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The Wronskian of discrete methods in linear systems

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SUMMARY

In the past decade it has been suggested that the use of superposition of particular solutions technique may be employed to solve linear systems with considerable programming advantage over the more widely used method of superposition of homogeneous and particular solutions, when solving numerically multi-point boundary-value problems. The present article on analytical expression for the discretization errors of the Wronskian, induced by the discretization errors of the particular solutions, is found for linear systems of ordinary differential equations when single-step methods of numerical integration of the Runge-Kutta type are used. It is shown that the analysis of this error can, in some cases, give useful information in the estimation of optimum integration step size in the sense that minimum errors, discretization plus round-off, are attained during integration.

1. Introduction

Except for a few cases where analytical solutions can be obtained, boundary-value problems involving a system of ordinary differential equations have to be solved by a discrete, approximate, numerical procedure. In the case of linear systems, the determination of the unknown initial conditions for which the system satisfy the imposed boundary conditions, can be computed fairly efficiently when the superposition of homogeneous and/or particular solutions technique is employed. If the system is nonlinear, some linearization procedure can be used and the superposition technique can be employed on the linearized form of the system, Bellman et al. [1].

In recent years Childs et al. [2] suggested that the superposition of particular solutions method (see also Fox [3]), may be employed to solve linear systems with considerable programming advantage over the more widely used technique of superposition of homogeneous and particular solutions. Moreover, they have found that the method may provide some indication of round-off error by an analysis of the behavior of the Wronskian of the numerical solution with respect to the step size of the numerical integration and time (the independent variable).

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In this article an analytical expression for the discretization error of the Wronskian (induced by the discretization errors of the particular solutions), is found for linear systems of ordinary differential equations when single-step methods of numerical integration of the Runge-Kutta type are used. It is shown that the analysis of the behavior of this error can, in some cases, give useful information in the estimation of optimum integration step size in the sense that minimum errors (discretization plus round-off) are attained during integration.

2. Superposition of particular solutions

Consider the linear system of ordinary differential equations and associated boundary conditions

$$\dot{\mathbf{y}} = A(t)\mathbf{y}(t) + \mathbf{r}(t), \tag{1a}$$

$$\sum_{k=1}^{n} b_{ik} y_k(t_i) = \beta_i \qquad (i = 1, 2, \ldots, M) \tag{1b}$$

where $\mathbf{y} = (y_1, \ldots, y_n)$ is the n-dimensional vector of the dependent variables, $A(t)$ is a $(n \times n)$ square matrix with variable (or constant) elements and $r = (r_1, \ldots, r_n)$ is a vector function of the independent variable t. Equations (1b) represent M boundary conditions occurring at times t_i. The dot notation is used to denote differentiation with respect to t.

A solution of (1) by the superposition of particular solutions technique is sought superimposing appropriate particular solutions such that if k is the number of unknown initial conditions in (1), we superimpose $(k+1)$ particular solutions $\mathbf{p}^j = (p_1^j, \ldots, p_n^j)$ $(j = 0, 1, \ldots, k)$ which satisfy equation (1a), i.e. it is assumed that

$$\mathbf{y} = \sum_{j=0}^{k} c_j \mathbf{p}^j \tag{2}$$

and

$$\dot{\mathbf{p}}^j = A\mathbf{p}^j + \mathbf{r}, \tag{3a}$$

$$\mathbf{p}^j(0) = \boldsymbol{\alpha}^j, \qquad (j = 0, 1, \ldots, k) \tag{3b}$$

where $\boldsymbol{\alpha}^j$ is an appropriate initial-value vector for the jth particular solution.

Taking equations (2) and (3a) into (1a) we obtain the auxiliary condition which the superposition constants c_j must satisfy

$$\sum_{j=0}^{k} c_j = 1. \tag{4}$$

Substituting equation (2) into (1b) and interchanging the two summation operators we obtain

$$\sum_{j=0}^{k} c_j \sum_{k=1}^{n} b_{ik} p_k^j(t_i) = \beta_i \qquad (i = 1, \ldots, M) \tag{5}$$

If we define the vector $\boldsymbol{\beta}' = (1, \beta_1, \ldots, \beta_M)$ and the matrix $E = (e_{ij})$ such that

$$\begin{aligned} e_{1j+1} &= 1, && (j = 0, 1, \ldots, k) \\ e_{i+1j+1} &= \sum_{k=1}^{n} b_{ik} p_k^j(t_i), && (i = 1, 2, \ldots, M) \end{aligned} \tag{6}$$

equations (4) and (5) can be combined to form the matrix equation

$$E\mathbf{c} = \boldsymbol{\beta}' \tag{7}$$

where $\mathbf{c} = (c_0, c_1, \ldots, c_k)$ is the vector of the superposition constants c_j which can be determined by solving equation (7). If $k < M$ (number of initial conditions smaller than the number of imposed boundary conditions) we still can obtain a solution for $\mathbf{c}$ by meeting the boundary conditions in a least-squares sense, for example. It is assumed that, in the case $k = M$, E is not singular.

