Numerical Solution of Differential Equations I

Endre Süli

Mathematical Institute
University of Oxford
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Lecture 9

Stiff problems

Consider an initial-value problem for a *system* of m ODEs:

$$\mathbf{y}' = \mathbf{f}(x, \mathbf{y}), \qquad \mathbf{y}(a) = \mathbf{y}_0, \tag{1}$$

where $\mathbf{y} = (\mathbf{y}_1, \ldots, \mathbf{y}_m)^{\mathrm{T}}$.

A linear k-step method for the numerical solution of (1) is

$$\sum_{j=0}^{k} \alpha_j \mathbf{y}_{n+j} = h \sum_{j=0}^{k} \beta_j \mathbf{f}_{n+j}, \qquad \text{where } \mathbf{f}_{n+j} = \mathbf{f}(x_{n+j}, \mathbf{y}_{n+j}). \tag{2}$$

Suppose, for simplicity, that $\mathbf{f}(x, \mathbf{y}) = A\mathbf{y} + \mathbf{b}$ where $A \in \mathbb{R}^{m \times m}$ is a constant matrix and $\mathbf{b} \in \mathbb{R}^m$ is a constant (column) vector.

Then (2) becomes

$$\sum_{j=0}^{k} (\alpha_j I - h\beta_j A)\mathbf{y}_{n+j} = h\sigma(1)\mathbf{b}, \tag{3}$$

where $\sigma(1) = \sum_{j=0}^{k} \beta_j \, (\neq 0)$ and I is the $m \times m$ identity matrix.

Let us suppose that the eigenvalues λ_i, $i = 1, \ldots, m$, of the matrix A are distinct. Then, there exists a nonsingular matrix H such that

$$HAH^{-1} = \Lambda = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \lambda_m \end{bmatrix}. \qquad (4)$$

Define $\mathbf{z} = H\mathbf{y}$ and $\mathbf{c} = h\sigma(1)H\mathbf{b}$. Then (3) becomes

$$\sum_{j=0}^{k} (\alpha_j I - h\beta_j \Lambda)\mathbf{z}_{n+j} = \mathbf{c}, \qquad (5)$$

or, in component-wise form,

$$\sum_{j=0}^{k} (\alpha_j - h\beta_j \lambda_i) z_{n+j,i} = c_i,$$

where $z_{n+j,i}$ and c_i, $i = 1, \ldots, m$, are the components of $\mathbf{z}_{n+j}$ and $\mathbf{c}$ respectively. Each of these m equations is completely decoupled from the other $m-1$ equations.

Thus we are now in the setting of the previous lecture where we considered linear multistep methods for a single ODE.

However, there is a new feature here: because the numbers λ_i, $i = 1, \ldots, m$, are eigenvalues of the matrix A, they need not be real numbers. As a consequence the parameter $\bar{h} := h\lambda$, where λ is any of the m eigenvalues, can be a complex number.

This leads to the following modification of our earlier definition of absolute stability.

Definition

A linear k-step method is said to be **absolutely stable** in an open set $\mathcal{R}_A$ of the complex plane if, for all $\bar{h} \in \mathcal{R}_A$, all roots r_s, $s = 1, \ldots, k$, of the stability polynomial $\pi(r, \bar{h})$ associated with the method satisfy $|r_s| < 1$. The set $\mathcal{R}_A$ is called the **region of absolute stability** of the method.

Clearly, the interval of absolute stability of a linear multistep method is a subset of its region of absolute stability.

Exercise

a) *Find the region of absolute stability of Euler's explicit method when applied to* $y' = \lambda y$, $y(x_0) = y_0$, $\lambda \in \mathbb{C}$, $\mathrm{Re}\ \lambda < 0$.

b) *Suppose that Euler's explicit method is applied to the second-order differential equation*

$$y'' + (1-\lambda)y' - \lambda y = 0, \qquad y(0) = 1, \quad y'(0) = -\lambda - 2,$$

rewritten as a first-order system in the vector $(u, v)^{\mathrm{T}}$, *with* $u = y$ *and* $v = y'$, $\lambda \in \mathbb{C}$, $\mathrm{Re}\ \lambda < 0$, *and let* $|\lambda| \gg 1$.

