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Explicit Method for Parameter Identification

M. Tadi*
University of Illinois at Chicago, Chicago, Illinois 60607
and
Herschel Rabitz†
Princeton University, Princeton, New Jersey 08544

Parameter identification of dynamical systems through a new method that treats the unknown parameters as time dependent is reported. With appropriate observational data, the unknown system parameters are guided from an arbitrary initial condition to their true value at a final time. An explicit equation describing the time evolution of the parameters is obtained by minimizing the error along the trajectory. The method leads to an iterative algorithm, which is described in detail. Numerical results with the method indicate that accurate estimates of the unknown parameters can be obtained.

I. Introduction

THIS paper presents a new method for parameter identification of dynamical systems. This activity falls in the general domain of inverse problems where the interest is to obtain the unknown system parameters from the given output measurement of the system. In many applications there is a nonlinear relationship between the measured output and the desired system unknowns. The inverse problem is further complicated by the fact that the measured data will contain noise and are often insufficient to uniquely specify a solution. A number of techniques have been developed to treat such problems. A brief summary of results for systems described by ordinary differential equations can be found in, for example, Refs. 1 and 2. These approaches include the method of least squares, stochastic least squares, maximum likelihood, and a number of other variations. These schemes have also been applied to dynamical systems governed by partial differential equations.[3,4] A generalized class of linear inversion methods has been applied to a number of physical systems involving replacement of the nonlinear relationship between the observed data and the unknowns with a linear approximation. A comprehensive review of this approach can be found.[5,6]

Of particular interest are direct inversion schemes for continuous systems that are based on regularization.[7] In this paper, we approach the parameter identification problem for systems governed by ordinary differential equations in a way that permits a similar treatment of the problem. We then use regularization to stabilize the inversion. The method leads to an explicit differential equation for the unknown parameters, which is used in an iterative algorithm. In this paper, we do not address the question of system *identifiability*.[8] We present a method that can be used to estimate the parameters for systems that are identifiable.

The paper is organized as follow. In Sec. II, we present the general algorithm along with a number of numerical examples. Section III considers an extension of the method to a broader class of systems, including further numerical results, and Sec. IV is devoted to conclusions.

II. Identification Equations

Consider a dynamical system given by

$$\dot{x} = f(x, q), \qquad x(0) = x_0 \tag{1}$$

$$y = c^T x \tag{2}$$

where $x \in R^n$, $f \in R^n$, $q \in R^m$, and $y \in R^1$. For simplicity, we assume that the observation y is linear in the state x and one dimensional (i.e., a scalar function of time). The problem posed here consists of estimating the system parameter vector q based on the measured observation $y(t)$. The approach is based on expanding the problem and allowing the parameters in the vector q to be time dependent. The unknown parameters are guided from an arbitrary initial value $q(0) = q_0$ at time $t = 0$ to the final value q at a suitable final time $t = T$. Such a trajectory for the unknown parameters is obtained by minimizing the error difference between the model prediction and observation during the time $t = [0 : T]$. We search for the parameters in the class of admissible functions in $[0 : T]$ so that $q(0)$ is arbitrary and $q(T)$ is q along with $\dot{q}(T) = 0$. This poses an optimal inverse problem, the solution of which is the optimal $q(t)$, $t \in [0 : T]$. The desired trajectory minimizes the error between the actual data and the response obtained from the system given by

$$J = \int_0^T \left[\frac{1}{2}(y - c^T x)^2\right] \mathrm{d}t \tag{3}$$

The direct solution to the above minimization problem is almost always unstable. However, treating the parameters $q(t)$ as time dependent allows us to regularize the inversion. Therefore, we seek to minimize a cost functional given by

$$J = \int_0^T \left[\frac{1}{2}(y - c^T x)^2 + \frac{1}{2}\alpha\dot{q}^T\dot{q}\right] \mathrm{d}t \tag{4}$$

where we are also minimizing the time derivative of q. The latter stabilizing term also directly introduces time dependency into the parameters. The cost functional is minimized subject to the equation of motion, Eq. (1). Using Lagrange multipliers, we can form an unconstrained minimization problem. The modified objective functional is given by

$$J = \int_0^T \left[\frac{1}{2}(y - c^T x)^2 + \frac{1}{2}\alpha\dot{q}^T\dot{q} + \lambda^T(\dot{x} - f)\right] \mathrm{d}t \tag{5}$$

where $\lambda \in R^n$ is the vector of Lagrange multipliers. Necessary minimization conditions are obtained by setting the first variation of J equal to zero. It follows that

$$\delta J = \int_0^T [-(y - c^T x)c^T\delta x + \alpha\dot{q}^T\delta\dot{q} + \delta\lambda^T(\dot{x} - f) + \lambda^T(\delta\dot{x} - \delta f)]\,\mathrm{d}t = 0 \tag{6}$$

The variation in f is given by

$$\delta f = \frac{\partial f}{\partial x}\delta x + \frac{\partial f}{\partial q}\delta q \tag{7}$$

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*Visiting Assistant Professor, Department of Mathematics and Statistics.

