EUROPEAN JOURNAL OF PURE AND APPLIED MATHEMATICS
Vol. 10, No. 2, 2017, 157-166
ISSN 1307-5543 – www.ejpam.com
Published by New York Business Global

Nonlinear Least Squares Estimation of the Shifted Gompertz Distribution

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Abstract. The focus of this paper is the existence of the best nonlinear least squares estimate for the shifted Gompertz distribution. As a main result, two theorems on the existence of the least squares estimate are obtained, as well as their generalization in the l_p norm ($1 \le p < \infty$).

2010 Mathematics Subject Classifications: 65D10, 65C20, 62J02

Key Words and Phrases: Shifted Gompertz distribution, nonlinear least squares, least squares estimate, l_p-norm estimate, existence problem

1. Introduction

The shifted Gompertz distribution was introduced by Bemmaor [3] in 1994 as a model of adoption of innovations. The cumulative distribution function (CDF) of the random variable T having the shifted Gompertz distribution is given by

$$F(t;a,b) = \begin{cases} (1-\mathrm{e}^{-bt})\,\mathrm{e}^{-a\,\mathrm{e}^{-bt}}, & t > 0 \\ 0, & t \le 0. \end{cases} \tag{1}$$

The parameters $a > 0$ and $b > 0$ are called the shape parameter and the scale parameter, respectively. More information on statistical properties of the shifted Gompertz distribution can be found in Bemmaor [3] and Jiménez and Jodrá [12].

Note that the shifted Gompertz distribution can be interpreted as the distribution of the maximum of two independent random variables, one of which has an exponential distribution with parameter $b > 0$ and the other one has a Gumbel distribution with parameters $a > 0$ and $b > 0$.

In practice, the unknown parameters of the shifted Gompertz distribution are not known in advance and must be estimated from a random sample. There is no unique way to estimate the unknown parameters and many different statistical methods have been proposed in the literature, such as the maximum likelihood method, the method of

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moments, the method of percentiles and the Bayesian method. But, since each of these methods has some advantages and disadvantages, several other methods are proposed to estimate the unknown parameters in the shifted Gompertz distribution. For example, maximum likelihood method is very efficient for large samples, but not so efficient with small samples. A very popular method for parameter estimation is the least squares (LS) method. This method usually gives very good estimates even for small data sets. Numerical methods for solving the nonlinear LS problem are described in Dennis and Schnabel [9] and Gill et al. [10]. Before starting an iterative procedure, one should ask whether an LS estimate exists. In the case of nonlinear LS problems, it is still extremely difficult to answer this question (see [2, 5, 19, 20]). Results on the existence of the LS estimate for some special classes of functions other than the shifted Gompertz distribution can be found in [6, 7, 8, 14, 16, 17, 21].

In this paper, we consider the nonlinear weighted LS parameter estimation problem for the shifted Gompertz distribution. Our focus is on the existence of the corresponding best LS estimate. To the best of our knowledge, there is no paper focused on this existence problem. In Section 2, we briefly describe the LS method and show that it is possible that the LS estimate for the shifted Gompertz distribution does not exist (Proposition 1). As our main results, we present two theorems (Theorem 1 and Theorem 2) on the existence of the LS estimate for the shifted Gompertz distribution, as well as their generalizations (Theorem 3 and Theorem 4) in the l_p norm ($1 \le p < \infty$).

This paper is motivated by the paper of Jiménez Torres [13], where LS estimation for the log-transformed shifted Gompertz distribution was considered.

2. Estimation of the shifted Gompertz distribution

In this section, we first formulate the LS fitting problem for the shifted Gompertz distribution and then present two theorems on the existence of the least squares estimate, as well as their generalizations in the l_p norm ($1 \le p < \infty$).

2.1. LS fitting problem for the shifted Gompertz distribution

Suppose we are given the data (w_i, t_i, y_i), $i = 1, \dots, n$, $n > 2$, where

$$0 < t_1 < t_2 < \dots < t_n$$

denote the values of the independent variable (observations of the nonnegative shifted Gompertz random variable T, arranged in their increasing order),

$$0 < y_1 < y_2 < \dots < y_n < 1$$

are the respective estimators of the empirical CDF, and $w_i > 0$ are some data weights. Since the shifted Gompertz random variable T is nonnegative and numbers y_i denote empirical CDF values, the above two conditions are natural.

