2 - Ordinary Differential Equations 2

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1 Linear multi-step methods

In previous lecture we have talked about one-step methods: they calculate $\hat{y}_{n+1}$ using the previous step $\hat{y}_n$. More general methods include (linear) multi-step methods: they calculate $\hat{y}_{n+1}$ using the previous k steps $\hat{y}_n, \ldots, \hat{y}_{n-k}$. More formally, given a sequence of equally spaced mesh points $t_n = nh$ with step size h, a linear k-step method reads

$$\sum_{j=-1}^{k} \alpha_j \hat{y}_{n-j} = h \sum_{j=-1}^{k} \beta_j f(t_{n-j}, \hat{y}_{n-j}) \tag{1}$$

for some properly chosen coefficients α_j and β_j (with $\alpha_{-1} = 1$). There exists many systematic ways of generating (meaningful) linear multi-step methods, such as Backward Differentiation (BDF) methods and Adams methods.

1.1 Backward differentiation methods

These methods are defined by the formula

$$\sum_{j=-1}^{k} \alpha_j \hat{y}_{n-j} = h f(t_{n+1}, \hat{y}_{n+1})$$

The coefficients α_j are determined by imposing the method to have the highest order of consistency possible.

Question: What is the backward differentiation formula for $k = 0, 1, 2$?

1.2 Adams

Adams methods use quadrature (i.e. approximation of integrals) formula to evaluate $\hat{y}_n$ using the integral form of the ODE:

$$y_{n+1} - y_n = \int_{t_n}^{t_{n+1}} f(s, y(s))\, ds$$

To approximate the integral above Adams method replace f with its interpolating polynomial at nodes $y_n, \dots, y_{n-k}$. For example, taking $k = 0$ corresponds to simply approximate $f(s, y(s)) \simeq f(t_n, y_n)$ for $s \in [t_n, t_{n+1}]$; then one gets

$$y_{n+1} - y_n = \int_{t_n}^{t_{n+1}} f(s, y(s))\, ds \simeq \int_{t_n}^{t_{n+1}} f(t_n, y_n)\, ds = h f(t_n, y_n)$$

That is, we recovered Explicit Euler's method. For $k = 1$, we approximate f with its interpolating polynomial at nodes t_n, t_{n-1}, i.e. $f(s, y(s)) \simeq f(t_n, y_n) + (f(t_{n-1}, y_{n-1}) - f(t_n, y_n))\frac{s-t_n}{t_{n-1}-t_n}$. The methods then reads

$$\begin{aligned}
\hat{y}_{n+1} - \hat{y}_n &= \int_{t_n}^{t_{n+1}} \left[f(t_n, \hat{y}_n) + (f(t_{n-1}, \hat{y}_{n-1}) - f(t_n, \hat{y}_n)) \frac{s - t_n}{t_{n-1} - t_n} \right] ds \\
&= h f(t_n, \hat{y}_n) + [f(t_{n-1}, \hat{y}_{n-1}) - f(t_n \hat{y}_n)] \frac{h^2}{-2h} \\
&= \frac{h}{2} [3 f(t_n, \hat{y}_n) - f(t_{n-1}, \hat{y}_{n-1})] \qquad (2)
\end{aligned}$$

2 Convergence analysis

In the first lecture, we saw that two simple conditions (namely consistence and Lipschitzianity of the one-step operator Φ) guaranteed convergence of one-step methods. A similar analysis holds for linear multi-step methods; in this case convergence is guaranteed if and only if two fundamentals properties hold: *consistence* and *zero-stability*.

2.1 Consistency

Consistency of linear k-step methods is defined in the same way as for one step methods. We define the truncation error for formula (1) as

$$T_n = \frac{\sum_{j=-1}^{k} \alpha_j y_{n-j} - h \sum_{j=-1}^{k} \beta_j f(t_{n-j}, y_{n-j})}{h \sum_{j=-1}^{k} \beta_j}$$

Again, this is the error that comes from approximating the true solution at one time step using formula (1). A method is said to be consistent if the truncation error satisfies $T(h) = \sup_{0 \le n \le T/h} T_n = o(1)$ as $h \to 0$.

Question: Show that the Adams method defined in (2) satisfies $T(h) = O(h^2)$.

