

Least orthogonal absolute deviations problem for generalized logistic function *

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Abstract. *We consider the existence of optimal parameters for generalized logistic model by least orthogonal absolute deviations, and prove the existence of such optimal solution, under the monotonicity condition on the data.*

Key words: *generalized logistic function, least orthogonal absolute deviations, total least squares*

Sažetak. **Najmanja ortogonalna apsolutna odstupanja za generaliziranu logističku funkciju.** *Razmatra se problem egzistencije optimalnih parametara za generaliziranu logističku funkciju u smislu najmanjih ortogonalnih apsolutnih odstupanja, te dokazuje egzistenciju takvog optimalnog rješenja, uz uvjet monotonosti podataka.*

Ključne riječi: *generalizirana logistička funkcija, najmanja ortogonalna apsolutna odstupanja, najmanji potpuni kvadrati*

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1. Introduction

The generalized logistic function

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

is often used in applied research (see [5], [13]). It is the solution of the so-called Nelder's model

$$y' = cy \left(1 - \left(\frac{y}{A} \right)^\gamma \right), \quad A, \gamma > 0,$$

(see [8]). The constant $A > 0$ denotes the saturation level, and the constant $\gamma > 0$ is the so-called asymmetry coefficient (see [10]).

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The unknown parameters b, c have to be determined on the basis of the given data (w_i, t_i, f_i) , $i = 1, \dots, m$ ($m > 2$), where t_i are the measured values of the independent variable, f_i are the measured values of the dependent variable, and $w_i > 0$ are the data weights.

In the case when only the measured values f_1, \dots, f_m of the dependent variable contain unknown additive errors ε_i , the estimation of the parameters b, c is usually done in the sense of ordinary least squares, i.e. the L_2 -norm (see [3], [6]), by minimizing the functional

$$G(b, c) = \sum_{i=1}^m w_i \left(f_i - \frac{A}{(1 + be^{-c\gamma t_i})^{1/\gamma}} \right)^2.$$

Some results on the existence problem for generalized logistic function in the sense of ordinary least squares can be found in [2], [5], [10].

The least squares criterion is most suitable in cases where errors are normally distributed with mean zero and variance $\sigma^2 I$. When errors do not follow the normal (Gaussian) distribution, the use of other L_p -norms ($p \neq 2$) is recommended (see [3]).

In general case, significant errors exist both in measurements t_i of the independent variable and in measurements f_i of the dependent variable ([1]). If one assumes that t_i has the unknown additive error δ_i and f_i has the unknown additive error ε_i , then we have the model

$$f_i = \frac{A}{(1 + be^{-c\gamma t_i})^{1/\gamma}} + \varepsilon_i, \quad i = 1, \dots, m,$$

and the parameters b, c can be estimated by the total least squares approach (see [1], [4]), which leads to minimization of the functional

$$T(b, c, \delta_1, \dots, \delta_m) = \sum_{i=1}^m w_i \left(\left(f_i - \frac{A}{(1 + be^{-c\gamma t_i})^{1/\gamma}} \right)^2 + \delta_i^2 \right). \quad (2)$$

Note that $T(b, c, \delta_1, \dots, \delta_m)$ is the weighted sum of squares of the distances from the data points to the curve Γ_f , where $t \mapsto f(t; b, c) = \frac{A}{(1 + be^{-c\gamma t})^{1/\gamma}}$.

In this paper we consider the existence problem of optimal parameters for the generalized logistic function in the sense of the least orthogonal absolute deviations (LOAD, see [9], [12]). The LOAD approach leads to minimization of the weighted sum of orthogonal distances from measurement points to the model function (see [7]). In this case, the problem of estimating the parameters b and c is reduced to the problem of minimizing the functional

$$F(b, c, \delta) = \sum_{i=1}^m w_i \sqrt{\left(f_i - \frac{A}{(1 + be^{-c\gamma t_i})^{1/\gamma}} \right)^2 + \delta_i^2}, \quad (3)$$

where $\delta = [\delta_1, \dots, \delta_m]^T \in \mathbb{R}^m$. We are going to prove, for monotonic data, the existence of a point (b^*, c^*, δ^*) which minimizes the functional F . The idea of the proof is based on [7] and [11].

2. The existence problem

Assume we are given the data (w_i, t_i, f_i) , $i = 1, \dots, m$, $m > 2$, $t_1 < t_2 < \dots < t_m$. Further, suppose that $f_i > 0$, $i = 1, \dots, m$, and that we apply the generalized logistic model function. Let us observe that if $f_1 \leq f_2 \leq \dots \leq f_m$, then it is appropriate to describe such data by an increasing function. Also, if $f_1 \geq f_2 \geq \dots \geq f_m$, then it is suitable to use a decreasing function.

With regard to the existence problem of optimal parameters b^* , c^* of the generalized logistic function in the sense of least orthogonal absolute deviations, we have the following theorem.

