Linearization—an Efficient Alternate for the Estimation of Parameters

E. J. SCHLOSSMACHER

Department of Energy Engineering
University of Illinois at Chicago Circle
Chicago, Illinois 60680

A fundamental problem in the area of mathematical modeling is that of determining the parameters which cause a set of experimental data to fit a proposed differential model in some optimal fashion. When the dimension of a model is small, it is often possible to solve the system of equations explicitly and to use the resulting algebraic system in a linear or nonlinear least squares analysis to directly find the unknown parameters. As the complexity of the system increases, however, it often is impossible to solve the differential equations explicitly, and one is forced to estimate the unknown parameters directly from the differential system.

Several methods exist for estimating unknown parameters in ordinary differential equations. A very powerful approach recently presented by Bellman et al. (1967) and Lee (1968) uses an iterative quasilinearization algorithm to estimate parameters in both linear and nonlinear ordinary differential equations. The technique, however, requires large amounts of computer time when the number of parameters to be estimated is large. This is due to the parallel fashion in which the unknown parameters are adjoined to the original system of equations. The technique to be presented in the next section, hereafter referred to as the linearization technique or algorithm, overcomes the dimensionality problem associated with the quasilinearization technique by not adjoining the unknown parameters in a parallel fashion. The resulting algorithm is a discretized version of the Gauss-Newton iterative procedure applied to the parameter estimation problem. An additional consequence of the proposed procedure is that a region of convergence larger than that possible with the quasilinearization technique is obtained.

DEVELOPMENT OF THE LINEARIZATION TECHNIQUE

The parameter estimation problem is concerned with finding a vector of parameters $\mathbf{c}$ in the differential equation

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{c}) \tag{1}$$

which will minimize the quadratic expression

$$I = \sum_{k=1}^{N} [\mathbf{x}(k) - \mathbf{w}(k)]' \mathbf{Q} [\mathbf{x}(k) - \mathbf{w}(k)] . \tag{2}$$

Linearizing about some known trajectory $\mathbf{x}_s$, Equation (1) becomes

$$\dot{\mathbf{y}} = \mathbf{A}(\mathbf{x}_s, \mathbf{c}_s)\mathbf{y} + \mathbf{B}(\mathbf{x}_s, \mathbf{c}_s)\mathbf{v} \tag{3}$$

where

$$\mathbf{A}(\mathbf{x}_s, \mathbf{c}_s) = [\partial \mathbf{f}(\mathbf{x}, \mathbf{c})/\partial \mathbf{x}]_s$$

$$\mathbf{B}(\mathbf{x}_s, \mathbf{c}_s) = [\partial \mathbf{f}(\mathbf{x}, \mathbf{c})/\partial \mathbf{c}]_s$$

Since the data to be fit are presented at specific points in time, Equation (3) is discretized to

$$\mathbf{y}(k+1) = \varphi(k)\mathbf{y}(k) + \Delta(k)\mathbf{v} \qquad k = 0, 1, 2, \ldots\ldots, N \tag{4}$$

while Equation (2) becomes

$$I = \sum_{k=1}^{N} [\mathbf{y}(k) - \mathbf{w}_s(k)]' \mathbf{Q} [\mathbf{y}(k) - \mathbf{w}_s(k)] . \tag{5}$$

The solution of Equation (4) at any time step k is

$$\mathbf{y}(k) = \left[\prod_{i=0}^{k-1} \varphi(i) \right] \mathbf{y}(0) + \left[\sum_{i=0}^{k-1} \left\{ \prod_{j=i+1}^{k} \varphi(j) \right\} \Delta(i) \right] \mathbf{v} \tag{6}$$

$$\varphi(j) = \mathbf{I} \quad \text{for} \quad j \geq k$$

Substituting Equation (6) into Equation (5) yields an expression which can be differentiated with respect to the control vector and solved for $\mathbf{v}$ to yield the optimal estimate $\mathbf{v}^0$.