†Professor of Chemistry, Frick Laboratory.

Furthermore, the terms $\dot{q}^T\delta\dot{q}$ and $\lambda^T\delta\dot{x}$ can be integrated by parts. Thus, the first variation of the cost functional is given by

$$\delta J = \int_0^T \left[-(y - c^T x)c^T \delta x - \alpha \ddot{q}^T \delta q + \delta\lambda^T(\dot{x} - f) - \dot{\lambda}^T \delta x - \lambda^T \left(\frac{\partial f}{\partial x}\delta x + \frac{\partial f}{\partial q}\delta q \right) \right] \mathrm{d}t + \delta\lambda^T \delta x|_0^T + \dot{q}\,\delta q|_0^T = 0 \tag{8}$$

The initial conditions x_0 and q_0 are specified implying that $\delta x|_0 = \delta q|_0 = 0$. It is also assumed that $\dot{q}(T) = 0$. After grouping the terms in the preceding integral, the first variation of J is given by

$$\delta J = \int_0^T \left\{ \left[-(y - c^T x)c^T - \dot{\lambda}^T - \lambda^T \frac{\partial f}{\partial x} \right] \delta x - \left[\alpha \ddot{q}^T + \lambda^T \frac{\partial f}{\partial q} \right] \delta q + \delta\lambda^T [\dot{x} - f] \right\} \mathrm{d}t = 0 \tag{9}$$

The variations δx, $\delta\lambda$, and δq are arbitrary; therefore, the first-order necessary conditions for mininization are given by

$$c(y - c^T x) + \dot{\lambda} + \frac{\partial f^T}{\partial x}\lambda = 0 \tag{10}$$

$$\alpha \ddot{q} + \frac{\partial f^T}{\partial q}\lambda = 0 \tag{11}$$

$$\dot{x} = f(x, q) \tag{12}$$

where the appropriate boundary conditions are given by

$$x(0) = x_0, \qquad \lambda(T) = 0, \qquad q(0) = q_0, \qquad \dot{q}(T) = 0 \tag{13}$$

These equations pose a two-point boundary value problem. Consider the special case in which the rank of the matrix $\partial f/\partial q$ is equal to m and the matrix $(\partial f/\partial q)(\partial f^T/\partial q)$ can be inverted. Section III will relax this condition. Then we can eliminate λ from the preceding system of equations and obtain an explicit relation for the parameters q. Premultiply Eq. (11) first by $\partial f/\partial q$ and then by Q^{-1}, where $Q = (\partial f/\partial q)(\partial f^T/\partial q)$ is a full rank matrix. Then Eq. (11) can be solved for λ:

$$\lambda = -Q^{-1}\frac{\partial f}{\partial q}\frac{\mathrm{d}^2 q}{\mathrm{d}t^2}\alpha \tag{14}$$

Using Eq. (10) we can obtain a relation for $\dot{\lambda}$:

$$\dot{\lambda} = -c(y - c^T x) + \frac{\partial f^T}{\partial x}Q^{-1}\frac{\partial f}{\partial q}\frac{\mathrm{d}^2 q}{\mathrm{d}t^2}\alpha \tag{15}$$

We next differentiate Eq. (11) with respect to time:

$$\alpha\frac{\mathrm{d}^3 q}{\mathrm{d}t^3} + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial f}{\partial q}\right)^T \lambda + \frac{\partial f^T}{\partial q}\dot{\lambda} = 0 \tag{16}$$

We can now substitute for λ and $\dot{\lambda}$ from Eqs. (14) and (15) and obtain an equation for the unknown parameters q given by

$$\frac{\mathrm{d}^3 q}{\mathrm{d}t^3} + \left[\frac{\partial f^T}{\partial q}\frac{\partial f^T}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial f}{\partial q}\right)^T \right] Q^{-1}\frac{\partial f}{\partial q}\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} - \frac{1}{\alpha}\frac{\partial f^T}{\partial q}c(y - c^T x) = 0 \tag{17}$$