When solving the initial-value problems for the particular solutions (3), the use of the following set of initial-condition vectors is suggested:

$$\mathbf{p}^0(0) = (\alpha_1^0, \ldots, \alpha_n^0), \tag{8}$$

$$\mathbf{p}^i(0) = (\alpha_1^0, \ldots, \alpha_i^0 + \delta_i, \ldots, \alpha_n^0) \qquad (i = 1, \ldots, n) \tag{9}$$

where $(\alpha_1^0, \ldots, \alpha_n^0)$ is the initial-value vector for the base particular solution $\mathbf{p}^0(t)$. If the number of unknown initial conditions is equal to the order of the system ($k = n$), the determinant made up of the column vectors

$$\begin{aligned} \mathbf{q}^i &= (1, p_1^i, p_2^i, \ldots, p_n^i), \\ D(t) &= D(\mathbf{q}^0, \mathbf{q}^1, \ldots, \mathbf{q}^n), \end{aligned} \tag{10}$$

becomes, after subtracting the first column from the others,

$$D(t) = D(\mathbf{z}^1, \mathbf{z}^2, \ldots, \mathbf{z}^n) \tag{11a}$$

where $\mathbf{z}^i = \mathbf{p}^i - \mathbf{p}^0$ $(i = 1, \ldots, n)$. This is recognized as being the Wronskian of the corresponding homogeneous system of (1). From Abel's equation for the Wronskian (cf. for example Petrovsky [4]),

$$D(t) = D(0) \exp\left[\int_0^t \text{trace } [A(\xi)]\, d\xi\right] \tag{11b}$$

where

$$D(0) = \delta_1 \delta_2 \ldots \delta_n$$

is obtained from equations (8), (9) and (11a). The linear independence of the particular solutions is guaranteed if $\delta_i \neq 0$ $(i = 1, \ldots, n)$, since, in this case, $D(t) \neq 0$. With the use of the initial conditions (8) and (9) the Wronskian value can be obtained fairly accurately if the integration in equation (11b) is performed with sufficient accuracy.

3. The discretization error of the solution of the differential equations

When a numerical solution is sought for the system of equations (1), two sources of error are introduced during the computation. The first is the discretization error due to the numerical approximation for the derivatives, which are usually estimated from a Taylor-series expansion. The second is the round-off error which is due to the fact that in most cases the numbers cannot be calculated with infinite precision because of the limited accuracy of any computing equipment.

In this work an analytical expression is sought for the discretization error of the Wronskian, induced by the discretization errors of the particular solutions of the system, when single-step methods of numerical integration are used. As will be shown later, for some cases, the analysis of the behavior of the error of discretization of the Wronskian may give useful information in the estimation of optimum integration step, in the sense that minimum errors (discretization plus round-off) are attained during integration.

In order to obtain an expression for the discretization error of the Wronskian, an estimation of the error of the particular solutions is needed.

Let us consider the corresponding homogeneous system of (3)

$$\dot{\mathbf{z}} = A\mathbf{z} = \mathbf{f}(t, \mathbf{z}), \qquad \mathbf{z}(0) = \mathbf{z}_0. \tag{12}$$

A single-step method of solution of (12) is given by the formula

$$\begin{aligned} \mathbf{z}_0 &= \mathbf{z}(0), \\ \mathbf{z}_{n+1} &= \mathbf{z}_n + h\boldsymbol{\Phi}(t, \mathbf{z}_n, h) \qquad (n = 0, 1, 2, \ldots) \end{aligned} \tag{13}$$

where h is the integration step and $\boldsymbol{\Phi}(t, \mathbf{z}_n, h)$ is the increment function, Henrici [5], and a lower subscript refers to the 'time level'.

