NORTH-HOLLAND

A Method for Solving the Parameter Identification Problem for Ordinary Differential Equations of the Second Order

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ABSTRACT

We give a method for solving the parameter identification problem for ordinary differential equations of the second order using a noninterpolated moving least squares method. The method is tested in two practical examples.

1. INTRODUCTION

The mathematical model in applied sciences is often defined by a system of differential equations. In this paper we deal with models that can be described by a single or several ordinary differential equations of the second order. The model usually contains some unknown parameters, which are to be determined from the given data in order to minimize the differences between the actual (i.e., experimental) values and the values given by the model. This problem is known in the literature as the Parameter Identification Problem. If the differential equations can be integrated, one obtains

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functions-models with a certain number of parameters, which are then determined by the least squares method from the given data. In general, the solution of the system of differential equations describing the mathematical model cannot be described by elementary functions, but one still has to determine the optimal parameter values in the model.

For simplicity we assume that we are dealing with a problem involving one differential equation. Suppose that some theoretical model is described by an ordinary differential equation of the second order:

$$\frac{d^2y}{dt^2} = f(t,\, y(t),\, y'(t), \mathbf{p}), \tag{1.1}$$

where $\mathbf{p} = (p_1, \dots, p_n)^T$ is the vector of n real parameters. In addition, we know the experimental data $(t_i,\ y_i)$, $i = 1, \dots, m$, where $0 \leqslant t_1 < \cdots < t_m \leqslant T$ usually denote time, and positive real numbers $y_1, \dots, y_m > 0$ denote approximate values of the searched function $y(t)$ at the data points $t_1, \dots, t_m$. Usually we have $m \gg n$. According to the given data one has to determine the optimal parameter values $\mathbf{p}^* = (p_1^*, \dots, p_n^*)^T$, which minimize the functional:

$$F(\mathbf{p}) = \sum_{i=1}^{m} [\, y_i - y(t_i, \mathbf{p})]^2. \tag{1.2}$$

The parameter identification problem for the system of ordinary differential equations of the second order is similarly defined.

Note that in general the solution of (1.1) need not be an elementary function. Therefore the problem is usually stated as follows:

find reasonable values for $\mathbf{p}$ *so that for suitably chosen initial conditions, the solution of* (1.1) *fits the given data.*

The next two examples illustrate the parameter identification problem in ordinary differential equation of the second order.

EXAMPLE 1.1. Enzyme effusion problem (see, e.g., Hemker and Kok [1], Van Domselaar and Hemker [2], Van Domselaar [3], Varah [4]):

$$\begin{aligned} y_1' &= p_1 \cdot (27.8 - y_1) + \frac{p_4}{2.6} \cdot (y_2 - y_1) \\ &\quad + \frac{4991}{t\sqrt{2\pi}} \exp\left(-0.5 \cdot \left(\frac{\ln(t) - p_2}{p_3} \right)^2 \right) \\ y_2' &= \frac{p_4}{2.7} \cdot (y_1 - y_2) \end{aligned} \tag{1.3}$$

is a model of enzyme effusion into the blood after a heart infarct. According to the given data (see Table 1 in Section 4) one has to estimate the parameter values p_1, p_2, p_3, p_4 in the model. Since in this case we know only the data on the function y_1, we are going to calculate y_2 from the first equation in the system (1.3) and substitute it into the second equation. In this way we obtain a second order differential equation for the function y_1 where $\left(\textit{with the notation } w := \dfrac{\ln(t) - p_2}{p_3} \right)$ the function f is defined by:

$$f(t, y, y', \mathbf{p}) = -\frac{5.3}{7.02} p_4 y' - p_1 y' + \frac{p_1 p_4}{2.7}(27.8 - y)$$
$$+\frac{1991}{t^2}\left(\frac{p_4}{2.7}t - 1 - \frac{w}{p_3}\right)\exp\left(-\frac{w^2}{2}\right). \tag{1.4}$$

Example 1.2. According to the given data (t_i, y_i), $i = 1, \dots, m$ (see Table 3 in Section 4) one has to estimate the parameter values p_1, p_2, p_3, p_4 of the function

$$y(t, \mathbf{p}) = p_1 \cdot \exp(p_3 t) + p_2 \cdot \exp(p_4 t) \tag{1.5}$$

by minimizing the functional (1.2). The function f is linear with respect to p_1, p_2 and nonlinear with respect to p_3, p_4. In this case the problem of minimization of the functional (1.2) is the so-called separable problem (see Golub and Pereyra [5] or Ruhe and Wedin [6]).

There is another way to solve the above problem (see Hemker [1], Mühlig [7, 8], Van Domselaar and Hemker [2]):

The functions $p_1 \cdot \exp(p_3 t)$ and $p_2 \cdot \exp(p_4 t)$ solve the second-order differential equation

$$y'' - (p_3 + p_4) \cdot y' + p_3 \cdot p_4 \cdot y = 0, \tag{1.6}$$

from which we can estimate the parameters p_3 and p_4 by solving the parameter identification problem for (1.6).

Solving the linear least squares problem

$$F(p_1, p_2) = \sum_{i=1}^{m} \left[y_i - p_1 \cdot \exp(p_3 t) - p_2 \cdot \exp(p_4 t)\right]^2, \tag{1.7}$$

we obtain the parameters p_1 and p_2.

There are several methods for solving the parameter identification problem for ordinary differential equations of the first order: Finite Differences (see e.g., Bard [9], Mühlig [7]), Integration of Data (see Bard [9]), Initial Value Approach (see Bard [9], Bock [10], Brewer, Burns and Cliff [11], Hemker and Kok [12], Varah [4, 13], Williams [14]), Smooth the Data (see e.g., Mühlig [7, 8], Swartz and Bremermann [15], Varah [4]), Multiple Shooting Approach (see, e.g., Bock [10], Deuflhard and Bader [16]). The parameter identification problem for ordinary differential equations of the second order is studied by Mühlig [7] and Varah [4].

