Least Squares Estimation for a Class of Non-Linear Models

IRWIN GUTTMAN
Universite de Montreal[1]

VICTOR PEREYRA
Universidad Central de Venezuela

and

HUGO D. SCOLNIK
Fundacion Bariloche, Argentina

A new method for determining least squares estimators for certain classes of non-linear models is discussed. The method is an extension of a variable projection method of Scolnik (1970), and involves the minimization of a modified functional. The feature of minimizing this modified functional is that for a certain class of non-linear models, called the constant-coefficients case, only one half the parameters are involved initially. To find the estimators of the remaining parameters is straight forward and relatively easy. This new two step-procedure is shown to be equivalent to the over-all least squares procedure. We also discuss the case of a class of models called the variable coefficients class. For this case, we formulate a new algorithm for determining the estimators which makes use of approximate confidence regions for the parameters.

KEY WORDS

Least Squares
Non-linear
Variable-projection Method
Constant Coefficients
Confidence Regions

1. INTRODUCTION

We consider in this paper the analysis of models which are essentially "linear combinations" of certain non-linear functions. In contrast to the methods of the general literature that have appeared on this topic, our analysis exploits the simple structure of models belonging to this class, which, however, are sufficiently general to cover a wide variety of applications. One such class of models is

$$\eta = \sum_{i=1}^{k} a_i \phi_i(\mathbf{t}; \alpha_i), \tag{1.1}$$

where the ϕ_i are given non-linear functions of their arguments, and where $\mathbf{t} = (t_1, \cdots, t_m)'$.

[1] Present address: University of Toronto.

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We will be concerned with the problem of estimating the α_i and a_i in the least squares sense, and we will suppose that, for this purpose, there is available n independent observations $y_1, \cdots, y_u, \cdots, y_n$, taken at the points $\mathbf{t}_1, \cdots, \mathbf{t}_u, \cdots, \mathbf{t}_n$, respectively, where

$$E(y_u) = \eta_u, \qquad \text{Var}(y_u) = \sigma^2 \tag{1.2}$$

with

$$\eta_u = \sum_{i=1}^{k} a_i \phi_i(\mathbf{t}_u ; \alpha_i). \tag{1.3}$$

Examples of (1.1) are many and well known; see for instance, Moore and Zeigler (1959).

The class of models (1.1) will be referred to as the *constant coefficients* case, in contrast with another class of models to be considered, the *variable coefficient* case:

$$\eta = \sum_{i=1}^{k} a_i(\boldsymbol{\alpha})\phi_i(\mathbf{t}; \alpha_i), \tag{1.4}$$

where the $a_i(\boldsymbol{\alpha})$ are now known functions of their arguments. An example of this type of model that occurs in chemical reaction theory (see Box and Lucas (1959)) is

$$\eta = \frac{\theta_1}{\theta_1 - \theta_2} e^{-\theta_1 t} - \frac{\theta_1}{\theta_1 - \theta_2} e^{-\theta_2 t}. \tag{1.5}$$

In the next sections of this paper, we propose a new method of handling the estimation problems incurred for the above classes of models. The method is based on the work of Scolnik (1970), who considers the analysis of the particular model

$$\eta = \sum_{i=1}^{k} a_i t^{\alpha_i}, \tag{1.6}$$

where the α_i are not necessarily integers. We extend Scolnik's work to the more general case (1.1), providing a proof (Theorem 2.1) for the equivalence between the minimization of a modified functional and the one we are interested in. This modified functional has actually half the number of parameters the original one had, this being the most important feature of the method (see also Osborne (1970) on this aspect).

In section 5 we extend the method of Scolnik for minimizing the variable projection functional, to the present case, giving a different presentation which includes some significant improvements(*).

In section 4 we propose an entirely new algorithm for handling the variable coefficient case, which coupled with the use of approximate confidence regions, shows great promise as a tool for the solution of this type of problem. We think that this algorithm deserves further investigating and testing.

The following notational conventions will be used throughout this paper. For any function of $\mathbf{t}$, $f(\mathbf{t})$, we will denote by $\mathbf{f}$, the vector obtained by evaluating $f(\mathbf{t})$ at each of the $\mathbf{t}_u$, $u = 1, \cdots, n$, that is

$$\mathbf{f} = (f(\mathbf{t}_1), \cdots, f(\mathbf{t}_n))'. \tag{1.7}$$

For any function $g(\mathbf{t}; \boldsymbol{\xi})$, with $\boldsymbol{\xi} = (\xi_1, \cdots, \xi_q)'$ we denote by $\nabla g(\mathbf{t}; \boldsymbol{\xi})$, the gradient vector defined as

$$\nabla g(\mathbf{t}; \boldsymbol{\xi}) = \left(\frac{\partial g}{\partial \xi_1}, \cdots, \frac{\partial g}{\partial \xi_q}\right)' \tag{1.8}$$

(*) We would like to acknowledge here the contribution of Mr. A. Pérez, of the Fundación Bariloche, to the algorithm described at the end of section 5.

