Numerical Solutions to PDE's

Mathematical Modelling Week 5
Kurt Bryan

Introduction

Let's start by recalling a simple numerical scheme for solving ODE's. Suppose we have an ODE $u'(t) = f(t, u(t))$ for some unknown function $u(t)$ (f is specified), with initial condition $u(0) = u_0$. Choose some small number h_t, the so-called *stepsize*, and use it to approximate $u'(t)$ as

$$u'(t) \approx \frac{u(t + h_t) - u(t)}{h_t}$$

a *finite-difference* approximation to the derivative of u. The smaller h_t is, the better the approximation.

Now define $t_i = ih_t$ and also $u(t_i) = u_i$. Take the original DE and replace t with t_i, $u(t_i)$ with u_i, and the derivative $u'(t_i)$ with the appropriate finite difference approximation to obtain

$$\frac{u_{i+1} - u_i}{h_t} \approx f(t_i, u_i).$$

This can be re-arranged into

$$u_{i+1} \approx u_i + h_t f(t_i, u_i). \tag{1}$$

Equation (1) gives us a recipe for approximating $u(t)$. We start off knowing $u_0 = u(0)$. We can use (1) to approximate $u_1 = u(h_t)$. With an estimate of u_1, we can then approximate u_2, and then u_3 and so on. This is just good old Euler's method.

There are much more sophisticated ways to solve ODE's, but philosophically they all work in pretty much the same way: Knowing the value of u_i (and maybe early values), we attempt to extrapolate the solution into the future by making use of the DE. The same idea works for PDE's.

Finite Differencing for PDE's

Consider the advection equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0 \tag{2}$$

for some function $u(x,t)$ on the half-line $x > 0$ with boundary and initial conditions

$$\begin{aligned} u(x,0) &= f(x), \qquad (3)\\ u(0,t) &= g(t), \qquad (4) \end{aligned}$$

for some functions $f(x)$ and $g(t)$. The number c is the wave speed and is a positive constant. Although u can be found explicitly, we are going to consider a numerical method for approximating u. For a more complicated equation in which c is no longer constant, or even depends on u, a numerical solution will be the only option.

Let's suppose that we're interested in the solution on the interval $0 \leq x \leq 1$. We will replace the partial derivatives of u by finite-difference approximations. Choose $n+1$ equally spaced points $x_0, x_1, \ldots, x_n$ in the interval $[0,1]$ of the form $x_i = i/n$. Let $h_x = 1/n$ denote the spacing between the points. Let's also divide time t up into increments h_t by setting $t_j = h_t j$ where h_t is some "small" number. The partial derivatives for u can then be approximated as

$$\begin{aligned} \frac{\partial u}{\partial t}(x_i,t_j) &\approx \frac{u(x_i,t_{j+1}) - u(x_i,t_j)}{h_t},\\ \frac{\partial u}{\partial x}(x_i,t_j) &\approx \frac{u(x_i,t_j) - u(x_{i-1},t_j)}{h_x}. \end{aligned}$$

As h_x and h_t get smaller the approximations typically get better—they're $o(h_x)$ and $o(h_t)$, at least if u is differentiable enough. Let's use the notation u_{ij} to mean $u(x_i,t_j)$. In this case we have

$$\begin{aligned} \frac{\partial u}{\partial t}(x_i,t_j) &\approx \frac{u_{i,j+1} - u_{ij}}{h_t},\\ \frac{\partial u}{\partial x}(x_i,t_j) &\approx \frac{u_{ij} - u_{i-1,j}}{h_x}. \end{aligned}$$

Take these expressions and substitute them into the advection equation (and replace "≈" with "=") to obtain