In this paper we combine two methods: Integration of Data and Smooth the Data. Using the given data (t_i, y_i), $i = 1, \dots, m$, we approximate the searched function y by some smooth function ξ, and the derivative y' by ξ'. This idea appeared in Swartz and Bremermann [15]. In order to determine the smooth function ξ, Varah [4] uses the least squares cubic spline (see also De Boor [17]), and Mühlig [7, 8] uses B-splines. There are also other methods (see e.g. Eubank [18], Yoshimoto [19]).

We use the moving least squares methods (see Farwig [17, 20–22], Lancaster and Salkauskas [23, 24]) for determining the smooth function ξ on the basis of the data (t_i, y_i), $i = 1, \dots, m$ (see the next Section). Then we can choose some new points τ_i, $i = 1, \dots, M$, and replace the differential equation (1.1) using the trapezoidal rule on the right-hand side by a system of, in general, nonlinear equations in the indeterminates $p_1, \dots, p_n$ (see Section 3). Usually we have $M \gg n$, and we solve this system in the sense of least squares.

Once we determine, in some way, the reasonable value for $\mathbf{p}$, we are left with the problem of initial conditions for the equation (1.1). The initial conditions may or may not be given in advance. One possibility is to choose those values for the initial values, which minimizes the integrated residual (1.2) (see Varah [4]). Another possibility is to introduce new parameters:

$$\mu = \xi(\tau_1), \qquad \nu = \xi'(\tau_1). \tag{1.8}$$

2. MOVING LEAST SQUARES METHODS

We are given some experimental data (t_i, y_i), $i = 1, \dots, m$, where $0 \leqslant t_1 \leqslant \cdots \leqslant t_m \leqslant T$ denote time, and $y_1, \dots, y_m > 0$ are positive real numbers representing some approximate values of the searched function $y(t)$ at time $t_1, \dots, t_m$. The goal is to find an approximation Sy to the function y, such that its graph is as close as possible to the given data, and that the derivative of the function Sy at $t_1, \dots, t_m$ approximates the derivative of the searched function sufficiently well. The function Sy has to be smooth. For this purpose we shall modify the well known moving least squares methods for interpolating a function (see Farwig [17, 20–22], Lancaster and Salkauskas [23, 24], McLain [25], Shepard [26]).

To every point (moment) t_i we assign a positive weight function $v_i \in C^2([0,\ T])$, so that its value drops with the distance from the point t_i.

In a neighborhood of the point t_i, $i = 1, \ldots, m$, we approximate the function y by the local approximant:

$$LS_{t_i}^q y(x) = \sum_{j=0}^{q} a_j(t_i) \cdot b_j(x), \qquad q < m, \tag{2.1}$$

where $a_0(t_i),\ a_1(t_i), \ldots,\ a_q(t_i)$ are the coefficients and $b_0,\ b_1, \ldots,\ b_q$ denote the basis functions with the properties: (i) $b_0 \equiv 1$; (ii) $b_j \in C^2([0,\ T])$, $j = 0, \ldots, q$; (iii) $b_0,\ b_1, \ldots,\ b_q$ are linearly independent over the set $\{t_1, \ldots, t_m\}$.

For every $i \in \{1, \ldots, m\}$ we are going to determine the unknown coefficients $a_0(t_i),\ a_1(t_i), \ldots,\ a_q(t_i)$ by solving the following linear least squares problem:

$$\sum_{k=1}^{m} \left(\sum_{j=0}^{q} a_j(t_i) \cdot b_j(t_k) - y_k \right)^2 \cdot v_k(t_i) \to \min. \tag{2.2}$$

We can solve the linear least squares problem (2.2) by applying the QR decomposition to the equation (see e.g. Björck [27]):

$$\mathbf{P}^{\frac{1}{2}}(t_i) \cdot \mathbf{J} \cdot \mathbf{a}(t_i) = \mathbf{P}^{\frac{1}{2}}(t_i) \cdot \mathbf{y}, \tag{2.3}$$

where $\mathbf{P}(t_i) = \operatorname{diag}(v_1(t_i), \ldots, v_m(t_i))$ and

$$\mathbf{J} = \begin{bmatrix} 1 & b_1(t_1) & \cdots & b_q(t_1) \\ \vdots & \vdots & \cdots & \vdots \\ 1 & b_1(t_m) & \cdots & b_q(t_m) \end{bmatrix},$$

$$\mathbf{a}(t_i) = \begin{bmatrix} a_0(t_i) \\ \vdots \\ a_q(t_i) \end{bmatrix}, \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}. \tag{2.4}$$

Namely, diagonal matrix $\mathbf{P}(t_i)$ is regular for every t_i. On the other side, the basis functions $b_0 \equiv 1,\ b_1, \dots, b_q$ are linearly independent over the set $\{t_1, \dots, t_m\}$ and therefore the matrix $\mathbf{P}^{\frac{1}{2}}(t_i)\mathbf{J}$ is of full column rank.

In solving the linear least squares problem (2.3), i.e., (2.4), for every $i \in \{1, \dots, m\}$ we can define the modified Shepard's approximant as a convex combination of the $L_{t_i}^q y$:

$$S^q y(t) = \sum_{i=1}^{m} L_{t_i}^q y(t) \cdot w_i(t), \qquad w_i(t) = u_i(t) \cdot \left(\sum_{j=1}^{m} u_j(t) \right)^{-1}, \tag{2.5}$$

where u_i are continuous weight functions, which are not necessarily the same as the weight functions v_i used in (2.2).

It is easy to show that $S^q y \in C^2([0,\ T])$. Namely, from (2.3) we have:

$$\mathbf{a}(t_i) = \left(\mathbf{J}^T \cdot \mathbf{P}(t_i) \cdot \mathbf{J}\right)^{-1} \cdot \mathbf{J}^T \cdot \mathbf{P}(t_i) \cdot \mathbf{y}, \tag{2.6}$$

and, because $v_i,\ w_i,\ b_j \in C^2([0,\ T])$, it follows that $S^q y \in C^2([0,\ T])$.