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Finally, we denote by $Jg(\xi)$, the Jacobian matrix of the functions $g(\mathbf{t}_u\ ;\ \xi)$, $u = 1, \cdots, n$, with respect to the variables ξ, that is

$$Jg(\xi) = \left(\frac{\partial g(\mathbf{t}_u\ ;\ \xi)}{\partial \xi_i}\right), \qquad u = 1, \cdots, n, \quad j = 1, \cdots, q. \tag{1.9}$$

Whenever possible we shall suppress the arguments of the various functions involved.

2. The Variable Projection Method

Referring to either a model of type (1.1) or (1.4), let R be the set of all vectors $\boldsymbol{\alpha} = (\alpha_1, \cdots, \alpha_k)'$, for which the $\boldsymbol{\phi}_i$', $i = 1, \cdots, k$, form a linearly independent set. We assume that R is nonempty. For any $\boldsymbol{\alpha} \in R$, define the vectors $\mathbf{e}_1, \mathbf{e}_2, \cdots, \mathbf{e}_k$, as an orthonormalized basis for the space spanned by $(\boldsymbol{\phi}_1, \cdots, \boldsymbol{\phi}_k)$, which we now denote as $S(\boldsymbol{\alpha})$.

The orthogonal projection of any vector $\mathbf{w}$ on the space $S(\boldsymbol{\alpha})$ is obtained by means of the operator $P(\boldsymbol{\alpha})$ defined by

$$P(\boldsymbol{\alpha})\mathbf{w} = P\mathbf{w} = \sum_{i=1}^{k} \langle \mathbf{w}, \mathbf{e}_i \rangle \mathbf{e}_i\ , \tag{2.1}$$

where $\langle \mathbf{w}, \mathbf{e}_i \rangle = \mathbf{w}'\mathbf{e}_i$ denotes the scalar product of the vectors $\mathbf{w}$ and $\mathbf{e}_i$. Since $\boldsymbol{\eta}$, (see (1.1)-(1.4)-(1.7)) is a vector in S, by definition, we then have that $\boldsymbol{\eta} = P\boldsymbol{\eta}$.

We consider now the model (1.1). We would like to find, on the basis of the sample information described in section 1, the least squares estimators of $\boldsymbol{\beta}$, that is, we wish to minimize

$$r_2(\boldsymbol{\beta}) = \|\mathbf{y} - \boldsymbol{\eta}\|^2 = (\mathbf{y} - \boldsymbol{\eta})'(\mathbf{y} - \boldsymbol{\eta}), \tag{2.2}$$

or, since $\boldsymbol{\eta} = P\boldsymbol{\eta}$, we wish to minimize

$$\|\mathbf{y} - \boldsymbol{\eta}\|^2 = \|\mathbf{y} - P\boldsymbol{\eta}\|^2 \tag{2.2a}$$

In what follows, we denote these estimates of $\boldsymbol{\beta}$ by $\boldsymbol{\beta}^*$, i.e.,

$$m_2 = r_2(\boldsymbol{\beta}^*) = \min r_2(\boldsymbol{\beta}) \tag{2.2b}$$

Now note that (2.2a) is compact notation for

$$\left\| \mathbf{y} - \sum_{i=1}^{k} \langle \boldsymbol{\eta}, \mathbf{e}_i \rangle \mathbf{e}_i \right\|^2 = \left\| \mathbf{y} - \sum_{i=1}^{k} a_i \boldsymbol{\phi}_i \right\|^2 \tag{2.2c}$$

We would like to simplify this functional without affecting the least squares estimates too much, and for this we propose the minimization of the following modified functional, viz

$$r_1(\boldsymbol{\alpha}) = \left\| \mathbf{y} - \sum_{i=1}^{k} \langle \mathbf{y}, \mathbf{e}_i \rangle \mathbf{e}_i \right\|^2 \tag{2.3}$$

which is obtained replacing $\boldsymbol{\eta}$ by $\mathbf{y}$ in (2.2c). We will denote the estimate of $\boldsymbol{\alpha}$ obtained from (2.3) by $\hat{\boldsymbol{\alpha}}$, that is,

$$m_1 = r_1(\hat{\boldsymbol{\alpha}}) = \min r_1(\boldsymbol{\alpha}). \tag{2.3a}$$

