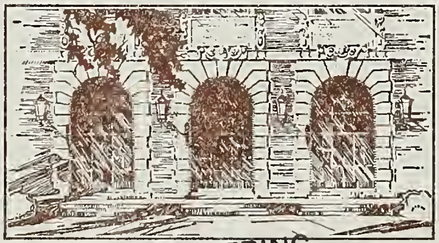

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NUMERICAL METHODS FOR THE IDENTIFICATION OF DIFFERENTIAL EQUATIONS

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ABSTRACT

Numerical methods are given for finding unknown functions contained in ordinary differential equations when a solution of the equation is known. These are iterative methods giving a best fit to the ℓ_2 norm to the known solution, which may contain random errors. A stability requirement on the numerical methods is proved.

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1. Introduction

This paper considers an inverse problem in differential equations, that of identifying ordinary differential equations given their solution. Such a procedure may be of use as an aid in building mathematical models to describe observed phenomena.

Since many different equations may have the same solution, the problem is ill posed and cannot be solved in this generality. It is therefore necessary to restrict the problem to cases where the form of the equation is given but it contains arbitrary functions. The goal is then to identify these functions. This puts the problem in a form concrete enough to be amenable to solution by numerical methods. For example, an attempt to verify the inverse square law of gravitation might start with the equation (in one dimension)

$$x''(t) = f[x(t)]$$

and using suitable data for x would identify the function f numerically to give tabular values of the function

$$f(x) = k/x^2.$$

In order to simplify the problem, it is assumed that each unknown function is a function only of the dependent variable or one of its derivatives. This avoids the more difficult problem of identifying functions of two or more variables.

If $\underset{\sim}{f}$ represents the unknown functions to be determined, let $E(\underset{\sim}{f}) = ||\underset{\sim}{x}_{\underset{\sim}{f}} - \hat{\underset{\sim}{x}}||^2$, where $\underset{\sim}{x}_{f}$ is the solution to the equations (the initial conditions are ignored for the moment) and $\hat{\underset{\sim}{x}}$ the observed data. Iterative methods are used to minimize E over all f for which the solution x_f exists. In general only a local minimum can be found but by adding a "regularization" term, of the form $[c_o||\tilde{f}||^2 + c_1||\tilde{f}'||^2]$, to the error functional this problem is overcome. If the observed solution $\hat{\tilde{x}}$ contains random errors, this also has the effect of smoothing $\tilde{f}$.

To solve the problem numerically, each f must be replaced by a finitie element approximation $f(x) \simeq f_n(x) = \sum_{i=1}^{n} q_i \phi_{i,n}(x)$ where the $\{\phi_{i,n}\}$ are a given, linearly independent set (in the examples given they are splines). It is shown that, under certain conditions, the f_n giving the optimal value of E approaches that obtained by minimizing over all f as n increases.

The stability of multi-step methods for solving differential equations is considered from the point of view of estimating not the difference between the computed and the exact solutions for a given equation, x and X respectively, but between equations which have x and X as their solutions.

2. Solution Methods

Linear problems can be reduced immediately to a corresponding system of linear algebraic equations. For example, a system of n variables $\frac{dx}{dt} = Ax$ has the solution

$$x(t) = e^{At}x(0) = (e^{A})^{t}x(0)$$
$$= \Phi^{t}\ x(0) \qquad \text{(say)} \tag{1}$$

if $x_i = x(i)$ then

$$x_{i+1} = \Phi\ x_i . \tag{2}$$

Taking a set of n of these equations yields the matrix equation

$$[x_1, x_2, \ldots, x_n] = \Phi[x_o, x_1, \ldots, x_{n-1}], \tag{3}$$

from which Φ, and hence A, may be found, provided the last matrix is non-singular. Φ can only be found to within a similarity transformation. For the case where the observed x's certain random errors, this problem has been extensively studied (Lee [6]).

