situations. Therefore Lewandowsky [4] suggested the following modification of (1.2):

$$\frac{dy}{dt} = cy\left[1 - \left(\frac{y}{A}\right)^{\gamma}\right], \quad c > 0, \ \gamma > 0, \tag{1.4}$$

which has the solution

$$f(t) = \frac{A}{(1 + be^{-c\gamma t})^{1/\gamma}}, \quad c > 0, \ \gamma > 0. \tag{1.5}$$

For $\gamma = 1$ the function (1.5) becomes the logistic function, and for $\gamma \neq 1$ it is an asymmetric S-function.

Definition 1.1. We say that the S-function f with the inflection point $I(t_I, y_I)$ is *negatively asymmetric* if the following holds:

$$f(t_I) < \tfrac{1}{2}[f(t_I + t) + f(t_I - t)], \quad \forall t \in \mathbb{R}, \tag{1.6}$$

and it is *positively asymmetric* if the opposite inequality holds.

Remark 1.2. From the definition it is clear that the function (1.5) is negatively (respectively positively) asymmetric, provided $y_I < \frac{1}{2}A$ (respectively $y_I > \frac{1}{2}A$).

It is shown in [4] that if $\gamma < 1$ (respectively $\gamma > 1$), then the function (1.5) is negatively (respectively positively) asymmetric. Therefore γ is called the *asymmetry coefficient*.

In [4] Lewandowsky suggests that the negatively asymmetric function be used to describe phenomena of relatively short duration span (e.g., fashion products), and the positively asymmetric functions for phenomena of relatively longer duration span (e.g., the personal car demand).

The saturation level A is a constant which may represent the biological maximum (e.g., of the yield of a specific farm crop) or the economic maximum (e.g., the maximal profitable production). The asymmetry coefficient γ is determined from one's experience and depends on the particular problem (see [4]).

The parameters b and c have to be determined from the experimental data (p_i, t_i, f_i), $i = 1, \ldots, m$, where t_i denotes the independent variable, f_i the respective function value and p_i is the data weight.

In this paper we solve the existence problem of this special nonlinear least-squares problem, and the example at the end of the paper is worked out using the modified Levenberg–Marquardt's method with regulated step (see [1–3,5]), based on my own software modified for PCs.

2. Existence of the best approximation

Given are the data (p_i, t_i, f_i), $i = 1, \ldots, m$, where the p_i are some positive weights and $t_1 < \cdots < t_m$. Furthermore, since the numbers f_i usually denote the quantity of something, we may assume that $f_1, \ldots, f_m > 0$.

Consider the class of functions

$$f(t;b,c) = \frac{A}{(1+be^{-c\gamma t})^{1/\gamma}}, \quad b>0, \quad c>0, \tag{2.1}$$

where $A>0$ and $\gamma>0$ are constant.

We look for an ordered pair $(b^\star, c^\star)$ of real numbers, which minimizes the function

$$F(b,c) = \frac{1}{2}\sum_{i=1}^{m} p_i \left[f_i - \frac{A}{(1+be^{-c\gamma t_i})^{1/\gamma}}\right]^2. \tag{2.2}$$

If we denote the set

$$\mathcal{B} = \{(b,c)\in\mathbb{R}^2\colon\ b>0, c>0\},$$

then the problem can be defined as follows.

Does there exist a pair of numbers $(b^\star, c^\star)\in\mathcal{B}$, such that

$$F(b^\star,c^\star) = \inf_{(b,c)\in\mathcal{B}} F(b,c)?$$

The following example shows that the above problem does not always have a solution.

Example 2.1. The function F defined in (2.2) does not always have its minimum in the set $\mathcal{B}$.

We give an example. Let $f_1 = \cdots = f_m = 1$. Then $F(A^\gamma - 1, 0) = 0$. Since $F(b,c) \geqslant 0$ for all $(b,c)\in\mathcal{B}$, this means that the global minimum of F is on the boundary of $\mathcal{B}$. But this means that the function (2.1) is the constant function $t \to 1$, which is ruled out by requiring $c>0$.