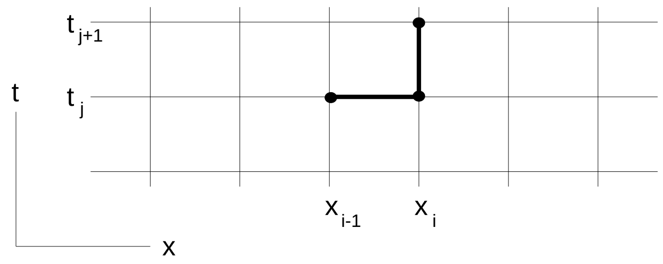
$$\frac{u_{i,j+1} - u_{ij}}{h_t} + c\frac{u_{ij} - u_{i-1,j}}{h_x} = 0.$$

Notice how this finite-difference equation mirrors the original differential equation. We can solve for $u_{i,j+1}$ as

$$u_{i,j+1} = \left(1 - c\frac{h_t}{h_x}\right) u_{ij} + c\frac{h_t}{h_x} u_{i-1,j}. \tag{5}$$

Equation (5) is the basis of a reasonable numerical method for computing the solution to the original differential equation. Repeated application of (5) let's us estimate the solution $u(x,t)$ at any later time. For example, we know $u(x,0) = f(x)$, where f is a given function, so that $u_{i,0} = f(x_i)$ is known for all i from 0 to n. We can estimate $u(x_i, t_1) \approx u_{i,1}$ for $1 \le i \le n$ by using (5) with $j = 0$; all terms on the right side are known. We compute $u_{0,1}$ from the boundary condition, as $u_{0,1} = g(h_t)$. Once the numbers $u_{i,1}$ are known we apply equation (5) with $j = 1$ to compute $u_{i,2}$, and then $u_{i,3}$, etc., while using the boundary condition to compute $u_{0,j+1}$. Such a method for solving a PDE is called an *explicit time-marching* method—repeated application of (5) marches the solution forward in time.

Here's a graphical way to look at what we're doing.



This figure is called the *stencil* for the numerical method, and it pictorially illustrates what equation (5) is doing—estimating $u(x_i, t_{j+1})$ in terms of $u(x_i, t_j)$ and $u(x_{i-1}, t_j)$.

Exercises:

1. Explain why the scheme in equation (5) is exact (for the advection equation) if we choose h_t and h_x so that $c\frac{h_t}{h_x} = 1$.

2. Take $c = 2$, $f(x) \equiv 0$, and $g(t) = \frac{1}{2}\sin(5t)$. Use $h_x = 0.1$ and $h_t = 0.04$ in the scheme (5) and solve out to $t = 1$ for $0 < x < 1$. You may find the Maple notebook on the class web site useful, or you can write your own code—it's easy!

   Plot the solution for several times from $t = 0$ to $t = 1$. Change h_t to 0.1 and repeated the process, solving out to time $t = 1.0$. What happens?

3. Suppose that instead of Dirichlet boundary conditions at $x = 0$ we have a Neumann condition
$$\frac{\partial u}{\partial x}(0, t) = g(t).$$
   How should this be implemented numerically?

Stability

Problem 2 illustrates that there's something more to know about implementing equation (5); in certain circumstances the method may will numerically unstable.

One way to understand the problem is via linear algebra. Let $\mathbf{u}^j$ denote the column vector $[u_0, u_1, \ldots, u_n]^T$ (where ^{T} is transpose). Then the iteration in j embodied by equation (5) can be cast as

$$\mathbf{u}^{j+1} = \mathbf{A}\mathbf{u}^j + \mathbf{g}_j$$

where

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ \alpha & 1-\alpha & 0 & 0 & \cdots & 0 \\ 0 & \alpha & 1-\alpha & 0 & \cdots & 0 \\ & & & \vdots & & \\ 0 & 0 & \cdots & 0 & \alpha & 1-\alpha \end{bmatrix}$$

with $\alpha = \frac{ch_t}{h_x}$ and $\mathbf{g}^j = [g(jh_t), 0, \cdots, 0]^T$.