For the remainder of this paper only nonlinear equations will be discussed. For simplicity only a single equation containing one unknown function is considered, although the results may be extended to systems. Usually it will be sufficient to consider the special equation

$$\frac{dx}{dt} = f(x(t)) \tag{4}$$

The problem may be solved by minimizing the error functional

$$E(f) = ||x_f - \hat{x}||^2 \tag{5}$$

where $\hat{x}(t)$ is the observed solution and

$x_f(t)$, $o \leq t \leq T$, is the solution of

$$\begin{cases} \frac{dx}{dt} = f(x(t)) \\ x(0) = x_o \end{cases} \tag{6}$$

for all pairs f, x_o for which a unique solution is obtained. (x_f should be written, more precisely, as $x_{(f,\ x_o)}$ but no confusion is caused by dropping the x_o). The norm used is given by

$$||y||^2 = \int_o^T \{y(t)\}^2\ dt \tag{7}$$

In order to solve the problem numerically, it must be parameterized in the form

$$f(x) = \sum_{i=1}^{n} q_i\ \phi_i(x) \tag{8}$$

where $\{\phi_i\}_{i=1}^{n}$ is a fixed linearly independent set.

Let some set of n parameters $\{q_i\}_{i=1}^{n}$, with n fixed, together with the initial condition $x(0) = x_o$ form the set over which otimization is to take place. If x_o is equated with q_o, a set of $n + 1$ parameters $\{q_i\}_{i=o}^{n}$ must be found. The discrete problem may be stated as

$$\begin{aligned} &\text{minimize } E(q) = ||x_q - \hat{x}||^2 \\ &\text{where } ||y||^2 = \int_o^T y^2(t)\ dt \end{aligned} \tag{9}$$

$$\begin{cases} \frac{dx}{dt} = \sum_{i=1}^{n} q_i\ \phi_i\ (x(t)) \\ x(0) = q_o \end{cases} \tag{10}$$

If the function E is convex then its minimum can be found by solving the set of equations

$$\nabla E(q) = 0.$$

Lack of convexity may cause convergence to a local minimum, also, if the solution is not unique, difficulty may be experienced in obtaining convergence from the iterative method used. To avoid these difficulties, a regularization term of the form $\alpha W[f]$ may be added to E, where

$$W[f] = c_o||f||^2 + c_1||f'||^2, \quad c_o, c_1 \geq 0 \tag{11}$$

c_o and c_1 not both being zero and $\alpha>0$. Norms on the function f are given by $||g||^2 = \int_a^b \{g(x)\}^2 dx, I \equiv [a, b]$. The effect of this is twofold, if α is large enough, $E_\alpha(q) = ||x_q - \hat{x}||^2 + \alpha W[\sum_{i=1}^{n} q_i \phi_i]$ is a convex functional and secondly if the data $\hat{x}$ contain random errors, it will have a smoothing effect on the solution.

To obtain the derivatives of E with respect to q_i,

$$\frac{\partial E}{\partial q_i} = \int_o^T [x(t) - \hat{x}(t)] \frac{\partial x(t)}{\partial q_i} dt \tag{12}$$

The quantities $\frac{\partial x}{\partial q_i}$ satisfy a differential equation obtained from the original equation by differentiating it with respect to q_i.

$$\begin{aligned} \frac{\partial}{\partial q_i}\left(\frac{dx}{dt}\right) &= \frac{d}{dq_i}(f(x(t)) \\ &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial q_i} + \frac{\partial f}{\partial q_i}. \end{aligned} \tag{13}$$

Assuming the order of differentiation can be changed, and setting $\frac{\partial x}{\partial q_i} \equiv \delta_i$

$$\frac{d}{dt}\,\delta_i(t) = \frac{\partial f}{\partial x}(x)\;\delta_i(t) + \frac{\partial f}{\partial q_i}(x) \tag{14}$$

$$\frac{\partial f}{\partial x}(x) = \frac{\partial}{\partial x}\sum_{j=1}^{n} q_j\;\phi_j(x) = \sum_{j=1}^{n} q_j\;\phi_j'(x) \tag{15}$$

and

$$\frac{\partial f}{\partial q_i}\,(x) = \frac{\partial}{\partial q_i}\sum_{j=1}^{n} q_j\;\phi_j(x) = \phi_i(x) \tag{16}$$

The initial condition being $\delta_i(0) = 0$.