We note that the a_i's are not involved at all in (2.3), which implies that since we are dealing with model (1.1), that we have decreased consideration, for the moment, of 1/2 the number of parameters. Of course, we also need estimates of the a_i's. Our procedure for this is as follows: having obtained the estimate $\hat{\boldsymbol{\alpha}}$ by

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minimizing (2.3), we would then find estimates $\hat{a}_i$'s of the a_i's by standard linear least squares, that is, by minimizing

$$r_3(\mathbf{a}) = \left|\left|\mathbf{y} - \sum_{i=1}^{k} a_i \boldsymbol{\phi}_i(\hat{\alpha}_i)\right|\right|^2, \tag{2.4}$$

so that we will have

$$m_3 = r_3(\hat{\mathbf{a}}) = \min r_3(\mathbf{a}). \tag{2.4a}$$

We denote the combined estimator $(\hat{\alpha}, \hat{a})$ by $\hat{\boldsymbol{\beta}}$.

This new 2-step procedure raises the question as to whether the estimate $\hat{\boldsymbol{\beta}}$ is in some sense, close to the estimate $\hat{\boldsymbol{\beta}}^*$. Our answer to this question is, not only are they close, but they are *equal*, as shown in Theorem 2.1, for which we need the following lemma.

Lemma 2.1. $m_1 \leq m_2$

Proof. For any fixed $\boldsymbol{\alpha}$ and $\mathbf{a}$, we have

$$\begin{aligned} ||\mathbf{y} - \mathbf{n}||^2 &= ||(\mathbf{y} - P\mathbf{y}) + (P\mathbf{y} - \mathbf{n})||^2 \\ &= ||\mathbf{y} - P\mathbf{y}||^2 + ||P\mathbf{y} - \mathbf{n}||^2 + 2\langle P\mathbf{y} - \mathbf{n}, \mathbf{y} - P\mathbf{y}\rangle. \end{aligned}$$

But $P\mathbf{y} - \mathbf{n} \in S(\boldsymbol{\alpha})$, and $\mathbf{y} - P\mathbf{y}$ is a vector that is easily seen to be orthogonal to $S(\boldsymbol{\alpha})$, so that $\langle P\mathbf{y} - \mathbf{n}, \mathbf{y} - P\mathbf{y}\rangle = 0$. Hence, we have that

$$r_2(\boldsymbol{\alpha}, \mathbf{a}) = r_1(\boldsymbol{\alpha}) + ||P\mathbf{y} - \mathbf{n}||^2, \tag{2.5}$$

which implies that

$$r_1(\boldsymbol{\alpha}) \leq r_2(\boldsymbol{\beta}) \tag{2.6}$$

with equality if and only if $P\mathbf{y} = \mathbf{n}$. From (2.6), we have

$$m_1 \leq r_2(\boldsymbol{\beta}) \tag{2.7}$$

for all $\boldsymbol{\beta}$, from which the lemma follows.

We may now state and prove the following theorem.

Theorem 2.1 Assuming unique minimums for the functionals r_1 and r_2 in $R \times E^k$, then

$$\boldsymbol{\beta}^* = \hat{\boldsymbol{\beta}}. \tag{2.8}$$

Proof. We note first, that for any given fixed $\boldsymbol{\alpha} \in R$, we have that $r_1(\boldsymbol{\alpha})$ and $\min_{\mathbf{a}} r_2(\boldsymbol{\alpha}, \mathbf{a})$ are both equal to the square of the norm of the vector $\mathbf{y} - P\mathbf{y}$, a vector which is orthogonal to $S(\boldsymbol{\alpha})$. Hence

$$m_2 = \min_{\boldsymbol{\alpha}, \mathbf{a}} r_2(\boldsymbol{\alpha}, \mathbf{a}) \leq \min_{\mathbf{a}} r_2(\boldsymbol{\alpha}, \mathbf{a}) = r_1(\boldsymbol{\alpha}) \tag{2.9}$$

so that

$$m_2 \leq \min_{\boldsymbol{\alpha}} r_1(\boldsymbol{\alpha}) = m_1 . \tag{2.10}$$

But from Lemma 2.1 and (2.10), we have $m_2 = m_1$, and the uniqueness of the minima proves the theorem.

We defer the discussion of estimation in the variables coefficients case until section 4. We turn now to a discussion of the construction of confidence regions for $\boldsymbol{\beta}$ and $\eta(\mathbf{t})$ based on the estimators $\hat{\boldsymbol{\beta}}$.

