FITTING FUNCTIONAL EQUATIONS TO EXPERIMENTAL DATA

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1. Introduction

Much of mathematical analysis is devoted to the problem of predicting the future behavior of a system, given a descriptive equation and the current state. This is surprising since a basic scientific problem in such fields as physics, engineering, biology and economics is that of determining the structure of a system, given various observations over time [1-6]. In the past, such system identification or inverse problems were solved by trial and error or by simple approximations. Modern computing machines have dramatically altered the picture with their ability to integrate systems of several thousand differential equations given a complete set of initial conditions. Many types of functional equations may be converted into systems of ordinary differential equations. This means that wide classes of direct problems can be solved as initial-value problems.

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This also means that a great many inverse problems may be computationally resolved. Let the equations which describe a particular process be a system of differential equations. The unknown structure of the process is reflected in unknown system parameters which appear in the differential equations or in the initial conditions. These parameters are to be estimated on the basis of observations of the process. The identification problem takes the form of a nonlinear boundary-value problem. This can be solved by a variety of methods. One that has been shown to be quite effective is described below.

2. Illustrative Example

Consider a system undergoing a process which may be described by the scalar differential equation

\[ x = g(x, a), \]

where \( a \) is an unknown system parameter, and the initial state

\[ x(0) = c \]

is also unknown. Suppose that at the time \( t_i \) the system is observed to be in the state \( b_i, i = 1, 2, \ldots, N; t_{i+1} - t_i \). Neither the observations nor the theory of Eq. (1) need be perfect, so in general

\[ x(t_i) = b_i, \quad i = 1, 2, \ldots, N. \]
To fit the theoretical equation (1) to the experimental data, we wish to determine the constants $a$ and $c$ so that we minimize $S$, the sum of the squares of the deviations

$$S = \sum_{i=1}^{N} \left[ x(t_i) - b_i \right]^2.$$  

Frequently this can be done using a quadratically convergent successive approximation scheme. Let $x_0(t)$, $a_0$ and $c_0$ be the current approximations to the optimal function $x(t)$ and the parameters $a$ and $c$. The new approximations are obtained by considering the linearized equation

$$\dot{x}_1 = g(x_0, a_0) + (x_1 - x_0)g_x(x_0, a_0) + (a_1 - a_0)g_a(x_0, a_0).$$

The solution of this equation may be written in the form

$$x_1(t) = p(t) + c_1 h(t) + a_1 q(t), \quad 0 \leq t \leq t_N,$$

where the functions $p$, $h$, and $q$ are solutions of the linear initial-value problems

$$\dot{p} = g_x(x_0, a_0)p + g(x_0, a_0) - x_0 g_x(x_0, a_0) - a_0 g_a(x_0, a_0), \quad p(0) = 0,$$

$$\dot{h} = g_x(x_0, a_0)h, \quad h(0) = 1,$$

$$\dot{q} = g_x(x_0, a_0)q + g_a(x_0, a_0), \quad q(0) = 0, \quad t_1 \leq t \leq t_N.$$
The functions \( p, h \) and \( q \) are readily determined numerically. Then the constants \( c_1 \) and \( a_1 \) are determined by minimizing the expression

\[
E = \sum_{i=1}^{N} \left\{ p(t_i) + c_1 h(t_i) + a_1 q(t_i) - b_i \right\}^2,
\]

which involves solving the linear algebraic equations

\[
\frac{\partial E}{\partial c_1} = 0, \quad \frac{\partial E}{\partial a_1} = 0.
\]

The process is repeated until a sufficiently small change takes place from one step to the next. In this way, frequently, the differential equation may be fitted to the experimental data [4].

3. Other Functional Equations

Systems of ordinary differential equations may be fitted to the data in the manner just described. So may functional equations which can be reduced exactly or approximately to systems of ordinary differential equations. The wave equation, for example,

\[
\frac{u_{tt}}{u_{xx}} = c^2(x)u_{xx}
\]

can be reduced to ordinary differential equations either by taking Laplace transforms or by using the semi-discretization technique. This leads to the possibility of identifying inhomogeneous media through observation of wave propagation processes [7]. The reduction of differential-difference equations to ordinary differential
equations and the estimation of time lags are discussed in [5]. Even integral equations may be converted into initial value problems [8]; this leads to the computational solution of many inverse problems in multiple scattering [6].

4. Discussion

The least squares criterion of the above example may be replaced by some other criterion, such as a minimax condition [9], depending on the statistical nature of the problem and any a priori estimates that are available.

If the nonlinear Eq. (1) represents a large system of differential equations with complicated right-hand sides, the forming of the partial derivatives needed in the linearized equations could be a formidable task. A method for the computer evaluation of partial derivatives of functions given analytically has been described by Wengert [10] and shown to be useful in orbit determination [11].

The linearized differential equations may be unstable. The method of invariant imbedding provides a reformulation in terms of an initial-value problem for stable differential equations [12]. Invariant imbedding also obviates the need to solve linear algebraic equations, another source of difficulty, by enabling the unknown constants to be directly determined.
If the data are continuously received, an invariant imbedding method for sequential filtering may be employed [13, 14].
REFERENCES