REMARK 3.1. The moving least squares method was developed in the last 20 years as a method for interpolating a function $f: \mathbf{R}^s \to \mathbf{R}$, for which we know the values at the points $x_1, \dots, x_m \in \mathbf{R}^s$ (see Farwig [17, 20–22], Franke [28], Lancaster and Salkauskas [23, 24]). If we define the weight function $v_i: \mathbf{R}^s \to \mathbf{R}$ in such a way that it has a singularity at the point x_i, this will guarantee the interpolation conditions $L_{t_i}^q f(x_i) = f(x_i)$, $i = 1, \dots, m$. The weight function v_i with singularity at x_i is usually defined as the inverse distance weight function $v_i(x) = \|x - x_i\|^{-p}$, $p > 1$, where $\|\cdot\|$ denotes the Euclidean norm. For the basis functions one usually takes $b_j(x) = x^j$ (McLain's method) or the Taylor polynomial terms $b_j(x,\ t) = (x - t)^j$ (Farwig's method), etc. If $q = 0$, moving least squares reduces to Shepard's interpolation formula:

$$Sf(x) = \sum_{i=1}^{m} f(x_i) \cdot w_i(x), \qquad w_i(x) = v_i(x) \cdot \left(\sum_{j=1}^{m} v_j(x) \right)^{-1}, \tag{2.7}$$

(see Shepard [26]), for which the following holds: $0 \leqslant w_i(x) \leqslant 1$, $\sum_{i=1}^m w_i(x) = 1$, $w_i(x_k) = \delta_{ik}$, $Sg = g$ for every polynomial g of degree $\leqslant q$, as well as some other properties (see e.g. Farwig [17, 20–22], Salkauskas [12]).

3. SOLVING THE PARAMETER IDENTIFICATION PROBLEM USING THE NONINTERPOLATING MOVING LEAST SQUARES METHOD

Again, to keep things simple, we are going to consider the parameter identification problem for a single differential equation of the second order:

$$\frac{d^2y}{dt^2} = f(t, y(t), y'(t), \mathbf{p}), \tag{3.1}$$

where the parameters $\mathbf{p} = (p_1, \ldots, p_n)^T$ are to be determined according to data (t_i, y_i), $i = 1, \ldots, m$, by minimizing the functional:

$$F(\mathbf{p}) = \sum_{i=1}^{m} [y_i - y(t_i, \mathbf{p})]^2. \tag{3.2}$$

Since in general it is not possible to represent the function y occurring in the functional (3.2) by elementary or some other known functions, we reformulate the problem as follows:

find reasonable values $\hat{\mathbf{p}}$ *for* $\mathbf{p}$, *such that for suitably chosen initial conditions the function* $y(t, \hat{\mathbf{p}})$ *fits the given data.*

The realization of this principle goes like this:

Step 1.

According to the data (t_i, y_i), $i = 1, \ldots, m$, we approximate the searched function y by applying the moving least squares method with the modified Shepard's approximant (2.5), where we take:

$$b_0 \equiv 1, \qquad b_j(x) = x^j, \qquad j = 1, \ldots, q \tag{3.3}$$

for the basis functions.

We define the weight functions by:

$$v_i(t) = \exp\left(-\frac{1}{2}\left(\frac{t - t_i}{\sigma_i}\right)^2\right), \qquad i = 1, \ldots, m, \tag{3.4}$$

where $\sigma_i > 0$ are real constants that regulate, in some neighborhood of the data points t_i, the influence of the data (t_i, y_i) on the value of the searched

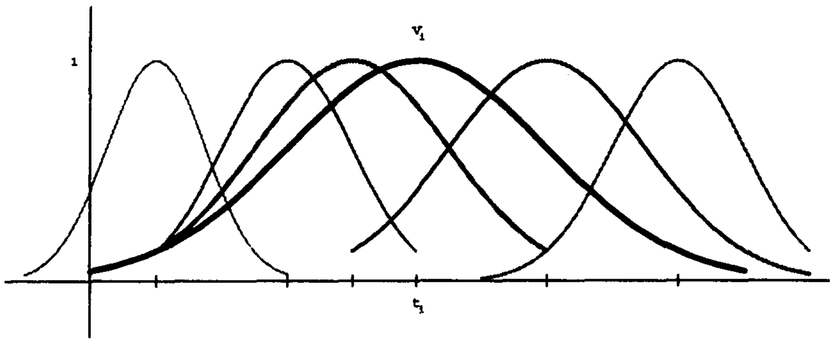


FIG. 1. Weight functions.

function y (see Figure 1). A larger σ_i means a larger extent of influence of the ith data. One possibility for the definition of the numbers σ_i is the following:

$$\sigma_i = s \cdot \Delta_i, \qquad (s > 0), \tag{3.5}$$

where

$$\Delta_i = \begin{cases} |t_2 - t_1|, & i = 1 \\ \max\{|t_i - t_{i-1}|, |t_i - t_{i+1}|\}, & i = 2, \ldots, m-1 \\ |t_m - t_{m-1}|, & i = m \end{cases} \tag{3.6}$$

If $s = 1$, then at least three data with weights of at least 0.6 affect the local approximant in a neighborhood of the point t, and hence the respective local approximant (2.1) can be calculated. The value of parameter s in (3.5) will be chosen according to the dispersion of data. Taking $s < 1$ will emphasize the local values of the data, while taking $s > 1$ will keep the tendency of the data to fluctuate. Since only the "future" ("past") affects the value of the local approximant in a neighborhood of the first (respectively, last) data point, the approximation of the searched function y, as well as of its derivative, will here be less accurate. The whole of this problematics is illustrated by examples in Section 4. This choice of the weight functions v_i will guarantee that the conditions required in Section 2 are satisfied.