There are many different ways to derive estimators y_i for the empirical CDF corresponding to the sample data $t_1 < t_2 < \ldots < t_n$. Most commonly used estimators can be expressed in the following form (see [15, 18]):

$$y_i = \frac{i-c}{n+1-2c}, \quad i = 1, \ldots, n,$$

for some real number c, $0 \le c < 1$. Some alternatives are as follows: $y_i = \frac{i}{n+1}$ (*mean rank* estimator, $c = 0$), $y_i = \frac{i-0.5}{n}$ (*median rank* estimator, $c = 0.5$), $y_i = \frac{i-0.3}{n+0.4}$ (*Benard's median rank* estimator, $c = 0.3$).

The goal of the LS method (see e.g. [2, 5, 10, 19, 20]) is to choose the unknown parameters of the shifted Gompertz distribution (1) such that the weighted sum of squared distances between the model and the data is as small as possible. More precisely, the unknown parameters a and b have to be estimated by minimizing the functional

$$S(a,b) = \sum_{i=1}^{n} w_i [F(t_i; a, b) - y_i]^2 \tag{2}$$

on the set (parameter space)

$$\mathcal{P} := \{(a,b) \in \mathbb{R}^2 : a, b > 0\}.$$

A point $(a^\star, b^\star) \in \mathcal{P}$ such that $S(a^\star, b^\star) = \inf_{(a,b)\in\mathcal{P}} S(a,b)$ is called the least squares estimate (LS estimate), if it exists (see e.g. [5, 8, 10, 19, 20]).

The following proposition shows that there exist data such that the LS estimate for the shifted Gompertz distribution (1) does not exist.

Proposition 1. *Let (w_i, t_i, y_i), $i = 1, \ldots, n, n \ge 3$, be the data. If the data are such that the points (t_i, y_i), $i = 1, \ldots, n$, all lie on some exponential curve $g(t) = 1 - \mathrm{e}^{-b_0 t}$, $b_0 > 0$, then the LS estimate does not exist.*

Proof. Since $S(a,b) \ge$ for all $(a,b) \in \mathcal{P}$, and

$$\lim_{a\to 0^+} S(a, b_0) = \lim_{a\to 0^+} \sum_{i=1}^{n} w_i [(1 - \mathrm{e}^{-b_0 t_i})\, \mathrm{e}^{-a\,\mathrm{e}^{-b_0 t_i}} - y_i]^2 = \sum_{i=1}^{n} w_i [(1 - \mathrm{e}^{-b_0 t_i}) - y_i]^2 = 0,$$

it is easy to conclude that $\inf_{(a,b)\in\mathcal{P}} S(a,b) = 0$. Furthermore, since the graph of any shifted Gompertz distribution (1) intersects the graph of exponential function $g(t) = 1 - \mathrm{e}^{-b_0 t}$ in at most two points, and $n \ge 3$, it follows that $S(a,b) > 0$ for all $(a,b) \in \mathcal{P}$, and hence the best LS estimate does not exist. □

2.2. The LS existence theorem for the shifted Gompertz distribution

The following theorem gives a necessary and sufficient condition on the data which guarantee the existence of the LS estimate for the shifted Gompertz distribution. First, we introduce one notation. Let $E^\star$ be an infimum of the weighted sum of squares for the exponential function (distribution) $g(t) = 1 - \mathrm{e}^{-bt}$ $(b > 0)$, i.e.,

$$E^\star = \inf_{b>0} E(b),$$

where

$$E(b) = \sum_{i=1}^{n} w_i[(1 - \mathrm{e}^{-bt_i}) - y_i]^2.$$

Theorem 1 (Necessary and sufficient condition)**.** *Suppose that the data* (w_i, t_i, y_i)*,* $i = 1, \dots, n$*,* $n \geq 3$*, satisfy conditions* $0 < t_1 < t_2 < \dots < t_n$ *and* $0 < y_i < 1$*,* $i = 1, \dots, n$*. Then the LS estimate for the shifted Gompertz distribution (1) exists if and only if there is a point* $(a_0, b_0) \in \mathcal{P}$ *such that* $S(a_0, b_0) \leq E^\star$*.*

By using Theorem 3.1 from Jukić [14], it is easy to show that there exists a $\beta^\star > 0$ such that $E(\beta^\star) = E^\star$. Therefore, in other words, under the assumptions of the theorem, the LS estimate exists if and only if there is at least one shifted Gompertz distribution which is in an LS sense as good as or better than the best exponential distribution.