Therefore, to ensure the existence of the minimum of the function F, it is necessary to require that the data satisfy some conditions. It will be shown that the property of preponderant increase is playing an important role (see [9]).

Definition 2.2. The data (p_i, t_i, f_i), $i=1,\ldots,m$, are said to have the *preponderant increase* (respectively *decrease*) *property* if the slope of the associated linear trend is positive (respectively negative). If this coefficient is equal to zero, then the data is said to be *preponderantly stationary*.

Remark 2.3. In [9] it is shown that the condition of the preponderant increase is equivalent to the corresponding Chebyshev inequality

$$\sum_{i=1}^{m} p_i t_i f_i \sum_{i=1}^{m} p_i - \sum_{i=1}^{m} p_i t_i \sum_{i=1}^{m} p_i f_i > 0, \tag{2.3}$$

and that the condition of preponderant increase is weaker than the condition of increase

$$f_1 \leqslant f_2 \leqslant \cdots \leqslant f_m \quad \& \quad f_1 < f_m.$$

The next theorem gives the same sufficient conditions which assure that the function F reaches its minimum in $\mathcal{B}$.

Theorem 2.4. *Let the data (p_i, t_i, f_i), $i = 1, \dots, m$, be given. Denote*

$$\omega = \sum_{i=1}^{m} p_i, \qquad \sigma = \sum_{i=1}^{m} p_i f_i, \qquad f_p = \frac{\sigma}{\omega}, \qquad t_p = \frac{1}{\omega}\sum_{i=1}^{m} p_i t_i,$$
$$\omega_+ = \sum_{t_i > t_p} p_i, \qquad \sigma_+ = \sum_{t_i \geqslant t_p} p_i f_i, \qquad f_p^+ = \frac{\sigma_+}{\omega_+},$$

and let (i) *the data fulfil Chebyshev's inequality* (2.3), (ii) $f_i \leqslant A$, $i = 1, \dots, m$. *Then,* (I) *if*

$$f_p^+ \leqslant \sqrt{\frac{\omega}{\omega_+}} f_p, \tag{2.4a}$$

there exists a pair $(b^\star, c^\star) \in \mathcal{B}$ which minimizes the function F defined by (2.2) *on $\mathcal{B}$;*
(II) *if*

$$f_p^+ > \sqrt{\frac{\omega}{\omega_+}} f_p \tag{2.4b}$$

and

$$f_p^+ + \sqrt{f_p^{+2} - \frac{\omega}{\omega_+} f_p^2} \leqslant A, \tag{2.5}$$

there also exists a pair $(b^\star, c^\star) \in \mathcal{B}$ which minimizes the function F on $\mathcal{B}$.

Proof. If we substitute

$$\tau_i = t_i - t_p, \quad i = 1, \dots, m, \tag{2.6}$$

the function F takes the form

$$F(b, c) = \Phi(\beta, c) = \frac{1}{2}\sum_{i=1}^{m} p_i \left[f_i - \frac{A}{(1 + \beta e^{-c\gamma\tau_i})^{1/\gamma}} \right]^2, \tag{2.7}$$

where $\beta = b e^{-c\gamma t_p}$. The function Φ is of the same type as F, and since the map $(b, c) \mapsto (b e^{-c\gamma t_p}, c)$ is a bijection of $\mathcal{B}$ into $\mathcal{B}$, our problem is equivalent to the following one.