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3. Confidence Regions Pertaining to the Constant Coefficients Model

In section 2, we have given a procedure for obtaining estimates $\hat{\beta}$ of the parameter β of model (1.1), and it turned out that $\hat{\beta} = \beta^*$, where β^* is the least squares estimate of β. In this section, we develop (approximate) confidence regions for (i) the parameters β and (ii) the function $\eta(\mathbf{t})$, under the assumption of normality of the y_u's.

So suppose that in addition to the assumptions of independence of the y_u's, where the y_u's satisfy (1.2) and (1.3), that the y_u's are normally distributed. As is well known (see for example Box and Hunter (1965), and pages 274 and 299 of Draper and Smith (1966), amongst others), an approximate 100 $(1 - \gamma)\%$ confidence region C for β under the assumptions of this paper, is given by

$$C(\beta) = \left\{\beta \;\middle|\; ||\mathbf{y} - \mathbf{n}(\beta)||^2 \leq ||\mathbf{y} - \mathbf{n}(\beta^*)||^2 \left[1 + \frac{2k}{n - 2k} F_\gamma\right]\right\}, \tag{3.1}$$

where F_γ denotes the point exceeded with probability γ when using the Snedecor-F distribution with $(2k, n - 2k)$ degrees of freedom. But, under the assumptions of Theorem 2.1, we have that the region (3.1) can be written as

$$C(\beta) = \left\{\beta \;\middle|\; ||\mathbf{y} - \mathbf{n}(\beta)||^2 \leq m_1\left[1 + \frac{2k}{n - 2k} F_\gamma\right]\right\}. \tag{3.2}$$

We turn now to the estimation of η when $\mathbf{t} = \mathbf{t}_0$, that is, to the estimation of

$$\eta(\mathbf{t}_0) = \sum_{i=1}^{k} a_i \phi_i(\mathbf{t}_0 \,;\, \alpha_i). \tag{3.3}$$

Now we have that $\hat{\beta}$ are least squares estimators of β, so that a natural (point) estimator of "the response $\eta(\mathbf{t}_0)$" is

$$\hat{y}_{\mathbf{t}_0} = \hat{\eta}(\mathbf{t}_0) = \sum_{i=1}^{k} \hat{a}_i \phi_i(\mathbf{t}_0 \,;\, \hat{\alpha}_i). \tag{3.4}$$

Under the assumption that, for all $\mathbf{t}$, the function $\phi_i(\mathbf{t}, \alpha_i)$ is a one-one function of α_i, $i = 1, \cdots, k$, then, as is well known, the normality of the y_u's implies that $\hat{y}_{\mathbf{t}_0}$ is the maximum likelihood estimator of $\eta(\mathbf{t}_0)$.

To provide ourselves with a confidence "belt" for the response $\eta(\mathbf{t})$ at any value of $\mathbf{t}$, we have, as is well known (see for example, page 61 of Draper and Smith (1966)), that

$$\frac{\sqrt{(n - 2k)}\,(\hat{y}_{\mathbf{t}} - \eta(\mathbf{t}))}{\sqrt{m_1 Q(\mathbf{t}; \hat{\beta})}} \doteq t_{n-2k}, \tag{3.5}$$

where

$$Q(\mathbf{t}; \hat{\beta}) = (\nabla \mathbf{n})'[(J(\mathbf{n}))'(J(\mathbf{n}))]^{-1}(\nabla \mathbf{n}), \tag{3.6}$$

with $\nabla \mathbf{n} = \nabla \mathbf{n}(\mathbf{t}; \hat{\beta})$ the $(2k \times 1)$ vector with jth component given by

$$\frac{\partial \eta(\mathbf{t}; \hat{\beta})}{\partial \beta_j}, \tag{3.6a}$$

and where the $(n \times 2k)$ matrix $J(\mathbf{n})$ has as its uth row

$$(\nabla \eta(\mathbf{t}_u \,;\, \hat{\beta}))'. \tag{3.6b}$$

Hence, an approximate 100 $(1 - \gamma)\%$ confidence "belt" for $\eta(\mathbf{t})$ is

$$[\hat{y}_{\mathbf{t}} \pm \sqrt{m_1 Q(\mathbf{t}; \hat{\beta})}\; t_{\gamma/2}/(n - 2k)], \tag{3.7}$$

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where $t_{\gamma/2}$ is the point exceeded with probability $\gamma/2$ when using the Student-t distribution with $(n - 2k)$ degrees of freedom.

