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# NOTE ON THE NUMERICAL TREATMENT OF SECOND-ORDER DIFFERENTIAL EQUATIONS

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P-439

October 7, 1953



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# NOTE ON THE NUMERICAL TREATMENT OF SECOND-ORDER DIFFERENTIAL EQUATIONS

by

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A variety of methods exist for treating numerically second-order differential equations of the general form

$$\frac{d^2\phi(x)}{dx^2} = F\left[x,\phi(x)\right] , \qquad (1)$$

supplemented by boundary conditions

(i) $\phi(x) = \alpha$ at $x = a$

(ii) $\frac{d\phi(x)}{dx} = \beta$ at $x = a$

These methods have a common defect, however, being all basically extrapolation procedures which involve replacing the second-order differential by a suitable second difference. This feature of "extrapolation" throws some question on the reliability of error estimates deduced from these methods. The situation would be more satisfactory if the solution of equation (1) could be performed by a completely implicit scheme. It has been found that such a simple possibility exists.

The present scheme proceeds by converting the differential equation into an integral equation, which is effected by a double

integration ~~of equation (1).~~

$$\phi(x) = \alpha + \beta(x-a) + \int_a^x dy \int_a^y dz\ F\ [z,\phi(z)] \qquad (2)$$

The equation is not conveniently handled in this form; however, an integration by parts of the last term gives

$$\phi(x) = \alpha + \beta(x-a) + \int_a^x dy(x-y)\ F\ [y,\phi(y)] \quad . \qquad (3)$$

In this form the equation is particularly well suited for numerical treatment. There are two reasons for this: first, that while $\phi(x)$ at x occurs on both sides of the equation, it occurs with zero weight on the right hand side and hence admits of an explicit determination of $\phi(x)$, and second, the integral in equation (3) involves x only in an inessential way so that the integral may be separated into two integrals, neither of which contains x in the integrand. This means that equation (3) may be integrated explicitly with a simple accumulation over values of $\phi(x)$ on the interval (a,x).

In the numerical treatment of equation (3) the integral is replaced by a sum. If the sum is given by a k-point integration formula, equation (3) reduces to the difference equation

$$\phi(x_n) = \alpha + \beta(x_n-a) + \left[x_n P(x_n) - Q_n(x_n)\right] \quad , \qquad (4)$$

where

$$P(x_n) = \sum_{j=n-k}^{n} \sigma_j \; F\left[x_j, \phi(x_j)\right] + P(x_{n-k}) \qquad (5)$$

$$Q(x_n) = \sum_{j=n-k}^{n} \sigma_j x_j \; F\left[x_j, \phi(x_j)\right] + Q(x_{n-k}) \quad , \qquad (6)$$

and the coefficients $\sigma_j$ arise from the specific integration formula which is being used. The latter also determines the accuracy of the integration. For the tranezoidal rule, the error is of the order of the square of the interval size, while for Simpson's rule it is the fourth power, which is equivalent to that of the familiar Runge-Kutta method.

In order to start the integration of the difference equation (4) it is necessary to specify the values of $\phi(x)$, $P(x)$ and $Q(x)$ at the first (k-1) points of the integration. This requires an analytic approximation about the starting point $x = a$. This is accomplished by first expanding $F\left[x,\phi(x)\right]$ as a power series in x and then determining $\phi(x)$, $P(x)$, and $Q(x)$ from this series. Thus let

$$F\left[x,\phi(x)\right] = \sum_{\ell=0}^{\infty} \frac{A_\ell}{\ell!} (x-a)^\ell \quad , \qquad (7)$$

where

$$A_\ell = \frac{d^\ell}{dx^\ell} F\left[x,\phi(x)\right] \Bigg|_{x=a} \quad . \qquad (8)$$

The evaluation of $A_\ell$ is carried out directly with the aid of the expressions

$$\phi(a) = \alpha \tag{9}$$

$$\phi'(a) = \beta \tag{10}$$

$$\phi''(a) = F(a,\alpha) \tag{11}$$

$$\phi''(x) = F\ [x,\phi(x)] \tag{12}$$

which follow immediately from equation (1) and its associated boundary conditions. Equation (7) when substituted into

$$P(x) = \int_a^x dy F\ [y,\phi(y)] \tag{13}$$

$$Q(x) = \int_a^x dyy\ F\ [y,\phi(y)] \tag{14}$$

and

$$\phi(x) = \alpha + \beta(x-a) + [xP(x) - Q(x)]\ , \tag{15}$$

constitute the required formulas to initiate the integration. Of course, one retains only those terms of equation (7) which are consistent with the accuracy of the integration formula.

The method presented here has been applied in detail to the specific case in which (1) is the well known Fermi-Thomas equation. In addition, for this case, the analytic simplicity of the integral formulation has been exploited to obtain approximate solutions. These results will be reported elsewhere.