As it stands now, the boundary conditions on Eq. (17) are $q(0) = q_0$ and $\dot{q}(T) = 0$ from Eq. (13) along with $\ddot{q}(T) = 0$ from Eqs. (13) and (14). However, the special nature of the ultimate solution $q(t) \equiv q$ being a constant suggests that we have the freedom to convert Eq. (17) into an initial value problem. Thus, the inversion is started with $q(0) = q_0$, $\dot{q}(0) = 0$, and $\ddot{q}(0) = 0$. Upon successful solution of Eq. (17), the original two-point boundary conditions will be satisfied. It is noted that by setting $\alpha = 0$, one eliminates the term that was added to the cost functional in Eq. (4) to regularize the inversion. In that case, the preceding equation simplifies to only the last term on the left-hand side, which in general cannot be stably used to solve for the unknown parameters q. Introducing regularization results in an explicit relation for the unknown parameter q. This equation should be solved simultaneously with the equation of motion, Eq. (1). At every iteration, Eq. (17) brings the assumed values for the parameters $q(0)$ closer to their true value. The procedure is then as follows.

Algorithm

1) Choose a time T, a positive constant α, and a set of arbitrary initial values for the parameters q_0. The derivatives $\dot{q}(0)$, $\ddot{q}(0)$ at the initial time can be chosen to be zero.

2) Use the initial conditions and integrate Eq. (17) simultaneously with the equation of motion (1) forward until time T.

3) Use the current value of $q(T)$ as the initial condition for q together with the zero initial conditions on the derivatives $\dot{q}(0)$, $\ddot{q}(0)$ and integrate the system of equation from $t = 0$ forward until $t = T$ and, thereby, obtain new estimates for the parameters $q(T)$.

4) Repeat processes 2 and 3 until the error [i.e., the first term in the cost functional in Eq. (4)] is arbitrarily small and convergence is obtained.

The procedure is iterative and the only restriction so far is that the matrix Q can be inverted. We next use a number of simple numerical examples to demonstrate the method.

Example 1

Consider a simple first-order one-dimensional system given by

$$\dot{x} = -0.2x + q, \qquad y = x, \qquad q = 0.2 \tag{18}$$

The problem is to estimate the system parameter q based on the measurement y. This problem is simple enough that a mere substitution of x for y in Eq. (18) would immediately give q; nevertheless, it still serves as a good illustration of the algorithm. For this system, Eq. (17) simplifies to

$$\frac{\mathrm{d}^3 q}{\mathrm{d}t^3} - 0.2\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} - \frac{1}{\alpha}(y - x) = 0 \tag{19}$$

We set $\alpha = 10$ and choose the final time to be $T = 10$. Figure 1 shows the convergence of the unknown parameter q as a function of the number of iterations. Results are given for three different initial conditions. The method is quite robust to the choice of the initial condition. The actual trajectories for $q(t)$ in all the examples in the paper are monotonic at every level of iteration. This simple behavior is connected with the fact that the convergent solution is a constant, $q(t) = q$.

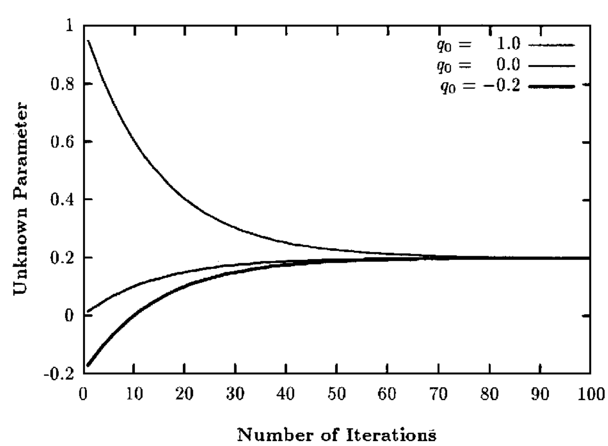

Fig. 1 Unknown parameter as a function of the number of iterations. The unknown parameter is $q = 0.2$. Convergence is shown for three different initial conditions.

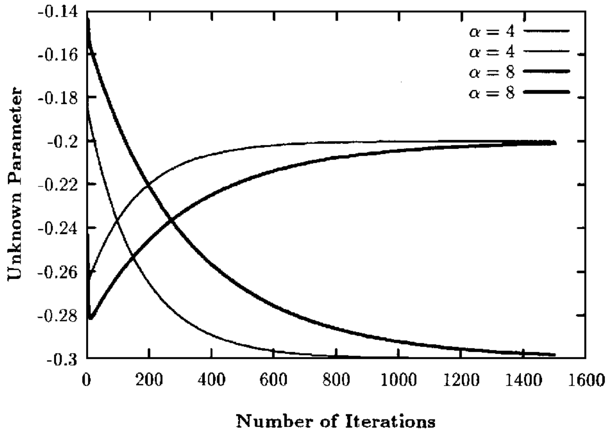

Fig. 2 Unknown parameters as a function of the number of iterations. The unknown parameters are $q_1 = -0.3, q_2 = -0.2$. Convergence is shown for two different values of α.

