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A New Method for the Estimation of Parameters in Differential Equations

A new objective function for estimating parameters in differential equations, based upon a weighted least squares criterion for the residuals of these equations, is presented. The use of Lobatto quadrature in combination with the collocation technique reduces the original problem to one of minimizing a simple algebraic expression with respect to a series of unknowns. The method can be applied to different types of differential equations as shown by a series of examples and leads to very good estimates. It becomes particularly useful for systems which are linear in the parameters and for which all states are observable since in this case the usual convergence problem is avoided. The gain in computation time when compared with classical methods is significant.

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SCOPE

Most chemical engineering problems are modeled by complex sets of algebraic or differential equations. In the common problem of engineering analysis the outputs of a model are calculated for given values of the parameters. Contrary to this direct problem the inverse situation often occurs, that is, when measurements of the outputs can be performed without knowing values of the parameters. The form of the model itself is usually obtained from a priori knowledge on the nature of the process. In this grey box problem, the unknown parameters are identified or estimated from an analysis of the output data. This is performed by selecting an appropriate objective function based upon deviations of the observation equations. The parameters are calculated by use of an algorithm for minimization of the objective function, which often involves a problem of convergence. Methods derived from the general gradient techniques are most commonly encountered, calling for repetitive and time-consuming solutions of the differential equations.

In this investigation a new criterion based upon the residuals of the differential equations is presented. The application of the Lobatto quadrature formulas with appropriate weighting functions in combination with the collocation technique leads to a simple algebraic expression for the objective function. The parameters can then be estimated in the same way as for systems described by algebraic equations.

CONCLUSIONS AND SIGNIFICANCE

The use of quadrature formulas and the collocation technique for approximating objective functions for parameter estimation reduces significantly the complexity of the problem. An algebraic expression is obtained, which has to be minimized with respect to a series of unknowns. By defining an objective function based upon residuals of the differential equations instead of upon deviations from the observation equations, it is possible to eliminate part of the unknowns, since constraints derived from boundary conditions and from observation equations are usually linear with respect to the unknowns. Repetitive solution of the differential equations, typical for classical methods, is avoided, and the computation time for obtaining estimates of the parameters is drastically reduced. Because of the general validity of the objective criterion and of the two approximation techniques, no a priori restrictions

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are to be imposed on the form or the number of differential equations or of the boundary conditions. The method becomes particularly useful whenever the so-called "collocation equations" derived from the differential equations are linear with respect to the unknowns since then a linear least squares problem arises making the estimation of the parameters very straightforward, and the convergence problem, typical of the classical methods, disappears.

After introducing the two approximations, continuous observations of the state variables are made superfluous, and it suffices to perform measurements at the quadrature nodes. Remarkable is the fact that these nodes are not equidistant.

From a series of examples it is clear that the accuracy of the estimates depends upon the weighting function and the order n of the approximation, as well as upon errors in the data. If exact data for the observed variables are available, more accurate estimates are obtained for increasing n, which is in agreement with the excellent accuracy of collocation solutions and of quadrature formulas for increasing order of approximation. In fact, the accuracy of the results for sufficiently large n is limited only by the machine accuracy of the computer used to calculate the estimates, and in the case of collocation equations which are nonlinear with respect to the unknowns, also by the algorithm for minimization of the objective function. However, slight errors normally disturb the data, and a value $n = 6$ suffices since a further increase does not improve the results. In the latter case the accuracy depends upon the magnitude of the errors in the data, showing larger deviations from the exact estimates than in the case of the classical least squares method. For data subject to errors a weighting function emphasizing these parts of the integration interval where no information from boundary conditions is available gives better results for the different examples investigated.

Because of its simplicity the method can be used for a fast comparison of the validity of different mathematical models for a given process whenever the a priori knowledge of the system does not completely specify the form of the equations.