Theorem 1. *Let the given data (w_i, t_i, f_i) , $i = 1, \dots, m$, $m > 2$, $t_1 < \dots < t_m$, be such that $0 < f_i < A$, $\forall i$.*

(i) *If $f_1 \leq f_2 \leq \dots \leq f_m$, then there exists a point $(b^*, c^*, \delta^*) \in S \times \mathbb{R}^m$,*

$$S = \{(b, c) \in \mathbb{R}^2 : b > 0, c \geq 0\},$$

at which the functional F defined by (3) attains its infimum on the set $S \times \mathbb{R}^m$.

(ii) *If $f_1 \geq f_2 \geq \dots \geq f_m$, then there exists a point $(b^*, c^*, \delta^*) \in D \times \mathbb{R}^m$,*

$$D = \{(b, c) \in \mathbb{R}^2 : b > 0, c \leq 0\},$$

at which the functional F defined by (3) attains its infimum on the set $D \times \mathbb{R}^m$.

Proof. Case (i). Since $F \geq 0$, there exists $F^* := \inf_{(b,c,\delta) \in S \times \mathbb{R}^m} F(b, c, \delta)$.

(If $f_1 = f_2 = \dots = f_m$, then $F\left(\left(\frac{A}{f_1}\right)^\gamma - 1, 0, \mathbf{0}\right) = 0$, and the functional F has its global minimum for $b = \left(\frac{A}{f_1}\right)^\gamma - 1$, $c = 0$, $\delta = \mathbf{0}$; hence, the assertion of theorem was proved. So, let us suppose further that $f_1 < f_m$.)

Let (b_n, c_n, δ^n) be a sequence in $S \times \mathbb{R}^m$ such that

$$F^* = \lim_{n \rightarrow \infty} F(b_n, c_n, \delta^n) = \lim_{n \rightarrow \infty} \sum_{i=1}^m w_i \sqrt{\left(f_i - \frac{A}{(1 + b_n e^{-c_n \gamma (t_i + \delta_i^n)})^{1/\gamma}}\right)^2 + (\delta_i^n)^2}. \quad (4)$$

Note that the sequences (δ_i^n) , $i = 1, \dots, m$, are bounded. If it were not, we would have $\limsup_n F(b_n, c_n, \delta^n) = \infty$, which contradicts the assumption (4).

We are going to show, by contradiction, that the sequence (c_n) is also bounded. Assume that the sequence (c_n) is unbounded. By the Bolzano-Weierstrass theorem, we may assume (without loss of generality, by taking appropriate subsequence if necessary) that $c_n \rightarrow \infty$ and

$$\lim_{n \rightarrow \infty} \delta_i^n = \delta_i^*, \quad i = 1, \dots, m.$$

But, let us show that the infimum of the functional F cannot be attained in such way. We are going to find a point in $S \times \mathbb{R}^m$ at which the functional F defined by (3) attains a value which is smaller than $\lim_{n \rightarrow \infty} F(b_n, c_n, \delta^n)$.

Denote $M := \{1, \dots, m\}$. Note that when $c_n \rightarrow \infty$, sequences $(b_n e^{-c_n \gamma (t_i + \delta_i^n)})$, $i \in M$, (or respectively, without loss of generality, their corresponding subsequences) have the following property:

If $\lim_{n \rightarrow \infty} b_n e^{-c_n \gamma (t_{i_0} + \delta_{i_0}^n)} = r < \infty$ for some $i_0 \in M$, then $\lim_{n \rightarrow \infty} b_n e^{-c_n \gamma (t_i + \delta_i^n)} = 0$ for every $i \in M$ such that $t_i + \delta_i^* > t_{i_0} + \delta_{i_0}^*$.

Namely, if $t_i + \delta_i^* > t_{i_0} + \delta_{i_0}^*$, then

$$\lim_{n \rightarrow \infty} b_n e^{-c_n \gamma (t_i + \delta_i^n)} = \lim_{n \rightarrow \infty} b_n e^{-c_n \gamma (t_{i_0} + \delta_{i_0}^n)} \cdot \lim_{n \rightarrow \infty} e^{-c_n \gamma (t_i + \delta_i^n - t_{i_0} - \delta_{i_0}^n)} = 0.$$

Similarly, if $\lim_{n \rightarrow \infty} b_n e^{-c_n \gamma (t_{i_0} + \delta_{i_0}^n)} = \infty$ for some $i_0 \in M$, then $\lim_{n \rightarrow \infty} b_n e^{-c_n \gamma (t_i + \delta_i^n)} = \infty$ for $i \in M$ such that $t_i + \delta_i^* < t_{i_0} + \delta_{i_0}^*$.