The linearized estimation procedure can now be outlined as follows:

1. Assume initial values for the unknown parameters, form the vector $\mathbf{c}_s$, and generate the trajectory $\mathbf{x}_s$.
2. Calculate the $\mathbf{A}(\mathbf{x}_s, \mathbf{c}_s)$ and $\mathbf{B}(\mathbf{x}_s, \mathbf{c}_s)$ matrices as a function of $\mathbf{x}_s$ for the linearized system of Equation (3).
3. Discretize this set of linear equations by calculating the $\varphi(k)$ and $\Delta(k)$ matrices to produce a system which can be described by Equation (4).
4. Using the appropriate $\varphi(k)$ and $\Delta(k)$ matrices calculate a revised estimate of the unknown parameters $\mathbf{c}^{j+1} = \mathbf{c}_s + \mathbf{v}^0$, after calculating $\mathbf{v}^0$.
5. Repeat steps 1 thru 4 by letting $\mathbf{c}^{j+1}$ be the new $\mathbf{c}_s$ until $|\mathbf{c}^{j+1} - \mathbf{c}^j| < \epsilon$.

NUMERICAL EXAMPLES

Nonlinear Differential Models

Cuenod and Sage (1968) illustrate the quasilinearization algorithm by estimating the unknown parameter c in the differential equation

$$\dot{x} = -cx^2 \tag{7}$$

given the initial condition $x(0) = 0.5$, a measured point $w = (1/6)$ at $t = 2$, and an initial guess for c of 3.0. This differential kinetic model describes a second-order reaction of the form

$$2A \rightarrow B$$

The quasilinearization algorithm begins by adjoining the equation $\dot{c} = 0$ to a linearized form of Equation (7) and ends up with a set of simultaneous equations which are solved to yield a new estimate of the unknown parameter. Bellman's paper gives the explicit details of this procedure. The iteration sequence which results from the application of the quasilinearization algorithm to this scalar example is presented in Table 1.

The linearization technique proposed in this work proceeds for this problem as follows. First, Equation (7) is linearized to

$$\dot{y} = (-2c_s x_s)y + (-x_s^2)v . \tag{8}$$

Discretization of this equation is accomplished by evaluating the coefficients of y and v in Equation (8) at some value of the state x_A,

$$x_A = [x(0) + x(2)]/2 . \tag{9}$$

Performing the appropriate mathematical operations yields

an expression identical to Equation (4), so following the rest of the procedure outlined in the previous section for this estimation problem yields the sequence of iterations also presented in Table 1.

It should be noted that while the quasilinearization algorithm converged to the best estimate of the unknown parameter faster than the linearization approach, the number of the equations that were integrated per iteration was different for each technique. The quasilinearization approach required the simultaneous integration of three equations. The linearization procedure required the integration of only one equation to generate the $\mathbf{x}_s$ trajectory. The calculation of the matrix exponential necessary for formation of the discretized system is essentially equivalent to an integration, so it will be considered as one. Thus the linearization procedure required two integrations. The computer times required for the application of each estimation algorithm to this problem are approximately the same, since the greater number of integrations required by the quasilinearization technique balanced with the greater number of iterations required by the linearization procedure to reach the same degree of convergence. (The degree of convergence used for all the examples in this work was $(c^{j+1} - c^j)/c^{j+1} < \epsilon$. Each table presents the ϵ used for that particular example.) In general, the quasilinearization technique requires the integration of only $2n$ equations.

Table 1. Comparison of the Quasilinearization and Linearization Iteration Sequences for $(\dot{x} = -cx^2)$, $\epsilon = 10^{-4}$

J	c_J Linearization technique	c_J Quasilinearization technique
0	3.000000	3.000000
1	2.180733	1.647464
2	2.047452	2.000832
3	2.013188	2.000336
4	2.003719	2.000044
5	2.001053	2.000044
6	2.000299	
7	2.000085	
8	2.000025	

Table 2. Comparison of the Iteration Sequences for the Nonlinear System of Equation (10), $\epsilon = 10^{-4}$

