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Differential Quadrature and Long-Term Integration*

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1. Introduction

The term "quadrature," as ordinarily used, applies to the approximate evaluation of an integral

$$\int_0^1 f(x) dx \cong \sum_{i=1}^N w_i f(x_i). \tag{1}$$

In Refs. [1 and 2] it was shown that this technique could be utilized in a simple and systematic fashion to obtain the computational solution of non-linear differential-integral equations derived from applications of the theory of invariant imbedding to transport processes. The foregoing approximation technique, however, can be extended to far more general linear functionals. Thus, we can write

$$f'(x_i) \cong \sum_{i=1}^{N} a_{ij} f(x_i), \quad i = 1, 2, ..., N,$$
 (2)

with the coefficient matrix (a_{ij}) determined in various fashions. We call this procedure "differential quadrature." In Ref. [3] we indicated how this provided a new approach to the identification of parameters in systems described by various types of functional equations, a method quite different from the procedure based on the use of quanlinearization.

In general, we can contemplate the systematic use of various approximation

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techniques to eliminate transcendental operations. This is part of a general theory of closure of operations, a theory which has become increasingly significant with the introduction of the hybrid computer [5]. In this paper we wish to indicate how these ideas offer a new technique for the numerical solution of initial value problems for ordinary and partial differential equations with particular relevance to certain difficult questions arising from long-term integration.

2. Long-Term Integration

Consider the vector equation

$$y' = g(y), y(0) = c,$$
 (1)

where y is an N-dimensional vector, and suppose that it is desired to calculate y(T). A finite difference approximation (crude version),

$$w(t + \Delta) - w(t) = g(w(t)) \Delta, \qquad w(0) = c, \tag{2}$$

 $t=0, \Delta, 2\Delta,...$, leads to an algorithm well-suited to the nature of the contemporary digital computer. Starting with the initial value w(0)=c, we can use (2) in an interative fashion to calculate in turn $w(\Delta)$, $w(2\Delta),...$, and so on. We expect that $w(n\Delta) \cong y(n\Delta)$.

If T, the point in time at which the value of y is desired, is large, the foregoing procedure has several drawbacks. In the first place, we encounter the problem of numerical stability. An accumulation of evaluation and round-off errors may seriously contaminate w(T), and even obscure the actual value.

Secondly, if $T \gg 1$ and $\Delta \ll 1$, the fact that $[T/\Delta]$ steps are required may create an exorbitant execution time. This can be a serious consideration in connection with various "on-line" decision processes of the type that occur in weather prediction and medical diagnosis.

Thirdly, even if the stability problem is resolved and the time requirements are acceptable, the procedure nevertheless still possesses some esthetic handicaps. Often, the mathematical model of the original physical process is known to be rather "rough and ready." What is desired from the equation then, is a reasonable estimate of the functional values at a few grid points rather than any highly accurate determination of the entire set of values $\{w(k\Delta)\}$.

In Ref. [4] we discussed the use of the Laplace transform to meet the foregoing objections, considering both linear and nonlinear equations. In Ref. [5] we presented a use of nonlinear extrapolation. Here we wish to examine the general application of differential quadrature.

3. Differential Quadrature

Let the points $0 = t_0 < t_1 < t_2 < \cdots < t_N$ be selected and the coefficient matrix $A = (a_{ij})$ be chosen so that

$$y'(t_i) \cong \sum_{j=1}^{N} a_{ij} y(t_j). \tag{1}$$

There are several ways of doing this based upon the method of least squares, methods akin to Gaussian quadrature, and the emerging theory of splines.

The equation of (2.1) then becomes

$$\sum_{j=1}^{N} a_{ij} y(t_j) \cong g(y(t_i)), \qquad i = 1, 2, ..., N.$$
 (2)

We can now proceed in several ways. To begin with, we can consider the system of equations

$$\sum_{j=1}^{N} a_{ij} y(t_j) = g(y(t_i)), \qquad i = 1, 2, ..., N,$$
(3)

as a method of determining $y(t_i)$. Secondly, we can use a least squares technique. Thirdly, we can use a Chebyshev norm and apply linear and nonlinear programming techniques.

4.
$$g(y)$$
 Linear

If g(y) = By, an application of the least squares technique leads to the problem of the solution of a linear system of equations. In a number of cases we can employ intrinsic properties of the physical process to determine a regularization, or "penalty," function to ensure a well-conditioned system; cf. Ref. [4].

If a Chebyshev norm is employed, linear programming techniques can be used.

5. g(y) Nonlinear

If g(y) is nonlinear, the minimization problem associated with a least squares procedure requires some use of successive approximations. One way to obtain a good initial approximation is to use a low-order differential

quadrature, where the minimization process is easy to carry out, plus interpolation. This is a method proposed in Ref. [4] in another connection.

6. PARTIAL DIFFERENTIAL EQUATIONS

The method can be applied to various classes of partial differential equations reducing them to ordinary differential equations and then to finite-dimensional systems. Consider, for example, the equation

$$u_t = g(u, u_x), \quad u(x, 0) = h(x).$$
 (1)

Write

$$u_x \Big|_{x=x_i} = \sum_{j=1}^{N} a_{ij} u(x_j, t), \quad i = 1, 2, ..., N,$$
 (2)

where $x_1 < x_2 < \cdots < x_N$, and consider the associated system of ordinary differential equations

$$v_{i}' = g\left(v_{i}(t), \sum_{j=1}^{N} a_{ij}v_{j}(t)\right), \quad v_{i}(0) = h(x_{i}),$$
 (3)

where

$$v_i \simeq u(x_i, t), \qquad i = 1, 2, ..., N.$$

We can eliminate the t derivative if desired with a repeated application of this procedure. Alternatively, a Buvnov-Galerkin technique can be used to find an approximate solution of (3) [5].

Numerical examples illustrating the different possibilities will be presented subsequently.

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