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NOTE

Errors in the Numerov and Runge-Kutta Methods

We consider the numerical solution of the Schrödinger equation

$$u''(x) = f(x)\,u(x) \tag{1}$$

by the Numerov [1] and Runge-Kutta [2] methods. Blatt [1] has asserted that the Numerov method is clearly superior to the Runge-Kutta method, because of the higher-order truncation error in the Numerov method. (The truncation error in the Numerov method is of order h^6, where h is the step length.)

The purpose of this note is to point out that this strong conclusion is unjustified, since the cumulative errors in the fourth-order Runge-Kutta method [2] (with truncation errors of order h^5) and the Numerov method are in fact of the same order—in each case the cumulative error at a fixed value of x is of order h^4.

Consider first the Runge-Kutta method, using the notation

$$u_j = u(x_j), \quad u'_j = u'(x_j).$$

In advancing the solution through a single step, from x_{j-1} to x_j say, the Runge-Kutta method uses u_{j-1} and u'_{j-1} as initial value data, and predicts approximate values of u_j and u'_j. (The considerations here apply equally whether we use the direct Runge-Kutta method for a second-order differential equation, or the method for a pair of first-order differential equations.) Let R_j and S_j be the (truncation) errors in u and u', respectively, incurred in integrating from x_{j-1} to x_j. Then the cumulative error in u after n steps is [3]

$$\begin{aligned}\Delta u(x_n) &= \sum_{j=1}^{n} [\chi'(x_j)\,R_j - \chi(x_j)\,S_j] \\ &\approx \frac{1}{h}\int_{x_0}^{x_n} [\chi'(x)\,R(x) - \chi(x)\,S(x)]\,dx,\end{aligned} \tag{2}$$

where $\chi(x)$ is the solution of the (adjoint) equation $\chi'' = f\chi$, subject to $\chi(x_n) = 0$, $\chi'(x_n) = 1$. In the fourth-order Runge-Kutta method [2], the truncation errors $R(x)$ and $S(x)$ are both of order h^5. It follows immediately from (2) that the cumulative error $\Delta u(x)$ is of order h^4.

local error

$\frac{1}{h}(h^5)$

cumulative vs local error

The Numerov method has a different structure, in that first derivatives are not considered, and the initial-value data for the calculation of u_j is provided by u_{j-1} and u_{j-2}. Equation (2) is therefore inapplicable. That the cumulative error is again of order h^4 may, however, be inferred from the fact that the Numerov method is equivalent to a second difference equation, or more directly by reference to a particular example. A convenient example is the differential equation

$$u''(x) = -u(x), \tag{3}$$

with the initial conditions

$$u(0) = 0, \quad u'(0) = 1, \tag{4}$$

which has the exact solution $u(x) = \sin x$. With starting values $u(0) = 0$, $u(h) = \sin h$, the Numerov method yields the result [4]

$$u(x) = \sin h \sin \lambda x / \sin \lambda h,$$

where

$$\lambda = \frac{1}{h} \cos^{-1}\left(\frac{12 - 5h^2}{12 + h^2}\right)$$
$$= 1 + h^4/480 + \cdots,$$

Same h^4 error in Num & RK

hence the cumulative error is

$$\Delta u(x) = (h^4/480)(\sin x - x \cos x) + \cdots, \tag{5}$$

which is manifestly of order h^4.

The magnitudes of the errors in the two methods have been explored for the differential equation (3) with initial conditions (4), and the results are shown in Table I, with N denoting the Numerov method, and RK the direct fourth-order Runge-Kutta method for a second-order differential equation. The Numerov errors agree with (5), and the Runge-Kutta errors show approximately the required h^4 dependence. It is seen that the Numerov method is only slightly superior if the same step length is used in both methods. However, the Runge-Kutta method

TABLE I

CUMULATIVE ERRORS MULTIPLIED BY 10^8

x	$\sin x$	N ($h = 0.1$)	RK ($h = 0.1$)	RK ($h = 0.2$)
0.8	0.71735609	3	56	911
1.6	0.99957360	22	53	904
2.4	0.67546318	51	−17	−224
3.2	−0.05837414	65	−103	−1649
4.0	−0.75680250	39	−126	−2104
4.8	−0.99616461	−29	−47	−892

requires values of $f(x)$ in (1) at the half-way points, thus if $f(x)$ requires extensive calculation, or is available only in tabular form, then the reasonable comparison is between Numerov $h = 0.1$ and Runge-Kutta $h = 0.2$ results. On that basis, the Numerov method is clearly superior.

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References

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4. Reference [3], Section IV–K.

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