Does there exist a pair of numbers $(b^\star, c^\star) \in \mathcal{B}$, such that

$$\Phi^\star = \Phi(\beta^\star, c^\star) = \inf_{(\beta, c) \in \mathcal{B}} \Phi(\beta, c)?$$

Note that because of (2.6) we have

$$\sum_{i=1}^{m} p_i \tau_i = 0, \tag{2.8}$$

and the condition for the preponderant increase property (Chebyshev's inequality (2.3)) becomes simply

$$\sum_{i=1}^{m} p_i \tau_i f_i > 0. \tag{2.9}$$

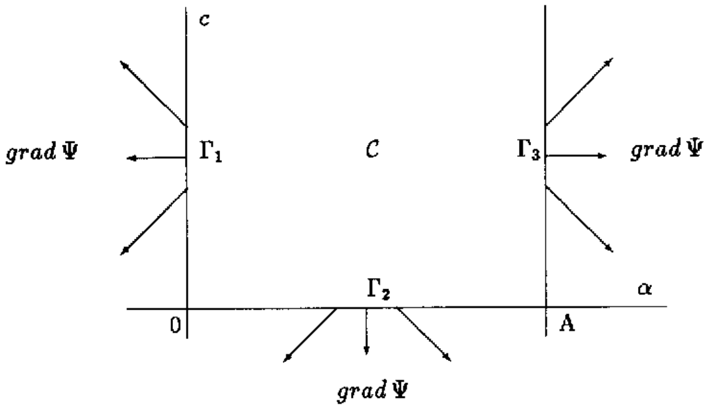

Fig. 1. The behavior of the function Ψ on the boundary ∂C of the set C.

The substitution

$$\alpha = \frac{A}{(1+\beta)^{1/\gamma}}, \quad \alpha \in (0, A), \tag{2.10}$$

reduces the problem to the following one.

Does there exist a pair $(\alpha^\star, c^\star) \in C = \{(\alpha, c) \in \mathbb{R}^2\colon\ 0 < \alpha < A, c > 0\}$ *such that*

$$\Psi^\star = \Psi(\alpha^\star, c^\star) = \inf_{(\alpha,c)\in C} \Psi(\alpha, c),$$

where

$$\Psi(\alpha, c) = \Phi(\beta, c) = \frac{1}{2}\sum_{i=1}^{m} p_i \left[f_i - \frac{\alpha A}{(\alpha^\gamma + (A^\gamma - \alpha^\gamma)\mathrm{e}^{-c\gamma\tau_i})^{1/\gamma}} \right]^2 ? \tag{2.11}$$

After the performed transformations, the function f became

$$g(t; \alpha, c) = \frac{\alpha A}{(\alpha^\gamma + (A^\gamma - \alpha^\gamma)\mathrm{e}^{-c\gamma\tau_i})^{1/\gamma}}. \tag{2.12}$$

The existence of a minimum for Ψ on the set C will ensure the existence of a minimum of Φ, and hence of F, on the set B.

We investigate first the behavior of Ψ on the boundary ∂C of the set C, which we write as $\partial C = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$, where (see Fig. 1)

$$\Gamma_1 = \{(\alpha, c) \in \overline{C}\colon\ \alpha = 0\}, \qquad \Gamma_2 = \{(\alpha, c) \in \overline{C}\colon\ c = 0\}, \qquad \Gamma_3 = \{(\alpha, c) \in \overline{C}\colon\ \alpha = A\}.$$

We investigate the behavior of Ψ on ∂C by means of its gradient

$$\operatorname{grad} \Psi = \begin{bmatrix} \dfrac{\partial \Psi}{\partial \alpha} \\[2mm] \dfrac{\partial \Psi}{\partial c} \end{bmatrix} = -A \sum_{i=1}^{m} p_i \frac{\mathrm{e}^{-c\gamma\tau_i}}{\Delta_i^{1/\gamma+1}} \left(f_i - \frac{\alpha A}{\Delta_i^{1/\gamma}} \right) \begin{bmatrix} A^\gamma \\ \alpha(A^\gamma - \alpha^\gamma)\tau_i \end{bmatrix}, \tag{2.13}$$

where

$$\Delta_i = \alpha^\gamma + (A^\gamma - \alpha^\gamma)\mathrm{e}^{-c\gamma\tau_i}, \quad i = 1, \ldots, m.$$

