13.6. Stability of linear multistep methods.

Definition: 1st and 2nd characteristic polynomial of a multistep method:

$$\rho(z) = z^{p+1} - \sum_{i=0}^{p} a_i z^{p-i}, \qquad \sigma(z) = \sum_{i=-1}^{p} b_i z^{p-i}.$$

The linear multistep method is consistent if $\rho(1) = 0$ and $\rho'(1) = \sigma(1)$. The first identity is obvious. The second implies

$$(p+1) - \sum_{i=0}^{p} (p-i)a_i = \sum_{i=-1}^{p} b_i.$$

Hence

$$p(1 - \sum_{i=0}^{p} a_i) + 1 - \sum_{i=0}^{p} (-i)a_i - \sum_{i=-1}^{p} b_i = 0.$$

Since the first term in the sum is zero, then so is the second.

Definition: The linear multistep method is said to be zero-stable (satisfy the root condition) if no root of the characteristic polynomial $\rho(z)$ has modulus greater than one and if every root of modulus one is simple.

Theorem 13. A necessary condition for convergence of a linear multistep method is that it be zero-stable.

Proof. We only give the proof in the case that the roots of $\rho(z)$ are real simple roots. If the method is convergent, then it is convergent for the IVP y' = 0, y(0) = 0, whose solution is y(x) = 0. For this problem, the method becomes $y_{n+1} = \sum_{i=0}^{p} a_i y_{n-i}$. If the method is convergent, then by (i), for any x > 0,

$$\lim y_n^h = 0, \quad n \to \infty, \quad h \to 0, \quad nh = x$$

for all solutions $\{y_n\}$ of the difference equation satisfying (ii) $\lim_{h\to 0} y_k(h) = 0, k = 0, \ldots, p$. We first show that all roots have modulus ≤ 1 . Let z = r be a real root of $\rho(z)$. Then $y_n = r^n$ is a solution of the difference equation and so is $y_n = hr^n$. Note that this second solution satisfies (ii). Hence, (i) must hold, i.e., $\lim_{n\to\infty} xr^n/n = 0$. Now

$$\lim_{n \to \infty} xr^n / n = x \lim_{n \to \infty} r^n / n = 0$$

if $0 \leq |r| \leq 1$. If r > 1, using L'Hospital's rule,

$$x \lim_{n \to \infty} r^n / n = x \lim_{n \to \infty} r^n \ln r / 1 = \infty.$$

A similar result hold if r < -1. Hence for (i) to hold, we require $|r| \le 1$.

Theorem 14. A necessary and sufficient condition for a linear multistep method to be convergent is that it be consistent and zero-stable.

Proof. We have shown these conditions are necessary. The proof of sufficiency can be found in Henrici: Discrete Variable Methods in Ordinary Differential Equations. \Box

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Example: Midpoint rule: $y_{n+1} = y_{n-1} + 2hf_n$. Then p = 1, $a_0 = 0$, $a_1 = 1$, $b_{-1} = 0$, $b_0 = 2$, $b_1 = 0$. Hence $\sum_{i=0}^{p} a_i = 1$ and $-\sum_{i=0}^{p} ia_i + \sum_{i=1}^{p} b_i = -1 + 2 = 1$, so the method is consistent. To check zero-stability, we find the roots of the characteristic polynomial $\rho(z) = z^{p+1} - \sum_{i=0}^{p} a_i z^{p-i} = z^2 - a_1 = z^2 - 1$. The roots are $z = \pm 1$. Since both roots have modulus 1 and both are simple, the method is zero-stable. Hence, the method is convergent.

Question: How high an order can be achieved in a (p+1) step method if it is consistent and zero-stable? In seeking high order methods, we automatically get consistency; zero-stability poses a more difficult constraint. Recall that a (p+1) step method has (2p+3) coefficients, p+1 a_i s and p+2 b_i 's. If the method is explicit, this number is reduced by one. Hence, we can expect at most order 2p + 2 for an implicit method and 2p + 1 for an explicit method (recall that if a method has order r, it is exact for all polynomials of degree $\leq r$). However, the following result is known.

Theorem 15. (Dahlquist) No zero-stable p + 1 step linear multistep method can have order exceeding p + 2 when p is even or exceeding p + 3 when p is odd.

A zero-stable p+1 step method which has order p+3 is called an optimal method. It can be shown that for an optimal method, all the roots of $\rho(z)$ lie on the unit circle.

Example: Simpson's rule: $y_{n+1} = y_{n-1} + (h/3)[f_{n+1} + 4f_n + f_{n-1}]$. Since p = 1, this is a two-step method. The local truncation error is $-(1/90)h^5y^{(5)}(\xi)$. It is a fourth order method, so Simpson's rule is an optimal method. However, we shall see that Simpson's rule has computational disadvantages that make it unsuitable as a general purpose method. These disadvantages are shared by all optimal order methods. Hence, we will not choose the coefficients in a multistep method solely to achieve maximum order.

