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INVERSE PROBLEMS FOR NONLINEAR, LARGE DIFFERENTIAL SYSTEMS.(U)

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INTERIM SCIENTIFIC REPORT

Title of Research: Inverse Problems for Nonlinear, Large Differential Systems.

Principal Investigator: Jaime Milstein

Department of mathematics
University of Southern California
Los Angeles, California 90007

Air Force Office of Scientific Research Grant AFOSR 80-0243

Abstract

Research completed includes the following:

The dynamics of a system of nonlinear ordinary differential equation depends on the constant coefficients (parameters) of the system. Identifying these coefficients from the solution curves defines an inverse problem. A method to determine the values of the parameters from a finite number of solution curves was developed and implemented. The method consist of two major algorithmic procedures: (1) A derivative free nonlinear optimization, and (2) An error analysis of the parameters found.

The Optimization Algorithm [1]

The nonlinear optimization algorthm utilizes random vector as directions of search to find an optimun point. The components of the random vector are independently generated from a Gaussian distribution. Two interpolating schemes are used; (a) lagrangian polynomial approximations, (b) and spline approximations. The method is iterative and has fast convergence when used on problem having many variables (more than ten). The algoirthm is capable of finding an optimun point even when the function F to be optimized is not available in closed form, but rather only values of F at discrete points can be obtained. Moreover, derivatives of F are not available. This kind of functions are typical when dealing with inverse problems where a set of parameters has to be determine from a finite number of discrete points on the solution curves. [2]

The method does not require "close" estimates of the optimun point, and it is easy to implement and use. The algorithm was tested on several dynamical systems and nonlinear functions in many variables, such as a model of gluconeogeneris having 31 parameters, [3]. Also, the "Rosenbrook" function of 50 variables [4] and the "Powell singular" function [5] which has the characteristic that precisely at its minimum value the Jacobian becomes singular (this is the reason that Gradient methods fail to converge to the minimum). The results on the test problems showed the versatility of the method, and its superior performance compare to often algorithms [1].

The Error Analysis [6]

An important aspect in the parameter estimation technique is the validation of the parameters found by the optimization technique. Small perturbations in the observations $y(t_r)$, $r = 1,\ldots,m$ can result in a percentage error that can vary greatly (by orders of magnitude) between parameters. Thus I performed an error analysis of the parameter values to determine the validity of the results. The methods can be outline as follows: Denote by $K \varepsilon R^p$ the best estimate found by optimizing the function F, let $[\dot{X}]_s = [f(X,K,t)_s, [X(0)]_s = [C]_s$ describe the system for the s^{th} initial condition, and let

$$[\dot{D}(t)]_s = [A(t)]_s \, [D(t)]_s + [B(t)]_s , \qquad [D(0)]_s = 0$$

be the corresponding variational system, where

$$[A(t)]_s = \left[\frac{\partial f_i}{\partial x_i}\right]_s , \quad [B(t)]_s = \left[\frac{\partial f_i}{\partial k_j}\right]_s , \quad [D(t)]_s = \left[\frac{\partial x_i}{\partial k_j}\right]_s .$$

We integrate the variational system at $t_1, \ldots t_m$ and form the matrix H such that

$$H = \sum_{s=1}^{\ell} \sum_{r=1}^{\ell} \left([D(t_r)]_s\right)^T [W_r]_s [D(t_r)]_s ,$$

where W_r is a weighting function for each data point.

Then $\sigma^2_{k_i}$, the expected variance for the i^{th} parameter, is given by

$$\sigma^2_{k_i} = (H_{ii})^{-1} .$$

To minimize the probability of making a mistake during the derivation of $[\dot{D}(t)]_s$, I implemented an algorithm that uses automated symbol manipulation to formally obtain the $[\partial f_i/\partial k_i)]_s$, $[(\partial f_i/\partial x_i)]_s$, and the necessary sum and product of such matrices [6].

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(1) Milstein, J., The Inverse Problem: Estimation of kinetic parameters Springer Verlag lecture notes in "Modelling of Chemical Reaction Systems" Editors, K. Ebert, P. Deuflhard, W. Jager. #18, 1981.

(2) Milstein, J., and Bremermann, H., A Mathematical Model of the Calvin Photosynthesis Cycle, Journal of Mathematical Biology 7, 99-116 (1979).

(3) Milstein, J., Modelling and Parameter Identification of Insulin Action on Gluconeogenesis, proceeding of the International Conference in Modelling Methodologies, Editor, B. Ziegler, North Holland, Dec. (1978).

(4) Deuflhard, P. "Recent Advances in Multiple Shooting Techniques", in Computational Techniques for Ordinary Differential Equations, ed. by L. Gladwell/Sayers (Academic press, New York 1980) p. 217.

(5) Milstein J. "A Derivative Free Optimization Algorithm for Functions of Many Variables". Submitted to the IMA Journal of Applied Mathematics.

(6) Milstein, J., Error Estimates for Rate Constants of Inverse Problems, S.I.A.M. Applied Mathematics, Vol. 35, N.3. Nov. (1978).

Manuscripts in Preparation

(1) J. Milstein. A nonlinear derivative free optimization algorithm using conjugate random directions , to be submitted to the Siam Journal of Applied Math.

(2) J. Milstein Finding multiple equilibrium points in chemical kinetics. (To be submitted to Journal of Mathematical Biology.

(3) J. Milstein Mathematical modelling of unstable inverse problems (To be submitted to Siam Journal of Applied math.)

Interaction.

(1) Gave a seminar at U.C. Berkeley May 12/81, on *A new mathematical approach for the law of mass action.*

(2) Invited speaker to the international conference on modelling of chemical reaction systems held in Heidelberg, Germany, Sept. 1980.

(3) I am interacting with Professor Naremdra Goel of S.U.N.Y. Binghampton, on reconstructing dynamical systems from observation points.

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The dynamics of a system of nonlinear ordinary differential equation depends on the constant coefficients (parameters) of the system. Identifying these coefficients from the solution curves defines an inverse problem. A method to determine the values of the parameters from a finite number of solution curves was developed and implemented. The method consist of two major algorithmic procedures (1) A derivative free nonlinear optimization, (2) An error analysis of the parameters found.

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