4. The Variable Coefficients Case

In this section, we propose a new iterative procedure for the variable coefficients case. This new procedure utilizes confidence regions for deciding when to terminate the procedure.

Specifically, suppose η is of the form

$$\eta(\mathbf{t}; \boldsymbol{\alpha}) = \sum_{i=1}^{k} a_i(\boldsymbol{\alpha})\phi_i(\mathbf{t}, \alpha_i), \tag{4.1}$$

where the $a_i(\boldsymbol{\alpha})$ are k given functions of $\boldsymbol{\alpha}$. To find an estimate of $\boldsymbol{\alpha}$ based on the data $\{y_u\}$ observed at $\{\mathbf{t}_u\}$, $u = 1, \cdots, n$, we proceed as in section 2. Thus, we wish to minimize, over $(\boldsymbol{\alpha})$, the functional

$$r_4(\boldsymbol{\alpha}) = ||\mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\alpha})||^2. \tag{4.2}$$

We assume that there is a unique minimum m_4 at, say, the point $\boldsymbol{\alpha}^*$, that is

$$m_4 = r_4(\boldsymbol{\alpha}^*) = \min_{\boldsymbol{\alpha}} r_4(\boldsymbol{\alpha}). \tag{4.3}$$

We note the similarity of the functional (4.2) for the model (4.1), with the functional r_2 defined in (2.2)—indeed, we would write

$$r_4(\boldsymbol{\alpha}) = r_2(\boldsymbol{\alpha}, \mathbf{a}(\boldsymbol{\alpha})). \tag{4.4}$$

Now $r_4(\boldsymbol{\alpha})$, or $r_2(\boldsymbol{\alpha}, \mathbf{a}(\boldsymbol{\alpha}))$ is a very complicated non-linear function of $\boldsymbol{\alpha}$. However, guided by the identity (4.4), we will proceed by minimizing the functional $r_1(\boldsymbol{\alpha})$ defined in (2.3), which of course, yields the estimate $\hat{\boldsymbol{\alpha}}$ of $\boldsymbol{\alpha}$. We note that Lemma 2.1 still holds, that is

$$m_1 = r_1(\hat{\boldsymbol{\alpha}}) = \min_{\boldsymbol{\alpha}} r_1(\boldsymbol{\alpha}) \leq m_4 . \tag{4.5}$$

However, since the parameters $\mathbf{a}(\boldsymbol{\alpha})$ are not free, Theorem 2.1 has no meaning in this situation. Thus we cannot assert that $\hat{\boldsymbol{\alpha}} = \boldsymbol{\alpha}^*$, as in the constant coefficients case discussed in section 2 and 3.

Now if we did have available the least squares estimate $\boldsymbol{\alpha}^*$, and if the normality assumption of the y's discussed earlier holds, then an (approximate) $1 - \gamma$ confidence region for $\boldsymbol{\alpha}$ would be given by

$$C(\boldsymbol{\alpha}) = \{\boldsymbol{\alpha} \mid ||\mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\alpha})||^2 \leq m_4[1 + kF_{k,n-k;\gamma}/(n - k)]\} \tag{4.6}$$

Of course, we do not have $\boldsymbol{\alpha}^*$ nor $m_4 = r_4(\boldsymbol{\alpha}^*)$. But from (4.5) we have a lower bound, m_1 , which is computable, for m_4 , so that the region

$$C_1(\boldsymbol{\alpha}) = \{\boldsymbol{\alpha} \mid ||\mathbf{y} - \boldsymbol{\eta}(\boldsymbol{\alpha})||^2 \leq m_1[1 + kF_{k,n-k,\gamma}/(n - k)]\} \tag{4.7}$$

lies entirely within the region $C(\boldsymbol{\alpha})$ given by (4.6). Therefore, we can use as a criterion of the suitability of the estimate $\hat{\boldsymbol{\alpha}}$, whether $\hat{\boldsymbol{\alpha}}$ belongs to $C_1(\boldsymbol{\alpha})$. The region $C_1(\boldsymbol{\alpha})$ is not, of course, of level $1 - \gamma$, but has some level, say $1 - \gamma' \leq 1 - \gamma$. In the case that $\hat{\boldsymbol{\alpha}}$ does not lie in the region $C_1(\boldsymbol{\alpha})$, it can be still utilized as a reasonable starting value for any iterative procedure to minimize the functional $r_4(\boldsymbol{\alpha})$. The region $C_1(\boldsymbol{\alpha})$ could then be used to interrupt the iteration at any stage for which the iterate $\boldsymbol{\alpha}^{(r)}$ first lies in $C_1(\boldsymbol{\alpha})$.