Remark 1. *It can be easily shown that if* $\partial S/\partial a < 0$ *evaluated at* $a = 0$ *and* $b = b_0 = \operatorname{argmin} E(b)$*, then there exists a point* $(a, b_0) \in \mathcal{P}$ *such that* $S(a, b_0) < E^\star$*, which according to the Theorem 1 ensure the existence of the least squares estimate for the shifted Gompertz distribution.*

The next lemma will be used in the proof of Theorem 1.

Lemma 1. *Suppose we are given the data* (t_i, y_i)*,* $i = 1, \dots, n$*,* $n > 2$*, such that* $0 < t_1 < t_2 < \dots < t_n$ *and* $0 < y_i < 1$*,* $i = 1, \dots, n$*. Let* $w_i > 0$*,* $i = 1, \dots, n$*, be some weights. Given any real number* $\tau_0 > 0$*, let*

$$\Sigma_{\tau_0} := \sum_{t_i < \tau_0} w_i y_i^2 + \sum_{t_i > \tau_0} w_i (1 - y_i)^2.$$

Then there exists a point in $\mathcal{P}$ *at which functional* S *defined by (2) attains a value less than* Σ_{τ_0}*.*

The summation $\sum\limits_{t_i<\tau_0}$ (or $\sum\limits_{t_i>\tau_0}$) is to be understood as follows: the sum over those indices $i \leq n$ for which $t_i < \tau_0$ (or $t_i > \tau_0$). If there are no such points t_i, the sum is empty; following the usual convention, we define it to be zero.

Proof. Let $\tau_0 > 0$ be given. If $\tau_0 \neq t_i$, for each index i in the range 1 to n, let ξ_0 be an arbitrary number from the interval $(0, 1)$, and otherwise, if $\tau_0 = t_i$ for some i, let $\xi_0 = y_i$. Define function $a : \left(\frac{1}{\tau_0} \ln \frac{1}{1-\xi_0}, \infty\right) \to \mathbb{R}$

$$a(b) = \ln\left(\frac{1 - \mathrm{e}^{-b\tau_0}}{\xi_0}\right) \mathrm{e}^{b\tau_0}.$$

It is easy to verify that $a(b)$ is positive, and therefore $(a(b), b) \in \mathcal{P}$. Let us now associate with each real $b \in \left(\frac{1}{\tau_0} \ln \frac{1}{1-\xi_0}, \infty\right)$ a shifted Gompertz distribution function

$$F(t; a(b), b) = \begin{cases} (1 - \mathrm{e}^{-bt})\, \mathrm{e}^{-\ln\left(\frac{1-\mathrm{e}^{-b\tau_0}}{\xi_0}\right) \mathrm{e}^{-b(t-\tau_0)}}, & \text{if } t > 0 \\ 0, & \text{if } t \leq 0. \end{cases}$$

By a straightforward calculation, it can be verified that

$$F(\tau_0; a(b), b) = \xi_0 \tag{3}$$

and

$$\lim_{b \to \infty} F(t; a(b), b) = \begin{cases} 0, & \text{if } 0 < t < \tau_0 \\ 1, & \text{if } t > \tau_0. \end{cases}$$

Due to this, we may assume that for every sufficiently large $b > 0$,

$$\begin{aligned} &0 < F(t_i; a(b), b) < y_i, && \text{if } 0 < t_i < \tau_0 \\ &y_i < F(t_i; a(b), b) < 1, && \text{if } t_i > \tau_0. \end{aligned} \tag{4}$$

Hence, for every sufficiently large $b > 0$ it follows from (3) and (4) that

$$\begin{aligned} S(a(b), b) &= \sum_{i=1}^{n} w_i [F(t_i; a(b), b) - y_i]^2 \\ &= \sum_{t_i < \tau_0} w_i [F(t_i; a(b), b) - y_i]^2 + \sum_{t_i > \tau_0} w_i [F(t_i; a(b), b) - y_i]^2 \\ &< \sum_{t_i < \tau_0} w_i y_i^2 + \sum_{t_i > \tau_0} w_i (1 - y_i)^2 = \Sigma_{\tau_0}. \end{aligned}$$

This completes the proof of the lemma. □

Proof of Theorem 1.