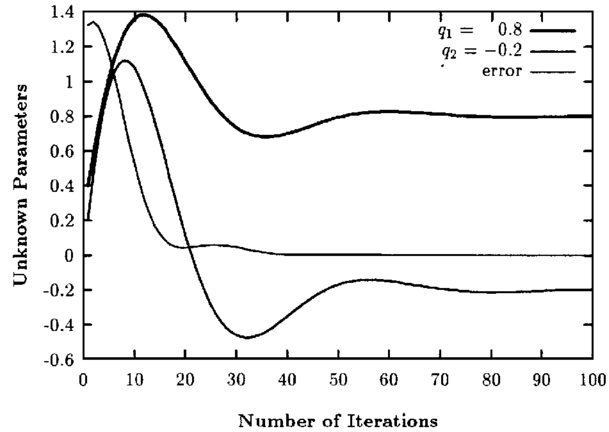

Fig. 3 Unknown parameters as a function of the number of iterations. The error at each iteration is also shown as a function of the number of iterations.

Example 2

We next consider a one-dimensional system given by

$$\dot{x} = q_1 x + q_2, \qquad y = x, \qquad q_1 = -0.3, \qquad q_2 = -0.2 \tag{20}$$

For this case there are two unknown parameters to be identified. The matrix $(\partial f / \partial q) = [x \quad 1]$ is rank deficient, but the matrix $Q = (x^2 + 1)$ can be inverted. The components λ, $\dot{\lambda}$, which are scalars, are obtained from Eqs. (11) and (12), and we can obtain explicit relations for the unknown parameters given by

$$\frac{d^3 q_1}{dt^3} - (x^2+1)^{-1}\left(x\frac{d^2 q_2}{dt^2} + \frac{d^2 q_2}{dt^2}\right) q_2 - \frac{1}{\alpha} x(y - x) = 0 \tag{21}$$

$$\frac{d^3 q_2}{dt^3} + (x^2+1)^{-1}\left(x\frac{d^2 q_1}{dt^2} + \frac{d^2 q_2}{dt^2}\right) q_1 - \frac{1}{\alpha}(y - x) = 0 \tag{22}$$

We choose $T = 7$. Figure 2 shows the convergence of the parameters for two different values of α. The convergence is faster for the case $\alpha = 4$ in comparison to the case $\alpha = 8$. Increasing the parameter α in the cost functional Eq. (4) limits the value of the time derivative of q_i along the trajectory from $t = 0 \to T$. For these cases $q_i(T)$ changes slightly from $q_i(0)$ and as a result the convergence is slower.

Example 3

We next consider a two-dimensional system given by

$$\dot{x}_1 = -x_2 + q_1 \tag{23}$$

$$\dot{x}_2 = x_1 - x_2 + q_2 \tag{24}$$

$$y = x_1, \qquad q_1 = 0.8, \qquad q_2 = -0.2 \tag{25}$$

Equation (17) simplifies to

$$\frac{d^3 q_1}{dt^3} + \frac{d^2 q_2}{dt^2} - \frac{1}{\alpha}(y - x_1) = 0 \tag{26}$$

$$\frac{d^3 q_2}{dt^3} - \frac{d^2 q_1}{dt^2} - \frac{d^2 q_2}{dt^2} = 0 \tag{27}$$

Figure 3 shows the convergence of the parameters as a function of the number of iterations. It also shows the error that is included in the cost functional in Eq. (4), which is to be minimized. At every iteration the error is given by

$$e = \int_0^T [y(t) - c^T x(t)]^2 dt \tag{28}$$

where $x(t)$ depends on the system's parameters that are computed along the trajectory by the algorithm. It is evident that the final convergence of q to its true value is governed by the remaining small error e at later iterations. This behavior suggests that the final values for the parameters obtained by the algorithm may be corrupted by the presence of the noise in the laboratory data. Filtering techniques need to be introduced for such cases, and this is a matter for further development.

For all of these cases, it was possible to invert the matrix Q. We next consider the situation in which the matrix Q cannot be inverted.

