Existence of optimal weighted least squares estimate for 3-parametric exponential model

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Abstract : Given a set of data $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ we present sufficient conditions which guarantee the existence of the weighted least squares estimate for a 3-parametric exponential function. To this end, we suggest a classification of the data based on their increasing or decreasing trend, and on their convexity or concavity form. We discuss a choice of the initial approximation and present a numerical example.

Key Words : weighted least squares, parametric exponential function, least squares estimate, existence problem, classification of data.

AMS Subject Classification : 65D10, 62J02.

1. Introduction

Very often in experimental research data $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ are obtained and we have to find a good model to fit them. In this paper we consider the 3-parametric exponential model

$$f(t; a, b, c) = a + be^{ct} \tag{1.1}$$

where a, b, and c are real parameters. These parameters will be estimated from the data $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ where the t_i's represent the values of the independent variable, the f_i's are the values of the measured function, and each ω_i is the weight associated to the data (t_i, f_i).

It is well known that such model are useful in different fields of applied research such that economy [14], biology [11], physics [15], chemistry [1], medicine [9], engineering [11, 13] and agriculture [4].

To estimate the parameters a, b, and c we use the weighted least squares method. We minimize the functional

$$F(a, b, c) = \frac{1}{2}\sum_{i=1}^{m} \omega_i \big(f(t_i; a, b, c) - f_i\big)^2 = \frac{1}{2}\sum_{i=1}^{m} \omega_i \big(a + be^{ct_i} - f_i\big)^2 \tag{1.2}$$

on $\mathbb{R}^3$ and we find the weighted least squares estimate (WLSE) given by

$$(a^*, b^*, c^*) = \arg\min_{(a,b,c)\in\mathbb{R}^3} F(a,b,c).$$

In the sequel we assume that $m \geq 3$ and the t_i's are strictly increasing

$$t_1 < t_2 < \cdots < t_m.$$

The goal of this paper is to present sufficient conditions for the existence of the WLSE for the 3-parametric exponential model (1.1) to complement the papers [5] and [6]. It appends that the proof contained in these papers contains some mistakes and we present a way to get the result correctly. Our approach is based on orthogonal polynomials to obtain a rough classification of the data and then deduce sufficient conditions for the existence of the WLSE. Other approaches concerning the existence of the WLSE exist. In particular, using the concept of "existence level", some theorems about the existence of the WLSE are obtained in [2] and [3].

In Section 2 we briefly review the polynomial least squares fitting and suggest an elementary classification of the data based on the coefficients of the best polynomial with respect to an orthogonal basis of polynomials. In Section 3 we present sufficient conditions for the existence of the weighted least square estimate for the 3-parametric exponential model. In Section 4 we suggest two ways to initialize the numerical algorithm to find the optimal solution. A numerical example follows in Section 5.

2. Polynomial least squares fitting and data classification

Let $\mathcal{P}_n$ be the set of polynomials of degree $\leq n$. In this section, we look for the best n-degree polynomial fitting to the data $\{(\omega_i, t_i, f_i)\}_{i=1}^m$. This polynomial is given by

$$p_n^* = \arg\min_{p\in\mathcal{P}_n} G(p)$$

where

$$G(p) = \frac{1}{2}\sum_{i=1}^m \omega_i \big(p(t_i) - f_i\big)^2.$$

This polynomial exists and is unique as long as $n+1 \leq m$. Indeed in this case

$$G(p) = \frac{1}{2}\|p - f\|^2$$

where $\|\cdot\|$ is the norm on $\mathcal{P}_n$ induced by the scalar product defined by

$$\langle p, q\rangle = \sum_{i=1}^m \omega_i p(t_i) q(t_i)$$

for any pair of polynomials p and q in $\mathcal{P}_n$. For the f_i's we use the notation $f_i = f(t_i)$ $(i = 1, ..., m)$. It is well known that p_n^* is characterized by the normal equations

$$\langle p_n^* - f, p\rangle = 0$$

for all $p \in \mathcal{P}_n$.

In this setting, we can find a sequence of orthogonal polynomials by applying the Gram-Schmidt orthogonalization process to the standard basis $\{1, t, t^2, \cdots, t^n\}$ of $\mathcal{P}_n$. These orthogonal polynomials are given by

$$q_0(t) = 1, \quad q_1(t) = t - \alpha_1,$$

and for $j \geq 2$

$$q_j(t) = (t - \alpha_j)q_{j-1}(t) - \beta_j q_{j-2}(t)$$

where

$$\alpha_j = \frac{\langle tq_{j-1}, q_{j-1}\rangle}{\langle q_{j-1}, q_{j-1}\rangle} \quad (j = 1, 2, 3, \ldots),$$

and

$$\beta_j = \frac{\langle tq_{j-1}, q_{j-2}\rangle}{\langle q_{j-2}, q_{j-2}\rangle} \quad (j = 2, 3, 4, \ldots).$$

Hence the best n-degree least squares polynomial p_n^* can be written as

$$p_n^*(t) = \sum_{j=0}^{n} \gamma_j^* q_j(t)$$

where

$$\gamma_j^* = \frac{\langle f, q_j\rangle}{\langle q_j, q_j\rangle} \quad (j = 0, 1, \ldots, n).$$

Let us observe that

$$p_n^*(t) = \gamma_n^* q_n(t) + p_{n-1}^*(t).$$

In the next section we will use the following result.