Step 2.

We approximate the derivative of the searched function y by the derivative of the modified Shepard's approximant (2.5). Then we have the following theorem.

THEOREM 1. *Let (t_i, y_i), $i = 1, \dots, m$, be the given data and*

$$S^q y(t) = \sum_{i=1}^{m} L_{t_i}^q y(t) \cdot w_i(t),$$
$$w_i(t) = v_i(t) \cdot \left(\sum_{j=1}^{m} v_j(t) \right)^{-1}, \qquad t \in [0, T] \tag{3.7}$$

be the modified Shepard's approximant where the weight functions v_j and the coefficients $a_j(t_i)$, $j = 0, \dots, q$, are given by (3.4) and (2.6), respectively. Then

$$\frac{d}{dt}(S^q y(t)) = \sum_{i=1}^{m} w_i(t) \left[\sum_{j=0}^{q} a_j(t_i) \big(\Omega_i(t) \cdot b_j(t) + b'(t) \big) \right], \tag{3.8}$$

where

$$\Omega_i(t) = \frac{t_i - t}{\sigma_i^2} - \sum_{j=1}^{m} w_j(t) \cdot \frac{t_j - t}{\sigma_j^2}. \tag{3.9}$$

If the basis functions are given by (3.3) then

$$\frac{d}{dt}(S^q y(t)) = \sum_{i=1}^{m} w_i(t) \left[\sum_{j=0}^{q} a_j(t_i) \big(t^j \cdot \Delta_i + j \cdot t^{j-1} \big) \right]. \tag{3.10}$$

PROOF. Since $v_i'(t) = v_i(t) \cdot (t_i - t)/\sigma_i^2$, it is easy to show that

$$w_i'(t) = w_i(t) \cdot \Omega_i(t), \tag{3.11}$$

where $\Omega_i(t)$ is given by (3.9). From (3.11) we deduce (3.8) and (3.10) ■

REMARK 3.2. It turns out that, in order to obtain a good approximation of the derivative of the function y, it suffices to take $q = 2$, i.e., we look for the local approximant of the form:

$$LS_{t_i}^2 y(t) = a_0(t_i) + a_1(t_i) \cdot t + a_2(t_i) \cdot t^2. \tag{3.12}$$

We denote by Sy the modified Shepard's approximant. Then

$$\frac{d}{dt}(Sy(t)) = \sum_{i=1}^{m} w_i(t)\left[\Delta_i\left(a_0(t_i) + a_1(t_i) \cdot t + a_2(t_i) \cdot t^2\right) + a_1(t_i) + 2 \cdot t \cdot a_2(t_i)\right]. \tag{3.13}$$

Step 3.

We can choose some new points τ_i, $i = 1, \dots, M$, from $[0, T]$ and replace the differential equation (1.1) using the trapezoidal rule on the right-hand side by a system of, in general, nonlinear equations in the indeterminates $p_1, \dots, p_n$:

$$S'(\tau_i) - S'(\tau_1) = \frac{1}{2} \sum_{r=1}^{i-1} \left[f(\tau_{r+1}, Sy(\tau_{r+1}), S'y(\tau_{r+1}), \mathbf{p}) + f(\tau_r, Sy(\tau_r), S'y(\tau_r), \mathbf{p})\right] \cdot(\tau_{r+1} - \tau_r), \qquad i = 2, \dots M. \tag{3.14}$$

Usually we have $M \gg n$ and we solve this system in the sense of least squares. We denote the least squares solution by $\hat{\mathbf{p}} = (\hat{p}_1, \dots, \hat{p}_n)$.

If the function f is linear in the parameters $p_1, \dots, p_n$, then we are dealing with a linear least squares problem, which always has a unique solution, and it can be obtained, e.g., by applying the QR-decomposition or Singular Value Decomposition (see e.g. Björck [27], Gill et al. [29] or Golub and Van Loan [30]). If the function f is nonlinear in the parameters $p_1, \dots, p_n$, then we are faced with a nonlinear least squares problem (see, e.g., Björck [27], Gill et al. [31] or Dennis and Schnabel [32]). If the function f is linear with respect to some parameters and nonlinear with respect to others, then one can apply some special methods for the so-called separable problems (see, e.g., Golub and Pereyra [5] or Ruhe and Wedin [6]).

Step 4.

Once we estimated the value for $\mathbf{p}$, we still need some suitable initial conditions in order to determine the function y from the equation (3.1). The initial conditions may or may not be given in advance. Following Varah [4], for the initial value we will take that value which minimizes the integrated residual (3.2). This means that one has to do a two-dimensional minimization of the function

$$F(\mu, \nu) = \sum_{i=1}^{m} \left[y_i - y_{\mu\nu}(t_i, \hat{\mathbf{p}}) \right]^2, \tag{3.15}$$

where $y_{\mu\nu}(t_i, \hat{\mathbf{p}})$ are the values of the function $y_{\mu\nu}$ obtained by solving the Cauchy's problem:

$$\frac{d^2y}{dt^2} = f(t, y(t), y'(t), \hat{\mathbf{p}}), \qquad y(t_1) = \mu, \qquad y'(t_1) = \nu. \tag{3.16}$$

4. NUMERICAL EXAMPLES

We will illustrate the discussed method for the parameter identification problems with two examples.

