Lecture # 27
The Method of Lines and Large Stiff Systems

To motivate our discussion, we consider the dimensionless heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad t \geq 0, x \in [0,1] \tag{1}$$

It is accompanied by the initial condition

$$u(x,0) = g(x)$$

and the boundary conditions

$$u(0,t) = u_L(t), \quad u(1,t) = u_R(t).$$

We can approximate this with a system of ordinary differential equations. Let

$$x_k = k\Delta x, \quad k = 0, \ldots, n+1$$

where $\Delta x = 1/n+1$. We then use the finite difference approximation

$$\frac{\partial^2 u(x_k,t)}{\partial x^2} = \frac{u(x_{k+1},t) - 2u(x_k,t) + u(x_{k-1},t)}{(\Delta x)^2} + O((\Delta x)^2)$$

We define the functions $u_k(t), k = 1, \ldots, n$ by

$$u_k(t) \approx u(x_k, t)$$

and then have them satisfy

$$u_k'(t) = \frac{u_{k+1})t) - 2u_k(t) + u_{k-1}(t)}{(\Delta x)^2}, \quad k = 1, \ldots, n$$

where the boundary conditions are enforced by

$$u_L(t) = u_0(t), \quad u_R(t) = u_{n+1}(t).$$

If we let

$$\mathbf{u}(t) = (u_1(t), \ldots, u_n(t))^T$$

then we have the system of ordinary differential equations

$$\mathbf{u}'(t) = A\mathbf{u}(t) + \boldsymbol{\phi}(t) \tag{2}$$

where

$$A = \begin{pmatrix} -2 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & -2 & 1 & \cdots & \cdots & \cdots & \cdots \\ 0 & 1 & -2 & 1 & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdot & \cdot & \cdots & \cdots & 1 & -2 & 1 \\ \cdot & \cdot & \cdot & \cdots & \cdots & 1 & -2 \end{pmatrix}$$

and

$$\boldsymbol{\phi}(t) = \frac{1}{(\Delta x)^2} \begin{pmatrix} u_L(t) \\ 0 \\ \vdots \\ 0 \\ u_R(t) \end{pmatrix}.$$

The initial conditions can be expressed as

$$\mathbf{u}(0) = \mathbf{g} = (g(x_1), \ldots, g(x_n))^T. \tag{3}$$

We can solve this system using methods for ordinary differential equations. There is not a lot of point in doing the time integration with extremely high accuracy. Stability is more important.

The eigenvalue/eigenvector decomposition of A can tell us a lot about this problem. Suppose A is diagonalizable (in this case it is even symmetric). Then

$$A = Y \Lambda Y^{-1}$$

where

$$Y = (\mathbf{y}_1, \ldots, \mathbf{y}_n)$$

is a matrix of eigenvectors. Consider first the case $\phi(t) = 0$ (corresponding to zero boundary conditions). Let

$$\mathbf{z}(t) = Y^{-1}\mathbf{u}(t).$$

Then $\mathbf{z}(t)$ satisfies the diagonal system of ordinary differential equations

$$\mathbf{z}'(t) = \Lambda \mathbf{z}(t).$$

where

$$\mathbf{z}(0) = \mathbf{h} = X^{-1}\mathbf{g}.$$

This has the solution

$$z_i(t) = h_i e^{\lambda_i t}.$$

Thus the general solution of the original ordinary differential equation is

$$\mathbf{u}_g(t) = Y\mathbf{z}(t) = \sum_{j=1}^{n} h_j \mathbf{y}_j exp(\lambda_j t).$$

If we instead let $g(x) = 0$ and solve for the *special* solution

$$\mathbf{u}_s(t) = A\mathbf{u}_s(t) + \phi(t)$$

where

$$\mathbf{u}_s(t) = 0,$$

then we have the contribution of the boundary conditions. The full solution of our system of ordinary differential equations is

$$\mathbf{u}(t) = \mathbf{u}_s(t) + \mathbf{u}_g(t).$$

For the discretized heat equation, the eigenvalues and eigenvectors of the matrix A are known. They are given by

$$\lambda_k = -2(1 - \cos(\frac{2\pi k}{n+1})/(\Delta x)^2$$

with

$$\mathbf{y}_k = (y_{1k}, \ldots, y_{nk})^T, \quad y_{ik} = \frac{2}{\sqrt{n}} \sin{(2\pi ik)}/(n+1).$$

We note that all of the λ_k are negative. For a large value of n, they will span quite a range. Thus some components of the general solution will decay much faster than others.