What choice of the step size $h \in (0, 1)$ *will guarantee absolute stability in the sense of the last definition?*

Solution:

a) For Euler's explicit method $\rho(z) = z - 1$ and $\sigma(z) = 1$, so that

$$\pi(z; \bar{h}) = \rho(z) - \bar{h}\sigma(z) = (z - 1) - \bar{h} = z - (1 + \bar{h}), \quad \bar{h} := h\lambda.$$

This has the root $r = 1 + \bar{h}$. Hence the region of absolute stability is

$$\mathcal{R}_A = \{\bar{h} \in \mathbf{C} \, : \, |1 + \bar{h}| < 1\},$$

which is an open unit disc centred at -1.

b) Now writing $u = y$ and $v = y'$ and $\mathbf{y} = (u, v)^{\mathrm{T}}$, the initial-value problem for the given second-order differential equation can be recast as

$$\mathbf{y}' = A\mathbf{y}, \qquad \mathbf{y}(0) = \mathbf{y}_0,$$

where

$$A = \begin{pmatrix} 0 & 1 \\ \lambda & \lambda - 1 \end{pmatrix} \quad \text{and} \quad \mathbf{y}_0 = \begin{pmatrix} 1 \\ -\lambda - 2 \end{pmatrix}.$$

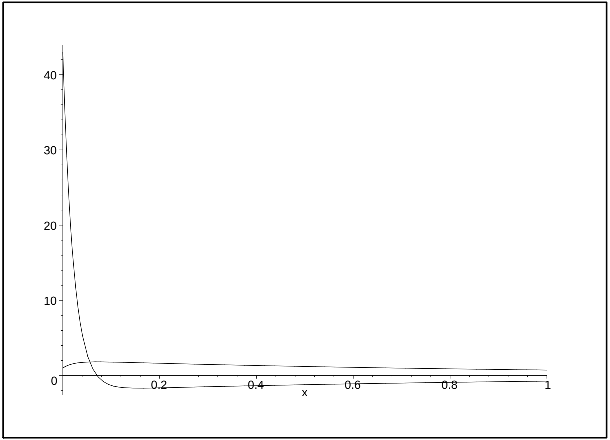
The eigenvalues of A are the roots of the characteristic polynomial of A,

$$\det(A - zI) = z^2 + (1 - \lambda)z - \lambda.$$

Hence, $r_1 = -1$ and $r_2 = \lambda$, and we deduce that the method is absolutely stable provided that $|1 + h\lambda| < 1$. It is an easy matter to show that

$$u(x) = 2\mathrm{e}^{-x} - \mathrm{e}^{\lambda x}, \qquad v(x) = -2\mathrm{e}^{-x} + \lambda \mathrm{e}^{\lambda x}.$$

The graphs of u and v are shown on the next slide for $\lambda = -45$. $\diamond$



v varies rapidly near $x = 0$ while u is slowly varying for $x > 0$ and v is slowly varying for $x > 1/45$. Nevertheless, we are forced to use a step size of $h < 2/45$ in order to ensure that the method is absolutely stable.

To ensure the absolute stability, the mesh size h may have to be chosen exceedingly small, $h < 2/(-\lambda)$, smaller than an accurate approximation of the solution for $x \gg 1/(-\lambda)$ would necessitate. Systems of differential equations which exhibit this behaviour are generally referred to as **stiff systems**.

Stiffness of an ODE is a concept that lacks a rigorous definition.[1]

A historic and pragmatic 'definition' by Curtis and Hirschfelder[2] reads: stiff equations are equations where the implicit Euler method works significantly better than the explicit Euler method.

[1] See G. Söderlind, L. Jay, and M. Calvo, *Stiffness 1952–2012: Sixty years in search of a definition.* BIT Numerical Mathematics, June 2015 55(2), 531–558.

[2] *Integration of stiff equations.* Proceedings of the National Academy of Sciences, March 1, 1952 38 (3) 235–243.

Stability of numerical methods for stiff systems

To motivate the various definitions of stability that follow, we begin with a simple example.