ESTIMATION OF PARAMETERS FOR SYSTEMS MODELED BY DIFFERENTIAL EQUATIONS

When the state variables of a system are governed by a set of differential equations, the observation equations determine the relationship between the output variables $\mathbf{y}$, the m state variables $\mathbf{x}$ and the S independent variables $\mathbf{t}$:

$$\mathbf{F}(\mathbf{y}, \mathbf{x}, \mathbf{t}) = \mathbf{0} \tag{1}$$

or

$$\mathbf{y} = \mathbf{f}(\mathbf{x}, \mathbf{t}) \tag{2}$$

The parameters are grouped into a vector $\mathbf{k}$ of dimension K, $\mathbf{k}$ entering the problem through the set of differential equations, which can be written in a very general way

$$\mathbf{L}(\mathbf{x}(\mathbf{t}), \mathbf{t}, \mathbf{k}) = \mathbf{0} \tag{3}$$

The operator $\mathbf{L}$ has the same dimension as $\mathbf{x}$ and contains several operations including differentiation with respect to the independent variables $\mathbf{t}$.

Two kinds of errors can be involved: measurement errors disturb the observation equations whereas dynamic errors enter through the system equations. The residuals are

$$\mathbf{e}(\mathbf{x}, \mathbf{t}) = \mathbf{F}(\mathbf{y}, \mathbf{x}, \mathbf{t}) \tag{4}$$

upon which a general objective function is based. The parameters are estimated by minimizing this objective function.

This estimation problem is much more complicated than in the case of algebraic equations (Seinfeld, 1970) since the residuals are not known as explicit functions of the parameters $\mathbf{k}$, but do depend upon them indirectly through the system equations. It is assumed that the system is observable, that is, there exists a unique set of parameters $\mathbf{k}$ from which the outputs can be obtained. The property of convergence of any algorithm solving the estimation problem will be accepted to be a sufficient condition for observability (Seinfeld, 1969).

Classical methods used to solve the estimation problem of differential equations (Rosenbrock and Storey, 1970; Lee, 1968) have the important disadvantage that repetitive solutions of a large set of differential equations are necessary, the number of which is determined by the dimensions of $\mathbf{x}$ and $\mathbf{k}$. This requires a substantial use of computation time, and the applicability of these methods is restricted to systems with small values for both dimensions. Because of this restriction several alternative methods have been proposed (for example, Seinfeld, 1970; Hwang and Seinfeld, 1972; Gavalas, 1973). A different approach will be presented here.

PROCEDURE FOR ESTIMATING PARAMETERS IN DIFFERENTIAL EQUATIONS

A new objective criterion will be defined based upon deviations of the differential equations:

$$\mathbf{e}(\mathbf{x}, \mathbf{t}, \mathbf{k}) = \mathbf{L}(\mathbf{x}(\mathbf{t}), \mathbf{t}, \mathbf{k}) \tag{5}$$

The moment matrix becomes

$$\mathbf{M}(\mathbf{x}, \mathbf{t}, \mathbf{k}) = \mathbf{e}(\mathbf{x}, \mathbf{t}, \mathbf{k})\ \mathbf{e}^T(\mathbf{x}, \mathbf{t}, \mathbf{k}) \tag{6}$$

from which the objective function is derived:

$$S(\mathbf{x}, \mathbf{k}) = \Psi[\mathbf{M}(\mathbf{x}, \mathbf{t}, \mathbf{k})] \tag{7}$$

Assuming that all variables t_s vary between 0 and 1, the weighted least squares criterion based upon a positive semidefinite matrix $\mathbf{Q}$ is

$$\Psi = \int_0^1 \int_0^1 \cdots \int_0^1 Tr\,[\mathbf{Q}(\mathbf{t})\ \mathbf{M}(\mathbf{x}, \mathbf{t}, \mathbf{k})]\ dt_1 \ldots dt_s \ldots dt_S \tag{8}$$

This objective function has to be minimized with respect to the functions $\mathbf{x}(\mathbf{t})$ and the parameters $\mathbf{k}$. The observation equations enter into the problem as constraints to the state functions $\mathbf{x}(\mathbf{t})$. This is without doubt as hard a mathematical problem as the minimization of the classical objective function. The application of two approximation techniques turns out to be a very useful simplification for the presented objective function, which is based upon a new conception of the deviations. First, the integrations involved in Equation (8) will be replaced by formulas for numerical quadrature. Secondly the residuals at the quadrature nodes will be approximated by means of the collocation technique using the quadrature nodes as collocation points.