First consider the part Γ_1 of $\partial\mathcal{C}$. For the first component of $\operatorname{grad}\Psi$ on Γ_1 we have

$$\operatorname{grad}_\alpha \Psi|_{\Gamma_1} = \frac{\partial\Psi}{\partial\alpha}\Big|_{\alpha=0} = -\sum_{i=1}^{m} p_i f_i e^{c\tau_i} < 0. \tag{2.14}$$

Therefore, regardless of the second component of $\operatorname{grad}\Psi$, the direction of the antigradient (i.e., of the fastest decrease) of Ψ on Γ_1 is going to be towards $\mathcal{C}$.

In order to investigate the behavior of Ψ on Γ_2, consider the second component of $\operatorname{grad}\Psi$. We have

$$\operatorname{grad}_c \Psi|_{\Gamma_2} = \frac{\partial\Psi}{\partial c}\Big|_{c=0} = \frac{\alpha^2(A^\gamma - \alpha^\gamma)}{A^\gamma}\sum_{i=1}^{m} p_i\tau_i - \frac{\alpha(A^\gamma - \alpha^\gamma)}{A^\gamma}\sum_{i=1}^{m} p_i\tau_i f_i. \tag{2.15}$$

Then for (2.8) and (2.9) we have $\operatorname{grad}_c \Psi|_{\Gamma_2} < 0$. This again means that the direction of the antigradient of Ψ on Γ_2 has the direction towards $\mathcal{C}$.

Finally, for the first component of $\operatorname{grad}\Psi$ on Γ_3 we have

$$\operatorname{grad}_\alpha \Psi|_{\Gamma_3} = \frac{\partial\Psi}{\partial\alpha}\Big|_{\alpha=A} = -\sum_{i=1}^{m} p_i(f_i - A)e^{c\gamma\tau_i} > 0. \tag{2.16}$$

The condition (ii) then shows that the direction of the antigradient of Ψ on Γ_3 is also towards $\mathcal{C}$.

The above considerations show that Ψ cannot reach its infimum on $\partial\mathcal{C}$. Since $\Psi \geqslant 0$, there is a sequence (α_n, c_n) in $\mathcal{C}$ such that

$$\Psi_n = \Psi(\alpha_n, c_n) = \inf_{(\alpha,c)\in\mathcal{C}} \Psi(\alpha, c).$$

We show that the sequence (α_n, c_n) is bounded. Assume the contrary. Because of the shape of the set $\mathcal{C}$, this means that the sequence (c_n) is not bounded. One can assume that $c_n \to +\infty$ (if not, take an appropriate subsequence). By the Bolzano–Weierstrass theorem we may assume that the sequence (α_n) converges (if not, take a convergent subsequence). Let $\alpha^\star = \lim_{n\to\infty}\alpha_n$, $\alpha^\star \in (0, A)$. Because $\tau_1 < \cdots < \tau_m$, we see for (2.8) that $\tau < 0$ and $\tau_m > 0$. Now it is easy to see that the sequence $g_n(\tau_i) = g(\tau_i; \alpha_n, c_n)$, $n \in \mathbb{N}$, where g was defined in (2.12), converges with the limit being

$$\delta_i = \begin{cases} 0, & \tau_i < 0, \\ \alpha^\star, & \tau_i = 0, \\ A, & \tau_i > 0. \end{cases}$$

The corresponding sequence $\Psi_n = \Psi(\alpha_n, c_n)$ converges with the limit being

$$\Psi_0 = \frac{1}{2}\sum_{\tau_i<0} p_i f_i^2 + \tfrac{1}{2}p_{i_0}(f_{i_0} - \alpha^\star)^2 + \frac{1}{2}\sum_{\tau_i>0} p_i(f_i - A)^2, \tag{2.17}$$

where

$$(p_{i_0}, t_{i_0}, f_{i_0}) = \begin{cases} i_0\text{th data}, & \text{if there exists a data with } t_i = t_p, \\ (0,0,0), & \text{otherwise.} \end{cases}$$

In order to show that the assumption that $c_n \to +\infty$, i.e., that the infimum of Ψ is obtained for $\alpha_n \to \alpha^\star$ and $c_n \to +\infty$, either we have to find a function of the type (2.12) which is, in the sense of least squares, better than g and which is at the point τ_i given by δ_i, or we have to find a point in $\mathcal{C}$ where the value of Ψ is smaller than Ψ_0 in (2.17).

