A note on the numerical integration of conservative systems of first-order ordinary differential equations

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Numerical integration of first-order conservative systems is also conservative. For practical computation this is a useful approximation within the effects of round-off error in application of the formulae. The result is invalidated when there is numerical instability and when finite arithmetic is used.

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The set of first-order ordinary differential equations

$$\frac{dy_i}{dx} = f_i(x, y_j), \quad i = 1, 2 \ldots m \tag{1}$$

represents a conservative system if the variables y_i satisfy a relationship of the form

$$\sum_i a_i y_i = C. \tag{2}$$

If several species are conserved there may be a number of such relationships. (2) is inherent in the form of the differential equations and arises from integration of the identity.

$$\Sigma_i a_i \frac{dy_i}{dx} \equiv 0. \tag{3}$$

In this note we show that if u_i are approximate solutions derived by use of any one of a number of commonly used numerical integration procedures then u_i also satisfy the relationship (2). u_i and y_i may differ as usual due to the truncation error of the integration formula. When finite arithmetic is used the relationship (2) is only approximately valid.

Finite-difference integration formulae in ordinate form may be written:

$$y_{i,n+1} = \sum_{j=0} \alpha_j y_{i,n-j} + h \sum_{k=0} \beta_k f_{i,n-k+1} + T_{i,n} \tag{4}$$

where h is the interval of integration and $T_{i,n}$ is the truncation error of the formula. If $\beta_0 = 0$, the formula is explicit, whereas for $\beta_0 \neq 0$ the formula is implicit. If $u_{i,n+1}$ is the function generated from (4) with neglect of $T_{i,n}$ and if y_i is conservative so that (3) is satisfied then we show that

$$\sum_i a_i u_{i,r} = C, \tag{5}$$

i.e. u_i is also a conservative system.

The proof is by induction.

If (5) is valid for $r \leqslant n$, then from (4) we have

$$\sum_i a_i u_{i,n+1} = \sum_i a_i \sum_j \alpha_j u_{i,n-j} + h \sum_i a_i \sum_k \beta_k f_{i,n-k+1}. \tag{6}$$

Using the conservation relations (3) and (5) for the given values we obtain

$$\sum_i a_i u_{i,n+1} = C \Sigma_j \alpha_j. \tag{7}$$

But,

$$\sum_j \alpha_j = 1 \tag{8}$$

is a necessary condition that u converges to y in the limit of small values of h and is satisfied by all integration formulae of the type (4). The result follows.

The conservation relations (1) and (3) may be used to prove a similar result for Runge-Kutta type formulae. For Taylor series methods, differentiated forms of the identity (3) enable the result to be obtained.

The significance of this result is that in numerical computation of such systems the conservation relation cannot be used as a guide to the accuracy of the solutions. Truncation errors in the formula (4) of arbitrary size may arise which do not invalidate the conservation relation for u.

Over one step we have

$$u_{i,n+1} = y_{i,n+1} - T_{i,n} \tag{9}$$

Clearly, since u and y are conservative, T is conservative so that

$$\Sigma_i a_i T_{i,n} = 0, \tag{10}$$

but $\sum_n T_{i,n}$, which represents the accumulated truncation error in u is not otherwise constrained and propagates in a manner dependent on the structure of the equations.

The phenomenon of numerical instability is associated with the replacement of a set of first-order equations by recurrence relations of higher order thus introducing spurious solutions. Numerical instability is present when these solutions grow faster than the true solutions of the differential equations. In practical computation the round-off procedure inevitably introduces components of the spurious solutions and instability may ensue. Round-off errors are random between limits and will vary in their effect from one equation of the set to another. The round-off procedure is not commutative with multiplication or addition so that exact relationships applying to the u_i now became inexact in an arbitrary fashion. In these circumstances the accuracy of the conservation relations may be used as an indication of the onset of numerical instability. We can not, however, use this relation as a test that truncation errors are negligible.

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