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Automatic Step-Size Control for Runge-Kutta Integration*

In a recent paper Chase[1] investigated the stability of various predictor-corrector methods. He showed among other things that during integration of the initial value problem $y' = -a \cdot y + b$, $y(0) = 0$, $a > 0$, the modified Hamming method exhibits instability at an integration step h with $h \cdot a \geq 0.85$. It can be shown that the well known fourth-order Runge-Kutta method[2] remains stable for all h with $h \cdot a \leq 2.78$.[3] Inasmuch as Hamming's method requires two derivative evaluations per time step, as against four for the Runge-Kutta method, stable integration from 0 to 1 requires a minimum of $2.35 \cdot a$ derivative evaluations for Hamming's method as against $1.44 \cdot a$ derivative evaluations for the Runge-Kutta method. Thus the extra derivative evaluations per single time step for the Runge-Kutta method do not seem as serious a drawback as might at first appear.

A more serious problem arises in automatic step-size control. While a measure of automatic step-size control is relatively easily implemented in predictor-corrector methods, through a comparison of predicted and corrected values[4], the Runge-Kutta method has been conspicuous until now for its lack of any efficient method for automatic step-size control. It is the purpose of this paper to provide at least a partial remedy for this condition.

To this end consider the initial value problem $Y' = F(t, Y)$, $Y(0) = Y_0$, where Y and F are vectors and, noting that $k_5 = k_1$ for time $t + h$, set $k_5 = hF(t + h, Y + k)$, where $k = (1/6)(k_1 + 2k_2 + 2k_3 + k_4)$. Following up a suggestion by Hamming[5] and generalizing Collatz's rule of thumb,[6] we try to estimate the local truncation error by means of a linear combination of the k_i, $i = 1, \cdots, 5$, and achieve a measure of error control by computing $|E|$, where $|E|$ is some norm of E and

$$E = \sum_{i=1}^{5} a_i k_i .$$

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To determine the a_i, we require that E approximate the local truncation error in the initial value problem $y' = ay + b$, $y(0) = y_0$ or, in what amounts to the same, in the system $Y' = AY + B$, $Y(0) = Y_0$, where A and B are constant. Computation shows that for $E_5 = k_1 - 2k_3 - 2k_4 + 3k_5$ we obtain

$$E_5 = \frac{h^5}{8} A^4 Y'(t).$$

On the other hand, the local truncation error E_0 is given by

$$E_0 = h^5 A^4 \left(\sum_{k=0}^{\infty} \frac{h^k A^k}{(k+5)!} \right) Y'(t).$$

Thus, apart from the factor in parentheses, E_5 represents the local truncation error. If only the first four k_i are to be used, the best one can achieve is to use $E_4 = k_1 + k_4 - 2k_3$, obtaining

$$E_4 = \frac{h^4}{4} A^3 Y'(t).$$

Let us set $E_2 = k_1 - k_2$, and $E_3 = k_2 - k_3$. Computation shows that

$$E_2 = \frac{-h^2}{2} A Y'(t), \quad \text{and} \quad E_3 = \frac{-h^3}{4} A^2 Y'(t).$$

Collatz's rule of thumb, as applied to the initial value problem $y' = -ay + c$, $a > 0$, $y(0) = 0$ with solution $(c/a)(1 - e^{-at})$, becomes $|k_2 - k_3|/|k_1 - k_2| \leq r$ with, say, $r = 0.05$. This leads to $|E_3|/|E_2| = a \cdot h/2 \leq 0.05$. Hence, in this case, the rule of thumb prescribes a uniform step size independent of the local truncation error. On the other hand one has $E_4 = (h^4/4)\, a^3 ce^{-at}$ and $E_5 = (h^5/8)\, a^4 ce^{-at}$. It is seen that both E_4 and E_5 prescribe variable time steps and that they prescribe smaller steps during the transient region and larger ones in the steady state portion. When E_4 is used, a step size change (i.e., halving or doubling the step size) causes the truncation error to change by approximately a factor of 32, whereas the indicated error is changed by a factor of 16. Thus E_4 forces smaller steps than are necessary during the transient region and permits larger steps than warranted during the steady state. E_5 is relatively free from this defect.

Returning to Collatz's rule of thumb, one finds that like E_4, E_2 and E_3 can be used by themselves for step-size control; however, numerical experiments indicate that the distortions of the local truncation error force excessively small steps during the transient portion and thus bring about an attendant increase in derivative evaluations. As an unexpected advantage, both E_4 and E_5 seem to detect and control numerical instability in the steady state region.

In addition to its primary use the proposed step-size control can also be used to provide starting values and a proper initial integration step for those multi-step methods which are not self-starting. At the same time, it is to be noted that the error criteria advanced here may, in certain instances, provide only a partial remedy. Thus, for example, when $F(t,y)$ is independent of y, one obtains $E_4 = E_5 \cong h^3/4y^{(3)}(t)$ whereas the actual truncation error is of order $h^5\, y^{(5)}(t)$.

References

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