Assume first that $(a^\star, b^\star) \in \mathcal{P}$ is the best LS estimate, and then show that $S(a^\star, b^\star) \leq E^\star$. In order to do this, first note that for all $a, b > 0$,

$$S(a^\star, b^\star) \leq S(a, b) = \sum_{i=1}^{n} w_i [(1 - \mathrm{e}^{-bt_i})\, \mathrm{e}^{-a\, \mathrm{e}^{-bt_i}} - y_i]^2,$$

from where, taking the limit as $a \to 0$, it follows that

$$S(a^\star, b^\star) \leq \sum_{i=1}^{n} w_i [(1 - \mathrm{e}^{-bt_i}) - y_i]^2.$$

From the last inequality and the definition of $E^\star$ we obtain that $S(a^\star, b^\star) \leq E^\star$, so that it is enough to set $(a_0, b_0) = (a^\star, b^\star)$.

Let us show the converse of the theorem. Suppose that there is a point $(a_0, b_0) \in \mathcal{P}$ such that $S(a_0, b_0) \le E^\star$. Since functional S is nonnegative, there exists $S^\star := \inf_{(a,b)\in\mathcal{P}} S(a, b)$. It should be shown that the best LS estimate exists, i.e., that there exists a point $(a^\star, b^\star) \in \mathcal{P}$ such that $S(a^\star, b^\star) = S^\star$. To do this, first note that

$$S^\star \le S(a_0, b_0) \le E^\star$$

If $S^\star = S(a_0, b_0)$, to complete the proof it is enough to set $(a^\star, b^\star) = (a_0, b_0)$. Hence, we can further assume that

$$S^\star < S(a_0, b_0) \le E^\star. \tag{5}$$

Let (a_k, b_k) be a sequence in $\mathcal{P}$, such that

$$\begin{aligned} S^\star &= \lim_{k\to\infty} S(a_k, b_k) = \lim_{k\to\infty} \sum_{i=1}^{n} w_i[F(t_i; a_k, b_k) - y_i]^2 \\ &= \lim_{k\to\infty} \sum_{i=1}^{n} w_i[(1 - \mathrm{e}^{-b_k t_i})\,\mathrm{e}^{-a_k \mathrm{e}^{-b_k t_i}} - y_i]^2. \end{aligned}$$

Without loss of generality, in further consideration we may assume that sequences (a_k) and (b_k) are monotone. This is possible because the sequence (a_k, b_k) has a subsequence (a_{l_k}, b_{l_k}), such that all its component sequences (a_{l_k}) and (b_{l_k}) are monotone, and since $\lim_{k\to\infty} S(a_{l_k}, b_{l_k}) = \lim_{k\to\infty} S(a_k, b_k) = S^\star$.

As each monotone sequence of real numbers converges in the extended real number system $\bar{\mathbb{R}}$, denote

$$a^\star := \lim_{k\to\infty} a_k, \quad b^\star := \lim_{k\to\infty} b_k.$$

Note that $0 \le a^\star \le \infty$ and $0 \le b^\star \le \infty$, because $(a_k, b_k) \in \mathcal{P}$.

To complete the proof, it is enough to show that $(a^\star, b^\star) \in \mathcal{P}$, i.e., that $0 < a^\star < \infty$ and $0 < b^\star < \infty$. The continuity of the functional S will then imply that $S^\star = \lim_{k\to\infty} S(a_k, b_k) = S(a^\star, b^\star)$, which will complete the proof of the theorem.

Before continuing with the proof, let us note that Lemma 1 implies that

$$S^\star < \Sigma_{\tau_0}, \tag{6}$$

for arbitrary $\tau_0 > 0$.

It remains to show that $(a^\star, b^\star) \in \mathcal{P}$. The proof will be done in four steps. In Step 1, we will show that $b^\star \ne 0$. In Step 2, we will show that $b^\star \ne \infty$, which will imply that $0 < b^\star < \infty$. The proof that $a^\star \ne \infty$ will be done in Step 3. Finally, in Step 4 we will show that $a^\star \ne 0$.