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Of course, the difference between the region $C(\alpha)$ and $C_1(\alpha)$ is controlled by the difference between m_4 and m_1. But from (4.5) and the definition of m_4, we have that $m_1 \leq m_4 \leq r_4(\hat{\alpha})$, so that

$$\frac{m_4 - m_1}{m_1} \leq \frac{r_4(\hat{\alpha}) - m_1}{m_1} = b \tag{4.8}$$

where b can be easily computed. The size of b, gives us some information as to whether the region $C_1(\alpha)$ is a good substitute to $C(\alpha)$.

If $\hat{\alpha} \in C_1(\alpha)$, a reasonable point estimate of $\eta(\mathbf{t}) = \sum_{i=1}^{k} a_i(\alpha)\phi_i(\mathbf{t}; \alpha_i)$ is

$$\hat{\eta}(\mathbf{t}) = \sum_{i=1}^{k} a_i(\hat{\alpha})\phi i(\mathbf{t}; \hat{\alpha}_i). \tag{4.9}$$

The problem of finding a reasonable interval estimator when α^* is not known, is still an open question. The pitfall lies in the question of the behaviour of $Q(\mathbf{t}; \alpha)$ (see (3.6)) as α changes from α^* to $\hat{\alpha}$ etc.

5. The Minimization of the Non-Linear Projection Functional

As discussed in sections 2 and 4, the minimization of the functional $r_1(\alpha) = ||\mathbf{y} - P\mathbf{y}||^2$, where $P\mathbf{y} = \sum_{i=1}^{k} \langle \mathbf{y}, \mathbf{e}_i \rangle \mathbf{e}_i$ plays a key role in our procedures. This minimization may be done using any of the known standard methods (see for example Ortega and Rheinboldt (1970), or Daniel (1971)). Now some of these methods require the knowledge of the partial derivatives of $P^{\perp}\mathbf{y} = \mathbf{y} - P\mathbf{y}$. Due to the particular form of $P^{\perp}\mathbf{y}$, and following the ideas of Scolnik (1970), we are able to obtain expressions for these derivatives in simple closed form, which we now proceed to develop.

We recall that the $\mathbf{e}_i$ form an orthogonal basis for $S(\alpha)$, the space spanned by the vectors $\phi_i(\alpha_i)$. For the algebraic developments here, we choose that basis provided by the Gram-Schmidt process, that is

$$\tilde{\mathbf{e}}_i = \phi_i(\alpha_i) - \sum_{j=1}^{i-1} \langle \mathbf{e}_j, \phi_i(\alpha_i) \rangle \mathbf{e}_j , \tag{5.1}$$

$$\mathbf{e}_i = \tilde{\mathbf{e}}_i / ||\tilde{\mathbf{e}}_i||, \qquad i = 1, \cdots, k. \tag{5.1a}$$

We remark here that it is known that Gram-Schmidt is not a good numerical procedure, but it will be clear at the end of our development that *any* procedure to produce projections can be used in the actual computation. We shall obtain first the partial derivative with respect to α_k :

$$\frac{\partial P^{\perp}\mathbf{y}}{\partial \alpha_k} = -\frac{\partial P\mathbf{y}}{\partial \alpha_k} = -\frac{\partial}{\partial \alpha_k}[\langle \mathbf{y}, \mathbf{e}_k \rangle \mathbf{e}_k] = -\left(\left\langle \mathbf{y}, \frac{\partial \mathbf{e}_k}{\partial \alpha_k} \right\rangle \mathbf{e}_k + \langle \mathbf{y}, \mathbf{e}_k \rangle \frac{\partial \mathbf{e}_k}{\partial \alpha_k} \right), \tag{5.2}$$

where, as usual, the derivative of a vector function is the vector of derivatives of its components.

On the other hand, a simple computation shows that,

$$\frac{\partial \mathbf{e}_k}{\partial \alpha_k} = \frac{1}{||\tilde{\mathbf{e}}_k||} \left[\frac{\partial \tilde{\mathbf{e}}_k}{\partial \alpha_k} - \mathbf{e}_k \left\langle \frac{\partial \tilde{\mathbf{e}}_k}{\partial \alpha_k}, \mathbf{e}_k \right\rangle \right], \tag{5.3}$$

with

$$\frac{\partial \tilde{\mathbf{e}}_k}{\partial \alpha_k} = \frac{\partial \phi_k(\alpha_k)}{\partial \alpha_k} - \sum_{i=1}^{k-1} \left\langle \frac{\partial \phi_k(\alpha_k)}{\partial \alpha_k}, \mathbf{e}_i \right\rangle \mathbf{e}_i . \tag{5.4}$$