III. Extension to the Case When Q Is Singular

In this section, we consider the situation in which the matrix Q cannot be inverted. We consider the case when the rank k of the matrix $\partial f / \partial q$ is less than m. We can rearrange the matrix $\partial f / \partial q$ into two parts so that the upper portion is a matrix of rank k with the dimension $k \times m$, $(\hat{\partial} f / \partial q)$, and a lower portion that is a matrix of dimension $(n - k) \times m$. Accordingly, we split the vector of Lagrange multipliers into two parts. As a result, Eqs. (10) and (11) can be written as

$$\begin{bmatrix} \hat{c} \\ c \end{bmatrix} (y - c^T x) + \begin{bmatrix} \dot{\hat{\lambda}} \\ \dot{\lambda} \end{bmatrix} + \begin{bmatrix} \dfrac{\hat{\partial} f}{\partial x} \\ \dfrac{\partial f}{\partial x} \end{bmatrix}^T \begin{bmatrix} \hat{\lambda} \\ \lambda \end{bmatrix} = 0 \tag{29}$$

$$\alpha \ddot{q} + \begin{bmatrix} \dfrac{\hat{\partial} f}{\partial q} \\ \dfrac{\partial f}{\partial q} \end{bmatrix}^T \begin{bmatrix} \hat{\lambda} \\ \lambda \end{bmatrix} = 0 \tag{30}$$

We next set the Lagrange multipliers that correspond to the bottom portion of the matrix $\partial f / \partial q$ in Eq. (30) equal to zero. This operation permits obtaining an explicit relation for the Lagrange multipliers that are kept. This corresponds to including only k number of equations of motion as constraints in the modified objective functional in Eq. (5). We can then proceed as in the preceding section and obtain an explicit relation for the unknown parameter $q(t)$. At each iteration, the equation for $q(t)$ should be solved simultaneously with all of the equations of motion, and as a result the whole dynamics of the system is included in the process. It follows that the preceding equations simplify to

$$\hat{c}(y - c^T x) + \frac{\hat{\partial} f^T}{\partial x} \hat{\lambda} = 0 \tag{31}$$

$$\alpha \ddot{q} + \frac{\hat{\partial} f^T}{\partial q} \hat{\lambda} = 0 \tag{32}$$

The matrix $\hat{Q} \in R^{k \times k}$ is now given by

$$\hat{Q} = \frac{\hat{\partial} f}{\partial q} \frac{\hat{\partial} f^T}{\partial q} \tag{33}$$

In general, the rank of the matrix Q in the preceding section can at most be equal to the number of unknown parameters m. For singular cases for which the rank of the matrix $(\partial f/\partial q)(\partial f^T/\partial q)$ is equal to k, where $k < m$, we essentially keep the portion of the matrix $\hat{Q}$, which has a full rank of k and can be inverted. Following the steps in the preceding section, we can obtain an explicit relation for the unknown parameters q given by

$$\frac{\mathrm{d}^3 q}{\mathrm{d}t^3} + \left[\frac{\hat{\partial} f^T}{\partial q}\frac{\hat{\partial} f^T}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\hat{\partial} f}{\partial q}\right)^T\right]\hat{Q}^{-1}\frac{\hat{\partial} f}{\partial q}\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} - \frac{1}{\alpha}\frac{\hat{\partial} f^T}{\partial q}\hat{c}(y - c^T x) = 0 \tag{34}$$

An analogous procedure has recently been introduced to control a subspace of a full dynamical system.[9] We next consider a number of examples in which such an approach can be used to obtain an explicit relation for the parameters.

Example 4

Consider the two-dimensional Duffing equation

$$\dot{x}_1 = x_2 \tag{35}$$

$$\dot{x}_2 = -x_1 + q x_1^3 \tag{36}$$

$$y = x_1 + x_2, \qquad q_1 = 0.2 \tag{37}$$

with $n = 2$ and $m = 1$. For this case, the matrix $\hat{Q} = (x_1^3)(x_1^3)$ and Eq. (34) simplifies to

$$\frac{\mathrm{d}^3 q}{\mathrm{d}t^3} - 3\frac{x_2}{x_1}\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} - \frac{1}{\alpha}x_1^3(y - x_1 - x_2) = 0 \tag{38}$$

This equation corresponds to setting $\lambda_1 = 0$ in the objective functional and thus $k = 1$. This equation is solved simultaneously with the equations of motion, and as a result the whole dynamics is taken into account. Figure 4 shows the convergence of the unknown parameter for an arbitrary initial condition. The parameter α is chosen as 10 and $T = 6$.

We next consider the case in which the rank of the matrix $\partial f/\partial q$ is less than the number of unknown parameters. In the following example, only one Lagrange multiplier is used to obtain iterative equations for two unknown parameters.

