The Lecture Contains:

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A-stable linear multistep methods must be implicit, and have order not greater than two. The best known A-stable method is the Trapezoidal rule, which has the additional advantage of processing an asymptotic expansion in even powers of the step length i.e.

$$y(t;h) \sim y(t) + A_2 h^2 + A_4 h^4 + A_6 h^6 + \cdots$$

thus permitting efficient use of the extrapolation processes. Its disadvantage is that if a moderate step length is used in the initial phase, then fast decaying components of the theoretical solution are represented numerically by slowly decaying components, resulting in a slowly decaying oscillatory error. This difficultly can be avoided either by choosing a very small step length in the initial phase or by using a moderate step length and applying in the first few steps the same smooth procedure as is used in Gragg's method, that is, y_n is replaced by $\hat{y}_n$ here $\hat{y}_n = \frac{1}{4} y_{n+1} + \frac{1}{2} y_n + \frac{1}{4} y_{n-1}$.

This procedure preserves the form of the asymptotic expansion.

The class of linear one-step methods of order one is given by

$$y_{n+1} - y_n = h[(1-\theta) f_{n+1} + \theta f_n] \qquad (9.6)$$

often referred to as the 'θ– method'. It follows that this is A-stable if and only if $\theta \le \frac{1}{2}$. One way in which the free parameter θ may be used to effect is to achieve exponential fitting; a concept proposed by Liniger and Willoughby.

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Exponential Fitting

Definition: A numerical method is said to be exponentially fitted at a (complex) value λ_0 if, when the method is applied to the scalar test problem $y' = \lambda y,\ y(t_0) = y_0$, with exact initial conditions, it yields the exact theoretical solution in the case when $\lambda = \lambda_0$.

The method (9.6) applied to the above test equation yields

$$y_n = y_0 \left[\frac{1+\theta h \lambda}{1-(1-\theta) h \lambda}\right]^n$$

This coincides with the theoretical solution in the case $\lambda = \lambda_0$ if we choose θ such that $(1+\theta\lambda_0 h)/[1-(1-\theta)h\lambda_0] = e^{h\lambda_0}$,

or

$$\theta = -\frac{1}{h\lambda_0} - \frac{e^{h\lambda_0}}{1-e^{h\lambda_0}}.$$

Note that we can only exponentially fit the method (9.6) to one value of λ, whereas for a general stiff system, the Jacobian will have m eigenvalues. Strategies for choosing the value at which (9.6) should be exponentially fitted; when we have some a-priori knowledge of the distribution of the eigen values of the Jacobian are discussed by Liniger and Willoughby. If we have no such knowledge, Liniger proposes θ be chosen to minimize

$$\max_{-\infty \le h\lambda \le 0} \left| e^{h\lambda} - \frac{1+\theta h\lambda}{1-(1-\theta)h\lambda} \right|$$

The value of θ which achieves this minimization is $\theta = 0.122$.

There is no point is looking for A-stable methods in the one-parameter family of implicit linear two-step methods since they all have order at least three, and so cannot be A-stable. However, if we retain a second parameter, we may write the family in the form

$$y_{n+2} - (1+a)\,y_{n+1} + a\,y_n = h\left\{\left[\frac{1}{2}(1+a)+\theta\right]f_{n+1} + \left[\frac{1}{2}(1-3a)-2\theta\right]f_{n+1} + \theta\, f_n\right\} \quad (9.7)$$

which now has order two in general. It is shown by liniger that methods of this family are A-stable if and only if $-1 < a < 1$ and $a + 2\theta > 0$. (Note that the first of these conditions implies zero stability).

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Backward Differentiation Methods

Let us now consider linear multistep methods which are not necessarily A-stable, but are $A(\alpha)$-stable or stiffly stable. Since stiff stability implies $A(\alpha)$-stability for some α, we need, in view of the theorem, look only at implicit linear multistep methods. With the usual notation for the characteristic polynomials of a linear multistep method, the associated stability polynomial is $\pi(r,\bar{h}) = \rho(r) - \bar{h}\sigma(r)$. Both $A(\alpha)$ and stiff stability require that the roots of $\pi(r,\bar{h})$ be inside the unit circle when $\bar{h}$ is real and $\bar{h} \longrightarrow -\infty$. In this limit, the roots of $\pi(r,\bar{h})$ approach those of $\sigma(r)$, and it is thus natural to choose $\sigma(r)$ so that its roots lie within the unit circle. In particular, the choice $\sigma(r) = \beta_K\, r^K$, which has all its roots at the origin, is appropriate. The resulting class of methods

$$\sum_{j=0}^{K} \alpha_j\, y_{n+j} = h\, \beta_K\, f_{n+K} \qquad (9.7)$$

are known as the of backward differentiation methods . The coefficients of K^{th}order K-step method, of this class are given in the following table for $K = 1,2,\ldots,6$.

K	β_K	α_6	α_5	α_4	α_3	α_2	α_1	α_0
1	1						1	-1
2	$\frac{2}{3}$					1	$-\frac{4}{3}$	$\frac{1}{3}$
3	$\frac{6}{11}$				1	$-\frac{18}{11}$	$\frac{9}{11}$	$-\frac{2}{11}$
4	$\frac{12}{25}$			1	$-\frac{48}{25}$	$\frac{36}{25}$	$-\frac{16}{25}$	$\frac{3}{25}$
5	$\frac{60}{137}$		1	$-\frac{300}{137}$	$\frac{300}{137}$	$-\frac{200}{137}$	$\frac{75}{137}$	$-\frac{12}{137}$
6	$\frac{60}{147}$	1	$-\frac{360}{147}$	$\frac{450}{147}$	$-\frac{400}{147}$	$\frac{225}{147}$	$-\frac{72}{147}$	$\frac{10}{147}$

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Regions of absolute stability for these methods may be found is Gear; for $K = 1,2,\dots,6$, all regions are finite, and the corresponding methods are stiffly stable and $A(\alpha)$–stable.