Because of that, for the sequences $(b_n e^{-c_n \gamma (t_i + \delta_i^n)})$, $i \in M$, (or respectively, by the Bolzano-Weierstrass theorem, for their corresponding subsequences), we may assume that one of the two following cases appears when $c_n \rightarrow \infty$.

Subcase (i1). All the sequences $(b_n e^{-c_n \gamma (t_i + \delta_i^n)})$, $i \in M$, are unbounded and $\lim_{n \rightarrow \infty} b_n e^{-c_n \gamma (t_i + \delta_i^n)} = \infty$, $\forall i \in M$. In this case we have

$$F^* = \lim_{n \rightarrow \infty} F(b_n, c_n, \delta^n) = \sum_{i \in M} w_i \sqrt{f_i^2 + (\delta_i^*)^2} > \sum_{i \in M} w_i |f_i - f_1| = F\left(\left(\frac{A}{f_1}\right)^{1/\gamma} - 1, 0, \mathbf{0}\right),$$

which contradicts the assumption (4). Therefore, in this subcase the infimum of the functional F cannot be attained.

Subcase (i2). There exists at least one $i_0 \in M$ such that:

the sequence $(b_n e^{-c_n \gamma (t_{i_0} + \delta_{i_0}^n)})$ is bounded, $\lim_{n \rightarrow \infty} b_n e^{-c_n \gamma (t_{i_0} + \delta_{i_0}^n)} = r_{i_0} < \infty$ and

$$\lim_{n \rightarrow \infty} b_n e^{-c_n \gamma (t_i + \delta_i^n)} = \begin{cases} \infty, & \text{for } i \in K_-, \\ 0, & \text{for } i \in K_+, \end{cases}$$

where

$$K_- := \{i \in M : t_i + \delta_i^* < t_{i_0} + \delta_{i_0}^*\}, \quad K_+ := \{i \in M : t_i + \delta_i^* > t_{i_0} + \delta_{i_0}^*\}.$$

In order to show that the infimum of the functional F cannot be attained in such way, we are going to find a point in $S \times \mathbb{R}^m$ at which the functional F defined by (3) attains a value which is smaller than $F^* = \lim_{n \rightarrow \infty} F(b_n, c_n, \delta^n)$.

By using the notations $\tau^* := t_{i_0} + \delta_{i_0}^*$ and $K := \{i \in M : t_i + \delta_i^* = \tau^*\}$, we obtain

$$\lim_{n \rightarrow \infty} F(b_n, c_n, \delta^n) \geq \sum_{i \in K_-} w_i \sqrt{f_i^2 + (\delta_i^*)^2} + \sum_{i \in K} w_i |\delta_i^*| + \sum_{i \in K_+} w_i \sqrt{(f_i - A)^2 + (\delta_i^*)^2} =: F_0. \quad (5)$$

Let us show that there exists a point in the set $S \times \mathbb{R}^m$ at which the functional F attains value which is smaller than F_0 . For that purpose, let us define functions $\hat{b}(c)$, $\hat{\delta}_i(c)$, $i = 1, \dots, m$, from \mathbb{R}^+ to \mathbb{R} :

$$\hat{b}(c) = b_0 e^{c\gamma\tau^*},$$

$$\hat{\delta}_i(c) = \begin{cases} \delta_i^*, & i \in K_- \cup K_+ \\ \tau^* - t_i - \frac{1}{c\gamma} \ln \frac{(\frac{A}{f_i})^\gamma - 1}{b_0}, & i \in K, \end{cases}$$

where

$$b_0 = \begin{cases} \max\{(\frac{A}{f_i})^\gamma - 1 : i \in K \text{ \& } t_i \geq \tau^*\}, & \text{if } \{i \in K : t_i \geq \tau^*\} \neq \emptyset, \\ (\frac{A}{f_m})^\gamma - 1, & \text{if } \{i \in K : t_i \geq \tau^*\} = \emptyset. \end{cases}$$

From there it follows

$$\begin{aligned} F(\hat{b}(c), c, \hat{\delta}(c)) &= \sum_{i \in K_- \cup K_+} w_i \sqrt{\left(f_i - \frac{A}{(1 + b_0 e^{-c\gamma(t_i + \delta_i^* - \tau^*)})^{1/\gamma}}\right)^2 + (\delta_i^*)^2} \\ &\quad + \sum_{i \in K} w_i \left| \delta_i^* - \frac{1}{c\gamma} \ln \frac{(\frac{A}{f_i})^\gamma - 1}{b_0} \right|. \end{aligned} \quad (6)$$