Defining the truncation-error vector $\mathbf{e}(t)$ as

$$\mathbf{e}(t) = \mathbf{z}_n(t) - \mathbf{z}(t_n) \tag{14}$$

where $\mathbf{z}_n(t)$ is the exact vector obtained from (13) and $\mathbf{z}(t_n)$ the exact solution of (12) at $t_n = t_0 + nh$, an asymptotic formula for the magnified error

$$\mathbf{s}(t) = h^{-p}\mathbf{e}(t) \tag{15}$$

is given from the solution of

$$\dot{\mathbf{s}} = G(t)\mathbf{s} + \boldsymbol{\varphi}(t, \mathbf{z}), \qquad \mathbf{s}(0) = 0, \tag{16}$$

where

$$G(t) = \left(\frac{\partial f^i}{\partial z_j}(t, \mathbf{z})\right)$$

and

$$\boldsymbol{\varphi}(t, \mathbf{z}) = \frac{1}{p!}\frac{\partial^p \boldsymbol{\varphi}\,(t, \mathbf{z}, 0)}{\partial h^p} - \frac{1}{(p+1)!}\frac{d^p \mathbf{f}(t, \mathbf{z})}{dt^p} \tag{17}$$

where p is the order of integration of the numerical method (cf. Henrici [5]). For a linear system such as (12) it can be shown that $G(t) = A(t)$. The expression for $\boldsymbol{\varphi}(t, \mathbf{z})$, called by Henrici the principal-error function, is considerably more complex; it not only involves the function $\mathbf{f}(t, \mathbf{z})$ (equation (12)) but also the increment function $\boldsymbol{\Phi}(t, \mathbf{z}, h)$ which defines the numerical algorithm of integration.

Restricting our analysis to methods of integration of the Runge-Kutta type, the increment function for the second and fourth order methods are (cf. Henrici op. cit.):

(a) Runge-Kutta of order two,

$$\boldsymbol{\Phi} = (1-\lambda)\mathbf{f}(t, \mathbf{z}) + \lambda \mathbf{f}\left[t + \frac{h}{2\lambda}, \mathbf{z} + \frac{h}{2\lambda}\mathbf{f}(t, \mathbf{z})\right]; \tag{18}$$

(b) Runge-Kutta of order four (classical case),

$$\boldsymbol{\Phi} = \tfrac{1}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4) \tag{19}$$

where

$$\mathbf{k}_1 = \mathbf{f}(t, \mathbf{z}),$$

$$\mathbf{k}_2 = \mathbf{f}\left(t + \frac{h}{2}, \mathbf{z} + \frac{h}{2}\mathbf{k}_1\right),$$

$$\mathbf{k}_3 = \mathbf{f}\left(t + \frac{h}{2}, \mathbf{z} + \frac{h}{2}\mathbf{k}_2\right),$$

$$\mathbf{k}_4 = \mathbf{f}(t + h, \mathbf{z} + h\mathbf{k}_3).$$

The classical 'Improved Euler method' and 'Modified Euler method' are obtained by assigning to the parameter λ in (18) the values 0.5 and 1.0, respectively.

After some lengthy calculations, the principal error functions for the linear homogeneous system (12) are obtained from equation (17), (18) and (19) in the general form

$$\varphi(t, \mathbf{z}) = U(t)\,\mathbf{z} \tag{20}$$

where the matrix $U(t)$ takes the form:
(a) Runge-Kutta of order two,

$$U(t) = \left(\frac{1}{8\lambda} - \frac{1}{6}\right)(A'' + 2A'A) - \frac{1}{6}(AA' + A^3); \tag{21}$$

(b) Runge-Kutta of order four (classical case),

$$\begin{aligned} U(t) = {} & \frac{1}{2880}A'''' + \frac{1}{720}(A'''A - AA''') + \frac{1}{480}(A''A' - A'A'') \\ & + \frac{1}{480}(A''A^2 - 2AA''A + A^2A'') - \frac{1}{240}(A'^2A - 2A'AA' + 2AA'^2) \\ & + \frac{1}{240}(A^2A'A - AA'A^2) + \frac{1}{120}(A'A^3 - A^3A') - \frac{1}{120}A^5 \end{aligned} \tag{22}$$

where the primes denote derivation with respect to t. The equation for the principal-error function for the $\mathbf{z}^i$ solution is then reduced to (from equations (16) and (20)):

$$\dot{\mathbf{s}}^i = A\mathbf{s}^i + U\mathbf{z}^i, \qquad (i = 1, \ldots, k) \tag{23a}$$

$$\mathbf{s}^i(0) = 0. \tag{23b}$$

It should be remembered that since the Wronskian refers to the auxiliary initial-value problem, pertaining to the boundary-value problem (1a, b), the numerical difficulties in a neighborhood of a singular matrix E in (7) are not taken into account here. This situation will occur, for example, in the neighborhood of each eigenvalue of the boundary-value problem (1a, b) if $k = M$.