EXAMPLE 4.1. As the first example, consider the enzyme effusion problem (see Example 1.1) with the data given in Table 1. We define the influence of the data points on the value of the Shepard's approximant of y_1

TABLE 1

DATA FOR ENZYME EFFUSION PROBLEM

t	y_1	t	y_1	t	y_1	t	y_1
0.1	27.8	21.3	331.9	42.4	62.3	81.1	23.5
2.5	20.0	22.9	243.5	44.4	58.7	91.2	24.8
3.8	23.5	24.9	212.0	47.9	41.9	101.9	26.1
7.0	63.6	26.8	164.1	53.1	40.2	115.4	33.3
10.9	267.5	30.1	112.7	59.0	31.3	138.7	17.8
15.0	427.8	34.1	88.1	65.1	30.0	163.2	16.8
18.2	339.7	37.8	76.2	73.1	30.6	186.7	16.8

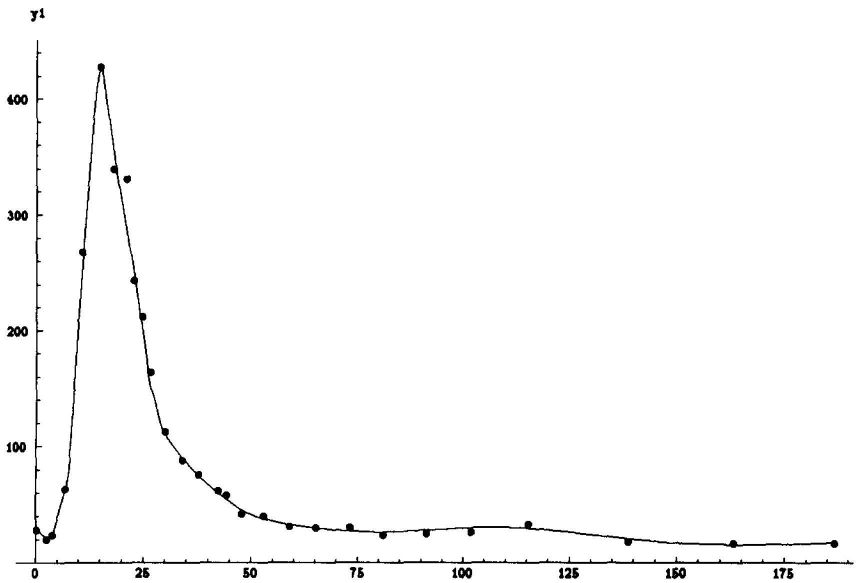


FIG. 2. Enzyme effusion problem: Sy_1.

by the parameter s, so that the data at the beginning have a preponderantly local character, while the later data have a preponderantly global character (see Figure 2).

Since the function f given by (1.4) is nonlinear in the parameters $p_1, \ldots, p_n$, we are going to solve a nonlinear least squares problem (3.14) by using the Gauss-Newton method with regulated steps (see, e.g., Dennis and Schnabel [32] or Gill et al. [31]).

The two-dimensional minimization of the functional (3.15) was done using the method of coordinate relaxation (see Ortega and Rheinboldt [33], p. 240).* In solving the Cauchy's problem (3.16) we employ the DIFSUB by Gear [34].

In Table 2 we show the results obtained by the moving least squares method for various choices of the numbers M and knots τ_i, by which the system (3.14) is defined. The sum of squares of residuals of the equation (3.14) is denoted by D.E. RES, the optimal initial condition value is denoted by OPTIMAL I.C., and the corresponding value of the functional (3.15) by INT. RES.

In Figure 3 we show the data and the graphs of the searched functions y_1 and y_2 obtained by solving (1.3) for optimal initial condition.

* The corresponding software for PC's is developed.

TABLE 2
RESULTS OBTAINED BY MOVING LEAST SQUARES METHOD

	Opt. parameters				Optimal i.c.		RES.	
# knots	p_1	p_2	p_3	p_4	$y_1(0.1)$	$y_2(0.1)$	D.E.	INT.
$M = 28$	0.3180	2.69001	0.41880	0.10350	22	38	643	5301.2
$M = 68$	0.3193	2.72109	0.41987	0.10303	22.9	40	966	5250.3
$M = 128$	0.3190	2.70100	0.41900	0.10310	22	39	3559	5076.6

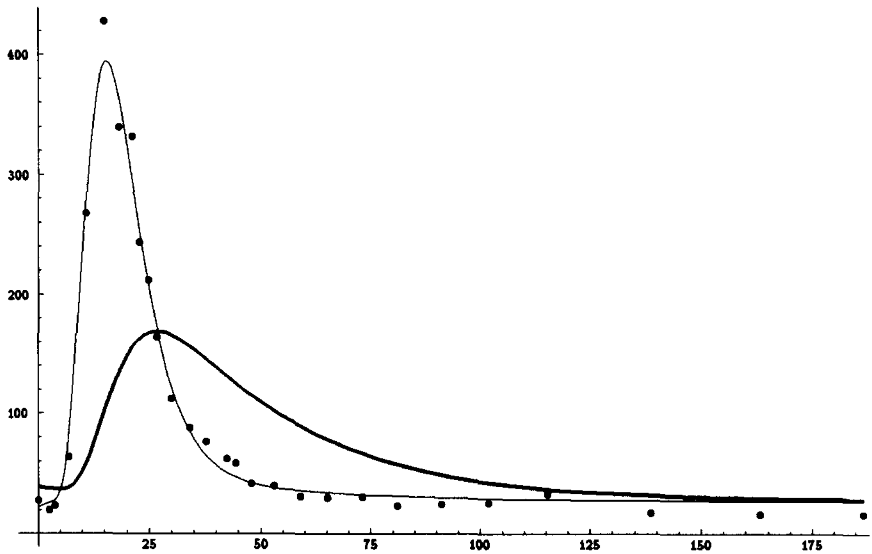


FIG. 3. Enzyme effusion problem: y_1 and y_2 for optimal initial condition ($M = 128$), (— y_1, — y_2).