Numerical Quadrature

The integrations can be performed using some functionals, known as numerical quadratures, based upon the knowledge of the integrand in a series of interpolation nodes (Villadsen, 1970). Several types of formulas exist depending upon the choice of the quadrature nodes and available data on the integrand. Since for systems of differential equations information is usually given at the end points through the boundary conditions, these points will be preselected as nodes for the quadrature.

The elements of the matrix $\mathbf{Q}(t)$ are chosen as

$$Q_{i,j}(t) = \delta_{i,j}\, w_1(t_1) \ldots\ldots w_s(t_s) \ldots\ldots w_S(t_S) \quad (9)$$

Thus all elements are zero, except on the main diagonal where the elements are all the same. With the above matrix, the objective function has to be evaluated by successive integrations with respect to the independent variables t_s ($s = 1, S$), each integration involving a weighting function $w_s(t_s)$ which is defined as

$$w_s(t_s) = (1 - t_s)^{\alpha_s}\, t_s^{\beta_s} \quad (10)$$

Both exponents α_s and β_s are nonnegative.

When using this weighting function the quadrature formula with a total number of n_s nodes can be made accurate for all polynomials of t_s with degree $\leq 2n_s - 3$. This is achieved by the Lobatto quadrature (Villadsen, 1970) obtained by selecting the nodes as the zeros of a polynomial of degree $(n_s - 2)$ belonging to a series of orthogonal polynomials with respect to the weighting function:

$$w_s{}^+(t_s) = (1 - t_s)^{\alpha_s+1}\, t_s^{\beta_s+1} \quad (11)$$

In addition the weights $H^s{}_{j_s}$ ($j_s = 1, n_s$) have to be evaluated in an appropriate way.

The following approximate expression for Ψ is obtained:

$$\Psi \doteq Tr \sum_{j_1=1}^{n_1} H^1{}_{j_1} \ldots \sum_{j_s=1}^{n_s} H^s{}_{j_s} \ldots \sum_{j_S=1}^{n_S} H^S{}_{j_S}\, \mathbf{M}\{\mathbf{e}[\mathbf{x}(t_{1,j_1} \ldots t_{S,j_S}), t_{1,j_1}, \ldots, t_{S,j_S}, \mathbf{k}]\} \quad (12)$$

This results in an approximation for the objective function:

$$S(\mathbf{x}, \mathbf{k}) \doteq S'\{\mathbf{e}[\mathbf{x}(t_{1,j_1} \ldots\ldots t_{S,j_S}), \mathbf{k}]\} \quad \begin{matrix} j_1 = 1, n_1 \\ \ldots\ldots \\ j_S = 1, n_S \end{matrix} \quad (13)$$

This approximation significantly reduces the complexity of the problem, requiring the knowledge of the residuals in Equation (5) only at $(n_1 \times n_2 \ldots\ldots \times n_S)$ quadrature nodes. Approximate expressions for these residuals as explicit functions of all $\mathbf{x}(t_{1,j_1} \ldots\ldots t_{S,j_S})$ are obtained by means of the collocation technique.

Collocation Technique

The collocation technique mainly consists in replacing all derivatives occurring in a given equation by approximate expressions at a series of collocation points, consisting of linear combinations of the values of the dependent variable v at the same points:

$$\left.\frac{dv}{dt_s}\right|_{t_S = t_{S,i}} = \sum_{j_s=1}^{n_s} A^{t_s}_{i,j_s}\, v_{j_s}$$

$$\left.\frac{d^2v}{dt_s^2}\right|_{t_S = t_{S,i}} = \sum_{j_s=1}^{n_s} B^{t_s}_{i,j_s}\, v_{j_s} \quad (15)$$

The matrices $\mathbf{A}^{t_s}$ and $\mathbf{B}^{t_s}$ can be calculated by very straight-forward procedures (Villadsen, 1972).

By the above technique, differential equations are replaced by a series of algebraic equations containing the unknown values of the variables at the collocation points. It has been shown by a series of applications in the chemical engineering field that the method is very accurate when taking the zeros of orthogonal polynomials as collocation points (Villadsen, 1972).