Lemma 2.1. $\langle p_{n-1}^* - f, t^n\rangle = -\gamma_n^* \|q_n\|^2$ *for* $n = 1, \ldots, m-1$.

Proof. Since $q_n(t) = t^n + \tilde{q}_{n-1}(t)$ where $\tilde{q}_{n-1}(t)$ is a polynomial of degree $\leq n-1$, we have

$$\begin{aligned}
\gamma_n^* \|q_n\|^2 &= \langle \gamma_n^* q_n, q_n\rangle \\
&= \langle p_n^* - p_{n-1}^*, q_n\rangle \\
&= \langle p_n^* - f, q_n\rangle + \langle f - p_{n-1}^*, q_n\rangle \\
&= -\langle p_{n-1}^* - f, t^n + \tilde{q}_{n-1}\rangle \\
&= -\langle p_{n-1}^* - f, t^n\rangle. \qquad \square
\end{aligned}$$

Lemma 2.2. *If the* q_j*'s are the orthogonal polynomials associated to* $\{(\omega_i, t_i)\}_{i=1}^m$*, the orthogonal polynomials* $\tilde{q}_j$*'s associated to* $\{(\omega_i, \tilde{t}_i = -t_i)\}_{i=1}^m$ *are given by*

$$\tilde{q}_j(t) = (-1)^j q_j(-t). \qquad \square$$

Definition 2.3. *The data* $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ *are said to be*
(i) *stationary if* $\gamma_1^* = 0$*;*
(ii) *essentially increasing, respectively decreasing, if* $\gamma_1^* > 0$*, respectively* $\gamma_1^* < 0$*;*
(iii) *essentially linear, if* $\gamma_2^* = 0$*;*
(iv) *essentially convex, respectively concave, if* $\gamma_2^* > 0$*, respectively* $\gamma_2^* < 0$. □

Remark 2.4. *If the data* $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ *are essentially increasing, resp. decreasing, then the data* $\{(\omega_i, -t_i, f_i)\}_{i=1}^m$ *are essentially decreasing, resp. increasing. Also if the data* $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ *are essentially convex, resp. concave, then the data* $\{(\omega_i, t_i, -f_i)\}_{i=1}^m$ *are essentially concave, resp. convex.* □

Let us define the following expression

$$f_{\bullet j} = \frac{\sum_{i=1, i\neq j}^m \omega_i f_i}{\sum_{i=1, i\neq j}^m \omega_i}$$

for $j = 1, ..., m$.

Definition 2.5. *The data* $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ *are said to be strongly regular if they are*
(i) *essentially increasing and convex, and* $f_m > f_{\bullet m}$ *and* $f_{m-1} > f_{\bullet m}$*, or*
(ii) *essentially decreasing and convex, and* $f_1 > f_{\bullet 1}$ *and* $f_2 > f_{\bullet 1}$*, or*
(iii) *essentially increasing and concave, and* $f_1 < f_{\bullet 1}$ *and* $f_2 < f_{\bullet 1}$*, or*
(iv) *essentially decreasing and concave, and* $f_m < f_{\bullet m}$ *and* $f_{m-1} < f_{\bullet m}$*.* □

3. Existence of the least squares estimate

In this section we discuss the weighted least squares estimate existence problem. We give conditions under which there exists a $(a^*, b^*, c^*) \in \mathbb{R}^3$ such that

$$(a^*, b^*, c^*) = \arg \min_{(a,b,c)\in\mathbb{R}^3} F(a, b, c).$$

It is necessary to add some conditions on the data for this existence problem as shown by the following example.

Example 3.1. *Suppose the data* $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ *are such that the data points* $\{(t_i, f_i)\}_{i=1}^m$ *are all on a given line* $y = kt + l$*.*

If $k = 0$ *hence* $l = f_i$ *for* $i = 1, ..., m$*, and let* $(a^*, b^*, c^*) \in \mathbb{R}^3$ *such that* $a^* + b^* e^{c^* t_i} = l$ *for* $i = 1, ..., m$*. Then*

$$a^* = l, b^* = 0, \, and \, c^* \in \mathbb{R}^3,$$

or

$$a^* + b^* = l, \, and \, c^* = 0,$$

are all optimal solutions such that $F(a^*, b^*, c^*) = 0$*.*

If $k \neq 0$*, since the graphs of* $y = f(t; a, b, c)$ *and* $y = kt + l$ *intersect in at most two points and* $m \geq 3$*, we have*

$$F(a, b, c) = \frac{1}{2} \sum_{i=1}^m \omega_i (a + b e^{ct_i} - f_i)^2 > 0.$$

But for

$$(a, b, c) = (f_0 - \frac{1}{c}, \frac{e^{-ckt_0}}{c}, ck) \in \mathbb{R}^3$$

where $f_0 = kt_0 + l$ *and* $c \neq 0$*, we have*

$$\begin{aligned}
\lim_{c\to 0} F(f_0 - \frac{1}{c}, \frac{e^{-ckt_0}}{c}, ck) &= \lim_{c\to 0} \frac{1}{2} \sum_{i=1}^m \omega_i (f_0 + \frac{e^{ck(t_i - t_0)} - 1}{c} - f_i)^2 \\
&= \frac{1}{2} \sum_{i=1}^m \omega_i (f_0 + k(t_i - t_0) - f_i)^2 \\
&= \frac{1}{2} \sum_{i=1}^m \omega_i (kt_i + l - f_i)^2 \\
&= 0.
\end{aligned}$$

Hence

$$\inf_{(a,b,c)\in\mathbb{R}^3} F(a, b, c) = 0$$

and the problem has no solution. □

To obtain an existence result we will assume that the data satisfy certain sufficient conditions. For example the data will be essentially increasing or decreasing and essentially convex or concave.