EXAMPLE 4.2. In Table 3 are given the data for no load loss y (in kW) for a generator, depending on the voltage U (in V) (see Mühlig [7]):

For the numerical reasons we introduce the transformation $t = (U - 425)/195$ and search for the function y in the form:

$$y(t, \mathbf{p}) = p_1 \cdot \exp(p_3 t) + p_2 \cdot \exp(p_4 t). \tag{4.1}$$

First we solve the parameter identification problem for differential equations (see Example 1.2):

$$y''(t) = f(t, y, y'; \alpha, \beta) = \alpha y' + \beta y. \tag{4.2}$$

TABLE 3
DATA FOR NO LOAD LOSS y

U	230	295	360	425	490	555	620
y	64.0	66.0	69.5	74.0	80.8	91.0	103.5
t	-1	$-2/3$	$-1/3$	0	$1/3$	$2/3$	1

In Figure 4 we show the derivative of the modified Shepard's approximant $S'y$ for $s = 0.5, 0.75, 1, 1.25, 1.5$. Since in this case the function f is linear in parameters, we are going to solve the system (3.14) by applying the QR-decomposition (see, e.g., Gill et al. [29] or Golub and Van Loan [30]).

Parameters p_3 and p_4 are the solutions of the quadratic equation:

$$p^2 - \alpha p - \beta = 0. \tag{4.3}$$

Then solving the linear least squares problem:

$$F(p_1, p_2) = \sum_{i=1}^{m} [y_i - p_1 \cdot \exp(p_3 t) - p_2 \cdot \exp(p_4 t)]^2 \to \min \tag{4.4}$$

we obtain the parameters p_1 and p_2.

In this way we reduce this very senzitive nonlinear least squares problem to two linear least squares problems.

In Table 4 we present the results obtained by the moving least squares method (M.L.S.) for various choices of parameter s, whereas in system (3.14) we used only the data points. Table 5 shows the results obtained by 201 equally spaced data points τ_i in $[-1, 1]$. Furthermore, one can also compare the results obtained by the Gauss-Newton method. The sum of squares of the residual of the equations (3.14) for the differential equation (4.2) is denoted by D.E. RES, and the value of the functional (3.2) for function (4.1) by INT. RES. Relative errors in parameters and minimizing functions (3.2) are also shown.

In Figure 5a we show the contour plot of the function:

$$F(p_3, p_3) = \sum_{i=1}^{m} [y_i - p_1^* \cdot \exp(p_3 t) - p_2^* \cdot \exp(p_4 t)]^2, \tag{4.5}$$

where the parameters p_1^* and p_2^* are obtained by solving the nonlinear least squares problem for the function (4.1). Values (p_3, p_4) from Table 4 are

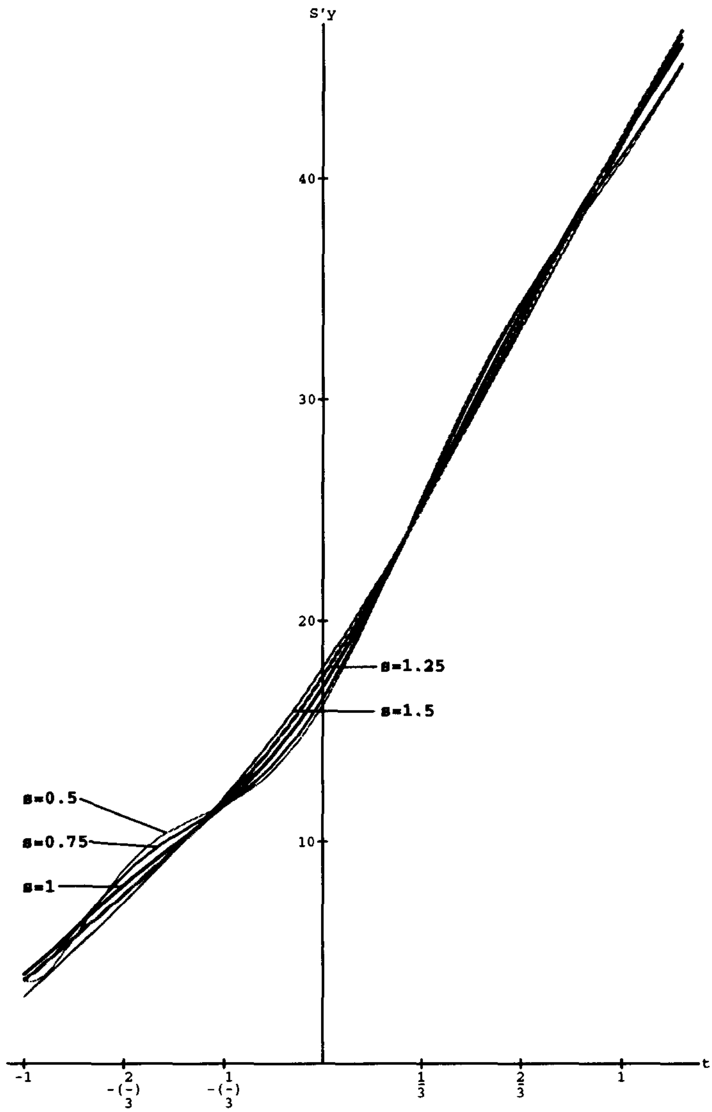
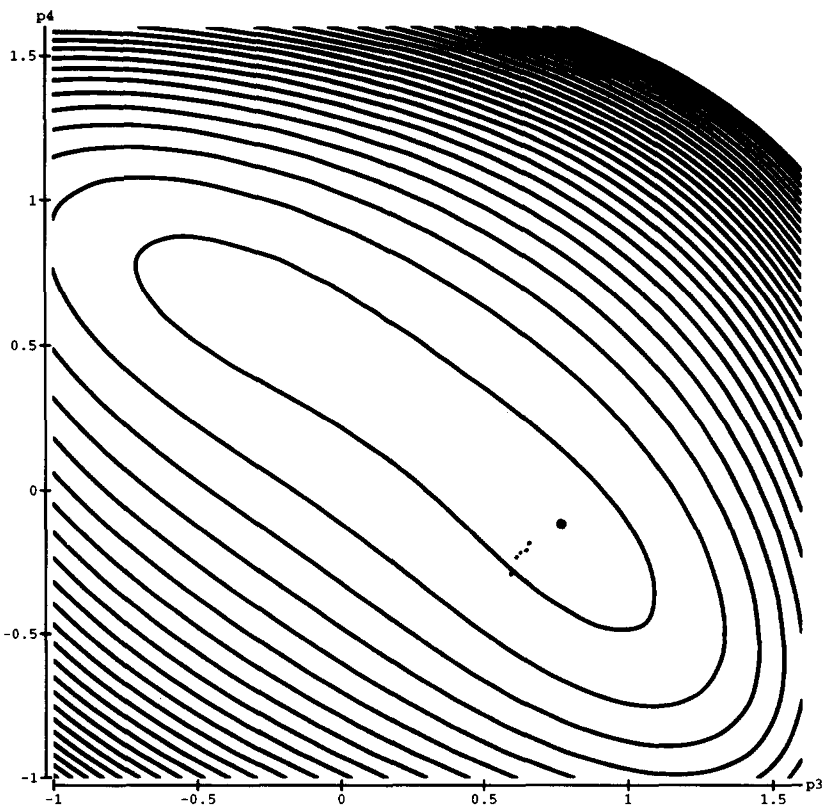