For q_o, the initial condition at $t = 0$,

$$\frac{d}{dt}\left(\frac{\partial x}{\partial q_o}\right) = \frac{\partial f}{\partial x}\frac{\partial x}{\partial q_o} + \frac{\partial f}{\partial q_o}\,, \tag{17}$$

but $^{\partial f}/\partial q_o = 0$ since q_o is simply the initial condition x_o. The initial condition $\frac{\partial x}{\partial q_o}$ at $t = 0$ is $\frac{\partial x_o}{\partial x_o} = 1$. If $\frac{\partial x}{\partial q_o} \equiv \delta_o$, equations (14) and (17) may be combined as

$$\frac{d}{dt}\,\delta_i(t) = \frac{\partial f}{\partial x}\,\delta_i(t) + \phi_i(x(t)) \tag{18}$$

where $\phi_o(x) \equiv 0$

with initial conditions

$\delta_o(0) = 1$

$\delta_i(0) = 0 \qquad\qquad i = 1, 2, \ldots, n$

The simplest minimization algorithm is the "steepest descent" method,

$$q^{k+1} = q^k + c_k p^k,$$

where $\quad p^k = -\nabla E(q^k)$

The scalar c_k being chosen so that

$$E(q^k + cp^k) \text{ is minimized over all } c>0.$$

Since E is assumed convex, at $c = c_k$

$$\frac{\partial E}{\partial c}(q^k + cp^k) = 0 \qquad (19)$$

Since we are minimizing a function of only one parameter, Newton's method may be used

$$c^{(i+1)} = c^{(i)} - \frac{\frac{\partial E}{\partial c}\Big|_{c = c^{(i)}}}{\frac{\partial^2 E}{\partial c^2}\Big|_{c = c^{(i)}}}$$

To calculate $^{\partial E}/_{\partial c}$, we have

$$E(q + cp) = \int_o^T (x_{q + cp} - \hat{x})^2 \, dt \qquad (20)$$

So, assuming the order of integration and differentiation can be interchanged

$$\frac{\partial E}{\partial c}(q + cp) = 2 \int_o^T (x_{q + cp} - \hat{x}) \frac{\partial x}{\partial c} \, dt \qquad (21)$$

The quantity $^{\partial x}/_{\partial c}$ may be obtained as the solution to a differential equation, in the case where $x' = f(x)$, $f(x) = \sum_{i=1}^{n} q_i \; \phi_i(x) + c \sum_{i=1}^{n} p_i \; \phi_i(x)$, therefore

$$\frac{d}{dt}\left(\frac{\partial x}{\partial c}\right) = \frac{\partial f}{\partial x}\frac{\partial x}{\partial c} + \frac{\partial f}{\partial c} \qquad (22)$$

and $$\frac{\partial f}{\partial c} = \sum_{i=1}^{n} p_i \; \phi_i(x)$$

Thus $^{\partial x}/_{\partial c}$ satisfies the same equation as $^{\partial x}/_{\partial q_i}$ except $\sum_{i=1}^{n} p_i \; \phi_i(x)$ replaces $\phi_i(x)$. The initial condition is $\frac{\partial x}{\partial c}\Big|_{t = o} = p_o$.

For the second derivative,

$$\frac{\partial^2 E}{\partial c^2}(q + cp) = 2\int_o^T \left(\frac{\partial x}{\partial c}\right)^2 dt + 2\int_o^T (x_{q+cp} - \hat{x}) \frac{\partial^2 x}{\partial c^2} dt \tag{23}$$

An equation for $\partial^2 x/\partial c^2$ may be found or the assumption made that x_{q+cp} is close to $\hat{x}$ and the second term ignored. Thus only one or two differential equations need be solved at each iteration of the calculation of c.