Let us consider the following subsets of $\mathbb{R}^3$

$$\begin{aligned} \mathcal{U}_{++} &= \{ (a,b,c) \in \mathbb{R}^3 \,|\, b \geq 0 \,\text{and}\, c \geq 0 \}, \\ \mathcal{U}_{+-} &= \{ (a,b,c) \in \mathbb{R}^3 \,|\, b \geq 0 \,\text{and}\, c \leq 0 \}, \\ \mathcal{U}_{-+} &= \{ (a,b,c) \in \mathbb{R}^3 \,|\, b \leq 0 \,\text{and}\, c \geq 0 \}, \\ \mathcal{U}_{--} &= \{ (a,b,c) \in \mathbb{R}^3 \,|\, b \leq 0 \,\text{and}\, c \leq 0 \}. \end{aligned}$$

The boundary of these subsets are

$$\begin{aligned} \partial\mathcal{U}_{++} &= \Gamma_b^+ \cup \Gamma_c^+, & \partial\mathcal{U}_{+-} &= \Gamma_b^+ \cup \Gamma_c^-, \\ \partial\mathcal{U}_{-+} &= \Gamma_b^- \cup \Gamma_c^+, & \partial\mathcal{U}_{--} &= \Gamma_b^- \cup \Gamma_c^-, \end{aligned}$$

where

$$\begin{aligned} \Gamma_b^+ &= \{ (a,b,0) \in \mathbb{R}^3 \,|\, b \geq 0 \}, \\ \Gamma_b^- &= \{ (a,b,0) \in \mathbb{R}^3 \,|\, b \leq 0 \}, \\ \Gamma_c^+ &= \{ (a,0,c) \in \mathbb{R}^3 \,|\, c \geq 0 \}, \\ \Gamma_c^- &= \{ (a,0,c) \in \mathbb{R}^3 \,|\, c \leq 0 \}. \end{aligned}$$

For the interior of a subset $\mathcal{U}$ of $\mathbb{R}^3$, defined by $\mathcal{U} \setminus \partial\mathcal{U}$, we will use the notation $\mathrm{Int}(\mathcal{U})$.

Theorem 3.2. *Let the data $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ be essentially convex ($\gamma_2^* > 0$) and strongly regular.*
(A) *If the data are essentially increasing ($\gamma_1^* > 0$) then there exists $(a^*, b^*, c^*) \in \mathrm{Int}(\mathcal{U}_{++})$ such that*

$$F(a^*, b^*, c^*) = \min_{(a,b,c)\in\mathcal{U}_{++}} F(a,b,c).$$

(B) *If the data are essentially decreasing ($\gamma_1^* < 0$) then there exists $(a^*, b^*, c^*) \in \mathrm{Int}(\mathcal{U}_{+-})$ such that*

$$F(a^*, b^*, c^*) = \min_{(a,b,c)\in\mathcal{U}_{+-}} F(a,b,c).$$

Proof. We assume that the t_i's are as follows

$$t_1 < t_2 = 0 < t_3 < \cdots < t_m.$$

(A) Since $F(a,b,c) \geq 0$ then

$$0 \leq \inf_{(a,b,c)\in\mathcal{U}_{++}} F(a,b,c) = F^* < +\infty.$$

Step 1. Let us show that F^* cannot be a value of F on the boundary $\partial\mathcal{U}_{++} = \Gamma_b^+ \cup \Gamma_c^+$. On Γ_b^+, $c = 0$ and

$$F(a,b,0) = \frac{1}{2}\sum_{i=1}^m \omega_i (a + b - f_i)^2 \geq \frac{1}{2}\sum_{i=1}^m \omega_i (\gamma_0^* - f_i)^2 = F_0.$$

This value can be obtained for any $(\tilde{a},\tilde{b},0)\in\Gamma_b^+$ such that $\tilde{a}+\tilde{b}=\gamma_0^*$ and $\tilde{b}\geq 0$. Also, because $\gamma_1^*>0$, and

$$\begin{aligned}\frac{\partial F}{\partial c}(\tilde{a},\tilde{b},0)\Big|_{\substack{\tilde{a}+\tilde{b}=\gamma_0\\ \tilde{b}>0}} &= \tilde{b}\sum_{i=1}^{m}\omega_i(\gamma_0^*-f_i)t_i\\ &= \tilde{b}\langle p_0^*-f,t\rangle\\ &= -\tilde{b}\gamma_1^*\|q_1\|^2\\ &< 0\end{aligned}$$

for $\tilde{b}>0$, there exists a point $(\tilde{a},\tilde{b},\tilde{c})\in \mathrm{Int}(\mathcal{U}_{++})$ such that

$$F(\tilde{a},\tilde{b},\tilde{c})\Big|_{\substack{\tilde{a}+\tilde{b}=\gamma_0^*\\ \tilde{b}>0}} < F(\tilde{a},\tilde{b},0)\Big|_{\substack{\tilde{a}+\tilde{b}=\gamma_0^*\\ \tilde{b}>0}} < F(a,b,0)\Big|_{(a,b,0)\in\Gamma_b^+}.$$

On Γ_c^+, $b=0$ and

$$\begin{aligned}F(a,0,c) &= \frac{1}{2}\sum_{i=1}^{m}\omega_i(a-f_i)^2\\ &\geq \frac{1}{2}\sum_{i=1}^{m}\omega_i(\gamma_0^*-f_i)^2\\ &\geq F(a,b,0)\Big|_{\substack{\tilde{a}+\tilde{b}=\gamma_0^*\\ \tilde{b}>0}}\\ &> F(\tilde{a},\tilde{b},\tilde{c})\Big|_{\substack{\tilde{a}+\tilde{b}=\gamma_0^*\\ \tilde{b}>0}}.\end{aligned}$$

Hence F^* cannot be attained on $\partial\mathcal{U}_{++}$.