FIG. 4. $S'y$ (s = 0.5, 0.75, 1, 1.25, 1.5).

TABLE 4

RESULTS OBTAINED BY MOVING LEAST SQUARES METHOD

Methods	Opt. parameters				Res.		Rel. error	
	p_1	p_2	p_3	p_4	D.E.	INT.	p	INT.
M.L.S. ($s = 0.5$)	43.1124	31.1964	0.60781	−0.26021	7.87	0.646	0.327	1.268
M.L.S. ($s = 0.75$)	41.5134	32.7882	0.62380	−0.24016	8.25	0.591	0.284	1.076
M.L.S. ($s = 1$)	39.4228	34.8719	0.64543	−0.21526	4.38	0.532	0.229	0.869
M.L.S. ($s = 1.25$)	40.9520	33.3094	0.63166	−0.23674	1.99	0.506	0.270	0.776
M.L.S. ($s = 1.5$)	45.8872	28.3297	0.58630	−0.30836	0.89	0.577	0.402	1.027
GN method	30.7168	43.4238	0.75930	−0.13435	—	0.285	—	—



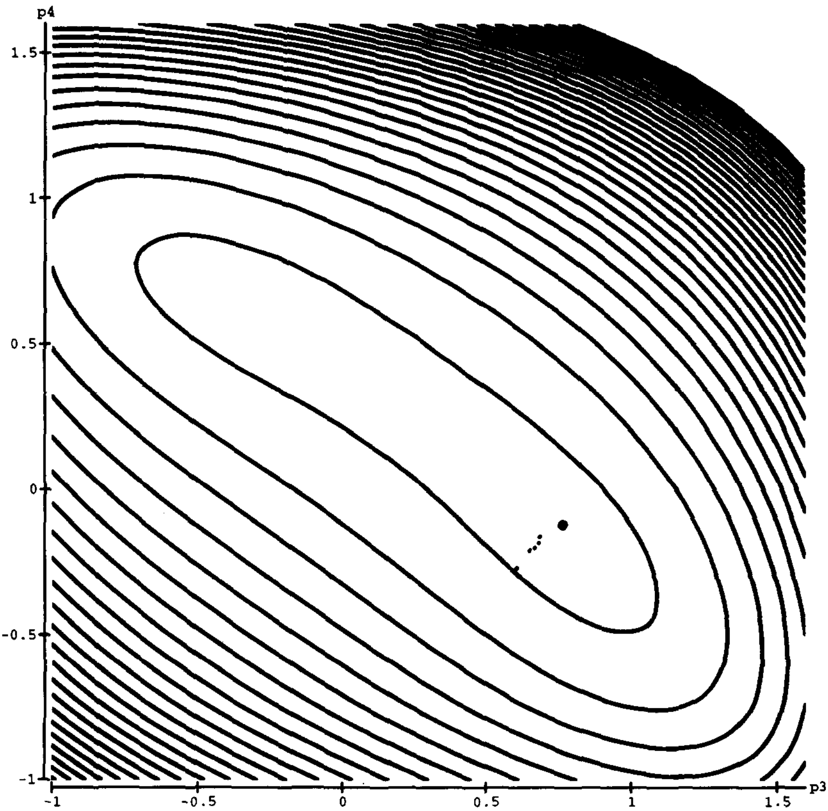
(a)

FIG. 5a. Contour plot of the function (4.5) and values (p_3, p_4) from Table 4.

TABLE 5

RESULT OF 201 EQUALLY SPACED DATA POINTS τ_i IN $[-1, 1]$

Methods	Opt. parameters				Res.		Rel. error	
	p_1	p_2	p_3	p_4	D.E.	INT.	p	INT.
M.L.S. ($s = 0.5$)	37.7479	36.4314	0.67023	−0.20551	305	0.353	0.186	0.241
M.L.S. ($s = 0.75$)	36.6454	37.5335	0.68261	−0.19309	205	0.338	0.157	0.187
M.L.S. ($s = 1$)	35.3570	38.8341	0.69676	−0.17805	94	0.331	0.123	0.162
M.L.S. ($s = 1.25$)	38.0648	36.1162	0.66665	−0.20902	40	0.359	0.195	0.262
M.L.S. ($s = 1.5$)	43.9805	30.1752	.60735	−0.28653	17	0.469	0.352	0.649
GN method	30.7168	43.4238	0.75930	−0.13435	—	0.285	—	—



(b)

FIG. 5b. Contour plot of the function (4.5) and values (p_3, p_4) from Table 5.

denoted by black dots. Analogously, in Figure 5b we show the contour plot for the function (4.5) and values (p_3, p_4) from Table 5.