Other algorithms may be obtained using different choices for p^k. For instance Newton's method

$$p^k = - \{H^k\}^{-1} \nabla E(q^k) \tag{24}$$

where H is a matrix with components

$$\begin{aligned} H_{ij} &= \frac{\partial^2 E}{\partial q_i \, \partial q_j} \\ &= 2\int_o^T \frac{\partial x}{\partial q_i} \frac{\partial x}{\partial q_j} dt \\ &+ 2\int_o^T (x - \hat{x}) \frac{\partial^2 x}{\partial q_i \, \partial q_j} dt. \end{aligned} \tag{25}$$

The equation for $\partial^2 x/\partial q_i \, \partial q_j$, for the case $x' = f(x)$ is

$$\begin{aligned} \frac{d}{dt}\delta^2_{ij} &= \frac{\partial^2 f}{\partial x^2}\delta_i \, \delta_j \\ &+ \frac{\partial f}{\partial x}\delta^2_{ij} \\ &+ \frac{\partial}{\partial x}\phi_i(x)\,\delta_j \\ &+ \frac{\partial}{\partial x}\phi_j(x)\,\delta_i \end{aligned} \tag{26}$$

where $\delta_i \equiv \frac{\partial x}{\partial q_i}$, $\delta^2_{ij} \equiv \frac{\partial^2 x}{\partial q_i \partial q_j}$

This however requires the solution of about $n^2/2$ equations, if $x - \hat{x}$ can be assumed small the second term may be neglected. This latter method (the Newton-Gauss method), works well in cases where $\hat{x}$ contains very little random error and a closely approximating x can be found.

A comparison of gradient methods for parameter estimation problems is given by Bard [2].

3. Stability Analysis

Consider our test equation $dx/dt = f(x)$ and suppose some numerical solution $\{X_i\}$, $i = 0, 1, 2, \ldots, n$ is obtained where X_i is the solution at $t = ih$. Let $X(t)$ be any function taking the values X_i at $t = ih$ and suppose $F(X)$ is some function satisfying $dX/dt = F(X)$. Let $x_i = x(ih)$.

The usual stability analysis is concerned with the behaviour of $X_i - x_i$ for increasing i (here called "stability in x"). Since we are concerned with the inverse problem it is necessary to find numerical methods for solving equations for which it can be shown that F is close to f. As the functions are evaluated only at the points $\{x_i\}$, the behaviour of $F(x_i) - f(x_i)$ is analyzed for increasing i. Roughly speaking, a method may be said to be "stable in f" if $F(x_i) - f(x_i)$ remains bounded. Our analysis is restricted to multistep methods.

The general k-step method of order q may be expressed in the form

$$\sum_{j=o}^{k} [\alpha_j \, x_{i-j} + h\beta_j \, f(x_{i-j})] = S_i \tag{27}$$

where $\quad S_i = C\, h^{q+1}\, x_i^{(q+1)} + 0(h^{q+2})$

and $\quad C = \sum_{j=o}^{k} [\frac{(-j)^q}{q!} \alpha_j + \frac{(-j)^{q-1}}{(q-1)!} \beta_j]$

Let

$$\rho(\xi) = \sum_{j=o}^{k} \alpha_j \, \xi^{k-j} \tag{28}$$

$$\sigma(\xi) = \sum_{j=o}^{k} \beta_j \, \xi^{k-j} \tag{29}$$

The condition that the method be weakly stable in x is that the roots of the equation

$$\rho(\xi) = 0 \tag{30}$$

lie within the unit circle or are on the unit circle (see Gear [4] §8.3. (The method is strongly stable (in x) if the roots lie within the unit circle except for the root $\xi = 1$). We show that a similar condition on the roots of $\sigma(\xi) = 0$ is required to ensure stability on f.

