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ABSTRACT

Linear multistep methods for the solution of the equation $y'' = f(t,y)$ are studied by means of the test equation $y'' = -\omega^2 y$, with ω real. It is shown that the order of accuracy cannot exceed 2 for an unconditionally stable method.

Consider a real second order differential system

(1) $$y'' = f(t,y).$$

We assume that all solutions of (1) are bounded. In the particular case of a diagonalizable linear autonomous system, $y'' = Ay$, this means that the eigenvalues must all be real and negative. We shall therefore consider the test equation,

(2) $$y'' = -\omega^2 y \ , \quad \omega \text{ positive} .$$

Consider a linear multistep method, ($t_n = t_o + nh$, h = step size)

(3) $$\alpha_k y_{n+k} + \dots + \alpha_1 y_{n+1} + \alpha_o y_n = h^2 (\beta_k f(t_{n+k}, y_{n+k}) + \dots + \beta_o f(t_n, y_n))$$

with the generating polynomials

(4) $$\rho(\zeta) = \sum_{j=o}^{k} \alpha_j \zeta^j \ , \quad \sigma(\zeta) = \sum_{j=o}^{k} \beta_j \zeta^j \ .$$

We say that the method (3) is <u>unconditionally stable,</u> if all solutions of the difference equation, when it is applied to the test equation (2) with any step size h , are bounded. A <u>necessary</u> condition for this is that the characteristic equation,

(5) $$\rho(\zeta) = -(\omega h)^2 \sigma(\zeta) \ ,$$

has <u>no root outside the unit circle for any real</u> ωh . This condition is equivalent to :

$\sigma(\zeta)/\rho(\zeta)$ must not be real and non-positive for $|\zeta| > 1$.

Then that branch of $(\sigma(\zeta)/\rho(\zeta))^{1/2}$ which takes positive values for $\zeta > 1$ exists and satisfies the condition,

(6) $$\mathrm{Re}\ (\sigma(\zeta)/\rho(\zeta))^{1/2} > 0 \quad \text{for} \quad |\zeta| > 1 .$$

We shall now investigate the accuracy of the method (3). Its order of accuracy is p , if for any function $y \in C^{p+2}$,

$$\alpha_k y(t_{n+k}) + \ldots + \alpha_1 y\ \text{it},,,) + \alpha_o y(t_n) -$$

$$- h^2(\beta_k y''(t_{n+k}) + \ldots + \beta_o y''(t_n)) \sim ch^{p+2}\ y^{(p+2)}(t_n) .$$

c and p are independent of y . In particular, by choosing $y(t) = e^t$ we obtain,

$$\rho(e^h) - h^2\sigma(e^h) \sim ch^{p+2}, \qquad (h30) ,$$

i.e., if we set $e^h = \zeta$,

$$\rho(\zeta) - (\log \zeta)^2\sigma(\zeta) \sim c\,(\zeta-1)^{p+2} , \quad (\zeta \to 1) .$$

Note that $\rho(\zeta) \sim \frac{1}{2} \rho''(1)(\zeta-1)^2$ and put $c' = 2c/\rho''(1)$. Then,

$$\sigma(\zeta)/\rho(\zeta) \sim (\log \zeta)^{-2} \cdot (1 - c'(\zeta-1)^p + o((\zeta-1)^p))$$

(7) $$(\sigma(\zeta)/\rho(\zeta))^{1/2} \sim (\log \zeta)^{-1}\ (1 - \tfrac{1}{2} c'(\zeta-1)^p + o((\zeta-1)^p)) ,$$

where $\log \zeta$ is the branch of the logarithmic function which is real when ζ is positive (and therefore positive when $\zeta > 1$).

It is convenient to perform the transformations,

$$\zeta = \frac{z+1}{z-1}\ , \quad \left(\sigma\left(\frac{z+1}{z+1}\right)/\rho\left(\frac{z+1}{z-1}\right)\right)^{1/2} = g(z)$$

Note that

(8) $$z = \frac{\zeta+1}{\zeta-1},\quad \frac{\sigma(\zeta)}{\rho(\zeta)} = \left(g\left(\frac{\zeta+1}{\zeta-1}\right)\right)^2 \quad .$$

The conditions (6) and (7) then become,

(6') $$\operatorname{Re} g(z) > 0 \text{ for } \operatorname{Re} z > 0\ ,$$

and, for $z \to \infty$,

$$g(z) = \left(\log \frac{z+1}{z-1}\right)^{-1}\left(1 - \frac{1}{2}\, c'\left(\frac{z}{2}\right)^{-p} + o(z^{-p})\right)\ ,$$

and since $\left(\log \frac{z+1}{z-1}\right)^{-1} = \frac{1}{2}\, z - \frac{1}{6}\, z^{-1} + \ldots$, we obtain,

(7') $$g(z) = \frac{1}{2}\, z\left(1 - \frac{1}{3}\, z^{-2} + O(z^{-4} - \frac{1}{2}\, c'\left(\frac{z}{2}\right)^{-p} + o(z^{-p})\right)\ .$$

The following lemma is often useful.

<u>Lemma</u>. Let $f(z)$ be analytic and have positive real part for $\operatorname{Re} z > 0$. Assume that $f(z) - (az+b) \to 0$ uniformly when $z \to \infty$ in the right half plane, $a \geq 0$, $\operatorname{Re} b \geq 0$. Then either $\operatorname{Re}(f(z)-az) > 0$ when $\operatorname{Re} z > 0$, or $f(z) - az$ is an imaginary constant, which is equal to zero, if $f(z) - az$ is real for at least one z.