For a sufficiently large positive c we have

$$\begin{aligned} \sqrt{(f_i)^2 + (\delta_i^*)^2} &> \sqrt{\left(f_i - \frac{A}{(1 + b_0 e^{-c\gamma(t_i + \delta_i^* - \tau^*)})^{1/\gamma}}\right)^2 + (\delta_i^*)^2}, \quad \text{for } i \in K_-, \\ \sqrt{(f_i - A)^2 + (\delta_i^*)^2} &> \sqrt{\left(f_i - \frac{A}{(1 + b_0 e^{-c\gamma(t_i + \delta_i^* - \tau^*)})^{1/\gamma}}\right)^2 + (\delta_i^*)^2}, \quad \text{for } i \in K_+. \end{aligned}$$

Further, by the property of monotonic data and by the definition of b_0 , it is not difficult to see that for a sufficiently large c

$$|\delta_i^*| \geq \left| \delta_i^* - \frac{1}{c\gamma} \ln \frac{(\frac{A}{f_i})^\gamma - 1}{b_0} \right|, \quad \text{for } i \in K.$$

Therefore, by comparing (5) and (6), from above inequalities it follows that for a sufficiently large positive c

$$F(\hat{b}(c), c, \hat{\delta}(c)) < F_0 \leq F^*,$$

which contradicts the assumption (4). This means that, when $c_n \rightarrow \infty$, the infimum of the functional F cannot be obtained.

Hence, the sequence (c_n) is bounded. By the Bolzano-Weierstrass theorem we may assume that the sequence (c_n) is convergent. Let $c_n \rightarrow c^*$.

Then, it follows from (3) that the sequence (b_n) is bounded, too. If not, i.e. if $b_n \rightarrow \infty$, it would be

$$\lim_{n \rightarrow \infty} F(b_n, c_n, \delta^n) \geq \sum_{i \in M} w_i |f_i| > \sum_{i=1}^m w_i |f_i - f_1| = F\left(\left(\frac{A}{f_1}\right)^\gamma - 1, 0, \mathbf{0}\right),$$

which contradicts the assumption (4). Analogously, we can assume that $b_n \rightarrow b^* \geq 0$.

By continuity of the functional F , we get

$$\inf_{(b,c,\delta) \in S \times \mathbb{R}^m} F(b, c, \delta) = \lim_{n \rightarrow \infty} F(b_n, c_n, \delta^n) = F(b^*, c^*, \delta^*).$$

Furthermore, for $b = 0$, $c \in [0, \infty)$ and $\delta \in \mathbb{R}^m$ we have

$$F(0, c, \delta) = \sum_{i=1}^m w_i \sqrt{(f_i - A)^2 + (\delta_i)^2} > \sum_{i=1}^m |f_i - f_m| = F\left(\left(\frac{A}{f_m}\right)^\gamma - 1, 0, \mathbf{0}\right).$$

Therefore, we conclude that $b^* > 0$, i.e. $(b^*, c^*) \in S$.

Case (ii). Let $c < 0$. Since

$$\sqrt{\left(f_i - \frac{A}{(1 + be^{-c\gamma(t_i + \delta_i)})^{\frac{1}{\gamma}}}\right)^2 + \delta_i^2} = \sqrt{\left(f_i - \frac{A}{(1 + be^{-(-c)\gamma(-t_i - \delta_i)})^{\frac{1}{\gamma}}}\right)^2 + (-\delta_i)^2},$$

and the data $(-t_i, f_i)$ $i = 1, \dots, m$ have the increasing property, this case reduces to *Case (i)*. \square

Let $A < 0$. Since the symmetrical expressions

$$\left(f_i - \frac{A}{(1 + be^{-c\gamma(t_i + \delta_i)})^{1/\gamma}}\right)^2 = \left((-f_i) - \frac{(-A)}{(1 + be^{-c\gamma(t_i + \delta_i)})^{1/\gamma}}\right)^2, \quad i = 1, \dots, m,$$

hold, from *Theorem 1*. we get the following corollary.

Corollary 1. *Let the given data (w_i, t_i, f_i) , $i = 1, \dots, m$, $m > 2$, $t_1 < \dots < t_m$, such that $A < f_i < 0$, $\forall i$.*

(i) If $f_1 \geq f_2 \geq \dots \geq f_m$, then there exists a point $(b^, c^*, \delta^*) \in S \times \mathbb{R}^m$, $S = \{(b, c) \in \mathbb{R}^2 : b > 0, c \geq 0\}$, at which the functional F defined by (3) attains its infimum on the set $S \times \mathbb{R}^m$.*

(ii) If $f_1 \leq f_2 \leq \dots \leq f_m$, then there exists a point $(b^, c^*, \delta^*) \in D \times \mathbb{R}^m$, $D = \{(b, c) \in \mathbb{R}^2 : b > 0, c \leq 0\}$, at which the functional F defined by (3) attains its infimum on the set $D \times \mathbb{R}^m$. \square*

Remark 1. *In the approximation problem for the generalized logistic function one can also show analogously that Theorem 1. is applicable in the case of the approximation by the total least squares criterion, i.e. Theorem 1. is applicable for the functional T defined by (2).*

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