4. The discretization error of the Wronskian

When evaluating the determinant (10) by a numerical method, the truncation error occurring in each one of the $\mathbf{z}^i$ $(i = 1, \ldots, n)$ particular solutions (12) will propagate through the determinant computation. Denoting by D_n the determinant value when evaluated numerically (admitting zero round-off error), and taking equation (14) into (10) we obtain

$$D_n(z_n^1, \ldots, z_n^n) = D(z^1 + e^1, \ldots, z^n + e^n) \tag{24}$$

which can be expanded in the form

$$\begin{aligned} D_n(z_n^1, \ldots, z_n^n) = {} & D(z^1, \ldots, z^n) + D_1(e^1, z^2, \ldots, z^n) + \ldots \\ & + D_i(z^2, \ldots, e^i, \ldots, z^n) + \ldots + D_n(z^2, \ldots, e^n) + \ldots \end{aligned} \tag{25}$$

or, from the magnified error definition (15), and equation (25),

$$\begin{aligned} D_e(t) &= D_n(z_n^1, \ldots, z_n) - D(z^1, \ldots, z^n) \\ &= h^p [D_1(s^1, z^2, \ldots, z^n) + D_2(z^1, s^2, \ldots, z^n) + \ldots \\ &\quad + D_n(z^1, \ldots, z^{n-1}, s^n)] + O(h^{2p}) \\ &= h^p \sum_{i=1}^{n} D_i(z^1, \ldots, s^i, \ldots, z^n) + O(h^{2p}) \end{aligned} \tag{26}$$

where the vector s^i (solution of (23)) constitutes the ith column of the determinant D_i.

If we now take the derivative of $D_e(t)$ and neglect the higher-order terms in (26) we come up with

$$\frac{dD_e}{dt} = h^p \sum_{i=1}^{n} D_i'(z^1, \ldots, s^i, \ldots, z^n) \tag{27}$$

where the primes denote derivative with respect to t. Since the derivative of an nth order determinant can be expressed as the sum of n determinants, the jth of which is obtained from the original determinant by differentiating its jth row (or column), we can substitute the jth row of the determinant in (27) by the following expression obtained from equations (12), (20), and (23),

$$\dot{z}_j^i = \sum_{k=1}^{n} a_{jk} z_k^i \tag{28}$$

and

$$\dot{s}_j^i = \sum_{k=1}^{n} a_{jk} s_k^i + \phi_j^i(t, z). \tag{29}$$

After some calculations we end up with the expression

$$\frac{dD_e}{dt} = \left(\sum_{i=1}^{n} a_{ii} \right) h^p \sum_{i=1}^{n} D_i(z^1, \ldots, s^i, \ldots, z^n) + h^p \sum_{i=1}^{n} D_i(z, \ldots, \phi^i(t, z), \ldots, z^n), \tag{30}$$

or, after taking equations (26) into (30) and defining the determinant

$$D_\phi(t) = \sum_{i=1}^{n} D_i(\mathbf{z}, \ldots, \boldsymbol{\varphi}^i(t, \mathbf{z}), \ldots, \mathbf{z}^n), \tag{31}$$

we obtain

$$\frac{dD_e}{dt} = \sum_{i=1}^{n} a_{ii} D_e + h^p D_\phi(t). \tag{32}$$

We now integrate (32), under the initial condition $D_e(0) = 0$ (see equations (23b) and (26)), and obtain

$$D_e(t) = h^p \exp \int_0^t tr[A(\xi)]\, d\xi \cdot \int_0^t D_\phi(\xi) \exp\left[-\int_0^t tr[A(\xi)]\, d\xi\right] d\xi \tag{33}$$

where $tr[A(t)]$ denotes the trace of matrix $A(t)$.