Linearization technique				Quasilinearization technique		
c_1	c_2	c_3	J	c_1	c_2	c_3
2.0000	2.0000	2.0000	0	2.0000	2.0000	2.0000
1.0198	0.8905	0.9401	1	0.9986	2.1940	0.6196
0.9978	1.0441	0.9924	2	1.1330	1.6130	0.9594
1.0019	1.0177	1.0034	3	0.9970	0.9095	1.0022
1.0007	0.9984	1.0006	4	0.9992	0.9973	1.0004
0.9998	0.9986	0.9999	5	0.9999	0.9998	1.0002
0.9998	0.9997	1.0001	6	0.9999	0.9998	1.0000
0.9998	0.9997	1.0001	7			

Sage (1969) determines that the region of convergence of the quasilinearization technique for this nonlinear example is $-1 \leq c \leq 5$. By using an appropriate Liapunov function it can be shown that the region of convergence for the technique proposed in this work is $-3 \leq c \leq \infty$.

The differential expression

$$\dot{x}_1 = -c_1x_1 + c_2x_2^2$$
$$\dot{x}_2 = c_1x_1 - (c_2 + c_3)x_2^2 \tag{10}$$

is the second nonlinear system considered. Following the estimation procedure outlined previously yields the results shown in Table 2. The raw data used in the estimation procedure were generated by using $c_1 = 1.0$, $c_2 = 1.0$, and $c_3 = 1.0$ in (10). Even though the linearization technique required more iterations than the quasilinearization approach, the linearization procedure was faster than the quasilinearization procedure by a factor of 2 because the iteration times integration factor (# iterations × # simultaneous equations) for quasilinearization was (2) (5) (6) = 60, while for the linearization approach it was (2) (2) (7) = 28.

Linear Differential Models

The linearization algorithm was applied to four linear differential models of the form $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{c})\mathbf{x}$. Linearizing these systems to

$$\dot{\mathbf{y}} = \mathbf{A}(\mathbf{c}_s)\mathbf{y} + \mathbf{B}(\mathbf{x}_s)\mathbf{v}, \tag{11}$$

where the $\mathbf{x}_s$ used for evaluating the $\mathbf{B}$ matrix is

$$x_s(i) = \{x_i(k+1) - x_i(k)\}/2$$

and discretizing the resulting equation yields

$$\mathbf{y}(k+1) = \varphi\mathbf{y}(k) + \Delta(k)\mathbf{v} \qquad k = 0, 1, 2, \ldots, N. \tag{12}$$

It should be noted that for this linear kinetic model the $\mathbf{A}(\mathbf{c}_s)$ matrix is constant with time, and hence, the φ matrix does not change with the time step. A comparison of the results obtained with the linearization and quasilinearization techniques when applied to these linear systems is shown in Table 3. In all cases the linearization technique required less computer time than the quasilinearization technique to converge to the best estimate of the unknown coefficients. In addition, the 2 × 3 model was used to illustrate the increased region of convergence obtained with the technique. For an initial value of $c_1 = c_2 = c_3 = 10.0$, the linearization technique converged to the correct answer in 10 iterations, while the quasilinearization algorithm diverged immediately.

DISCUSSION

The linearization technique presented in this work has been shown to be an efficient algorithm for the solution of

Table 3. Comparison of the Results for the Estimation Problems Defined by $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{c})\mathbf{x}$, Best Estimated Kinetic Coefficients, $c_i = 1.0$, Initial Estimates of the Unknown Coefficients, $\mathbf{c}_i = 2.0$ $\epsilon = 10^{-4}$

Order of model	Order of coefficient	No. iterations equations/iteration Quasilinearization	Linearization	No. iterations to convergence Quasilinearization	Linearization	Time factor/ iteration (quasi/linear)	Total time factor (quasi/linear)
2	2	8	4	6	5	1.8	2.2
2	3	10	4	6	8	2.1	1.6
3	3	15	6	6	6	2.9	2.9
3	4	18	6	6	6	3.3	3.3

parameter estimation problems. Since the quasilinearization technique has recently been proposed as an efficient and useful estimation procedure, this technique has been used as the basis of comparison for the results obtained with the linearization procedure. These comparisons show that the linearization procedure is particularly suited for the solution of large dimensioned linear problems because at most only the integration of $2n$ ordinary differential equations, where n is the dimension of the state vector, will be required per iteration. This differs from the quasilinearization algorithm for which the number of integrations involved is dependent on both the dimension of the differential system and the number of unknown parameters. The increased region of convergence obtained with the linearization procedure is characteristic of a Gauss-Newton procedure. Analysis of the difference between the quasilinearization and Gauss-Newton algorithms shows that the quasilinearization algorithm uses all the second-order variations of the performance criteria to generate a new estimate of the parameter, while the Gauss-Newton procedure uses only part of the second-order variation terms. This causes the linearization technique to converge at a slower rate but to be less sensitive to errors in the initial guesses of the unknown parameters.