Since in the above quadrature formulas zeros of orthogonal polynomials were preselected as nodes, expressions for the residuals of the differential equations at these points obtained through collocation will be very accurate, resulting in an accurate approximation for the objective function S':

$$S' \doteq S''[\mathbf{x}(t_{1,j_1} \ldots\ldots t_{S,j_S}), \mathbf{k}] \quad (16)$$

Thus whereas the first approximation (13) defines an objective criterion which is a function of the parameters $\mathbf{k}$ and of the residuals $\mathbf{e}$ at the nodes, the second approximation (16) transforms the criterion into a function of $\mathbf{k}$ and of the state variables $\mathbf{x}$ at the nodes. This leads to an objective function which is a simple algebraic expression with a total number of N unknowns, where N is defined by

$$N = K + (n_1 \times n_2 \times \ldots\ldots \times n_s \ldots\ldots \times n_S) \times m \quad (17)$$

Although for a given model the only real unknowns are the parameters, since the state variables can be calculated as soon as the parameters are found, both parameters and state variables are treated equivalently within the presented method and by minimization of the objective function S'' both classes of unknowns are determined simultaneously.

However, nothing has been said until now about the boundary conditions nor about the observation equations. Using the collocation technique the former equations can be reduced to algebraic equations containing the unknowns. By considering the observations only at the quadrature nodes, a similar remark holds for the second group of equations. This means that a set of algebraic equations is obtained, entering into the minimization problem as constraints to the unknowns. At least K of these constraints are required in order to have a unique solution to the minimization problem since the number of unknowns N exceeds the number of squares of the objective function by the value K. For many practical situations all these constraints are linear with respect to the unknowns, which makes the presented estimation method particularly useful since part of the unknowns can be eliminated before minimizing. A very common situation is when all state variables are measured at all nodes, reducing the problem to the minimization of the objective function with respect to the K unknown parameters $\mathbf{k}$. If these parameters occur linearly in the system equations, their calculation becomes extremely straightforward. In cases where the collocation equations are nonlinear with respect to the unknowns, there still exists a convergence problem, and the possibility of saving computation time depends upon the number of the unknowns and upon the form of the equations.

EXAMPLES

Three examples of different complexity will be studied. The first two examples intend to compare the ability of predicting accurate estimates for different weighting functions in the case of an initial value problem and of a two-point boundary value problem. The exponents of these

functions are given in Table 1. In the last example, described by a partial differential equation, both aspects are combined, and attention is given to the accuracy and the statistical properties of the method.

Example 1. Competitive Consecutive Reaction*

The reaction scheme

$$A + B \xrightarrow{k_1} C + E \tag{18}$$

$$A + C \xrightarrow{k_2} D + E \tag{19}$$

is governed by the following equations, when the initial concentrations of all components except A and B are zero:

$$\frac{dx_1}{dt} = (-k_1 + 2k_2)\, x_1 x_2 - k_2\, x_1^2 \tag{20}$$

$$\frac{dx_2}{dt} = -k_1\, x_1 x_2 \tag{21}$$

where x_1 and x_2 represent the concentration of A and B. The initial conditions are

$$x_1(0) = 1. \qquad x_2(0) = 1./2. \tag{22}$$

A time variation between zero and four is assumed. A new independent variable equal to $t/4$ is defined in order to reduce the interval to [0, 1].

Table 1. Exponents of the Weighting Functions

w	α	β
w_1	0	0
w_2	1	1
w_3	0	2
w_4	2	0

Table 2. Results of Estimation for System of Example 1. Accurate Data

w	n	k_1	k_2
w_1	5	0.974	1.027
	6	0.940	1.057
	7	0.953	1.057
	8	0.956	1.050
w_2	5	1.001	0.994
	6	0.988	0.993
	7	0.965	1.042
	8	0.959	1.023
w_3	5	0.992	1.022
	6	0.999	1.013
	7	0.991	1.008
	8	0.992	1.019
w_4	5	0.949	1.047
	6	0.903	1.125
	7	0.928	1.155
	8	0.966	1.003

Table 3. Results of Estimation of Parameters and States for System of Example 1. Weighting Function w_3

	n	k_1	k_2	$x_{2,1}$	$x_{2,2}$	$x_{2,3}$	$x_{2,4}$	$x_{2,5}$	$x_{2,6}$	$x_{2,7}$
Estimated	5	0.868	1.434	0.500	0.228	0.138	0.102	0.090		
Accurate		1.000	1.000	0.500	0.196	0.110	0.077	0.067		
Estimated	6	0.938	1.150	0.500	0.254	0.152	0.105	0.084	0.077	
Accurate		1.000	1.000	0.500	0.240	0.139	0.094	0.073	0.067	
Estimated	7	0.956	1.085	0.500	0.286	0.180	0.123	0.093	0.078	0.073
Accurate		1.000	1.000	0.500	0.278	0.170	0.115	0.086	0.072	0.067