Step 2. Now, let $\{a_n,b_n,c_n\}_{n=1}^{+\infty}$ be a sequence in $\mathcal{U}_{++}$ such that

$$0\leq \lim_{n\to+\infty}F(a_n,b_n,c_n)=\inf_{(a,b,c)\in\mathcal{U}_{++}}F(a,b,c)=F^*<+\infty.$$

Let

$$r_i(n)=a_n+b_ne^{c_nt_i}-f_i$$

for $i=1,...,m$.

Without loss of generality, whenever we have an unbounded sequence we may assume that it tends to $+\infty$ or to $-\infty$, because we can take a subsequence. Similarly, whenever we have a bounded sequence, we may assume it is convergent, otherwise by the Bolzano-Weierstrass theorem, we can take a convergent subsequence.

Let us show that the sequence $\{a_n,b_n,c_n\}_{n=1}^{+\infty}$ is bounded by showing that $F(a_n,b_n,c_n)$ cannot attain its infimum F^* in either the following two cases :

2.I $|a_n|\to+\infty$;
2.II $\lim_{n\to+\infty}a_n=a^*$ and $\lim_{n\to+\infty}(b_n+c_n)=+\infty$.

Case 2.I. Since

$$r_2(n)=a_n+b_n-f_2$$

we must have $\lim_{n\to+\infty}b_n=-\lim_{n\to+\infty}a_n$ and, from the fact that $b_n\geq 0$, it follows that $\lim_{n\to+\infty}a_n=-\infty$ and $\lim_{n\to+\infty}b_n=+\infty$. We can suppose that

$\lim_{n\to+\infty}(a_n+b_n) = l \in \mathbb{R}$ if not $\lim_{n\to+\infty} r_2^2(n) = +\infty$. If the sequence $\{c_n\}_{n=1}^{+\infty}$ is unbounded, then $\lim_{n\to+\infty} c_n = +\infty$. Take any t_{i_0} in $\{t_3, t_4, ..., t_m\}$, then $c_n t_{i_0} > 0$. Since $b_n > 0$ we have

$$a_n + b_n e^{c_n t_{i_0}} \geq a_n + b_n(1 + c_n t_{i_0}) = (a_n + b_n) + b_n c_n t_{i_0}$$

because $e^{c_n t_{i_0}} \geq 1 + c_n t_{i_0}$, and

$$\lim_{n\to+\infty} (a_n + b_n) + b_n c_n t_{i_0} = l + \infty = +\infty.$$

Hence $\lim_{n\to+\infty} c_n = \tilde{c} \geq 0$. If $\tilde{c} > 0$, as before we obtain $\lim_{n\to+\infty} a_n + b_n e^{c_n t_i} = +\infty$. If $\tilde{c} = 0$, from the mean value theorem we have

$$a_n + b_n e^{c_n t_i} = (a_n + b_n) + b_n c_n t_i e^{\theta_i(n) c_n t_i}$$

where $\theta_i(n) \in (0, 1)$ for all $i = 1, 2, ..., m$ and $n = 1, 2, ...$ If the sequence $\{b_n c_n\}_{n=1}^{+\infty}$ is unbounded, as before we obtain $\lim_{n\to+\infty} a_n + b_n e^{c_n t_i} = +\infty$. Hence $\{b_n c_n\}_{n=1}^{+\infty}$ is bounded and we can suppose that it converges to $k \geq 0$. It follows that

$$\lim_{n\to+\infty} a_n + b_n e^{c_n t_i} = l + k t_i$$

for $i = 1, ..., m$. Hence

$$\lim_{n\to+\infty} F(a_n, b_n, c_n) = \frac{1}{2}\sum_{i=1}^{m} \omega_i (l + k t_i - f_i)^2 = F_0 \geq \frac{1}{2}\sum_{i=1}^{m} \omega_i (p_1^*(t_i) - f_i)^2$$

where p_1^* is the best least squares polynomial of degree ≤ 1 for the data. We have

$$\begin{aligned} p_1^*(t) &= \gamma_0^* q_0(t) + \gamma_1^* q_1(t) \\ &= \gamma_0^* + \gamma_1^*(t - \alpha_1) \\ &= (\gamma_0^* - \gamma_1^* \alpha_1) + \gamma_1^* t \\ &= l^* + k^* t \end{aligned}$$

where $l^* = \gamma_0^* - \gamma_1^* \alpha_1$ and $k^* = \gamma_1^* > 0$. Let us choose any value $(\tau_0$ and define a continuous function $\phi : \mathbb{R} \mapsto \mathbb{R}$ by the formula

$$\phi(\lambda) = \begin{cases} \dfrac{1}{2}\displaystyle\sum_{i=1}^{m} \omega_i (k^*\tau_0 + \frac{e^{\lambda k^*(t_i - \tau_0)} - 1}{\lambda} - (f_i - l^*))^2 & \text{if} \quad \lambda \neq 0, \\ \dfrac{1}{2}\displaystyle\sum_{i=1}^{m} \omega_i (l^* + k^* t_i - f_i)^2 & \text{if} \quad \lambda = 0. \end{cases}$$