Step 1. Let us first show that $b^\star \ne 0$. We prove this by contradiction. Suppose to the contrary that $b^\star = 0$. First, note that for all $a_k, b_k \ge 0$ and for all $t \ge 0$

$$0 \le (1 - \mathrm{e}^{-b_k t})\,\mathrm{e}^{-a_k \mathrm{e}^{-b_k t}} \le 1 - \mathrm{e}^{-b_k t}. \tag{7}$$

Furthemore, since $b_k \to 0$, then

$$1 - \mathrm{e}^{-b_k t} \to 0,$$

and thus from inequalities (7) we have

$$F(t; a_k, b_k) = (1 - \mathrm{e}^{-b_k t})\,\mathrm{e}^{-a_k\,\mathrm{e}^{-b_k t}} \to 0, \quad \text{for all } t \geq 0.$$

Therefore, we would obtain that

$$S^\star = \lim_{k\to\infty} \sum_{i=1}^{n} w_i [F(t_i; a_k, b_k) - y_i]^2 = \sum_{i=1}^{n} w_i y_i^2 > \sum_{i=1}^{n-1} w_i y_i^2 = \Sigma_{t_n},$$

which contradicts (6). This means that in this way functional S cannot attain its infimum and we have proved that $b^\star \neq 0$.

Step 2. Let us now show that $b^\star \neq \infty$. We prove this by contradiction. Suppose to the contrary that $b^\star = \infty$. For each $i = 1, \ldots, n$, let us denote $l_i^\star := \lim_{k\to\infty} a_k e^{-b_k t_i}$. Now from the obvious inequalities

$$a_k e^{-b_k t_1} \geq a_k e^{-b_k t_2} \geq \cdots \geq a_k e^{-b_k t_n} \geq 0,$$

after taking the limit $k \to \infty$, we obtain

$$l_1^\star \geq l_2^\star \geq \cdots \geq l_n^\star \geq 0.$$

Note that only one of the following subcases can occur: (a) $l_i^\star = \infty$ for all $i = 1, \ldots, n$, (b) there exists an index i such that $0 \leq l_i^\star < \infty$.

Subcase (a) If $l_i^\star = \infty$ for all $i = 1, \ldots, n$, then $\lim_{k\to\infty} F(t_i; a_k, b_k) = 0$ for all i, and consequently we would have that $S^\star = \sum_{i=1}^{n} w_i y_i^2 > \Sigma_{t_n}$. As already shown in Step 1, in this way functional S cannot attain its infimum.

Subcase (b) Let $i_0 := \min\{i \mid 0 \leq l_i^\star < \infty\}$. Then for each $i > i_0$,

$$l_i^\star = \lim_{k\to\infty} a_k\,\mathrm{e}^{-b_k t_i} = \lim_{k\to\infty} a_k\,\mathrm{e}^{-b_k t_{i_0}}\,\mathrm{e}^{-b_k (t_i - t_{i_0})} = l_{i_0}^\star \lim_{k\to\infty} \mathrm{e}^{-b_k (t_i - t_{i_0})} = 0.$$

Thus

$$l_i^\star = \begin{cases} \infty, & \text{for all } i < i_0 \\ 0, & \text{for all } i > i_0, \end{cases}$$

and consequently

$$\lim_{k\to\infty} F(t_i; a_k, b_k) = \begin{cases} 0, & \text{for all } i < i_0 \\ 1, & \text{for all } i > i_0, \end{cases}$$

from where it follows that

$$S^\star = \lim_{k\to\infty} \sum_{i=1}^{n} w_i [F(t_i; a_k, b_k) - y_i]^2 \geq \sum_{t_i < t_{i_0}} w_i y_i^2 + \sum_{t_i > t_{i_0}} w_i (1 - y_i)^2 = \Sigma_{t_{i_0}}.$$

Again, this contradicts (6). Thus we have proved that $b^\star \neq \infty$.

Step 3. In this step, we will show that $a^\star \neq \infty$. We prove this by contradiction. Suppose to the contrary that $a^\star = \infty$. Then, as in Step 1, we would have that

$\lim_{k\to\infty} F(t; a_k, b_k) = 0$ for all $t \geq 0$, and as we have already shown, in that case functional S cannot attain its infimum.