Three estimation problems concerning the above model have been solved using the classical method (Berger, 1973). Two of these problems will be considered here, using the objective criterion:

$$S'' = \sum_{i=1}^{n} H_i \left\{ \left[\sum_{j=1}^{n} \frac{A^t_{i,j}}{4} x_{1,j} + (k_1 - 2k_2)\, x_{1,i} x_{2,i} + k_2\, x^2_{1,i} \right]^2 + \left[\sum_{j=1}^{n} \frac{A^t_{i,j}}{4} x_{2,j} + k_1\, x_{1,i}\, x_{2,i} \right]^2 \right\} \tag{23}$$

The index i refers to the nodes, whereas j is a summation index of the linear expressions obtained by collocating.

When experimental data on both x_1 and x_2 are available, a simple linear least squares problem with respect to k_1 and k_2 arises. Data were generated by integration of the Equations (20) and (21) using the Runge-Kutta-Gill algorithm for $k_1 = k_2 = 1$ and with the step length equal to 0.01. Values at the collocation points are obtained through linear interpolation of these results and are thus subject to small errors. The estimates obtained with different weighting functions and for variable n are given in Table 2. The best results are obtained with w_3 the value of which increases quadratically between zero and one when moving from left to right, putting more weight on that part of the interval where no information from boundary conditions is used. The erratic behavior with respect to n is caused by the errors in the data. By performing calculations for examples having analytical solutions, allowing for the evaluation of exact data, it was found that the accuracy of the estimates increases with increasing value of n, with the machine accuracy as the only limitation. Slight errors, however, suffice to produce the erratic behavior with respect to n, and an increase above the value 6 does not improve the results.

If only x_1 can be measured, all values $x_{2,i}$ $(i = 1, n)$ are additional unknowns except for the initial value. The unknowns can be found by any iterative procedure based upon the general gradient methods (Bard, 1970), and a problem of convergence arises. In Table 3 results are shown obtained by the Newton-Raphson method and with data containing small interpolation errors.

It is interesting to compare the number of operations involved at each step of the minimization of the objective function. In the conventional approach two state equations and four sensitivity equations have to be integrated. This

* A detailed description of the application of the method for parameter estimation for Example 1 has been deposited as Document No. 02321 with the National Auxiliary Publications Service (NAPS), c/o Microfiche publications, 305 E. 46 St., N. Y., N. Y. 10017 and may be obtained for $1.50 for microfiche or $13.50 for photocopies.

Table 4. Results of Estimation of State Variables for System of Example 2. Weighting Function w_2 and $n = 8$

i		1	2	3	4	5	6	7	8
x_{2i}	estimated	0.906	0.891	0.867	0.838	0.811	0.792	0.784	0.783
	accurate	0.912	0.896	0.872	0.843	0.815	0.795	0.786	0.784

could be done using the collocation technique. With seven collocation points a total number of 36 nonlinear collocation equations would have to be solved. When using the Newton-Raphson method this requires solving about 20 to 30 times a set of 36 linear equations in order to find the solution to the differential equations, which has to be done at each iteration. The method presented in this paper requires only a single solution of two linear equations for the fully observed system, and the repetitive solution of eight linear equations at each iteration for the partially observed system. In the latter example accuracy of the estimates depends upon the algorithm used to solve the nonlinear equations, more specifically upon its convergence and upon the criterion to stop the iterative procedure.