Let us look for such a point near Γ_2. On Γ_2 the function Ψ becomes

$$\Psi_1(\alpha) = \frac{1}{2}\sum_{i=1}^{m} p_i(f_i - \alpha)^2. \tag{2.18}$$

The function Ψ_1 has a minimum for $\alpha = f_p$. We shall show that the function Ψ has a value smaller than Ψ_0 at $T(f_p, 0)$. In fact, the point T lies on Γ_2, but because of (2.15) there is always a point in $\mathcal{C}$ where the value of Ψ is even smaller.

To do this, consider the difference

$$2[\Psi_0 - \Psi(f_p,0)] = 2f_p\sum_{i=1}^{m} p_i f_i - f_p^2\sum_{i=1}^{m} p_i + A^2\sum_{\tau_i>0} p_i - 2A\sum_{\tau_i>0} p_i f_i - 2\alpha^\star p_{i_0} f_{i_0} + p_{i_0}\alpha^{\star 2}. \tag{2.19}$$

From $p_{i_0}^{\star 2} \geqslant 0$ and $\alpha^\star < A$, we obtain

$$2[\Psi_0 - \Psi(f_p,0)] > A^2\omega_+ - 2A\omega_+ f_p^+ + \omega f_p^2. \tag{2.20}$$

The right-hand side of (2.20) can be considered a quadratic function in A, with the discriminant

$$D = 4\omega_+\left(\omega_+ f_p^{+2} - \omega f_p^2\right). \tag{2.21}$$

If (2.4a) holds, then $D \leqslant 0$, and since $\omega_+ > 0$, the whole graph of the quadratic function lies in the upper half-plane, i.e., we have

$$2[\Psi_0 - \Psi(f_p,0)] > 0. \tag{2.22}$$

If (2.4b) holds, then denote

$$h(x) = \omega_+ x^2 - 2\omega_+ f_p^+ x + \omega f_p^2. \tag{2.23}$$

Since the zeros of h are

$$x_{1,2} = f_p^+ \pm \sqrt{f_p^{+2} - \frac{\omega}{\omega_+} f_p^2},$$

and $\omega_+ > 0$, because of (2.5) we have again (2.22).

We now conclude that the sequence (c_n) is bounded, and therefore by the Bolzano–Weierstrass theorem we may assume that it converges (otherwise take a subsequence). Let $c^\star = \lim_{n\to\infty} c_n$, $c^\star \in (0, +\infty)$.

In that way we obtained a convergent sequence (α_n, c_n) with $\lim_{n\to\infty}(\alpha_n, c_n) = (\alpha^\star, c^\star)$. Note that $(\alpha^\star, c^\star)$ cannot lie on $\partial\mathcal{C}$ since the direction of the antigradient of Ψ is towards $\mathcal{C}$, and therefore $(\alpha^\star, c^\star) \in \mathcal{C}$. By continuity of Ψ we now have

$$\Psi(\alpha_n, c_n) \to \Psi(\alpha^\star, c^\star), \quad n \to +\infty. \qquad \square$$

Table 1

i	1	2	3	4
p_i	1	1	1	1
t_i	1	2	3	4
f_i	0.5	0.5	200	200

Remark 2.5. If we consider the case $m = 2k$, $k \in \mathbb{N}$, and $p_1 = \cdots = p_{2k} = 1$ and if the t_i are equidistant (which is often the case in practice), then condition (2.4a) becomes simply

$$f_{k+1} + \cdots + f_{2k} \leqslant (\sqrt{2}+1)(f_1 + \cdots + f_k).$$

This means in case of a "mild" preponderant increase, the data have to satisfy only condition (ii), while in case of more prevalent growth, the data have to satisfy also condition (2.5).