Step 4. It remains to show that $a^\star \neq 0$. Suppose to the contrary that $a^\star = 0$. Then $\lim_{k\to\infty} F(t; a_k, b_k) = 1 - \mathrm{e}^{-b^\star t}$ for all $t \geq 0$. In this case we would have

$$S^\star = \sum_{i=1}^{n} w_i \big[(1 - \mathrm{e}^{-b^\star t_i}) - y_i\big]^2 \geq E^\star,$$

which contradicts assumption (5). This means that in this way ($a^\star = 0$) functional S cannot attain its infimum. Thus we have provided that $a^\star \neq 0$, and herewith we have completed the proof of Theorem 1. □

From the curve fitting point of view, it makes sense to allow parameter a to be zero, i.e., to minimize functional S over the following set of parameters

$$\mathcal{P}_0 := \big\{(a, b) \in \mathbb{R}^2 : a \geq 0, b > 0\big\}.$$

The next theorem tells us that if that is of interest, then the corresponding LS estimate will exist.

Theorem 2. *Let the points* (w_i, t_i, y_i), $i = 1, \ldots, n$, $n > 2$, *be data such that* $0 < t_1 < t_2 < \ldots < t_n$ *and* $0 < y_i < 1$, $i = 1, \ldots, n$. *Then there exists a point* $(a^\star, b^\star) \in \mathcal{P}_0$ *such that*

$$S(a^\star, b^\star) = \inf_{(a,b)\in\mathcal{P}_0} S(a, b).$$

The proof of this theorem is omitted; it is the same for respective parts of the proof of Theorem 1, with the exception that we do not have to prove that $a^\star \neq 0$.

2.3. The l_p-norm existence theorem for the shifted Gompertz distribution

The LS problem is a nonlinear l_2-norm problem. During the last few decades an increased interest in alternative l_p-norm has become apparent (see e.g. [1] and [11]). For example, l_1-norm criteria are more suitable if there are wild points (outliers) in the data. Thus, instead of minimizing functional S, sometimes a more adequate criterion for estimation of unknown parameters a and b of the shifted Gompertz distribution (1) is to minimize the following functional:

$$S_p(a, b) = \sum_{i=1}^{n} w_i \big|F(t_i; a, b) - y_i\big|^p, \tag{8}$$

where p ($1 \leq p < \infty$) is an arbitrary fixed number. A point $(a^\star, b^\star) \in \mathcal{P}$ such that

$$S_p(a^\star, b^\star) = \inf_{(a,b)\in\mathcal{P}} S_p(a, b)$$

is called the best l_p*-norm estimate*, if it exists. For $p = 2$, the best l_2-norm estimate is the familiar weighted LS estimate.

To state the corresponding l_p-norm ($1 \le p < \infty$) generalizations of Theorems 1 and 2, we need an additional notation. Let

$$E_p^\star := \inf_{b>0} E_p(b), \quad \text{where } E_p(b) = \sum_{i=1}^{n} w_i |(1 - \mathrm{e}^{-bt_i}) - y_i|^p.$$

Obviously, $E^\star = E_2^\star$ and $S = S_2$. Again, by using Theorem 3.1 from Jukić [14], it is easy to show that there exists a $\beta^\star > 0$ such that $E_p(\beta^\star) = E_p^\star$.

Arguing in a similar way as in proofs of Lemma 1, Theorem 1 and Theorem 2, we can easily show the following l_p-norm generalizations of Theorem 1 and Theorem 2. To do this, it suffices to replace the l_2 norm by the l_p norm. Thereby all parts of the proofs remain the same.

Theorem 3 (Necessary and sufficient condition)**.** *Suppose that the data* (w_i, t_i, y_i), $i = 1, \ldots, n$, $n \ge 3$, *satisfy conditions* $0 < t_1 < t_2 < \ldots < t_n$ *and* $0 < y_i < 1$, $i = 1, \ldots, n$.. *Then functional* S_p *defined by (8) attains its infimum on* $\mathcal{P}$ *if and only if there is a point* $(a_0, b_0) \in \mathcal{P}$ *such that* $S_p(a_0, b_0) \le E_p^\star$.

Theorem 4. *Let the points* (w_i, t_i, y_i), $i = 1, \ldots, n$, $n > 2$, *be data such that* $0 < t_1 < t_2 < \ldots < t_n$ *and* $0 < y_i < 1$, $i = 1, \ldots, n$. *Then there exists a point* $(a^\star, b^\star) \in \mathcal{P}_0$ *such that*

$$S_p(a^\star, b^\star) = \inf_{(a,b)\in\mathcal{P}_0} S_p(a, b).$$

Acknowledgements

We would like to thank the referees for the useful comments and suggestions.

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