REFERENCES

1 P. W. Hemker, and J. Kok, A project on parameter identification in reaction kinetics, in Rep. NM-R9301, Centrum voor Wiskunde en Informatica, Amsterdam, 1993, pp. 38.

2 B. van Domselaar, and P. W. Hemker, Nonlinear parameter estimation in initial value problems, in Rep. NW 18/75, Mathematisch Centrum, Amsterdam, 1977, pp. 49.

3 B. van Domselaar, Een Mathematische Analyse van het Hertinfarct, in Rep. NN 4/74, Mathematisch Centrum, Amsterdam, 1974, pp. 19.

4 J. M. Varah, A spline least squares method for numerical parameter estimation in differential equations, *SIAM J. Sci. Stat. Comput.* 3:28–46 (1982).

5 G. H. Golub, and V. Pereyra, The differentation of pseudo-inverse and nonlinear least squares problems whose variable separate, *SIAM J. Numer. Anal.* 10:413–432 (1973).

6 A. Ruhe, and P. A. Wedin, Algorithms for separable nonlinear least squares problems, *SIAM Rev.* 22:318–337 (1980).

7 H. Mühlig, Parameteridentifikation bei Differentialgleichungen mit Hilfe von B-splines, *Wiss. Z. TU Dresden* 41:3–6 (1992).

8 H. Mühlig, Lösung praktischer Approximationsaufgaben durch Parameteridentifikation, *ZAMM* 73:T837–T839 (1993).

9 Y. Bard, *Nonlinear Parameter Estimation*, Academic Press, New York, 1974.

10 H. G. Bock, Recent advances in parameteridentification techniques for O.D.E., in *Numerical Treatment of Inverse Problems in Differential and Integral Equations*, (P. Deuflhard, Ed.), Heidelberg, 1983.

11 D. W. Brewer, J. A. Burns, and E. M. Cliff, Parameter identification for an abstract Cauchy problem by quasilinearization, *Q. Appl. Math.* 51:1–22 (1993).

12 K. Salkauskas, Moving least squares interpolation with thin-plate splines and radial basis functions, *Comput. Math. Appl.* 24:177–185 (1992).

13 J. M. Varah, On the conditioning of parameter estimation problems, in *Reliable Numerical Computation*, (M. G. Cox and S. Hammarling, Eds.), Oxford Science Publications, New York, 1990, pp. 187–195.

14 J. Williams, Approximation and parameter estimation in ordinary differential equations, in Algorithms for Approximation II, (J. C. Mason and M. G. Cox, Eds.), Chapman and Hall, London, 1990, pp. 395–403.

15 J. Swartz, and H. Bremermann, Discussion of parameter estimation in biological modelling: Algorithms for estimation and evaluation of the estimates, *J. Math. Biol.* 1:241–257 (1975).

16 P. Deuflhard, and G. Bader, Multiple shooting techniques revisited, in P. Deufhlard, Ed., *Numerical Treatment of Inverse Problems in Differential and Integral Equations*, Heidelberg, 1983, pp. 74–93.

17 R. Farwig, Multivariate interpolation of scattered data by moving least squares methods, in *Algorithms for Approximation*, (J. C. Mason and M. G. Cox, Eds.), Clarendon Press, Oxford, 1987, pp. 193–211.

18 R. L. Eubank, *Spline Smoothing and Nonparametric Regression*, Marcel Dekker, Inc., New York, 1988.

19 F. Yoshimoto, Least squares approximation by one-pass methods with piecewise polynomials, in *Algorithms for Approximation* (J. C. Mason and M. G. Cox, Eds.), Clarendon Press, Oxford, 1987, pp. 213–224.

20 R. Farwig, Rate of convergence of moving least squares interpolation methods: the univariate case, in *Progress in Approximation Theory* (P. Nevai and A. Pinkus, Eds.), Academic Press, 1991, pp. 313–327.

21 R. Farwig, Multivariate interpolation of arbitrary spaced data by moving least squares methods, *J. Comp. Appl. Math.* 16:79–93 (1986).

22 R. Farwig, Rate of convergence of Shepard's global interpolation formula, *Math. Comp.* 46:577–590 (1986).

23 P. Lancaster, and K. Salkauskas, Surfaces generated by moving least squares methods, *Math. Comp.* 37:141–158 (1981).

24 P. Lancaster, and K. Salkauskas, *Curve and Surface Fitting; An Introduction*, Academic Press, London, 1986.

25 D. H. McLain, Drawing contours from arbitrary data point, *Comput. J.* 17:318–324 (1974).

26 D. Shepard, A two-dimensional interpolation function for irregulary spaced data, *Proc. 23rd. Nat. Conf. ACM* (1968), pp. 517–524.

27 A. Björck, Least Squares Methods, in *Handbook of Numerical Analysis*, Vol. I, (P. G. Ciarlet and J. L. Lions, Eds.), Elsevier, New York, 1990, pp. 467–653.

28 R. Franke, Scattered data interpolation: test of some methods, *Math. Comp.* 38:99–106 (1982).

29 P. E. Gill, W. Murray, and M. H. Wright, *Numerical Linear Algebra and Optimization*, Vol. 1, Addison-Wesley, New York, 1991.

30 G. H. Golub, and C. F. van Loan, *Matrix Computations*, The J. Hopkins University Press, Baltimore, 1989.

31 P. E. Gill, W. Murray, and M. H. Wright, *Practical Optimization*, Academic Press, New York, 1981.

32 J. E. Dennis, Jr, and R. B. Schnabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Englewood Cliffs, N.J., 1983.

33 J. M. Ortega, and W. C. Rheinboldt, *Iterative Solutions of Nonlinear Equations in Several Variables*, Academic Press, New York, 1970.

34 C. W. Gear, *Numerical Initial Value Problems in Ordinary Differential Equations*, Prentice-Hall, Inc., Englewood Cliffs, N.J., 1971.