NOTATION

$\mathbf{A}(\mathbf{x}_s, \mathbf{c}_s)$ = matrix of dimension $n \times n$
$\mathbf{B}(\mathbf{x}_s, \mathbf{c}_s)$ = matrix of dimension $n \times m$
$\mathbf{c}$ = m dimensional vector of unknown parameters
$\mathbf{c}_s$ = nominal value of the vector c
$\mathbf{f}(\mathbf{x}, \mathbf{c})$ = arbitrary vector function of $\mathbf{x}$ and $\mathbf{c}$
j = iteration parameter
k = time step parameter
m = number of unknown parameters
n = dimension of the state vector
N = total number of time steps for the discretized system
$\mathbf{Q}$ = weighting matrix of dimension $n \times n$
$T(k)$ = length of the kth time interval
$\mathbf{u}$ = control vector of dimension m
$\mathbf{v}$ = normalized control vector: $\mathbf{v} = \mathbf{c} - \mathbf{c}_s$
$\mathbf{w}(k)$ = vector of observations of dimension n
$\mathbf{w}_s(k)$ = normalized value of the observation vector: $\mathbf{w}_s(k) = \mathbf{w}(k) - \mathbf{x}_s(k)$
$\mathbf{x}$ = state vector of dimension n
$\mathbf{x}(0)$ = initial value of the state vector
$\mathbf{x}_s$ = nominal value of the state
$\mathbf{y}$ = normalized state vector: $\mathbf{y} = \mathbf{x} - \mathbf{x}_s$
$'$ = denotes transpose of a vector or matrix
^{0} = denotes the optimal value of some quantity

Greek Letters

$\varphi(k)$ = transition matrix: $\varphi(k) = \exp(\mathbf{A}(\mathbf{x}_A, \mathbf{c}_s)^* T(k))$
$\varphi(-1) = In \times n$
$\Delta(k)$ = forcing function weighting matrix:
$$\Delta(k) = [\int \exp(\mathbf{A}(\mathbf{x}_A, \mathbf{c}_s)^* t) dt]\, \mathbf{B}(\mathbf{x}_A, \mathbf{c}_s)$$

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Simultaneous Mass Transfer and Equilibrium Chemical Reaction From Moving Bubbles: Film Theory

Y. T. SHAH

Department of Chemical Engineering
University of Pittsburgh, Pittsburgh, Pennsylvania 15213

Convective gas-liquid mass transfer in the presence of an equilibrium reaction was first analyzed by Olander (1960) for a quiescent gas-liquid system. Because of its practical significance, in this note we extend the analysis to cover mass transfer between a liquid and an ensemble of moving bubbles in the presence of a generalized liquid phase equilibrium chemical reaction involving one reactant and one product.

The analytical results for the mass transfer rate (or Sherwood number) from an ensemble of uniform bubbles are obtained. The analysis assumes the well-known cell model (Gal-Or, 1970), that is, the dispersed phase is distributed uniformly throughout the system so that everywhere in the system its volume fraction is Φ. A representative cell contains the same amount of liquid as the relative volume of liquid to particle volume in the entire assemblage. Hence, a mass transfer analysis of a spherical cell represents a similar analysis of the entire assemblage. The analysis considers various degree of internal circulation of bubbles.

THEORY

The reaction considered is

$$Y_A\, A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} Y_E\, E \tag{1}$$

wherein at equilibrium

$$K = \frac{E^n}{A^m} = \frac{k_1}{k_2} \tag{2}$$

K is the equilibrium constant; m and n are the orders of the reaction with respect to species A and E respectively. Y_A and Y_E are the stoichiometric coefficients and k_1 and