Assuming that equation (27) is used as a corrector and that sufficient iterations of the corrector are made then this equation holds for the computed X except that the truncation term is replaced by zero and some roundoff error is incurred.

$$\sum_{j=o}^{k} [\alpha_j X_{i-j} + h \beta_j f(X_{i-j})] = R_i \tag{31}$$

Equation (27) also holds for the solution X of $X' = F(X)$.

$$\sum_{j=o}^{k} [\alpha_j X_{i-j} + h \beta_j F(X_{i-j})] = T_i \tag{32}$$

where $T_i = (h^{q+1} X_i^{(q+1)} + 0(h^{q+2})$.

If we define $\Delta F_i = \Delta F(X_i) = F(X_i) - f(X_i)$, subtracting equation (31) from equation (32) gives

$$\sum_{j=o}^{k} h \beta_j \Delta F_{i-j} = T_i - R_i \tag{33}$$

This equation determines the difference between F and f at the solution points $\{X_i\}$. The analysis must be restricted to the set $\{\Delta F(X_i)\}$. A method will therefore be said to be stable in f if a perturbation ΔF_i will produce subsequent changes which do not increase step to step.

The general solution of the difference equation (33) may be found by taking any particular solution and adding to it any linear combination of solutions of the corresponding homogeneous equation

$$\sum_{j=o}^{k} h\,\beta_j\,\Delta F_{i-j} = 0. \tag{34}$$

A particular solution of (33) is

$$\Delta F_i = \sum_{j=k}^{i} \frac{(T_j - R_j)}{h}\, y_{i-j}$$

where y_i satisfies (Henrici [5] §5.2-1).

$$y_i = 0 \qquad o \leq i \leq k-1,$$

$$\sum_{j=o}^{k} h\,\beta_j\, y_{i-j} = \begin{cases} h \text{ for } i=k \\ 0 \text{ for } i>k \end{cases} \tag{35}$$

The general solution of equation (33) is therefore

$$\Delta F_i = \sum_{j=1}^{k} c_j\, z_{i,j} + \sum_{j=k}^{i} \frac{(T_j - R_j)}{h}\, y_{i-j}, \tag{36}$$

where the sequences $\{z_{i,j}\}$ $(j = 1, 2, \ldots, k)$ are the set of linearly independent solutions of the homogeneous equations, given by

$$z_{i,j} = r_j^{\,i}, \tag{37}$$

where r_j is a root of the equation

$$\sigma(r) = \sum_{j=o}^{k} \beta_j\, r^{k-j} = 0, \tag{38}$$

or, in the case where $\sigma(r) = 0$ has a root of multiplicity m then r^i, ir^i, i^2r^i, ..., $i^{m-1}r^i$ will be solutions. Since y_i satisfies the homogeneous difference equation for $i>k$, y_i is a linear combination of the $z_{i,j}$ for $i>k$. This proves the following result.

Theorem

A multi-step method is stable in f if and only if the roots of the equation

$$\sigma(\xi) = 0$$

lie within the unit circle or are simple on the unit circle.

A method may be said to be strongly stable in f if all the roots of $\sigma(\xi) = 0$ lie within the unit circle and weakly stable if any simple root lies on it.

The well known result of Dalquist [3] that a k-step method which is strongly stable (in x) is of order at most k+1 (for k even a weakly stable method of order k+2 is possible) may be extended to cover the case where stability in f is also required.

Theorem

A k-step method which is stable both in x and in f has order at most

k if k is even

k+1 if k is odd

Further if the method is of order k+1, it is weakly stable in both x and f.

Proof

The proof is similar to that used to obtain Dalquist's original result. The condition that the method be of order r is

$$\frac{\rho(\xi)}{\log(\xi)} + \sigma(\xi) = 0\ ((\xi-1)^r). \tag{39}$$

Making the transformation

$$\xi = \frac{1+z}{1-z}, \quad z = \frac{\xi-1}{\xi+1}$$

The interior of the unit circle in the ξ-plane maps into the left half of the z-plane

$$\text{Let} \qquad R(z) + \left(\frac{1-z}{2}\right)^k \rho\left(\frac{1+z}{1-z}\right)$$

$$\text{and} \qquad S(z) = \left(\frac{1-z}{2}\right)^k \sigma\left(\frac{1+z}{1-z}\right) \tag{40}$$

These are both polynomials of degree k in z. Except at $z = 1$ and $\xi = -1$ the roots of R and ρ, and of S and σ correspond. Since ρ and σ are stable, ξ such that $z = 1$ is not a root of $\rho(\xi) = 0$ or $\sigma(\xi) = 0$. The roots corresponding to $\xi = -1$ in the z-plane are at infinity and so decrease the order of R or S.