For simplicity let's assume we have zero boundary data, so $\mathbf{g}^j = \mathbf{0}$ for all j. Then we have simply

$$\mathbf{u}^j = \mathbf{A}^j\mathbf{u}^0.$$

We expect the process will be unstable (and in particular, errors will be magnified without bound) if $\mathbf{A}^j$ grows large in some sense.

One desirable feature is that $\mathbf{A}$ should have all eigenvalues of absolute value less than or equal to one. The reason for this is that the eigenvalues of $\mathbf{A}^j$ are of the form λ^j where λ is an eigenvalue of $\mathbf{A}$. If $|\lambda| > 1$ then the corresponding eigenvalue of $\mathbf{A}^j$ is large, and so errors which are not orthogonal to the eigenvector are multiplied.

It's easy to check that the eigenvalues of $\mathbf{A}$ are 0 (a simple eigenvalue if $\alpha \neq 1$) and $1 - \alpha$ (multiplicity n). Thus we definitely want $|1 - \alpha| \leq 1$, leading to $0 \leq \alpha \leq 2$, or $0 \leq \frac{ch_t}{h_x} \leq 2$. This is certainly a condition we should enforce on h_t and h_x.

But actually, that's not quite good enough. Suppose that $\mathbf{e}^j$ is the error in the jth stage of the computation. It would be preferable if $\mathbf{Ae}^j$ was no larger than $\mathbf{e}^j$, and this isn't quite the same as requiring the eigenvalues less than one.

Let $\|\mathbf{v}\|$ denote the Pythagorean length of the vector $\mathbf{v}$. Then we want $\|\mathbf{Ae}^j\| \leq \|\mathbf{e}^j\|$, or $\frac{\|\mathbf{Ae}^j\|}{\|\mathbf{e}^j\|} \leq 1$. Since we don't know what $\mathbf{e}^j$ is, we simple require that

$$\frac{\|\mathbf{Av}\|}{\|\mathbf{v}\|} \leq 1$$

for all vectors $\mathbf{v}$.

Now it's a fact from linear algebra (easy to prove) that the maximum value of $\frac{\|\mathbf{Av}\|}{\|\mathbf{v}\|}$ over all possible vectors $\mathbf{v}$ is exactly the largest eigenvalue of the matrix $\mathbf{AA}^T$. In the present case it's easy to compute that

$$\mathbf{AA}^T = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1-2\alpha+2\alpha^2 & \alpha-\alpha^2 & 0 & \cdots & 0 \\ 0 & \alpha-\alpha^2 & 1-2\alpha+2\alpha^2 & \alpha-\alpha^2 & \cdots & 0 \\ & & \alpha-\alpha^2 & \vdots & & \alpha-\alpha^2 \\ 0 & 0 & \cdots & 0 & \alpha-\alpha^2 & 1-2\alpha+2\alpha^2 \end{bmatrix}$$

The characteristic polynomial $p(\lambda)$ of this matrix is just λ times the characteristic polynomial of

$$\mathbf{A}_1 = \begin{bmatrix} 1-2\alpha+2\alpha^2 & \alpha-\alpha^2 & 0 & \cdots & 0 \\ \alpha-\alpha^2 & 1-2\alpha+2\alpha^2 & \alpha-\alpha^2 & \cdots & 0 \\ & \alpha-\alpha^2 & \vdots & & \alpha-\alpha^2 \\ 0 & \cdots & 0 & \alpha-\alpha^2 & 1-2\alpha+2\alpha^2 \end{bmatrix}$$

(just think about expanding the determinant of $\mathbf{A} - \lambda\mathbf{I}$ along the top row). The matrix $\mathbf{A}_1$ is n by n and can be written as $\mathbf{A}_1 = \mathbf{I} - (\alpha - \alpha^2)\mathbf{M}$ where

$$\mathbf{M} = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ & -1 & \vdots & & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{bmatrix}$$

Thus the eigenvalues of $\mathbf{A}_1$ are of the form $1 - (\alpha - \alpha^2)\lambda$ where λ is an eigenvalue of $\mathbf{M}$. To see this suppose that $\mathbf{M}\mathbf{v} = \lambda\mathbf{v}$ ($\mathbf{v}$ is an eigenvector of $\mathbf{M}$). Then $\mathbf{A}_1\mathbf{v} = (\mathbf{I} - (\alpha - \alpha^2)\mathbf{M})\mathbf{v} = (1 - (\alpha - \alpha^2)\lambda)\mathbf{v}$, i.e., $1 - (\alpha - \alpha^2)\lambda$ is an eigenvalue for $\mathbf{A}_1$.