Thus the form of $\mathbf{u}_g(t)$ is

$$(\mathbf{u}_g(t))_i = \frac{\sqrt{2}}{\sqrt{n}} \sum_{j=1}^{n} h_j \sin{(2\pi ik)}/(n+1) exp(\lambda_j t).$$

Since some components of the solution decay faster than others, one may have to solve the ODE for a long time before the long term solution $\mathbf{u}_s(t)$ dominates. At the same time, because of a large Lipschitz constant, Runge-Kutta and Adams methods will be required to take small steps.

The following 2×2 example illustrates this point.

Example 1

$$\begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix}' = \begin{pmatrix} -2 & 1 \\ 998 & -999 \end{pmatrix} \begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} + \begin{pmatrix} 2\sin\, t \\ 999(\cos\, t - \sin\, t) \end{pmatrix}$$

$$\begin{pmatrix} u_1(0) \\ u_2(0) \end{pmatrix} = \begin{pmatrix} 2 \\ 3 \end{pmatrix}.$$

The solution with these boundary conditions is

$$\begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} = 2\exp(-t) \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \begin{pmatrix} \sin\, t \\ \cos\, t \end{pmatrix}.$$

The general solution is

$$\begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} = \alpha_1 \exp(-t) \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \alpha_2 \exp(-1000t) \begin{pmatrix} 1 \\ -998 \end{pmatrix} + \begin{pmatrix} \sin\, t \\ \cos\, t \end{pmatrix}.$$

It has a fast transient (the $\exp(-1000t)$ *term) and a slow transient (the* $\exp(-t)$ *term). The fast transient gives it a large Lipschitz constant, forcing methods like the Runge–Kutta–Fehlberg or Adams methods to take small step sizes to obtain a stable solution, even though it fades quickly. The slow transient forces us to solve the ODE over a long time period to get to point where the long term solution dominates.*

Solving this with the Runge–Kutta–Fehlberg method with tolerence 0.01 *from* $[0, 10]$ *requires 3373 steps and over 20,000 function evaluations (Adams methods will not do much better). This is called the stiffness problem.*

It is common to use special methods for these problems. Below we give two "low accuracy" methods. They are:

The Backward Euler Method First order

$$\mathbf{x}_{n+1} = \mathbf{x}_n + h\mathbf{f}_{n+1}.$$

The Trapezoid Method Second order

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \frac{h}{2}(\mathbf{f}_n + \mathbf{f}_{n+1}).$$

Both a stable for arbitrary values of h. This is illustrated for the trapezoid method with the equation

$$\begin{aligned} x'(t) &= \lambda x(t), \quad \Re(\lambda) < 0 \\ x(0) &= x_0 \end{aligned}$$

The solution of this equation is

$$x(t) = x_0 e^{\lambda t}$$

and it should decay as $t \to \infty$.

If we solve this equation using the trapezoid rule we get

$$x_{n+1} = x_n + \frac{h\lambda}{2}(x_n + x_{n+1}).$$

Thus,

$$(1 - \frac{h}{2}\lambda)x_{n+1} = (1 + \frac{h}{2}\lambda)x_n$$

yielding

$$x_{n+1} = \left(\frac{1 + (h/2)\lambda}{1 - (h/2)\lambda}\right) x_n.$$

Thus

$$x_n = \left(\frac{1 + (h/2)\lambda}{1 - (h/2)\lambda}\right)^n x_0$$

and

$$\lim_{n\to\infty} x_n = 0$$

for all values of h.

For the linear problem (2)–(3), we have

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \frac{h}{2}A(\mathbf{u}_n + \mathbf{u}_{n+1}) + \frac{h}{2}[\boldsymbol{\phi}(t_n) + \boldsymbol{\phi}(t_{n+1})]$$

Each step is then the solution of the linear equation

$$(I - \frac{h}{2}A)\mathbf{u}_{n+1} = (I + \frac{h}{2}A)\mathbf{u}_n + \frac{h}{2}[\boldsymbol{\phi}(t_n) + \boldsymbol{\phi}(t_{n+1})].$$

In the case of the heat equation, this just involves the solution of a symmetric (and positive definite) tridiagonal system at each time step.