Equation (39) maps into

$$\frac{R(z)}{\log \{(1+z)/(1-z)\}} + S(z) = 0(z^r). \tag{41}$$

Following Gear [4] 10.2, let $R(z) = a_o + a_1 z + \ldots + a_k z^k$. Since $\xi = 1$ is a simple root of $\rho(\xi) = 0$, $z = 0$ is a simple root of $R(z) = 0$. Therefore, $a_o = 0$ and $a_1 \neq 0$.

Since ρ, and hence R, is a real polynomial, the roots of $R(z) = 0$ are either real, x_μ, or occur in conjugate pairs, $x_\nu \pm iy_\nu$ with non-positive real parts. Hence

$$R(z) = a\pi_\mu (z-x_\mu)\pi_\nu (z - x_\nu - iy_\nu)(z - x_\nu + iy_\nu)$$

$$= a\pi_\mu (z+|x_\mu|)\pi_\nu (z^2 + 2z|x_\nu| + x_\nu^2 y_\nu^2).$$

Therefore the signs of the non-zero a_i are all the same. Without loss of generality, take $a_1 > 0$, then $a_i \geq 0$, $i \geq 2$.

Similarly if

$$S(z) = b_o + b_1 z + \ldots + b_k z^k, \tag{42}$$

then all the b_i have the same sign since the roots of $S(z) = 0$ also have non-positive real parts.

If
$$\frac{z}{\log \{(1+z)/(1-z)\}} = \sum_{\mu=o}^{\infty} c_{2\mu} z^{2\mu}, \tag{43}$$

it may be shown that (Gear [4] §10.2)

$$c_o = \frac{1}{2}, \quad c_{2\mu} < 0, \quad \mu \geq 1.$$

Then
$$\begin{aligned} \frac{R(z)}{\log \{(1+z)/(1-z)\}} &= \sum_{m=1}^{k} a_m z^{m-1} \sum_{\mu=o}^{\infty} c_{2\mu} z^{2\mu}, \\ &= \sum_{n=o}^{\infty} r_n z^n, \text{ say} \end{aligned} \tag{44}$$

In order for the method to be of order p,

$$\sum_{n=o}^{\infty} r_n z^n + \sum_{n=o}^{k} b_n z^n = 0(z^p), \tag{45}$$

so that $r_n = -b_n$ for $n = 0, 1, 2, \ldots, p-1$

and hence the coefficients r_n must all have the same sign for 0 up to p-1.

Equating coefficients in equation (44)

$$r_o = c_o \, a_1$$

$$r_1 = c_o \, a_2$$

$$r_2 = c_o \, a_3 + c_2 \, a_1$$

$$r_3 = c_o \, a_4 + c_2 \, a_2$$

$$\vdots$$

$$r_k = \begin{cases} c_2 \, a_{k-1} + c_4 \, a_{k-3} + \dots + c_{k-2} \, a_3 + c_k a_1 & k \text{ even} \\ c_2 \, a_{k-1} + c_4 \, a_{k-3} + \dots + c_{k-3} \, a_4 + c_{k-1} a_2 & k \text{ odd} \end{cases}$$

Since c_o and a_1 are both > 0, $r_o > 0$. Therefore $r_1 \geq 0$ for r = 1, 2, ..., p-1. However, since a_1 0, $a_i \geq 0$ for $i \geq 2$ and $c_{2\mu} < 0$ for $\mu \geq 1$, $r_k < 0$ for k even and $r_k \leq 0$ for k odd. Therefore for k even, the method has maximum order k, and for k odd the method is limited to order k+1 by the requirement for stability in x .