To understand this issue, consider the problem y' = -y, y(0) = 1, whose exact solution is $y(x) = e^{-x}$. We apply the midpoint rule method $y_{n+1} = y_{n-1} + 2hf_n$, which in this case becomes $y_{n+1} + 2hy_n - y_{n-1} = 0$. Since this is a linear difference equation with constant coefficients, we solve it by first computing the roots of the characteristic polynomial $\rho(z) = z^2 + 2hz - 1 = 0$. Then $z = -h \pm \sqrt{1 + h^2}$, so the general solution has the form

$$y_n = C_1(-h + \sqrt{1+h^2})^n + C_2(-h - \sqrt{1+h^2})^n$$

Set $y_0 = 1$ and leave y_1 arbitrary for the moment and solve for C_1 and C_2 .

$$y_0 = 1 = C_1 + C_2,$$
 $y_1 = C_1(-h + \sqrt{1 + h^2}) + C_2(-h - \sqrt{1 + h^2}).$

Then

$$C_1 = \frac{1}{2} + \frac{y_1 + h}{2\sqrt{1 + h^2}}, \qquad C_2 = \frac{1}{2} - \frac{y_1 + h}{2\sqrt{1 + h^2}}$$

Inserting this result, we get

$$y_n = \left(\frac{1}{2} + \frac{y_1 + h}{2\sqrt{1 + h^2}}\right)(-h + \sqrt{1 + h^2})^n + \left(\frac{1}{2} - \frac{y_1 + h}{2\sqrt{1 + h^2}}\right)(-h - \sqrt{1 + h^2})^n.$$

If we compute the Taylor series of the function $f(h) = \sqrt{1+h^2}$ about h = 0, we get (since f'(0) = 0) that

$$f(h) = f(0) + hf'(0) + O(h^2) = 1 + O(h^2).$$

Hence, for h sufficiently small, the term $-h + \sqrt{1+h^2} = 1 - h + O(h^2) < 1$ and so $(-h + \sqrt{1+h^2})^n \to 0$ as $n \to \infty$. However, $|-h - \sqrt{1+h^2}| = 1 + h + O(h^2) > 1$, so that unless we choose y_1 so that $\frac{1}{2} - \frac{y_1+h}{2\sqrt{1+h^2}} = 0$, $\lim_{n\to\infty} |y_n| = \infty$.

The above is an example of numerical instability. The true solution $e^{-x} \to 0$ as $x = nh \to \infty$, while for fixed h the approximate solution $\to \infty$ as $n \to \infty$.

However, if we consider the convergence of the sequence $\{y_n^h\}$ as $h \to 0$, $n \to \infty$ and x = nh and make the assumption that $\lim_{h\to 0} y_1^h = y_0 = 1$, then

$$\lim_{h \to 0} \left(\frac{1}{2} + \frac{y_1 + h}{2\sqrt{1 + h^2}} \right) = 1, \qquad \lim_{h \to 0} \left(\frac{1}{2} - \frac{y_1 + h}{2\sqrt{1 + h^2}} \right) = 0.$$

Furthermore, for x = nh,

$$\lim_{h \to 0, n \to \infty} (-h + \sqrt{1 + h^2})^n = \lim_{h \to 0} [(-h + \sqrt{1 + h^2})^{1/h}]^x.$$

Let $y = \lim_{h \to 0} [(-h + \sqrt{1 + h^2})^{1/h}]$. Then

$$\ln y = \lim_{h \to 0} [\ln(-h + \sqrt{1 + h^2})/h] = \lim_{h \to 0} \frac{\frac{2h}{2\sqrt{1 + h^2}} - 1}{\sqrt{1 + h^2} - h} = -1.$$

Hence, $\ln y = -1$ so $y = e^{-1}$. Then

$$\lim_{h \to 0, n \to \infty} C_1 (-h + \sqrt{1 + h^2})^n = e^{-x}$$

Thus, the first part of the solution of the difference equation gives an approximation to the true solution of the differential equation. One can easily show that $|(-h - \sqrt{1 + h^2})^n| \leq e^x$. Hence, the second term is converging to zero, so the approximate solution is converging to the true solution.

To summarize, one root of the characteristic polynomial gives a solution that approximates the true solution. A second root gives a parasitic solution which for fixed h eventually blows up to give a bad overall approximation. Since the method converges, for any x and ϵ , one can find a value of h such that $|y_n^h - e^{-x}| < \epsilon$. However, since the parasitic solution grows like e^x , this h would have to be impractically small for any reasonable size x.