2.2 Zero-stability

The other property needed for convergence is zero-stability. What does zero-stability mean? It means that, for finite time intervals, the difference between two sequences given by formula (1) is going to be bounded by the difference on the sequence in the first k steps, as $h \to 0$ (in

other words, the error does not explode). It turns out (cfr. (Quarteroni et al., 2010), Section 11.6) that this is equivalent to the solutions to

$$\sum_{j=-1}^{k} \alpha_j \hat{y}_{n-j} = 0 \tag{3}$$

being bounded as $n \to \infty$, for any choices of $\hat{y}_0, \ldots, \hat{y}_k$ (this motivates the term *zero-stability*, as the above is the linear k-step method (1) applied to the ODE $\dot{y} = 0$). A standard result from discrete difference equations (cfr. (Quarteroni et al., 2010), Section 11.4) says that any solution to (3) is of the form

$$\hat{y}_n = \sum_{j=0}^{\ell} \left(\sum_{s=0}^{m_\ell - 1} \gamma_{sj} n^s \right) r_j^n$$

for some $\gamma_{sj} \in \mathbb{R}$, where the r_j's are the roots of the polynomial

$$p(z) = z^{k+1} + \alpha_0 z^k + \cdots + \alpha_{k-1} z + \alpha_k$$

and m_j is the multiplicity of root r_j. It follows that a method is zero-stable if and only if $|r_j| \leq 1$ for every j, and $|r_j| = 1$ implies $m_j = 1$.

Question: Prove Theorem 12.4 in (Süli and Mayers, 2003).

Question: Consider the Adams three-step method

$$\hat{y}_{n+3} = \hat{y}_{n+2} + h\left[\frac{23}{12} f(t_{n+2}, \hat{y}_{n+2}) - \frac{4}{3} f(t_{n+1}, \hat{y}_{n+1}) + \frac{5}{12} f(x_n, \hat{y}_n)\right]$$

Show that the characteristic polynomial for this method is given by $p(z) = z^3 - z^2$, and conclude that the method is zero-stable.

2.3 Dahlquist's equivalence theorem

Dahlquist's equivalence theorem says that for a method (1), if f is Lipschitz and the starting data consistent, if the method verifies $T(h) = O(h^p)$, then it converges if and only if it is zero-consistent, and in that case the error verifies $e(h) = O(h^p)$, as $h \to 0$.

3 Absolute stability

Last time we saw that even if a method is convergent, this does not imply that the numerical solution will stay bounded as $t_n \to \infty$, even if the actual solution does. One typically needs to impose conditions on the step size h. A way to formalize this concept is through the notion of absolute stability. Consider the ODE

$$\begin{aligned} \dot{y}(t) &= -\lambda y(t) \\ y(0) &= 1 \end{aligned}$$

The solution is given by $y(t) = \exp(-\lambda t)$. If $\mathrm{Re}(\lambda) < 0$, y goes to 0 as $t \to \infty$ increases; in the first lecture we saw that different methods require different bounds on h for this to happen. We can do the same kind of analysis for a linear multi-step method. Substituting $f(y) = -\lambda y$ in equation (1), we get

$$\sum_{j=-1}^{k} \alpha_j \hat{y}_{n-j} = -\lambda h \sum_{j=-1}^{k} \beta_j \hat{y}_{n-j} \quad \Rightarrow \quad \sum_{j=-1}^{k} (\alpha_j + \lambda h \beta_j) \hat{y}_{n-j} = 0$$

Therefore, we know that

$$\hat{y}_n = \sum_{j=0}^{\ell} \left(\sum_{s=0}^{m_\ell - 1} \gamma_{sj} n^s \right) r_j^n(\lambda h)$$

where $r_j(\lambda h)$ are the roots of the characteristic polynomial

$$p(z; \lambda h) = \sum_{j=-1}^{k} (\alpha_j + \lambda h \beta_j) z^{k-j}$$

The approximation $\hat{y}_n$ stays bounded for $n \to \infty$ if $|r_j(\lambda h)| \leq 1$ for all j's and $|r_j(\lambda h)| = 1$ implies $m_j = 1$; $y_n = o(1)$ as $n \to \infty$ if and only if $|r_j(\lambda h)| < 1$ for all j. The region

$$\mathcal{R} = \{\lambda h : |r_j(\lambda h)| < 1\}$$

is called *region of absolute stability*. Of course, different methods come with different regions of absolute stability. Their study is important for the case when we want to solve *stiff systems*, that are systems for which specific methods are forced to use small step-sizes to give a good approximation. These include, among others, systems such that the Jacobian of $\mathbf{f}$ has all of its eigenvalues with negative real part but with large ratio (in absolute value).

Adams methods In figure 1 are displayed the regions of stability (they are the regions included inside the curves) for Adams methods of order $k = 1, 2, 3$. We can see that region of stability decreases as the order increases. This indicates that such methods are not good for stiff problems.

Runge-Kutta In figure 2 are displayed the regions of stability (they are the regions included inside the curves) for Runge-Kutta methods of order $k = 1, 2, 3, 4$. In this case, the regions increase as the order increases; although they are still small compared to other methods.

Backward differentiation method In figure 3 are displayed the regions of stability (they are the regions included outside the curves) for BDF methods of order $k \in [6]$. We can see that these methods are better suited to stiff systems than the previous two. On the negative side, such methods are implicit and thus typically more computationally expensive than explicit methods.