Example 5

Consider a three-dimensional system given by

$$\dot{x}_1 = x_2 \tag{39}$$

$$\dot{x}_2 = x_3 \tag{40}$$

$$\dot{x}_3 = -q_1 \sin x_1 - q_2 x_1 \tag{41}$$

$$y = x_3, \qquad q_1 = -0.1, \qquad q_2 = 0.2 \tag{42}$$

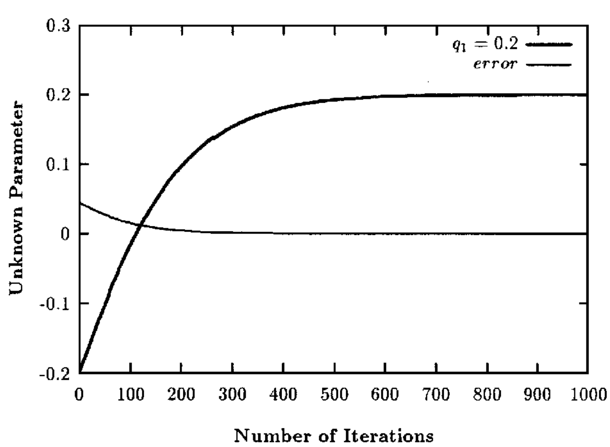

Fig. 4 Unknown parameter as a function of the number of iterations. The error at each iteration is also shown as a function of the number of iterations.

For this case, Eqs. (10) and (11) simplify to

$$\begin{bmatrix}\ddot{q}_1\\ \ddot{q}_2\end{bmatrix} + \frac{1}{\alpha}\begin{bmatrix}0 & 0 & -\sin x_1\\ 0 & 0 & -x_1\end{bmatrix}\begin{bmatrix}\lambda_1\\ \lambda_2\\ \lambda_3\end{bmatrix} = 0 \tag{43}$$

$$\begin{bmatrix}0\\0\\1\end{bmatrix}(y - x_3) + \begin{bmatrix}\dot{\lambda}_1\\ \dot{\lambda}_2\\ \dot{\lambda}_3\end{bmatrix} + \begin{bmatrix}0 & 0 & -q_1\cos x_1 - q_2\\ 1 & 0 & 0\\ 0 & 1 & 0\end{bmatrix}\begin{bmatrix}\lambda_1\\ \lambda_2\\ \lambda_3\end{bmatrix} = 0 \tag{44}$$

We next proceed as before and premultiply Eq. (43) by $\partial f/\partial q$, which simplifies to

$$\begin{bmatrix}0 & 0\\ 0 & 0\\ -\sin x_1 & -x_1\end{bmatrix}\begin{bmatrix}\ddot{q}_1\\ \ddot{q}_2\end{bmatrix} + \frac{1}{\alpha}\begin{bmatrix}0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & \sin^2 x_1 + x_1^2\end{bmatrix}\begin{bmatrix}\lambda_1\\ \lambda_2\\ \lambda_3\end{bmatrix} = 0 \tag{45}$$

The rank of the matrix $(\partial f/\partial q)(\partial f^T/\partial q)$ is equal to one, and it immediately follows that we need to set $\lambda_1 = \lambda_2 = 0$ and search for a solution for λ_3 that satisfies the preceding system of equations. It follows that

$$\dot{\lambda}_3 = -(y - x_3) \tag{46}$$

$$\alpha\frac{\mathrm{d}^2 q_1}{\mathrm{d}t^2} = \lambda_3 \sin x_1 \tag{47}$$

$$\alpha\frac{\mathrm{d}^2 q_2}{\mathrm{d}t^2} = \lambda_3 x_1 \tag{48}$$

We then proceed to differentiate the equations for the q values with respect to time and substitute for $\dot{\lambda}_3$ and λ_3 to obtain explicit relations for the unknown parameters given by

$$\frac{\mathrm{d}^3 q_1}{\mathrm{d}t^3} = x_2\frac{\cos x_1}{\sin x_1}\frac{\mathrm{d}^2 q_1}{\mathrm{d}t^2} - \sin x_1 (y - x_3) \tag{49}$$

$$\frac{\mathrm{d}^3 q_2}{\mathrm{d}t^3} = \frac{x_2}{x_1}\frac{\mathrm{d}^2 q_2}{\mathrm{d}t^2} - x_1(y - x_3) \tag{50}$$

At every iteration, the equations are solved simultaneously with the equations of motion. Figure 5 shows the convergence of the parameters for two different values of α. For this case, the final time is set at $T = 1$. The method is convergent for arbitrary initial conditions chosen for $q_i(0)$. It requires only that the initial condition on $x_1(0)$ be large. If the system is started from a small initial condition on $x_1(0)$, then $\sin x_1 \simeq x_1$, and the two unknown parameters could be combined into one. In that case, the system is not identifiable and when the algorithm is used the error increases with the number of iterations and the method fails to obtain a solution.