Let us observe that

$$\phi(\lambda) = F(k^*\tau_0 + l^* - \frac{1}{\lambda}, \frac{e^{-\lambda k^* \tau_0}}{\lambda}, \lambda k^*)$$

and

$$(k^*\tau_0 + l^* - \frac{1}{\lambda}, \frac{e^{-\lambda k^* \tau_0}}{\lambda}, \lambda k^*) \in \text{Int}(\mathcal{U}_{++})$$

for $\lambda > 0$. Its derivative is given by

$$\phi^{(1)}(\lambda) = \begin{cases} \displaystyle\sum_{i=1}^{m} \omega_i \Big(k^*\tau_0 + \frac{e^{\lambda k^*(t_i-\tau_0)} - 1}{\lambda} - (f_i - l^*) \Big) \Big(\frac{e^{\lambda k^*(t_i-\tau_0)}(\lambda k^*(t_i-\tau_0) - 1) + 1}{\lambda^2} \Big) & \text{if} \quad \lambda \neq 0, \\ \displaystyle\frac{(k^*)^2}{2} \sum_{i=1}^{m} \omega_i (l^* + k^* t_i - f_i)(t_i - \tau_0)^2 & \text{if} \quad \lambda = 0 \end{cases}$$

is also continuous on $\mathbb{R}$. But

$$\phi^{(1)}(0) = \frac{(k^*)^2}{2} \langle l^* + k^* t - f, (t-\tau_0)^2 \rangle = \frac{(k^*)^2}{2} \langle l^* + k^* t - f, t^2 \rangle = -\frac{(k^*)^2}{2} \gamma_2^* \|q_2\|^2.$$

Since $\gamma_2^* > 0$, it follows that $\phi^{(1)}(0) < 0$ and the function ϕ is decreasing on a neighborhood of $\lambda = 0$. Hence their exists a $\tilde{\lambda} > 0$ such that $\phi(\tilde{\lambda}) < \phi(0) \leq F_0$ and it follows that $F^* < F_0$ and the sequence $\{a_n\}_{n=1}^{+\infty}$ is bounded.

Case 2.II. Now we show that the sequence $\{(b_n, c_n)\}_{n=1}^{+\infty}$ is bounded. To show that we consider the 4 possible situations

(1) $b_n \to +\infty$ and $c_n \to +\infty$,
(2) $b_n \to +\infty$ and $c_n \to c^* \geq 0$,
(3) $b_n \to b^* > 0$ and $c_n \to +\infty$,
(4) $b_n \to b^* = 0$ and $c_n \to +\infty$.

For the cases (1), (2), and (3), we observe that $\{F(a_n, b_n, c_n)\}_{n=1}^{+\infty}$ diverge to $+\infty$ because $\lim_{n\to+\infty} r_2(n) = +\infty$. It remains to consider only the last case.

Let us assume that $\lim_{n\to+\infty} a_n = a^*$, $\lim_{n\to+\infty} b_n = b^* = 0$, and $\lim_{n\to+\infty} c_n = +\infty$. We also suppose that

$$\lim_{n\to+\infty} b_n e^{c_n t_m} = L < +\infty$$

because in the contrary $\lim_{n\to+\infty} r_m^2(n) = +\infty$. We have

$$\lim_{n\to+\infty} b_n e^{c_n t_i} = \lim_{n\to+\infty} b_n e^{c_n t_m} \lim_{n\to+\infty} e^{c_n (t_i - t_m)} = L \cdot 0 = 0$$

for $i = 1, ..., m-1$. Hence

$$\begin{aligned} F_1 &= \lim_{n\to+\infty} F(a_n, b_n, c_n) \\ &= \frac{1}{2} \sum_{i=1}^{m-1} \omega_i (a^* - f_i)^2 + \frac{1}{2} \omega_m (L - f_m)^2 \\ &\geq \frac{1}{2} \sum_{i=1}^{m-1} \omega_i (f_{\bullet m} - f_i)^2. \end{aligned}$$

We look for a point $(f_{\bullet m}, b', c')$ in $\mathrm{Int}(\mathcal{U}_{++})$ such that

$$F(f_{\bullet m}, b', c') < \frac{1}{2} \sum_{i=1}^{m-1} \omega_i (f_{\bullet m} - f_i)^2 \leq F_1.$$

Using the strong monotony for f_m, we consider the curve sketched in Figure 1 and defined by

$$\Gamma = \{\, (f_{\bullet m}, (f_m - f_{\bullet m})e^{-ct_m}, c) \in \mathcal{U}_{++} \,|\, c \geq 0\}.$$

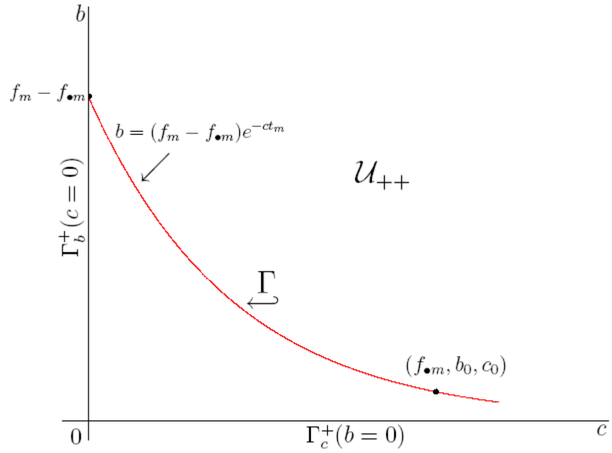


FIGURE 1. The curve Γ.