<u>Proof</u>. Let $-\infty < y < \infty$. Then, for $\operatorname{Re} z > 0$

$$\inf_{y} \varliminf_{z \to iy} \operatorname{Re}(f(z)-az) = \inf_{y} \varliminf_{z \to iy} \operatorname{Re} f(z) \geq 0 .$$

At infinity,

$$\lim_{z \to \infty} \operatorname{Re}(f(z)-az) = \operatorname{Re} b \geq 0 .$$

Then, by the minimum principle for harmonic functions, in the form given e.g., in [3, p. 203], either $\operatorname{Re}(f(z)-az) > 0$ for $\operatorname{Re} z > 0$ or $\operatorname{Re}(f(z)-az)$ is identically zero. In the latter case it follows from the Cauchy-Riemann equations that $\operatorname{Im}(f(z)-az) = \text{const.}$, and the lemma is proved.

<u>Remark.</u> The assumptions, $a \geq 0$, $\operatorname{Re} b \geq 0$ can be deduced from the other assumptions of the lemma.

By (6') and (7'), the lemma can be applied to the function $g(z)$. Hence $\operatorname{Re}(g(z) - \frac{1}{2} z) \geq 0$, but if $p > 2$ this is incompatible with the relation,

$$(7'') \qquad g(z) - \frac{1}{2} z = - \frac{1}{6} z^{-1} - \frac{1}{2} c' \left(\frac{z}{2}\right)^{1-p} + o(z^{\max(-2,1-p)})$$

since the dominant term for large $|z|$, i.e., $-\frac{1}{6} z^{-1}$, has a negative real part when $\operatorname{Re} z > 0$. <u>Hence $p \leq 2$.</u> If $p = 2$, then (7") can be true only if $-1/6 - c' \geq 0$, i.e., only if $c' \leq -1/6$. If $p = 2$ and $c' = -1/6$, then by (7"),

$$g(z) - \frac{1}{2} z = o(z^{-1}) , \qquad (z \to \infty)$$

If $g(z) - \frac{1}{2} z$ were not identically zero, it would behave like az^{-q}, say, for large z, where $q > 1$, $a \neq 0$, but then the real part could not be positive everywhere in the right half plane. Hence, if $p = 2$, $c' = -1/6$, then

$$g(z) = \frac{1}{2} z .$$

Then by (8),

$$\sigma(\zeta)/\rho(\zeta) = \frac{1}{4}(\zeta+1)^2/(\zeta-1)^2 .$$

The simplest pair (ρ,σ) which satisfies this equation is,

$$\rho(\zeta) = (\zeta-1)^2 , \ \sigma(\zeta) = \frac{1}{4}(\zeta+1)^2.$$

We would also multiply $\rho(\zeta)$ and $\sigma(\zeta)$ by a common factor $\varphi(\zeta)$, but this would only make the method (ρ,σ) more complicated without improving its accuracy.

So far we have only considered consequences of a necessary condition for unconditional stability. We therefore have to verify that the method generated by this particular pair (ρ,σ) is unconditionally stable. This follows from the fact that in this case the characteristic equation (5) has the solutions.

$$\zeta_1 = (1 + \frac{1}{2} i\omega h)/(1 - \frac{1}{2} i\omega h) , \ \zeta_2 = \bar{\zeta}_1 .$$

Since for $\omega h > 0$, $|\zeta_1| = |\zeta_2| = 1$, $\zeta_1 \neq \zeta_2$, the solutions of the difference equations are bounded. Hence, among the unconditinally stable formulas of the form (3), the local error is minimized, when

$$y_{n+2} - 2y_{n+1} + y_n = \frac{1}{4} h^2 (f(y_{n+2}) + 2f(y_{n+1}) + f(y_n)) . \tag{9}$$

This formula and its unconditional stability are mentioned by Richtmyer and Morton [7, p. 263] in connection with the solution of second order hyperbolic equations. Since ρ and σ are perfect squares, the method is equivalent to the linear multistep method for the first order system,

$$(10) \qquad \begin{aligned} y' &= z \\ z' &= f(t,y) \ , \end{aligned}$$

defined by

$$\rho(\zeta) = 5-1 \ , \ \sigma(\zeta) = \frac{1}{2}(\zeta+1$$

i.e. the trapezoidal method. Note that the system (10) is equivalent to the second order differential system (1). It is interesting to compare this with the well-known fact [1] that the trapezoidal has the smallest error constant of all A-stable linear multistep methods for first order systems.

We summarize our results:

THEOREM. The order of accuracy cannot exceed 2 for a linear multistep method of the form (2) which is unconditionally stable (in the sense defined on page 1). Among second order accurate methods the smallest error constant is obtained for the method defined by (9). This method is equivalent to the trapezoidal method for the first order system (10).

When this work was finished, R. Jeltsch made the writer aware of the article by Lambert and Watson [6] where a similar result is stated. The topic of their study is, however, not unconditional stability but periodicity, i.e. they require that all roots of (5) should have unit modulus which implies a restriction to even polynomials $r(z)$ and $s(z)$. Moreover, they omit the proof because it is lengthy.

Our theorem is similar to the old results, Dahlquist [1], that $p \leq 2$ for A-stable linear multistep methods for first order differential systems, but the proof is different. In fact, proofs along similar lines were given by Genin [4], Dahlquist [2] and Grigorieff [5, p 218].

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