Consider Euler's implicit method for

$$y' = \lambda y, \qquad y(0) = y_0, \qquad \text{where } \lambda \in \mathbb{C}.$$

The stability polynomial of the method is $\pi(z, \bar{h}) = \rho(z) - \bar{h}\sigma(z)$ where $\bar{h} = h\lambda$, $\rho(z) = z - 1$ and $\sigma(z) = z$.

Since the only root of the stability polynomial is $z = 1/(1 - \bar{h})$, we deduce that the method has the region of absolute stability

$$\mathcal{R}_A = \{\bar{h} \in \mathbb{C} : |1 - \bar{h}| > 1\}.$$

$\mathcal{R}_A$ includes the whole of the left open complex half-plane.

Definition (Dahlquist (1963))

A linear multistep method is said to be *A*-stable if its region of absolute stability, $\mathcal{R}_A$, contains the whole of the left open complex half-plane $\mathrm{Re}(h\lambda) < 0$.

Thus, for example, the implicit Euler method is *A*-stable.

As the next theorem shows, this definition is far too restrictive.

Theorem (Dahlquist (1963))

(i) *No* explicit *linear multistep method is A-stable.*

(ii) *The order of an A-stable* implicit *linear multistep method cannot exceed* 2.

(iii) *The second-order A-stable linear multistep method with smallest error constant is the trapezium rule.*

This motivates the following, less restrictive notion of stability.

Definition (Widlund (1967))

A linear multistep method is said to be $A(\alpha)$-**stable**, $\alpha \in (0, \pi/2)$, if its region of absolute stability $\mathcal{R}_A$ contains the infinite open wedge in the complex plane

$$W_\alpha = \{\bar{h} \in \mathbb{C} \,|\, \pi - \alpha < arg(\bar{h}) < \pi + \alpha\}.$$

A linear multistep method is said to be $A(0)$-**stable** if it is $A(\alpha)$-stable for some $\alpha \in (0, \pi/2)$.

A linear multistep method is A_0 stable if $\mathcal{R}_A$ includes the negative real axis in the complex plane.

Remark

If $\mathrm{Re}\,\lambda < 0$ *for a given* λ *then* $\bar{h} = h\lambda$ *either lies inside the wedge* W_α *or outside* W_α *for* all *positive* h.

Consequently, if all eigenvalues λ *of the matrix* A *happen to lie in some wedge* W_α *then an* $A(\alpha)$*-stable method can be used for the numerical solution of the initial-value problem without any restrictions on the step size* h.

In particular, if all eigenvalues of A *are real and negative, then an* $A(0)$ *stable method can be used.*

Theorem

(i) *No* explicit *linear multistep method is* $A(0)$*-stable.*

(ii) *The only* $A(0)$*-stable linear* k*-step method whose order exceeds* k *is the trapezium rule.*

(iii) *For each* $\alpha \in [0, \pi/2)$ *there exist* $A(\alpha)$*-stable linear* k*-step methods of order* p *for which* $k = p = 3$ *and* $k = p = 4$*.*

A different way of loosening the concept of A-stability was proposed by Gear (1969).

The motivation behind it is the fact that for a typical stiff problem the eigenvalues of the matrix A which produce the fast transients all lie to the left of a line $\mathrm{Re}\,\bar{h} = -a$, $a > 0$, in the complex plane, while those that are responsible for the slow transients are clustered around zero.

Definition (Gear (1969))

A linear multistep method is said to be **stiffly stable** if there exist positive real numbers a and c such that $\mathcal{R}_A \supset \mathcal{R}_1 \cup \mathcal{R}_2$ where

$$\mathcal{R}_1 = \{\bar{h} \in \mathbf{C} \,:\, \mathrm{Re}\,\bar{h} < -a\},$$
$$\mathcal{R}_2 = \{\bar{h} \in \mathbf{C} \,:\, -a \le \mathrm{Re}\,\bar{h} < 0,\ \ -c \le \mathrm{Im}\,\bar{h} \le c\}.$$

It is clear that stiff stability implies $A(\alpha)$-stability with

$$\alpha = \arctan(c/a).$$

More generally, we have the following chain of implications:

A-stability $\Rightarrow$ stiff-stability $\Rightarrow$ $A(\alpha)$-stability $\Rightarrow$ $A(0)$-stability $\Rightarrow$ A_0-stability.