Let

$$\psi(c) = F(f_{\bullet m}, (f_m - f_{\bullet m})e^{-ct_m}, c) = \frac{1}{2}\sum_{i=1}^{m} \omega_i (f_{\bullet m} + (f_m - f_{\bullet m})e^{c(t_i - t_m)} - f_i)^2.$$

Then

$$\lim_{c\to+\infty} \psi(c) = \frac{1}{2}\sum_{i=1}^{m-1} \omega_i (f_{\bullet m} - f_i)^2.$$

Also

$$\psi^{(1)}(c) = \sum_{i=1}^{m-1} \omega_i (f_{\bullet m} + (f_m - f_{\bullet m})e^{c(t_i - t_m)} - f_i)(f_m - f_{\bullet m})(t_i - t_m)e^{c(t_i - t_m)},$$

and if we consider the ratio

$$\frac{\psi^{(1)}(c)}{e^{c(t_{m-1}-t_m)}} = \sum_{i=1}^{m-1} \omega_i (f_{\bullet m} + (f_m - f_{\bullet m})e^{c(t_i - t_m)} - f_i)(f_m - f_{\bullet m})(t_i - t_{m-1})e^{c(t_i - t_{m-1})},$$

we have

$$\lim_{c\to+\infty} \frac{\psi^{(1)}(c)}{e^{c(t_{m-1}-t_m)}} = \omega_{m-1}(t_m - t_{m-1})(f_m - f_{\bullet m})(f_{m-1} - f_{\bullet m}) > 0$$

because the data are strongly monotonic. Hence $\psi^{(1)}(c) > 0$ for large enough c and there exists a $\bar{c}$ such that $\psi(c)$ is strictly increasing on $(\bar{c}, +\infty)$. Then there exists a $\tilde{c} \in (\bar{c}, +\infty)$ such that

$$\psi(\tilde{c}) = F(f_{\bullet m}, (f_m - f_{\bullet m})e^{-\tilde{c}t_m}, \tilde{c}) < \lim_{c\to+\infty} \psi(c) \leq F_1.$$

(B) From (A) we have a solution for the data $\{(\omega_i, -t_i, f_i)\}_{i=1}^m$. Then we only have to replace t by $-t$ in the model, which changes c by $-c$. □

We can also prove the following theorem for essentially concave data.

Theorem 3.3. *Let the data* $\{(\omega_i, t_i, f_i)\}_{i=1}^m$ *be essentially concave* ($\gamma_2^* < 0$) *and strongly regular.*
(A) *If the data are essentially increasing* ($\gamma_1^* > 0$) *then there exists* $(a^*, b^*, c^*) \in \mathrm{Int}(\mathcal{U}_{--})$ *such that*

$$F(a^*, b^*, c^*) = \min_{(a,b,c)\in\mathcal{U}_{--}} F(a, b, c).$$

(B) *If the data are essentially decreasing* ($\gamma_1^* < 0$) *then there exists* $(a^*, b^*, c^*) \in \mathrm{Int}(\mathcal{U}_{-+})$ *such that*

$$F(a^*, b^*, c^*) = \min_{(a,b,c)\in\mathcal{U}_{-+}} F(a, b, c). \qquad \square$$

4. Choice of the initial approximation

Numerical methods for minimizing the functional (1.2), which is a nonlinear weighted least squares problem, require an initial approximation $(a_0, b_0, c_0) \in \mathcal{U}$ which is as good as possible. A bad choice of the initial approximation can have bad consequences as a high number of iterations, a convergence to a local minimum or no convergence at all. A good initial approximation can leads to convergence in few iterations to the global minimum.

Here we compare two methods to find the initial approximation, both based on the choice of three points that represent the data and the model. We select three values (τ_k, φ_k) (for $k = 1, 2, 3$) and we solve the system of three nonlinear equations

$$\varphi_k = a + b e^{c\tau_k} \qquad (k = 1, 2, 3). \tag{4.1}$$

Under the condition that $\tau_2 = \frac{\tau_1+\tau_3}{2}$ we get

$$\begin{aligned}
a &= \varphi_1 - \frac{(\varphi_2-\varphi_1)^2}{\varphi_3 - 2\varphi_2 + \varphi_1},\\
b &= \frac{(\varphi_2-\varphi_1)^2}{\varphi_3 - 2\varphi_2 + \varphi_1}\Big(\frac{\varphi_2-\varphi_1}{\varphi_3-\varphi_2}\Big)^{2\tau_1/(\tau_3-\tau_1)},\\
c &= \frac{2}{\tau_3-\tau_1}\ln\Big(\frac{\varphi_3-\varphi_2}{\varphi_2-\varphi_1}\Big).
\end{aligned}$$