The determinant $D_\phi(t)$ in (31) represents the sum of n determinants, the ith of which has the vector $\boldsymbol{\varphi}^i(t, \mathbf{z})$ in its ith column. If we expand the ith determinant in terms of the elements of its ith column and rearrange the resulting n^2 terms, we obtain an expression for $D_\phi(t)$ in which we have a sum of n determinants such that

$$D_\phi(t) = \sum_{i=1}^{n} \det \begin{bmatrix} z_1^1 & z_1^2 & \ldots & z_1^n \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \phi_i^1 & \phi_i^2 & \ldots & \phi_i^n \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ z_n^1 & z_n^1 & & z_n^n \end{bmatrix} \tag{34}$$

where the ith row is made up of the ith elements of the $\boldsymbol{\varphi}^1, \boldsymbol{\varphi}^2, \ldots$ vectors and $\boldsymbol{\varphi}^i = (\phi_1^i, \ldots, \phi_n^i)$ is the principal error function corresponding to the $\mathbf{z}^i$ particular solution.

Substituting the expressions

$$\phi_j^i = \sum_{k=1}^{n} u_{jk} z_k^i \tag{35}$$

obtained from equation (20), into equation (34), and making use of Abel's equation (11b), we obtain

$$D_\phi(t) = \left(\sum_{k=1}^{n} u_{ii}\right) D(z^1, \ldots, z^n)$$

$$= tr[U(t)]\, D(0) \exp\left(\int_0^t tr[A(\xi)]\, d\xi\right). \tag{36}$$

Taking (36) into (33) we obtain

$$D_e(t) = h^p D(0) \left[\exp\left(\int_0^t tr[A(\xi)]\, d\xi\right)\right] \int_0^t tr[U(\xi)]\, d\xi$$

or

$$D_e(t) = h^p D(t) \int_0^t tr[U(\xi)]\, d\xi. \tag{37}$$

Finally, from equations (11a), (26) and (37)

$$D_n(t) = D(t)\,[1 + h^p \int_0^t tr[U(\xi)]\, d\xi] \tag{38}$$

which is a remarkably simple expression for the Wronskian of the numerical solution of (1), although the expression for the trace of matrix $U(t)$ might become quite involved, as seen in equations (21) and (22).

From equation (38) the relative truncation error of the Wronskian can be defined as

$$E_d(t) = \frac{D_n(t) - D(t)}{D(t)} = h^p \int_0^t tr[U(\xi)]\, d\xi. \tag{39}$$

In those cases where the elements of the matrix A, in (1), are constants, the trace of the matrix $U(t)$ is also constant. In these cases the trace can easily be determined from equations (21) or (22). Denoting then the value of the trace of U by σ, the relative truncation error of the Wronskian becomes

$$E_d(t) = (\sigma h^p)t \tag{40}$$

which indicates a linear behavior of $E_d(t)$ with respect to time for the case of constant A.

On the other hand, if A depends on t and an analytical solution is not available for the integral in (38), one must be careful in numerical applications since numerical quadrature will be required.

5. Numerical examples

In order to test the validity of the results obtained previously, as well as to see how these results can be used in the estimation of 'optimum' integration step h, let us study the following cases.

I. Bessel's equation of order zero

Consider the boundary-value problem

$$\frac{d^2x}{dt^2} + \frac{1}{t}\frac{dx}{dt} + x = 0, \tag{41}$$

$$x(2) = 0.9187378, \qquad x(8) = 0.4875767,$$

$$x(5) = 0.6042942, \qquad x(12) = 0.2358398,$$

where the boundary conditions were generated integrating equation (41) by the Runge-Kutta method of fourth order with a time step equal to 0.001 in double-precision (15 digits on the IBM-370/165 computer where the data were generated).

Equation (41) can be rewritten, defining $\mathbf{z} = (x, dx/dt)$, in the form

$$\frac{d\mathbf{z}}{dt} = A(t)\mathbf{z}$$

where

$$A(t) = \begin{bmatrix} 0 & 1 \\ -1 & -1/t \end{bmatrix}. \tag{42}$$

For the modified Euler method ($\lambda = 1$), equations (21) and (42) give

$$Tr[U(t)] = \frac{1}{2}\left[\frac{1}{t^3} - \frac{1}{t}\right] \tag{43}$$

and thus, equations (39) and (43) give the following expression for the relative error of the Wronskian for the interval of integration $(1, t)$,

$$E_d = \frac{1}{2}\left[\ln t + \frac{1}{2}\left(\frac{1}{t^2} - 1\right)\right] h^2. \tag{44}$$

The behavior of the discretization error of the Wronskian was analysed by integrating the system (41), with the boundary conditions being met in the least square sense. The modified Euler method of integration was employed with double-precision calculations, thus admitting a practically null round-off error for results with six or seven digits. The relative error is calculated, equation (39), by evaluating numerically, during the integration, the Wronskian of the system, equation (10), and its exact value, equation (11b). The results are shown in