Example 2. Nonisothermal-Nonadiabatic Tubular Reactor

A nonisothermal-nonadiabatic plug-flow tubular reactor in which an exothermic first-order reaction is going on is governed by the following dimensionless steady state equations for the temperature and reactant concentration (Hlavácek et al., 1971):

$$\frac{1}{Pe}\frac{d^2x_1}{dt^2} - \frac{dx_1}{dt} - \beta x_1 + B\,Da\,x_2 \exp\left(\frac{x_1}{1+\epsilon x_1}\right) = 0 \tag{24}$$

$$\frac{1}{Pe}\frac{d^2x_2}{dt^2} - \frac{dx_2}{dt} - Da\,x_2 \exp\left(\frac{x_1}{1+\epsilon x_1}\right) = 0 \tag{25}$$

with the boundary conditions

$$\text{at}\quad t=0\quad Pe\,x_1 = \frac{dx_1}{dt}\quad\text{and}\quad -Pe\,(1-x_2) = \frac{dx_2}{dt} \tag{26}$$

$$\text{at}\quad t=1\quad \frac{dx_1}{dt} = \frac{dx_2}{dt} = 0 \tag{27}$$

The kinetic and the transport parameters are normally unknown, giving rise to four unknown dimensionless parameters Da, ϵ, Pe, and β. The equations are nonlinear with respect to these unknowns.

Accurate data on x_1 and x_2 were generated by means of a shooting technique using the Runge-Kutta-Gill algorithm with the following values of the parameters: $k_1 = \epsilon = 0.050$, $k_2 = Da = 0.12$, $k_3 = 1/Pe = 1/2.0 = 0.50$, $k_4 = \beta = 2.0$, and $\mathbf{B} = 12.0$.

First it was assumed that data on both state variables were available. Neglecting the boundary conditions results were obtained by varying ϵ and calculating the remaining parameters as solutions of a linear least squares problem arising when ϵ is given. The objective criterion now is minimized by a one-dimensional search on the parameter ϵ. It was found that the weighting function w_2 gives most accurate results, putting maximum weight on the middle of the interval and zero weight on the boundary points. For $n = 8$ four significant figures of the estimates are exact.

In most real situations only the temperature is measured, and the values of all $x_{2,i}$ are additional unknowns. Neglecting the boundary conditions for x_2 the estimation procedure leads to the profile given in Table 4 when using w_2 and with $n = 8$. The results are remarkably good. The following estimates for the parameters were obtained: $\epsilon = 0.0505$, $Da = 0.1212$, $Pe = 1.961$, $\beta = 2.004$.

Example 3. Laminar-Flow Tubular Reactor

An isothermal laminar-flow tubular reactor is modeled by the following dimensionless equation for the concentration

$$-(1-t_2^2)\,t_2\frac{dx}{dt_1} + \beta\left(t_2\frac{d^2x}{dt_2^2} + \frac{dx}{dt_2}\right) - k\,t_2\,x = 0 \tag{28}$$

with the initial condition

$$x(0, t_2) = 1 \tag{29}$$

and the boundary conditions

$$\frac{dx}{dt_2}(t_1, 0) = \frac{dx}{dt_2}(t_1, 1) = 0 \tag{30}$$

Both independent variables t_1 and t_2 vary between zero and one.

The estimation of the kinetic parameter k from measurements on the state variable x is a time consuming task when using the classical methods involving solutions of the differential equations (Seinfeld, 1969). The estimation of k becomes extremely straight-forward when using the quadrature and collocation technique as will be explained below.

Accurate data on the profile obtained for $\beta = 0.10$ and $k = 1.0$ (Lapidus, 1962) are used. The values in the nodes are calculated through linear interpolation, and consequently are subject to errors.

Five nodes are taken for the t_1-interval based upon the weighting function w_3 which is optimal for initial-value problems. For the t_2-interval six nodes are considered corresponding to the function w_2 which is optimal for two-point boundary value problems. The objective function becomes

$$S'' = \sum_{i=1}^{6}\sum_{l=1}^{5} H_i^{t_2} H_l^{t_1} \Bigg\{ -(1-t_{2,i}^2)\, t_{2,i} \sum_{k=1}^{5} A_{1,k}^{t_1} x_{i,k} + \beta \Bigg[t_{2,i} \sum_{j=1}^{6} B_{i,j}^{t_2} x_{j,l} + \sum_{j=1}^{6} A_{i,j}^{t_2} x_{j,l} \Bigg] - k\,t_{2,i}\,x_{i,l} \Bigg\}^2 \tag{31}$$

Assuming that x can be observed at all nodes, the value of k follows from a single linear algebraic equation. An excellent estimate $k = 1.018$ was found. When the data are disturbed by Gaussian white noise with mean value zero and percent standard deviation of 10% produced numerically by a random number generator, an average value 0.953 with a percent standard deviation of 19% was found out of 16 runs.