1st method. Let $\omega = \Sigma_{i=1}^m \omega_i$ and set $0 < \alpha < 1/2$. We first choose j_1 and i_3 such that

$$1 = i_1 < j_1 \qquad \text{and} \qquad \sum_{i=i_1}^{j_1} \omega_i \approx \alpha\omega,$$

$$i_3 < j_3 = 1 \qquad \text{and} \qquad \sum_{i=i_3}^{j_3} \omega_i \approx \alpha\omega,$$

and we set

$$\tau_1 = \bar{t}_1 = \frac{\sum_{i=i_1}^{j_1}\omega_i t_i}{\sum_{i=i_1}^{j_1}\omega_i} \qquad \text{and} \qquad \varphi_1 = \overline{f}_1 = \frac{\sum_{i=i_1}^{j_1}\omega_i f_i}{\sum_{i=i_1}^{j_1}\omega_i}$$

$$\tau_3 = \bar{t}_3 = \frac{\sum_{i=i_3}^{j_3}\omega_i t_i}{\sum_{i=i_3}^{j_3}\omega_i} \qquad \text{and} \qquad \varphi_3 = \overline{f}_3 = \frac{\sum_{i=i_3}^{j_3}\omega_i f_i}{\sum_{i=i_3}^{j_3}\omega_i}.$$

Then we set $\tau_2 = \frac{\tau_1+\tau_3}{2}$ and we determine $1 \le i_2 \le j_2 \le m$ such that

$$\tau_2 \approx \bar{t}_2 = \frac{\sum_{i=i_2}^{j_2} \omega_i t_i}{\sum_{i=i_2}^{j_2} \omega_i} \qquad \text{and} \qquad \sum_{i=i_2}^{j_2} \omega_i \approx \alpha\omega$$

and we set

$$\varphi_2 = \overline{f}_2 = \frac{\sum_{i=i_2}^{j_2} \omega_i f_i}{\sum_{i=i_2}^{j_2} \omega_i}$$

We note by $(\bar{a}_0, \bar{b}_0, \bar{c}_0)$ the value obtained in solving (4.1).

2nd method. Let

$$p_2^*(t) = \gamma_0^* q_0(t) + \gamma_1^* q_1(t) + \gamma_2^* q_2(t)$$

be the best least squares polynomial approximation to the data. The idea is to use only the part of the parabola that best represents the data. This part of the parabola is on the left side or on the right side of the minimum or maximum point of the parabola.

If $\gamma_1^*\gamma_2^* < 0$, the data are essentially increasing and concave or essentially decreasing and convex (hence the left side is appropriate here), we set

$$t_{max} = \min\{t_m, \frac{\alpha_1+\alpha_2}{2} - \frac{\gamma_1^*}{2\gamma_2^*}\},$$

and

$$\begin{aligned} L_T &= t_m - t_1 \\ L_0 &= t_m - t_{max}, \\ L_1 &= t_{max} - t_1, \end{aligned}$$

then

$$\begin{aligned} \tau_1 &= t_1 + \lambda\Big(0.5 + \rho\frac{L_0}{L_T}\Big)L_1, \\ \tau_3 &= t_{max} - \lambda\Big(0.5 - \rho\frac{L_0}{L_T}\Big)L_1, \\ \tau_2 &= \frac{\tau_1+\tau_3}{2} = \frac{t_1+t_{max}}{2} + \lambda\rho\frac{L_0 L_1}{L_T} \end{aligned}$$

If $\gamma_1^*\gamma_2^* > 0$, the data are essentially increasing and convex or essentially decreasing and concave (hence the right side is appropriate here), we set

$$t_{min} = \max\{t_1, \frac{\alpha_1+\alpha_2}{2} - \frac{\gamma_1^*}{2\gamma_2^*}\},$$

and

$$\begin{aligned} L_T &= t_m - t_1 \\ L_0 &= t_{min} - t_1, \\ L_1 &= t_m - t_{min}, \end{aligned}$$

then

$$\begin{aligned}\tau_1 &= t_{min} + \lambda\Big(0.5 - \rho\frac{L_0}{L_T}\Big)L_1,\\ \tau_3 &= t_m - \lambda\Big(0.5 + \rho\frac{L_0}{L_T}\Big)L_1,\\ \tau_2 &= \frac{\tau_1+\tau_3}{2} = \frac{t_1+t_{max}}{2} - \lambda\rho\frac{L_0L_1}{L_T}.\end{aligned}$$

Finally, we set $\varphi_k = p_2^*(\tau_k)$ for $k = 1, 2, 3$. The parameters λ and ρ are such that $0 \le \lambda < 1$, $\rho \ge 0$ and $\Big(0.5-\rho\frac{L_0}{L_T}\Big)L_1 \ge 0$. We note by $(\hat{a}_0, \hat{b}_0, \hat{c}_0)$ the value obtained in solving (4.1).