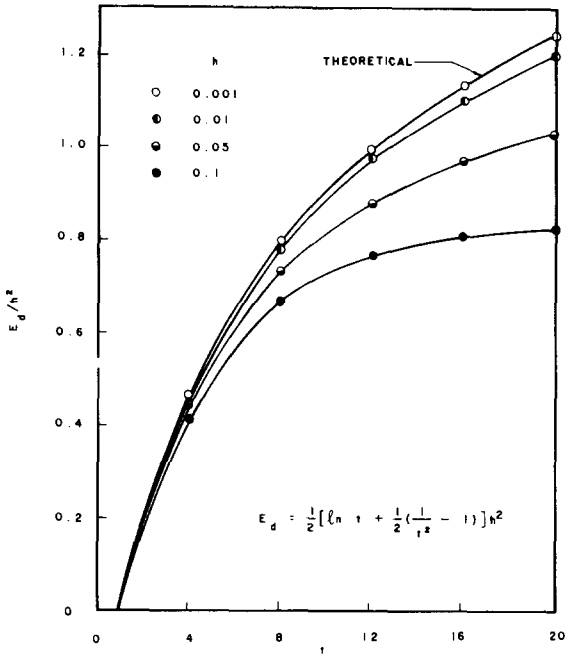

Figure 1. Discretization error of the Wronskian for Bessel's equation of order zero. Integration by the modified Euler method.

Figure 1 for integrations with several step values. It is seen that the results converge to equation (44) for small values of the step. This should be expected since the magnified error function given by equation (15) constitute an asymptotic expression for small steps.

A very interesting result was obtained in this study for the behavior of the discretization error of the Wronskian (calculated as described above), when single precision (six digits on the IBM-370/165 machine) was used. The results shown in Figure 2 indicate that for steps greater than 0.01 there is practically no round-off errors influence in the estimation of the discretization error of the Wronskian. On the other hand, for step values smaller than 0.01 the round-off errors dominate completely this calculation. In the same figure is plotted the behavior of the discretization and round-off errors of the integration of equation (41) with respect to the step size. The discretization errors were obtained by comparing the numerical solutions of (41) (average of twenty points) integrated with double precision arithmetic, for several values of h, and its exact solution. The round-off errors were obtained comparing the solutions of integrations in single and double precision; admitting, thus, the same discretization error during these integrations.

The analysis of the curves in Figure 2 indicates that the total minimum error (discretization plus round-off) during the integration process, which occur roughly in the intersection of the discretization and round-off error curves, can be estimated from the behavior of the discretization error of the Wronskian of the system. For the Bessel's equation (41) it is found that the 'optimum' integration step size, using single precision arithmetic, is about 0.01.

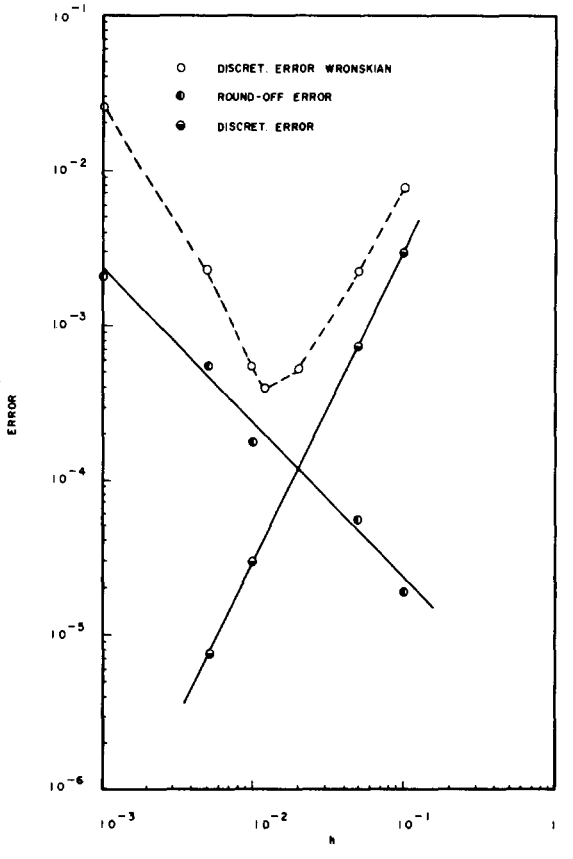

Figure 2. Error behavior with respect to the integration step for Bessel's equation of order zero.