When the method is of order k+1, (and k is odd), r_k must be zero and so $a_2 = a_4 \dots = a_{k-1} = 0$. Since a_o is also zero, R(z) is an odd polynomial. Further $r_1 = r_3 = \dots = r_k = 0$, so $b_1 = b_3 = \dots = b_k = 0$ and consequently S(z) is an even polynomial. Therefore if x + iy is a root of either R(z) = 0 or S(z) = 0 then so is -x-iy, but the roots of these equations must have non-positive real parts to satisfy the stability requirements and so all the roots lie on the imaginary axis. The root of both $\rho(\xi) = 0$ and $\sigma(\xi) = 0$ therefore all lie on the unit circle.

Example: If $\beta_o = 1$, $\beta_1 = \beta_2 = \beta_3 = \beta_4 = 0$, then all the roots of $\sigma(\xi) = 0$ are zero, and (directly from equation (33)),

$$\Delta F_i = \frac{T_i - R_i}{h}$$

This yields the fourth order four-step method,

j	0	1	2	3	4
α_j	-25/12	4	-3	4/3	-1/4
β_j	1	0	0	0	0

for which the roots of $\rho(\xi) = 0$ are 1, 0.3815, 0.2693 ± 0.04920i. The method is therefore strongly stable both in x and in f.

4. Test Problems

In the first example, an additional test was made in which the observed data were perturbed by adding random "noise". This was mainly to test the effect on the convergence rate.

Example 1

This is the simplest possible example, taking

$$\frac{dx}{dt} = f(x)$$

and input data of the form

$$x(t) = \frac{-1}{t+2}$$

specified on the interval [0,10] at discrete points distance .05 apart. This will give the solution

$$f(x) = x^2$$

on the interval (determined from the range of the observed data) $[-^1/2, -^1/12]$. A smoothing factor

$$\alpha[c_o \, ||f||^2 + c_1 \, ||f'||^2]$$

was introduced with $c_o = 0$, $c_1 = 1$ and α initially set to 10^{-2} and reduced by a factor of 10 at each iteration until a minimum of 10^{-9} was reached. The function f was approximated on the interval $[-^1/2, 0]$ by a natural spline with 8 equally spaced knots. (Natural splines are discussed in Ahlberg, Nilson and Walsh [1]).

At each iteration the value of the error functional and the

ℓ_2 norm of its gradient were produced. The programs were rerun after applying a random noise with zero mean and a variance of .01 to the input data. It may be noted that in all cases the function was better identified in the middle of the range where more data points were avilable than on the edges.

Table 1. x' = f(x) - no noise added to the observed x.

Iteration	$\|\|\nabla E\|\|$	E
1	6.77E-00	9.99E 02
2	5.56E-00	5.14E-02
3	4.91E-00	2.60E-02
4	1.04E-01	1.22E-04
5	7.09E-02	8.09E-06
6	2.54E-03	6.00E-08
7	7.76E-05	2.38E-09
8	6.89E-06	3.33E-11

x	computed	exact
-0.50	0.24993	0.25
-0.45	0.20250	0.2015
-0.40	0.16000	0.16
-0.35	0.12250	0.1225
-0.30	0.09000	0.09
-0.25	0.06250	0.0625
-0.20	0.04000	0.04
-0.15	0.02250	0.0225
-0.10	0.01000	0.01
-0.05	0.00252	0.0025
-0.00	0.00017	0

Table 2. $x' = f(x)$ - with noise added.

