Numerical Analysis – Lecture 13[1]

Technique 3.32 Inasmuch as no multistep method of order $p \geq 3$ may be A-stable, stability properties of BDF, say, are satisfactory for most stiff equations. The point is that in many stiff linear systems in applications the eigenvalues are not just in $\mathbb{C}^-$ but also well away from $\mathrm{i}\mathbb{R}$. *[Analysis of nonlinear stiff equations is difficult and well outside the scope of this course.]* All BDF methods of order $p \leq 6$ (i.e., all convergent BDF methods) share the feature that the linear stability domain $\mathcal{D}$ includes a wedge about $(-\infty, 0)$: such methods are said to be A_0*-stable.*

Example 3.33 Unlike multistep methods, implicit high-order RK may be A-stable. For example, recall the 3rd-order method

$$\begin{aligned}
\boldsymbol{k}_1 &= \boldsymbol{f}\left(t_n, \boldsymbol{y}_n + \tfrac{1}{4}h(\boldsymbol{k}_1 - \boldsymbol{k}_2)\right), \\
\boldsymbol{k}_2 &= \boldsymbol{f}\left(t_n + \tfrac{2}{3}h, \boldsymbol{y}_n + \tfrac{1}{12}h(3\boldsymbol{k}_1 + 5\boldsymbol{k}_2)\right), \\
\boldsymbol{y}_{n+1} &= \boldsymbol{y}_n + \tfrac{1}{4}h(\boldsymbol{k}_1 + 3\boldsymbol{k}_2).
\end{aligned}$$

from the last lecture. Applying it to $y' = \lambda y$, we have

$$\begin{aligned}
hk_1 &= h\lambda\left(y_n + \tfrac{1}{4}hk_1 - \tfrac{1}{4}hk_2\right), \\
hk_2 &= h\lambda\left(y_n + \tfrac{1}{4}hk_1 + \tfrac{5}{12}hk_2\right).
\end{aligned}$$

This is a linear system, whose solution is

$$\left[\begin{array}{c} hk_1 \\ hk_2 \end{array}\right] = \left[\begin{array}{cc} 1-\frac{1}{4}h\lambda & \frac{1}{4}h\lambda \\ -\frac{1}{4}h\lambda & 1-\frac{5}{12}h\lambda \end{array}\right]^{-1} \left[\begin{array}{c} h\lambda y_n \\ h\lambda y_n \end{array}\right] = \frac{h\lambda y_n}{1-\frac{2}{3}h\lambda+\frac{1}{6}(h\lambda)^2} \left[\begin{array}{c} 1-\frac{2}{3}h\lambda \\ 1 \end{array}\right],$$

therefore

$$y_{n+1} = y_n + \tfrac{1}{4}hk_1 + \tfrac{3}{4}hk_2 = \frac{1+\frac{1}{3}h\lambda}{1-\frac{2}{3}h\lambda+\frac{1}{6}h^2\lambda^2}y_n.$$

Let

$$r(z) = \frac{1+\frac{1}{3}z}{1-\frac{2}{3}z+\frac{1}{6}z^2}.$$

Then $y_{n+1} = r(h\lambda)y_n$, therefore, by induction, $y_n = [r(h\lambda)]^n y_0$ and we deduce that

$$\mathcal{D} = \{z \in \mathbb{C} \,:\, |r(z)| < 1\}$$

We wish to prove that $|r(z)| < 1$ for every $z \in \mathbb{C}^-$, since this is equivalent to A-stability. This will be done by a technique that can be applied to other RK methods. According to the *maximum modulus principle* from Complex Methods, if g is analytic in the closed complex domain $\mathcal{V}$ then $|g|$ attains its maximum on $\partial\mathcal{V}$. We let $g = r$. This is a rational function, hence its only singularities are the poles $2 \pm \mathrm{i}\sqrt{2}$ and g is analytic in $\mathcal{V} = \mathrm{cl}\,\mathbb{C}^- = \{z \in \mathbb{C} \,:\, \mathrm{Re}\, z \leq 0\}$. Therefore it attains its maximum on $\partial\mathcal{V} = \mathrm{i}\mathbb{R}$ and

$$\text{A-stability} \qquad \Leftrightarrow \qquad |r(z)| < 1, \quad z \in \mathbb{C}^- \qquad \Leftrightarrow \qquad |r(\mathrm{i}t)| \leq 1, \quad t \in \mathbb{R}.$$

In turn,

$$|r(\mathrm{i}t)|^2 \leq 1 \qquad \Leftrightarrow \qquad |1 - \tfrac{2}{3}\mathrm{i}t - \tfrac{1}{6}t^2|^2 - |1 + \tfrac{1}{3}\mathrm{i}t|^2 \geq 0.$$

[1]Please email all corrections and suggestions to these notes to `A.Iserles@damtp.cam.ac.uk`. All handouts are available on the WWW at the URL `http://www.damtp.cam.ac.uk/user/na/PartII/Handouts.html`.

But $|1-\frac{2}{3}\mathrm{i}t-\frac{1}{6}t^2|^2-|1+\frac{1}{3}\mathrm{i}t|^2=\frac{1}{36}t^4\geq 0$ and it follows that the method is A-stable.