Finally, if we settle for something less than $A(\alpha)$-stability, the methods proposed by Robertson are of interest. These comprise a one-parameter family obtained by taking the following linear combination of Simpson's rule and the two-step Adams-Moultan method:

$$(1-\alpha)\left[y_{n+2} - y_n - \frac{h}{3}(f_{n+2} + 4\, f_{n+1} + f_n)\right] + \alpha\left[y_{n+2} - y_{n+1} - \frac{h}{12}(\, 5f_{n+2} + 5\, f_{n+1} - f_n)\right],$$
$$0 \leq \alpha < 2$$

These methods have order three if $\alpha \neq 1$ and the regions of absolute stability are large, almost circular, regions in the half plane $\operatorname{Re} \bar{h} \leq 0$, the intervals of absolute stability being $[6\alpha/(\alpha-2), 0]$. (Note that as $\alpha \to 2,$ zero instability threatens). Such methods are appropriate for moderately stiff systems.

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Runge-Kutta methods for Stiff systems

Explicit Runge-Kutta methods have rather small regions of absolute stability. On the other hand it is rather easier to find A-stable implicit Runge-Kutta methods than to find A-stable implicit linear multistep methods. For example, Ehle has shown that Butcher's R-stage implicit Runge-Kutta methods of order 2 R, namely

$$y_{n+1} - y_n = h\,\phi(t_n, y_n, h)$$

$$\phi(t, y, h) = \sum_{r=1}^{R} C_r\, K_r$$

$$K_r = f\left(t + h\,a_r, y + h\sum_{s=1}^{R} b_{rs}\;K_s\right), r = 1,2,\ldots,R$$

$$a_r = \sum_{s=1}^{R} b_{rs}\;,\qquad r = 1,2,\ldots,R$$

[The functions K_r are no longer defined explicitly but by a set of R implicit equations, in general non linear.]

are all A-stable; thus there exist A-stable methods of this type of arbitrarily high order. L-stable implicit Runge-Kutta methods are also possible.

However, all such methods suffer a serious practical disadvantage in that the solution of the implicit nonlinear equations at each step is considerably harder to achieve in the case of implicit Runge-Kutta methods than in the case of implicit linear multistep methods. If we consider the R-stage fully implicit Runge-Kutta method given above, applied to a m-dimensional stiff system, then it is clear that the $K_r, r = 1,2,\ldots,R$ are also m-vectors. It follows that at each step we have to solve a system of m R simultaneous nonlinear equations by some form of Newton-iteration and this will converge only if we can find a suitably accurate initial iterate. This constitutes a formidable computational task.

If the Runge-Kutta method is semi-explicit, then the m R simultaneous equations split into R distinct sets of equations, each set containing m equations- a less daunting prospect. The class of semi-explicit methods developed by Butcher, namely [That an R-stage semi explicit method can attain higher order than an R-stage explicit method is demonstrated by the following fourth-order three-stage method quoted by Butcher]

$$y_{n+1} - y_n = \frac{h}{6}(K_1 + 4\,K_2 + K_3)$$

$$K_1 = f(x_n, y_n)$$

$$K_2 = f\left(x_n + \frac{1}{2}h, y_n + \frac{1}{4}\,h\,K_1 + \frac{1}{4}\,h\,K_2\right)$$

$$K_3 = f\,(x_n + h, y_n + h\,K_2)$$

are not, however, A-stable.

It is clear from the above discussion that our troubles with stiff systems are not over when we find as A-or L-stable method; the real test is the efficiency with which we can handle the resultant implicitness.

Problems

1. Find the stiffness ratio for the system

   $u' = -10u + 9V$

   $v' = 10u - 11V$

   What is the largest step length which can be used with a fourth order Runge-Kutta method?

2. Show that the Trapezoidal rule is A-stable and the backward Euler method is L-stable.
3. Consider a one-parameter family of one-step methods given by

   $y_{n+1} - y_n = h[(1-\theta)\, f_{n+1} + \theta\, f_n]$

   Find its order and investigate A-stability of the method.

4. Consider a two-parameter family of two step methods given by

   $y_{n+2} - (1+a)\, y_{n+1} + a\, y_n = h\left\{\left[\frac{1}{2}(1+a) + \theta\right] f_{n+1} + \left[\frac{1}{2}(1-3a) - 2\theta\right] f_{n+1} + \theta\, f_n\right\}$

   Find its order and investigate A-stability of the method.

5. Show that the Trapezoidal rule is exponentially fitted at 0, and the backward Euler method is exponentially fitted at $-\infty$..

6. Consider the backward differentiation methods

   $\sum_{j=0}^{K} \alpha_j\, y_{n+j} = h\, \beta_K\, f_{n+K}$

   for $K = 1,2$. Shows that these methods are A-stable.

7. Show that the following semi-explicit method of order two given by

   $y_{n+1} - y_n = \frac{h}{2}(K_1 + K_2)$

   with

   $K_1 = f(t_n, y_n)$

   $K_2 = f\left(t_n + h, y_n + \frac{1}{2}\, h\, K_1 + \frac{h}{2}\, K_2\right)$

   is A-stable.

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