And fortunately, the eigenvalues of $\mathbf{M}$ are known in closed form! The matrix $\mathbf{M}$ comes up a lot in finite difference methods. The eigenvalues of the n by n matrix $\mathbf{M}$ are given by $2(1 - \cos(k\pi/(n+1)))$ for $k = 1$ to $k = n$. Thus the eigenvalues of the matrix $\mathbf{A}$ are 0 and the n numbers $1 - (\alpha - \alpha^2)(1 - \cos(k\pi/(n+1)))$.

If we require that all of these eigenvalues have magnitude less than or equal to one we have

$$-1 \le 1 - (\alpha - \alpha^2)(1 - \cos(k\pi/(n+1))) \le 1.$$

This is easily rearranged to

$$0 \le (\alpha - \alpha^2)(1 - \cos(\frac{k\pi}{n+1})) \le 2.$$

Now since $-1 \le \cos \le 1$, the above inequality will be satisfied if $0 \le 2(\alpha - \alpha^2) \le 2$, leading immediately to $0 \le \alpha \le 1$ or

$$c\frac{h_t}{h_x} \le 1 \tag{6}$$

(since all quantities are positive, we needn't worry about the left inequality). Equation (6) is called the *Courant-Friedrich-Lewy* condition, or CFL condition for short. It's necessary (and sufficient) for the numerical scheme (for the advection equation with $c > 0$) to be stable.

The typical way the CFL condition is employed is as follows: We want to solve the advection equation with a certain spatial resolution, out to some time $t = T$. We thus choose h_x first. We then choose h_t in accordance to equation (6), and then march out in time to $t = T$ in steps of size h_t. The finer the spatial resolution required (smaller h_x) the smaller the time steps must be, with correspondingly greater computational burden.

If other "advection" like problems (such as in problem 4 below) there might not be a clear-cut choice for h_t. If, for example, c is variable, we might pick the smallest value for h_t dictated by the CFL condition (6).

4. Repeat problem 2 where c now depends on position, say $c(x) = 2 + \tanh(10(x - 0.5))$. Use $h_x = 0.1$. How small should you choose h_t? Show a graph of the solution at $t = 1$ with your choice for h_t.

5. Repeat problem 2 for the non-linear traffic flow equation

$$\frac{\partial u}{\partial t} + v_m \left(1 - \frac{2u}{u_m}\right) \frac{\partial u}{\partial x} = 0,$$

   where $u(x, t)$ is the traffic density at time t and position x, v_m is the maximum traffic velocity, and u_m is the maximum traffic density. For simplicity take $v_m = u_m = 1$. You'll need to work out the appropriate time marching scheme analogous to equation (5). Use $g(t) \equiv 0.2$ and $f(x) = 0.2$ for $x < 1/2$, $f(x) = 0$ for $x \geq 1/2$. Take $h_x = 0.1$ and try to find an appropriate choice for h_t—does the CFL condition help estimate a good choice?

   What is the physical interpretation of the initial conditions? What happens? Does it make sense?

6. Repeat the last problem but with $g(t) = 0.8$ and $f(x) = 0.8$ for $x < 1/2$, $f(x) = 0$ for $x \geq 1/2$. Can you make it work in any sensible way?

7. Repeat the last problem but with boundary condition $g(t) = 0$ and initial condition $f(x) = 0.5(1 + \tanh(10(x - 0.5)))$. What happens?