II. Two degrees of freedom system

Let us consider the solution of the linear system

$$\begin{aligned}
&\frac{d^2x}{dt^2} + 0.4\,\frac{dx}{dt} + 2x - 0.2\,\frac{dy}{dt} - y = 0,\\
&\frac{d^2y}{dt^2} + 0.2\,\frac{dy}{dt} + y - 0.2\,\frac{dx}{dt} - x = 5\sin 3t,\\
&x(3) = 1.980410, \quad x(7) = -1.777150, \quad x(12) = 1.526180,\\
&y(3) = 3.027660, \quad y(7) = -3.501270, \quad y(12) = 2.987220.
\end{aligned} \tag{45}$$

Defining the vectors $\mathbf{z} = (x, y, dx/dt, dy/dt)$ and $\mathbf{a} = (0, 0, 0, 5)$, this system can be rewritten in the form

$$\frac{d\mathbf{z}}{dt} = A\mathbf{z} + \mathbf{a}\sin 3t$$

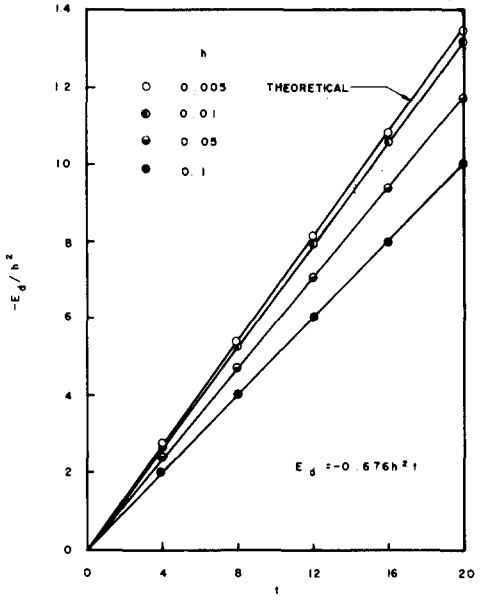

Figure 3. Discretization error of the Wronskian for the linear system (45). Integration by the modified Euler method.

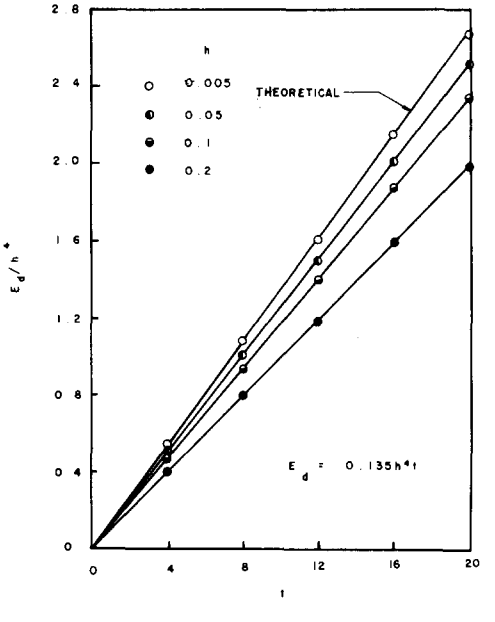

Figure 4. Discretization error of the Wronskian for the linear system (45). Integration by the fourth-order Runge-Kutta method.