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Replacing (5.3) and (5.4) in (5.2), and setting

$$\Psi_k = P^{\perp} \frac{\partial \phi_k(\alpha_k)}{\partial \alpha_k}$$

we finally obtain:

$$\frac{\partial P^{\perp}\mathbf{y}}{\partial \alpha_k} = -\frac{1}{||\tilde{\mathbf{e}}_k||} [\langle \Psi_k , \mathbf{y}\rangle \mathbf{e}_k + \langle \mathbf{y}, \mathbf{e}_k\rangle \Psi_k]. \tag{5.5}$$

Revising our procedure above we see that the gist of the question is to have as last variable that which we want to differentiate upon. But the order in which we take the vectors ϕ_i is immaterial in what the linear space spanned by them is concerned. Thus, for each $i = 1, \cdots, k$, we consider:

Vectors $(\phi_1 , \cdots , \phi_{i-1} , \phi_{i+1} , \cdots , \phi_k)$

$P_{k-1,i}$ = projection of ϕ_i on the $(k-1)$-dimensional subspace spanned by these vectors

$$\tilde{\mathbf{e}}_{(i)} = P^{\perp}_{k-1,i}\phi_i ; \qquad \mathbf{e}_{(i)} = \frac{\tilde{\mathbf{e}}_{(i)}}{||\tilde{\mathbf{e}}_{(i)}||} , \tag{5.6}$$

and formula (5.5) is now valid for any partial derivative when written in the form:

$$\frac{\partial P^{\perp}\mathbf{y}}{\partial \alpha_i} = -\frac{1}{||\tilde{\mathbf{e}}_{(i)}||} [\langle \Psi_i , \mathbf{y}\rangle \mathbf{e}_{(i)} + \langle \mathbf{y}, \mathbf{e}_{(i)}\rangle \Psi_i]. \tag{5.7}$$

In certain iterative processes, like the Gauss-Newton method or some of its variations, we also need the vector whose components are the scalar products:

$$\left\langle \frac{\partial P^{\perp}\mathbf{y}}{\partial \alpha_i} , P^{\perp}\mathbf{y} \right\rangle = -\frac{1}{||\tilde{\mathbf{e}}_{(i)}||} [\langle \Psi_i , \mathbf{y}\rangle \langle \mathbf{e}_{(i)} , P^{\perp}\mathbf{y}\rangle + \langle \mathbf{e}_{(i)} , \mathbf{y}\rangle \langle \Psi_i , P^{\perp}\mathbf{y}\rangle],$$

and since $\langle \mathbf{e}_{(i)} , P^{\perp}\mathbf{y}\rangle = 0$ we finally have the simple result

$$\left\langle \frac{\partial P^{\perp}\mathbf{y}}{\partial \alpha_i} , P^{\perp}\mathbf{y} \right\rangle = -\frac{\langle \mathbf{e}_{(i)} , \mathbf{y}\rangle}{||\tilde{\mathbf{e}}_{(i)}||} \cdot \langle \Psi_i , P^{\perp}\mathbf{y}\rangle. \tag{5.8}$$

Also we can obtain the $k \times k$ matrix of "normal equations", whose components, n_{ij} , are given by

$$n_{ij} = \left\langle \frac{\partial P^{\perp}\mathbf{y}}{\partial \alpha_i} , \frac{\partial P^{\perp}\mathbf{y}}{\partial \alpha_j} \right\rangle = \frac{1}{||\tilde{\mathbf{e}}_{(i)}|| \, ||\tilde{\mathbf{e}}_{(j)}||}$$

$$\cdot [\langle \Psi_i , \mathbf{y}\rangle \langle \Psi_j , \mathbf{y}\rangle \langle \mathbf{e}_{(i)} , \mathbf{e}_{(j)}\rangle + \langle \mathbf{y}, \mathbf{e}_{(i)}\rangle \langle \mathbf{y}, \mathbf{e}_{(j)}\rangle \langle \Psi_i , \Psi_j\rangle]. \tag{5.9}$$

We repeat now that the Gram-Schmidt form of the orthonormal vectors $\mathbf{e}_i$ was used for simplicity in the analytical manipulations, but that in the actual computation any numerically stable procedure can be used in order to produce the orthogonal projections needed in (5.6) through (5.9).

In fact, we can obtain the vectors $\mathbf{e}_{(i)}$ in a different fashion. Let Φ be the matrix whose columns are the vectors ϕ_i , $i = 1, \cdots, k$, and let Φ^+ be its Moore-Penrose pseudo inverse.