5. A numerical example

In this example we use the 3-parametric exponential model to fit $m = 100$ data points generated for $i = 1, ..., m$ by

$$\begin{aligned}t_i &= -10 + \frac{i}{5},\\ f_i &= -5 + 4e^{0.15t_i} + r_i,\\ r_i &\sim \mathcal{N}(0,\sigma) \qquad \text{for} \quad \sigma = 2,\end{aligned}$$

and the weights ω_i are given by the following assignment

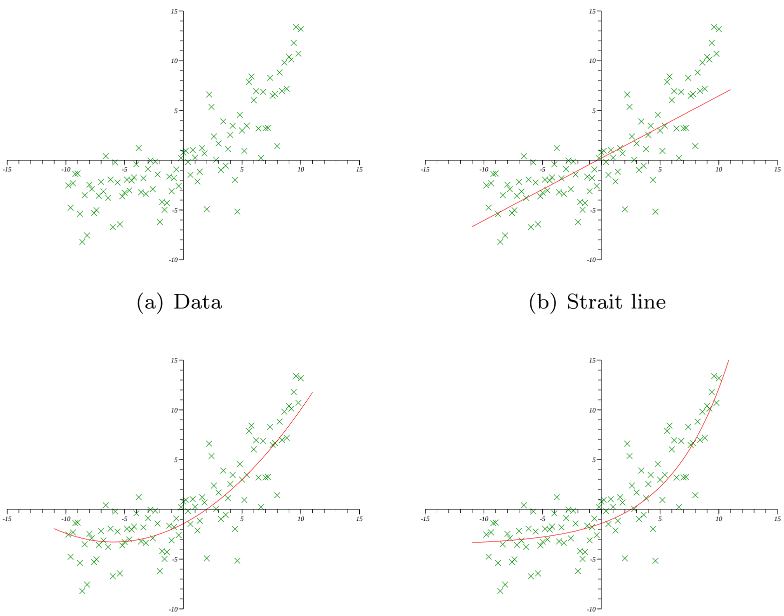
$$\omega_i = \begin{cases} 1 & \text{if} \quad 0 \le u_i < 0.30,\\ 2 & \text{if} \quad 0.30 \le u_i < 0.55,\\ 3 & \text{if} \quad 0.55 \le u_i < 0.75,\\ 4 & \text{if} \quad 0.75 \le u_i < 0.90,\\ 5 & \text{if} \quad 0.90 \le u_i \le 1.00,\end{cases}$$

where $u_i \sim \mathcal{U}[0,1]$ is a uniformly distributed random variable over $[0,1]$ and $r_i \sim \mathcal{N}(0,\sigma)$ is a normal random variable with mean $\mu = 0$ and standard deviation σ. The Levenberg-Marquardt's method [7], [8] has been used to find the optimal solution.

Model	Equation	optimal value	Optimal solution
Strait line	$y = \gamma_1^* q_1 + \gamma_0^* q_0$	1109.08	$\gamma_0^* = 0.19892$ $\gamma_1^* = 0.62588$
Parabola	$y = \gamma_2^* q_2 + \gamma_1^* q_1 + \gamma_0^* q_0$	816.32	$\gamma_0^* = 0.19892$ $\gamma_1^* = 0.62588$ $\gamma_2^* = 0.05245$
Exponential	$y = a^* + b^* e^{c^* t}$	758.95	$a^* = -3.58159$ $b^* = 2.17507$ $c^* = 0.19784$

Table 1. Optimal values of the best polynomial approximation of degree 1 and 2 and the exponential function $y = a + be^{ct}$.

To check the hypothesis of Theorem 3.2 and 3.3, Table 1 contains the coefficients of p_2^*. For this example, the data are essentially increasing $\gamma_1^* = 0.62588 > 0$ and



(a) Data (b) Strait line (c) Parabola (d) Exponential function

FIGURE 2. Graphic representations of the models of Table 1 with the data $\{(\omega_i, t_i, f_i)\}_{i=1}^{i=m}$.

essentially convex $\gamma_2^* = 0.05245 > 0$, hence the solution will be in $\mathrm{Int}(\mathcal{U}_{++})$. This table also contains the optimal value of the criteria $\frac{1}{2}\|p_i - f\|^2$for polynomials of degree $i = 1$ and $i = 2$. It also contains the optimal value and the optimal solution for the 3-parameters exponential model. Figure 2 contains the graphs of the data and the three models : strait line, parabola, and 3-parametric exponential model.

Initial approximation	$\bar{a}_0 = -3.72764$ $\bar{b}_0 = 2.06578$ $\bar{c}_0 = 0.21350$	$\hat{a}_0 = -4.94429$ $\hat{b}_0 = 3.77342$ $\hat{c}_0 = 0.13789$
$F(a_0, b_0, c_0)$	780.66	792.30
number of iterations	5	7
execution time (sec)	0.28	0.33
$\nabla F(x^*)$	$\begin{pmatrix} 1.283D-07 \\ 5.271D-07 \\ 1.570D-05 \end{pmatrix}$	$\begin{pmatrix} 2.462D-08 \\ -4.255D-07 \\ -7.609D-06 \end{pmatrix}$
Stopping criteria $\|\nabla F(x^*)\|_\infty \leq 0.5 \cdot 10^{-4}$	1.570D-05	7.609D-06

TABLE 2. Performance comparison of the method with respect to the two initial approximations.

In Table 2, we compare the performance of the method with respect to the choice of the initial solution determined by the two methods described in the preceding section. We have indicated the value of the criteria for the starting point, the number of iteration needed by the Levenberg-Marquardt's method to obtain the optimal solution using this initial approximation, and the time required to obtain the optimal solution. The sup norm of the gradient at the optimum and the stopping criteria. Let us observe that for the first choice with $\alpha = 1/5$, we get $\alpha\omega = 52.4$, $j_1 = 21$, $i_3 = 77$, $i_2 = 41$ et $j_2 = 60$. For the second choice the results given are for $\lambda = 3/8$ and $\rho = 2$.

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