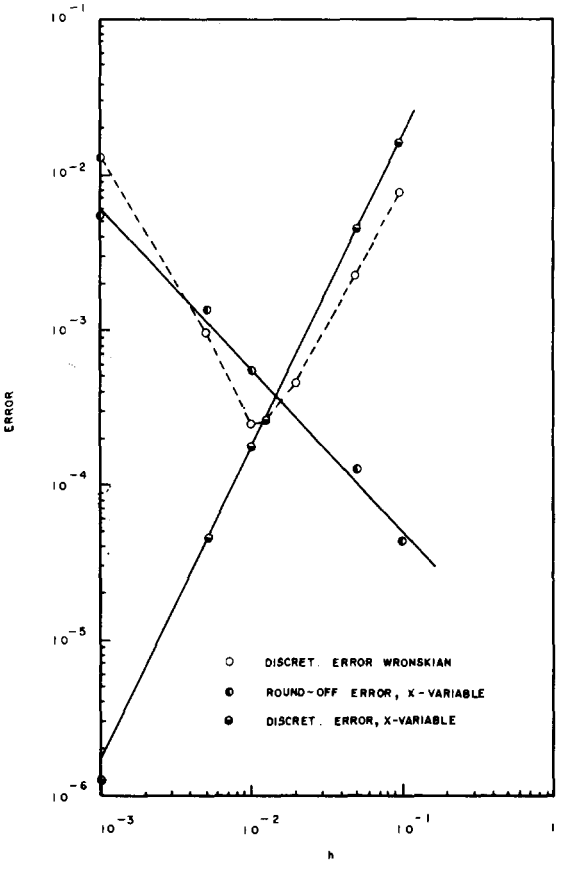

Figure 5. Error behavior with respect to the integration step for the linear system (45). Integration by the modified Euler method.

where

$$A = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -2 & 1 & -\cdot 4 & 2 \\ 1 & -1 & \cdot 2 & -\cdot 2 \end{bmatrix}. \tag{46}$$

Equations (21), (22), (39) and (46) give the following expression for the discretization error of the Wronskian for the modified Euler method and Runge-Kutta of fourth order:

$$E_d = -0.676\, h^2 t \quad \text{(Euler)}, \tag{47}$$

$$E_d = 0.135\, h^4 t \quad \text{(Runge-Kutta)}. \tag{48}$$

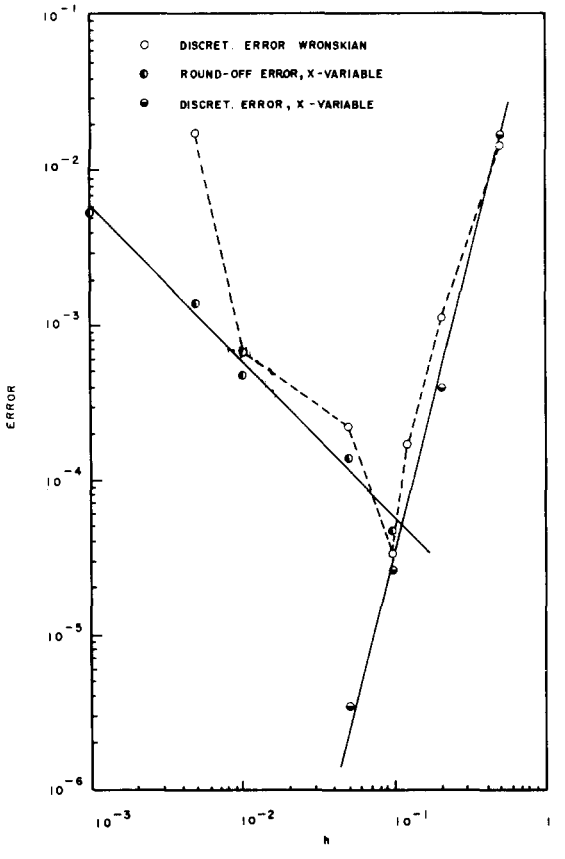

Figure 6. Error behavior with respect to the integration step for the linear system (45). Integration by the fourth-order Runge-Kutta method.

The behavior of these errors with respect to time (t) for this system is shown in Figures 3 and 4. The same procedure described for the solution of the Bessel's equation was used to obtain the curves indicated. Again, a remarkable agreement is found with the theoretical and numerical results for small values of h.

Figures 5 and 6 show the results of the error behavior for modified Euler and fourth-order Runge-Kutta integration methods, respectively. These results indicate that the discretization error of the Wronskian can also give for this case the 'optimum' integration step-size. For the modified Euler method, Figure 5 gives $h \simeq 0.01$; and for the fourth-order Runge-Kutta method Figure 6 gives $h \simeq 0.1$. In both cases single precision arithmetic is assumed to be employed during the numerical integration procedures.

6. Concluding remarks

A relatively simple expression was obtained for the discretization error of the Wronskian of linear systems for single-step numerical integration techniques. The results indicate that:

(i) the theoretical expressions for the error of the Wronskian (a scalar) agree fairly well with the numerical calculations; (ii) for linear systems with variable coefficients, the calculation of the error might become quite cumbersome, specially for higher-order methods; (iii) for linear systems with constant coefficients, the calculation of the error is very simple; (iv) from the analysis of the computed value of the Wronskian, during the integration procedure, its exact value (from Abel's equation), as well as from the expected error behavior of the error (obtained in this work), it is possible, in some cases, to estimate 'optimum' integration steps in the sense that the total error during the numerical computation is kept at a minimum value.

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