Example 2.6. The data are given in Table 1. For this data condition (2.4a) is not satisfied. Therefore it is not enough that the saturation level A be greater than 200 (by (ii)), but, in addition, the condition (2.5) has also to be satisfied, i.e., the saturation coefficient A has to be greater than 256. It was checked numerically that also in case $200 < A < 256$ the iteration process does not converge. But for $A = 260$ (and $\gamma = 0.5$) we have

$$b^* = 1989.08, \qquad c^* = 6.276\,11, \qquad F(b^*, c^*) = 1678.97.$$

The minimized function F is shown in Fig. 2.

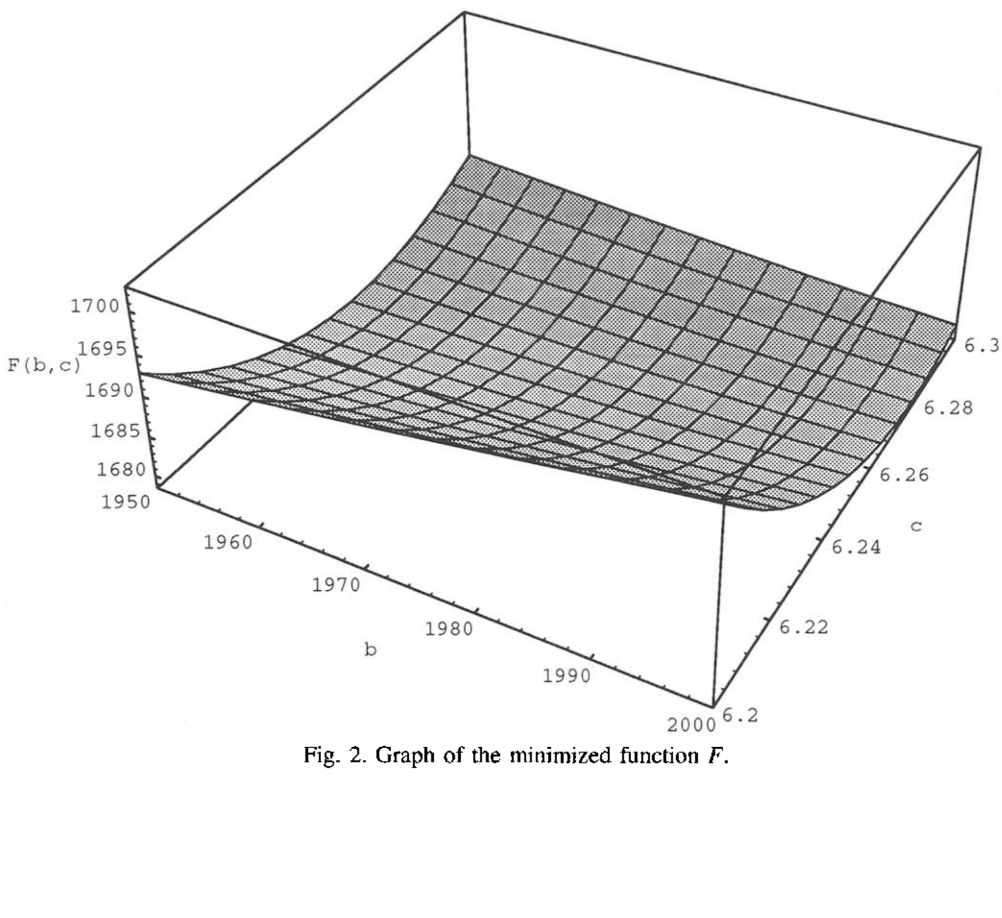

Fig. 2. Graph of the minimized function F.

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