If only the wall concentration is measured, there are twelve additional unknowns, namely, the values of x at the nodes for $i = 2$, 4 and $l = 2$, 5. Values at the other nodes are either directly given through the wall observations and through the initial conditions, or obtained as linear combinations of the unknown ordinates through the

Table 5. Results of Estimation of States for System of Example 3

Data obtained through interpolation

l \ i	1	2	3	4	5
1	1.000	0.725	0.488	0.335	0.260
2	1.000	0.717	0.477	0.329	0.251
3	1.000	0.677	0.418	0.278	0.210
4	1.000	0.597	0.313	0.202	0.148
5	1.000	0.502	0.231	0.147	0.106
6	1.000	0.456	0.210	0.134	0.096

Estimated values

l \ i	1	2	3	4	5
1	1.000	0.697	0.476	0.334	0.278
2	1.000	0.695	0.468	0.323	0.266
3	1.000	0.670	0.418	0.274	0.223
4	1.000	0.588	0.317	0.199	0.160
5	1.000	0.490	0.233	0.145	0.110
6	1.000	0.456	0.210	0.134	0.096

collocation equations replacing the boundary conditions (30). When varying k the other unknowns are found as the solution to a linear least squares problem. In this way the estimation is performed by a one-dimensional search on k for minimizing the objective function. A value 0.969 was found with the corresponding values of x given in Table 5, in comparison with the values obtained by linear interpolation of the accurate data. These estimates are very good. When the data at the wall are disturbed by noise with a standard deviation of 10%, an average value $k = 0.956$ was found with a percent standard deviation of 3.5% for a total number of 20 trials.

From the results it is clear that the presented method leads to a fast estimation of unknown parameters, although the speed of the procedure sacrifices some accuracy for data subject to errors. Slight errors indeed may cause rather large deviations for the estimates as compared to results obtained by the least squares method, which normally makes use of a larger number of data.

It is interesting to compare the number of operations involved in the presented method and in the standard technique. The superiority of the above procedure if data are available at all nodes is obvious. If only data at the wall are given both methods require a one-dimensional search for the parameter k. This can be done by the steepest descent method (Seinfeld, 1969), but usually a priori information on the parameter is available calling for the golden section technique for reduction of the original region of uncertainty. In the latter case both methods differ only by the number of operations performed for each new value of k. For the above described method this consists in the solution of twelve linear equations. When using the standard technique a linear partial differential equation has to be solved. With the finite difference method reported in the literature (Seinfeld, 1969) a large set of linear equations with tridiagonal matrix has to be solved repetitively. By using the collocation method for solving the differential equation a significant gain in computing time is possible since a set of 16 linear collocation equations results when considering the same nodes as before. In the latter case the above presented method is only slightly superior to the standard technique.

NOTATION

$\mathbf{A}$ = collocation matrix
$\mathbf{B}$ = collocation matrix
$\mathbf{e}$ = vector of deviations
$\mathbf{f}$ = vector of output functions
$\mathbf{F}$ = vector of observation equations
H = weights of quadrature formulas
i = index of quadrature node
j = summation index for quadrature
$\mathbf{k}$ = vector of parameters
K = dimension of $\mathbf{k}$
$\mathbf{L}$ = vector of operators
m = dimension of $\mathbf{x}$
$\mathbf{M}$ = moment matrix
n = number of quadrature nodes
N = number of unknowns
$\mathbf{Q}$ = positive semidefinite weighting matrix
r = index of observation
R = number of observations
s = index of components of $\mathbf{t}$
S = dimension of $\mathbf{t}$
$S(k)$ = objective function
S', S'' = approximations of the objective function
$\mathbf{t}$ = vector of independent variables
Tr = trace of a matrix
v = arbitrary dependent variable
w = weighting function
w^+ = weighting function determining the nodes
$\mathbf{x}$ = vector of state variables
$\mathbf{y}$ = vector of outputs

Greek Letters

α, β = exponents defining the weighting functions
$\delta_{i,j}$ = Kronecker delta
Ψ = criterion defining the objective function
σ = standard deviation
T = as superscript indicates matrix transpose

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