Iteration	$\|\|\nabla E\|\|$	
1	6.86E-00	1.01E-01
2	5.53E-00	5.87E-02
3	4.29E-00	2.72E-02
4	2.11E-00	5.18E-03
5	1.64E-01	1.21E-03
6	2.41E-01	9.90E-04
7	4.32E-02	9.38E-04
8	6.52E-03	9.32E-04
9	1.69E-03	9.32E-04

x	f(x) computed	f(x) exact
-0.50	3.93796E-01	0.25
-0.45	1.89431E-01	0.2015
-0.40	1.84711E-01	0.16
-0.35	1.03462E-01	0.1225
-0.30	8.22265E-02	0.09
-0.25	7.12669E-02	0.0625
-0.20	4.00412E-02	0.04
-0.15	2.53864E-02	0.0225
-0.10	1.01355E-02	0.01
-0.05	-5.73504E-02	0.0025
-0.00	-8.29363E-01	0

Example 2

This example uses a system of two equations with two unknown functions. Starting with the vector equation

$$\frac{d^2\tilde{x}}{dt^2} = \tilde{f}(x),$$

and splitting it into horizontal and vertical components x_1 and x_2, we try the equations

$$\frac{d^2x_1}{dt^2} = f_1\,(x_1)\,f_2\,(x_1^{\,2} + x_2^{\,2})$$

$$\frac{d^2x_2}{dt^2} = f_1\,(x_2)\,f_2\,(x_1^{\,2} + x_2^{\,2}).$$

If the original equation represents an inverse square law then we should obtain for the functions f_1 and f_2

$$f_1(x) = -kx$$
$$f_2(x) = \frac{1}{k}\,x^{-3/2}$$

where k is an arbitrary constant.

The non-uniqueness of f_1 and f_2 is handled by introducing a smoothing term

$$\alpha\,[c_o \sum_{i=1,2} ||f_i||^2 + c_1 \sum_{i=1,2} ||f'||]$$

into the error functional, with $c_o = c_1 = 1$. Again α was allowed to vary from 10^{-2} down to 10^{-9} when noise was not added to the data and down to 10^{-6} when it was. The exact solution is scaled so that the mean value for $f_2(x)$ is the same as the computed one.

Table 3.

Iteration		
1	5.72E2	7.19E-1
2	5.66E-1	1.70E-2
3	1.96E-1	9.77E-4
4	1.24E-2	1.91E-4
5	3.29E-2	1.37E-4
6	3.73E-2	1.01E-4
7	3.74E-2	6.66E-5
8	3.29E-2	4.00E-5
9	2.33E-4	1.02E-7

x	$f_1(x)$		x	$f_2(x)$	
	computed	exact		computed	exact
-0.23	0.1375	0.1924	1.00	1.2006	1.2153
-0.06	0.0457	0.0477	1.14	0.9870	1.0098
0.12	-0.0965	-0.0971	1.28	0.8302	0.8430
0.29	-0.2453	-0.2418	1.41	0.7111	0.7226
0.47	-0.3923	-0.3865	1.55	0.6170	0.6284
0.65	-0.5396	-0.5313	1.69	0.5426	0.5530
0.82	-0.6868	-0.6760	1.83	0.4848	0.4407
1.00	-0.8340	-0.8207	1.97	0.4414	0.4407
1.17	-0.9837	-0.9655	2.10	0.4097	0.3981
1.35	-1.1113	-1.1102	2.24	0.3859	0.3619
1.53	-1.1137	-1.2549	2.38	0.3763	0.3309

REFERENCES

[1] J. H. Ahlberg, E. N. Nilson and J. L. Walsh, The Theory of Splines and their Applications, Academic Press, 1967.

[2] Y. Bard, Comparison of Gradient Methods for the Solution of Nonlinear Parameter Estimation Problems, SIAM J. Numer. Anal. 7 (1970), pp. 157 - 186.

[3] G. Dalquist, Numerical Integration of Ordinary Differential Equations, Math. Scand. 4 (1956), pp. 33 - 50.

[4] C. W. Gear, Numerical Initial Value Problems in Ordinary Differential Equations, Prentice-Hall, 1971.

[5] P. Henrici, Discrete Variable Methods in Ordinary Differential Equations, Wiley, 1962.

[6] R. C. K. Lee, Optimal Estimation, Identification, and Control, M.I.T., 1964, Ch. 4.

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