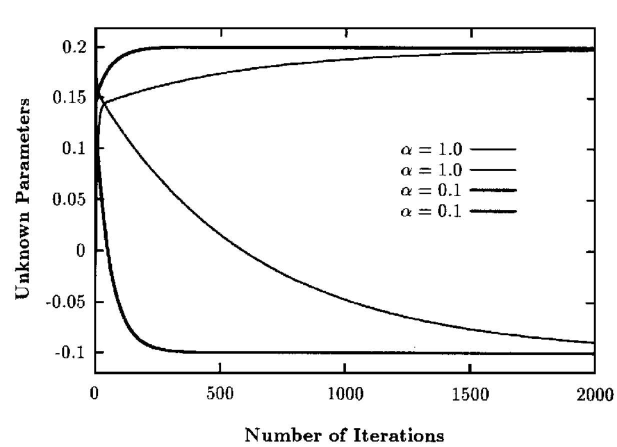

Fig. 5 Unknown parameters as a function of the number of iterations. The unknown parameters are $q_1 = -0.1, q_2 = 0.2$. Convergence is shown for two different values of α.

We next consider an example from reactions in chemical kinetics in which the unknown parameter is recovered from the actual experimental data obtained in the lab. Modeling and analysis of such systems are often encountered in aerospace combustion and propulsion systems.[10,11] For such systems the dynamics is modeled by a system of nonlinear ordinary differential equations that contain constant parameters known as rate constants. The rate constants determine the speed of the relative reactions and accurate knowledge of their value is important in the design and analysis of such systems. Here, we consider only one example to show the applicability of the new method.

Example 6

We consider a nonlinear system of equations given by

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = -r_1x_1x_2 + r_3x_2x_7 - r_6x_1x_9 - r_7x_1x_5 - r_9x_1x_7 - r_{10}x_1 - r_{16}x_1x_{10} + r_{17}x_3x_5$$

$$\frac{\mathrm{d}x_2}{\mathrm{d}t} = -r_1x_1x_2 - r_3x_7x_2 + r_5x_4x_{10}$$

$$\frac{\mathrm{d}x_3}{\mathrm{d}t} = r_1x_1x_2 - qx_3x_5 + r_5x_4x_{10} - r_8x_3x_7 - r_{11}x_3 - 2r_{14}x_3x_3 - r_{15}x_3x_{10} + 2r_{16}x_1x_{10} - r_{17}x_3x_5$$

$$\frac{\mathrm{d}x_4}{\mathrm{d}t} = r_1x_1x_2 + r_3x_2x_7 - r_5x_4x_{10}$$

$$\frac{\mathrm{d}x_5}{\mathrm{d}t} = -qx_3x_5 - r_7x_1x_5 - r_{17}x_3x_5$$

$$\frac{\mathrm{d}x_6}{\mathrm{d}t} = qx_3x_5 + r_8x_3x_7 + r_{14}x_3x_3 + r_{15}x_3x_{10}$$

$$\frac{\mathrm{d}x_7}{\mathrm{d}t} = qx_3x_5 - r_3x_7x_2 - r_4x_7x_9 + r_7x_1x_5 - r_8x_3x_7 - r_9x_1x_7 - r_{12}x_7$$

$$\frac{\mathrm{d}x_8}{\mathrm{d}t} = r_3x_2x_7 \qquad \frac{\mathrm{d}x_9}{\mathrm{d}t} = -r_4x_7x_9 - r_6x_1x_9 + r_{15}x_3x_{10}$$

$$\frac{\mathrm{d}x_{10}}{\mathrm{d}t} = r_4x_7x_9 - r_5x_4x_{10} + r_6x_1x_9 - r_{13}x_{10} - r_{15}x_{10}x_3 - r_{16}x_1x_{10}$$

$$\frac{\mathrm{d}x_{11}}{\mathrm{d}t} = r_4x_7x_9 + r_8x_3x_7 + r_9x_1x_7 \qquad \frac{\mathrm{d}x_{12}}{\mathrm{d}t} = r_7x_1x_5 + r_9x_1x_7$$

$$\frac{\mathrm{d}x_{13}}{\mathrm{d}t} = r_{14}x_3x_3 \qquad \frac{\mathrm{d}x_{14}}{\mathrm{d}t} = r_{17}x_3x_5$$