Since Φ is of full column rank by hypothesis, then Φ^+ is simply equal to $(\Phi'\Phi)^{-1}\Phi'$, and $\Phi^+\Phi = I$, the identity matrix of order k.

If we denote the ith row of Φ^+ by $(\phi_i^+)'$, the above relationship implies that

$$\langle \phi_i^+ , \phi_j\rangle = \delta_{ij} , \qquad i, j = 1, \cdots, k. \tag{5.10}$$

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Therefore, ϕ_i^+ is orthogonal to all ϕ_j , $j \neq i$, and we have

$$\mathbf{e}_{(i)} = \frac{\phi_i^+}{||\phi_i^+||} \tag{5.11}$$

In (5.7), (5.8), and (5.9), we also need $||\bar{\mathbf{e}}_{(i)}||$, the component of the vector ϕ_i in the direction $\mathbf{e}_{(i)}$. This quantity is easily obtained from the identity

$$||\bar{\mathbf{e}}_{(i)}|| = |\langle \phi_i , \mathbf{e}_{(i)} \rangle| = \left| \frac{1}{||\phi_i^+||} \langle \phi_i , \phi_i^+ \rangle \right| = 1/||\phi_i^+||. \tag{5.12}$$

It is now clear that in the formulas (5.7), (5.8) and (5.9), we can replace the vector $\mathbf{e}_{(i)}/||\bar{\mathbf{e}}_{(i)}||$ by the vector ϕ_i^+ .

Finally, we observe that there are numerically stable and efficient ways available for computing Φ^+ (see for instance, Golub (1970)).

6. Numerical Experiments

We present in this section some numerical examples that illustrate the performance of the methods proposed above.

For solving the nonlinear least squares problem (2.3) we have employed a relaxed form of the Gauss-Newton procedure (see Draper and Smith (1966), page 269), with the necessary derivatives calculated as indicated in section 5.

Problem I. The model in this application is $\eta = a_1 e^{\alpha_1 t} + a_2 e^{\alpha_2 t}$, and the following data has been used:

t	y
0.25	0.25
0.50	0.40
1.00	0.60
1.70	0.58
2.00	0.54
4.00	0.27

We took as initial guesses for the exponents: $\alpha_1 = -0.5$, $\alpha_2 = -2.5$. The initial value for the functional $r_1(\boldsymbol{\alpha})$ was 0.029, and after 4 iterations it stabilized at the value 0.001. The final value for the parameters was $\hat{\alpha}_1 = -0.443$, $\hat{\alpha}_2 = -1.258$. Solving the linear least squares problem (2.4) using these exponents gave the values $\hat{a}_1 = 1.645$, $\hat{a}_2 = -1.685$, for the remaining parameters. Let $F_{4,2;\gamma} = F_\gamma$. Then, with $\gamma = .05$, we have $(1 + 2F_\gamma) = 39.5$, and the 95% confidence region $C(\boldsymbol{\beta})$ given in (3.1) is now determined by using the fact that here the value of $39.5\, r_2(\boldsymbol{\beta}^*) = 0.04$.

Problem II. Here we consider the variable coefficients model given by (1.5) with the same data used in Problem I. Starting with $\alpha_1 = -4.0$, $\alpha_2 = -3.0$, the iterative process for the nonlinear projection algorithm converged in 6 iterations to practically the same exponents obtained for Problem I: $\hat{\alpha}_1 = -1.256$, $\hat{\alpha}_2 = -0.443$. The computed weights $\mathbf{a}(\hat{\boldsymbol{\alpha}})$ were: $a_1 = -1.545$, $a_2 = 1.545$. The values of the final sum of squares of residuals were: $r_1(\hat{\boldsymbol{\alpha}}) = 0.001$, $r_4(\hat{\boldsymbol{\alpha}}) = 0.004$.

Observe that in this case the order in which the parameters are taken *is* relevant. We chose the order which made the residual r_4 smallest. If the number of parameters (k) is large, this choice may be somewhat difficult and a better and faster criteria would have to be used.

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It is also worth mentioning that in this example it was necessary to take fractions of the Gauss-Newton correction step in order to obtain a norm reducing procedure. (This relaxation procedure was employed, of course, because of taking "bad" initial guesses).

With $\gamma = .05$, the condition for $\hat{\alpha}$ to belong to $C_1(\alpha)$ (see (4.7)) is that $r_4(\hat{\alpha}) \leq 0.0433$, which is amply satisfied. Thus the estimate given by the nonlinear projection method is appropriate, to a level of confidence of 95%.

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