3.1 Stiff systems

Question: Why does the definition of stiff problems depend on the ratio between maximum and minimum eigenvalue (as opposed to minimum eigenvalue only)?

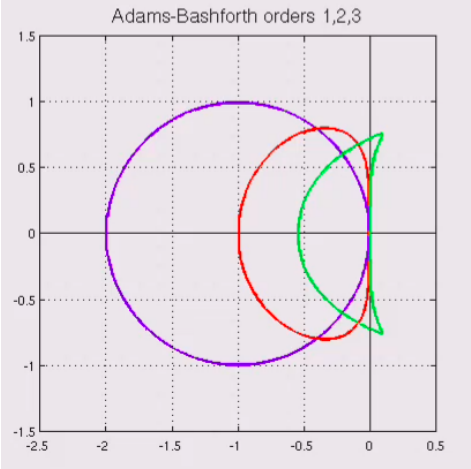

Figure 1: Regions of stability of Adams methods ($k = 1, 2, 3$).

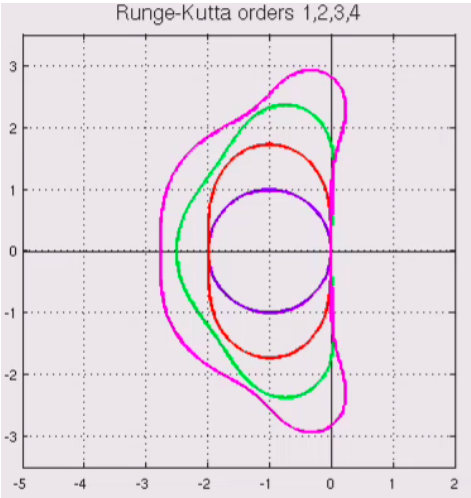

Figure 2: Regions of stability of Runge-Kutta methods ($k = 1, 2, 3, 4$).

We look more closely to a simple stiff system with $n = 2$. Consider the system

$$\dot{\mathbf{y}}(t) = \mathbf{A}\mathbf{y}(t)$$
$$\mathbf{y}(0) = \mathbf{y}_0$$

where $\mathbf{A} \in \mathbb{R}^{2\times 2}$ has eigenvalues $\lambda_1 = -1$, $\lambda_2 = -1000$ (and let $\mathbf{v}_1$, $\mathbf{v}_2$ the correspondent eigenvectors). The solution to this system reads

$$\mathbf{y}(t) = \alpha_1 e^{-t}\mathbf{v}_1 + \alpha_2 e^{-1000t}\mathbf{v}_2$$

for some $\boldsymbol{\alpha} \in \mathbb{R}^2$. Using Explicit Euler's method to approximate the solution we get

$$\mathbf{y}_0 = \alpha_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2$$
$$\hat{\mathbf{y}}_1 = \mathbf{y}_0 + h\mathbf{A}\mathbf{y}_0 = \sum_{i=1}^{2} \alpha_i(1 + h\lambda_i)\mathbf{v}_i$$

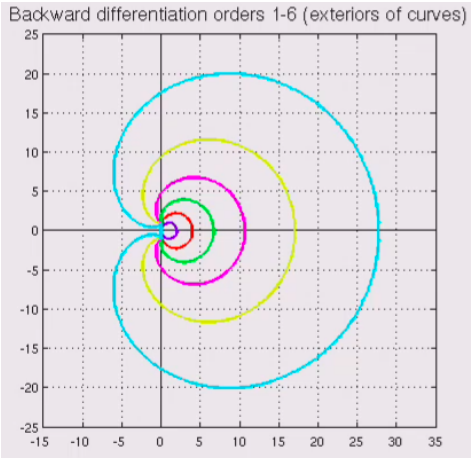

Figure 3: Regions of stability of BDF methods ($k \in [6]$).

Iterating, we get

$$\hat{\mathbf{y}}_n = \sum_{i=1}^{2} \alpha_i (1 + h\lambda_i)^n \mathbf{v}_i$$

We need to require $0 < 1 + h\lambda_i < 1$ for the solution to *well behave*, which in our case it implies $h < 10^{-3}$. Notice that this is required to have convergence for the $\mathbf{v}_2$ component of $\mathbf{y}(t)$. Nevertheless, this component is negligible in the actual solution, which instead dominated by $e^{-t}\mathbf{v}_1$. Here is the catch: we needed to impose a strict condition on h to properly approximate a negligible part of the solution. Of course this could have been avoided in this toy example, as we knew the exact solution, but it becomes relevant in practice when we deal with much more complicated system. This explains the importance for methods well suited to deal with stiff systems.

References

Quarteroni, A., R. Sacco, and F. Saleri
2010. *Numerical mathematics*, volume 37. Springer Science & Business Media.

Süli, E. and D. F. Mayers
2003. *An introduction to numerical analysis*. Cambridge university press.