where the states $x_1, \ldots, x_{14}$ are the concentrations of various species and $r_1, \ldots, r_{17}$ are the rate constants. This example is fully studied in Ref. 12. The rate constant q is the unknown parameter. The rest of the rate constants are given by $r_1 = 1.28E{-}10$, $r_3 = 4.0E{-}11$, $r_4 = 5.5E{-}12$, $r_5 = 8.3E{-}12$, $r_6 = 5.44E{-}15$, $r_7 = 6.69E{-}14$, $r_8 = 5.E{-}11$, $r_9 = 5.E{-}11$, $r_{10} = 10$, $r_{11} = 5$, $r_{12} = 10$, $r_{13} = 10$, $r_{14} = 1.99E{-}12$, $r_{15} = 6.4E{-}11$, $r_{16} = 7.0E{-}11$, and $r_{17} = 0.2E{-}12$. It is possible to measure the state variable x_3 in the lab, which is given in Fig. 6 (from Ref. 13). The parameter identification for this system is then to recover the parameter q based on the given laboratory data $y(t) = x_3(t)$. For this system, the matrix Q has the rank one and $(\partial f/\partial q) = -x_3x_5$. The only nonzero component of the Lagrange multiplier's vector is λ_3, and Eq. (34) simplifies to

$$\frac{\mathrm{d}^3q}{\mathrm{d}t^3} = \left(\frac{\dot{x}_3}{x_3} + \frac{\dot{x}_5}{x_5} - f_{1_{x_3}} - f_{3_{x_3}}\right)\ddot{q} - \frac{1}{\alpha}x_3x_5(y - x_3) \tag{51}$$

The initial conditions are given by $x_2 = 1.95E{+}12$, $x_3 = 2.65E{+}11$, $x_4 = 5.30E{+}11$, and $x_5 = 1.76E{+}13$. The rest of the variables are started from zero. The parameter α is chosen as 1×10^{10}. Figure 7 shows the convergence of the parameter for two different initial conditions. The converged value is in good agreement with the value $q = [(7.75 \pm 1.24) \times 10^{-12}]$ that was obtained in Ref. 13 by the curve-fitting least-squares method along with sensitivity analysis.

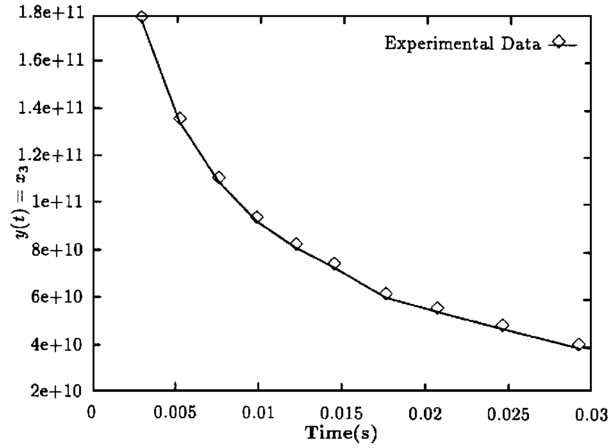

Fig. 6 Experimental measurement $y(t) = x_3(t)$ as a function of time (from Ref. 13).

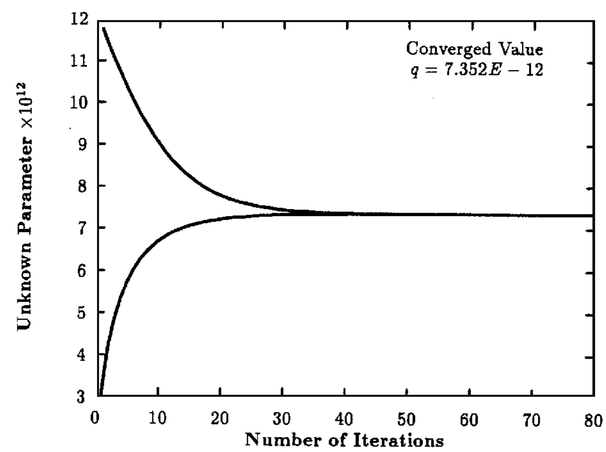

Fig. 7 Unknown parameter as a function of the number of iterations for two different initial conditions.

The method is in one respect similar to the homotopy or the continuation methods (Ref. 14 and references therein) in which a differential equation is obtained for the sought-after unknowns. In the present method, the explicit equation is obtained by introducing a new dynamics into the system and obtaining extremal trajectories along which the error is minimized. As a result, the error explicitly enters into the differential equation and, by choosing the appropriate initial conditions, for vanishing error the convergence is obtained.

IV. Conclusions

In this paper, we presented a new method for parameter identification. The approach is based on allowing the parameters to be time dependent. Regularization is used to stabilize the inversion. A minimization procedure is formulated to obtain the unknown parameters by minimizing the error during a period of time. An algorithm is presented that, at every iteration, integrates the differential equations for the parameters along with the equations of motion. A number of numerical results were presented to demonstrate the applicability of the method.

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