Example 3.34 It is possible to prove that the 2-stage *Gauss–Legendre method*

$$\begin{aligned}\boldsymbol{k}_1 &= \boldsymbol{f}(t_n+(\tfrac{1}{2}-\tfrac{\sqrt{3}}{6})h, \boldsymbol{y}_n+\tfrac{1}{4}h\boldsymbol{k}_1+(\tfrac{1}{4}-\tfrac{\sqrt{3}}{6})h\boldsymbol{k}_2),\\ \boldsymbol{k}_2 &= \boldsymbol{f}(t_n+(\tfrac{1}{2}+\tfrac{\sqrt{3}}{6})h, \boldsymbol{y}_n+(\tfrac{1}{4}+\tfrac{\sqrt{3}}{6})h\boldsymbol{k}_1+\tfrac{1}{4}h\boldsymbol{k}_2),\\ \boldsymbol{y}_{n+1} &= \boldsymbol{y}_n+\tfrac{1}{2}h(\boldsymbol{k}_1+\boldsymbol{k}_2)\end{aligned}$$

is of order 4. [You can do this for $y'=f(y)$ by expansion, but it becomes messy for $\boldsymbol{y}'=\boldsymbol{f}(t,\boldsymbol{y})$.] It can be easily verified that for $y'=\lambda y$ we have $y_n=[r(h\lambda)]^n y_0$, where $r(z)=(1+\frac{1}{2}z+\frac{1}{12}z^2)/(1-\frac{1}{2}z+\frac{1}{12}z^2)$. Since the poles of r reside at $3\pm\mathrm{i}\sqrt{3}$ and $|r(\mathrm{i}t)|\equiv 1$, we can again use the maximum modulus principle to argue that $\mathcal{D}=\mathbb{C}^-$ and the Gauss–Legendre method is A-stable.

Problem 3.35 The step size h is not some preordained quantity: it is a parameter of the method (in reality, many parameters, since we may vary it from step to step). The basic input of a well-written computer package for ODEs is not the step size but the *error tolerance:* the level of precision, as required by the user. The choice of $h>0$ is an important tool at our disposal to keep a local estimate of the error beneath the required tolerance in the solution interval. In other words, we need not just a *time-stepping algorithm*, but also mechanisms for *error control* and for amending the step size.

Technique 3.36 (*The Milne device*) Suppose that we wish to monitor the error of the trapezoidal rule

$$\boldsymbol{y}_{n+1}=\boldsymbol{y}_n+\tfrac{1}{2}h[\boldsymbol{f}(\boldsymbol{y}_n)+\boldsymbol{f}(\boldsymbol{y}_{n+1})]. \tag{3.11}$$

We already know that the order is 2. Moreover, substituting the true solution we deduce that

$$\boldsymbol{y}(t_{n+1})-\{\boldsymbol{y}(t_n)+\tfrac{1}{2}h[\boldsymbol{y}'(t_n)+\boldsymbol{y}'(t_{n+1})]\}=-\tfrac{1}{12}h^3\boldsymbol{y}'''(t_n)+\mathcal{O}\big(h^4\big)\,.$$

Therefore, the error in each step is increased roughly by $-\frac{1}{12}h^3\boldsymbol{y}'''(t_n)$. The number $c_{\mathrm{TR}}=-\frac{1}{12}$ is called the *error constant* of TR. To estimate the error in a single step we assume that $\boldsymbol{y}_n=\boldsymbol{y}(t_n)$ and subtract $\boldsymbol{y}(t_{n+1})=\boldsymbol{y}(t_n)+\frac{1}{2}h[\boldsymbol{y}'(t_n)+\boldsymbol{y}'(t_{n+1})]-\frac{1}{12}h^3\boldsymbol{y}'''(t_n)+\mathcal{O}\big(h^4\big)$ from the numerical method: this yields $\boldsymbol{y}_{n+1}-\boldsymbol{y}(t_{n+1})=c_{\mathrm{TR}}h^3\boldsymbol{y}'''(t_n)+\mathcal{O}\big(h^4\big)$. Similarly, each multistep method (but not RK!) has its own error constant. For example, the 2nd order 2-step Adams–Bashforth method

$$\boldsymbol{y}_{n+1}-\boldsymbol{y}_n=\tfrac{1}{2}h[3\boldsymbol{f}(t_n,\boldsymbol{y}_n)-\boldsymbol{f}(t_{n-1},\boldsymbol{y}_{n-1})], \tag{3.12}$$

has the error constant $c_{\mathrm{AB}}=\frac{5}{12}$.

The idea behind the *Milne device* is to use two multistep methods of the same order, one explicit and the second implicit (e.g., (3.12) and (3.11), respectively), to estimate the local error of the implicit method. For example, *locally,*

$$\begin{aligned}\boldsymbol{y}_{n+1}^{\mathrm{AB}} &\approx \boldsymbol{y}(t_{n+1})-c_{\mathrm{AB}}h^3\boldsymbol{y}'''(t_n)=\boldsymbol{y}(t_{n+1})-\tfrac{5}{12}h^3\boldsymbol{y}'''(t_n),\\ \boldsymbol{y}_{n+1}^{\mathrm{TR}} &\approx \boldsymbol{y}(t_{n+1})-c_{\mathrm{TR}}h^3\boldsymbol{y}'''(t_n)=\boldsymbol{y}(t_{n+1})+\tfrac{1}{12}h^3\boldsymbol{y}'''(t_n).\end{aligned}$$

Subtracting, we obtain the estimate

$$h^3\boldsymbol{y}'''(t_n)\approx -2(\boldsymbol{y}_{n+1}^{\mathrm{AB}}-\boldsymbol{y}_{n+1}^{\mathrm{TR}}),$$

therefore

$$\boldsymbol{y}_{n+1}^{\mathrm{TR}}-\boldsymbol{y}(t_{n+1})\approx -\tfrac{1}{6}(\boldsymbol{y}_{n+1}^{\mathrm{AB}}-\boldsymbol{y}_{n+1}^{\mathrm{TR}})$$

and we use the right hand side as an estimate of the local error.

Note that TR is a far better method than AB: it is A-stable, hence its *global* behaviour is superior. We employ AB *solely* to estimate the local error. This adds very little to the overall cost of TR, since AB is an explicit method.