MATH317 TWENTY-SECOND & TWENTY-FOURTH TUTORIAL

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1. Finite Difference Methods for PDEs

In many cases a problem will reduce to solving a given partial differential equation on a domain with initial data and some boundary conditions. There are many numerical methods for doing this. One of the most intuitive is the *finite difference concept* for PDEs. First we will look at two important examples. Later on we will study the stability of the schemes via matrix method and Von Neumann stability analysis.

The first equation that will come up is the *one-way wave equation*

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

Here c is a positive parameter modeling the wave speed. Some initial condition $u(x,0)$ has to be given. The second and more important equation is the *diffusion equation*

$$\frac{\partial u}{\partial t} - \kappa\frac{\partial^2 u}{\partial x^2} = 0.$$

The constant k is associated to the thermal diffusivity of the medium. Again, initial conditions and boundary conditions should be supplied.

2. Discretizing Time and Space

To be able to handle differential equations on a computer there is a need to discretize the data. Let us choose a time step Δt and a spatial step Δx. We are always going to assume $u = u(x,t)$, $t \geq 0$ and the spatial domain to be $x \in [0, L]$. Denote with u_j^n the value of u at time point n and spatial point j,

$$u_j^n = u(x_j, t_n) = u(j\Delta x, n\Delta t).$$

Let us assume $x_J = J\Delta x = L$. All calculations are going to take place on the grid on space-time we just came up with. Except for discretizing x, t and u we also need to transform the derivatives in our equation into finite differences. The formulas from the chapter on numerical differentiation will come in handy here. A short overview is presented below for spatial variables. Replacing x with t will get the formulas for the time derivative.

- Forward difference method for the first derivative
$$u'(x) = \frac{u(x+\Delta x) - u(x)}{\Delta x} + \mathcal{O}(\Delta x).$$
- Backward difference method for the first derivative
$$u'(x) = \frac{u(x) - u(x-\Delta x)}{\Delta x} + \mathcal{O}(\Delta x).$$
- Centered difference method for the first derivative
$$u'(x) = \frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} + \mathcal{O}(\Delta x)^2.$$
- Centered difference method for the second derivative
$$u''(x) = \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{(\Delta x)^2} + \mathcal{O}(\Delta x)^2.$$

3. Wave Equation Basics

For the wave equation there are a number of ways to discretize. Arguably the most obvious one is to construct an explicit scheme using a forward difference in time and a forward difference in space. In a formula we get
$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + c\frac{u_j^n - u_{j-1}^n}{\Delta x} = 0.$$
This method is called the *forward upward scheme* for the one-way wave equation. The error term associated to the method is $\mathcal{O}(\Delta t) + \mathcal{O}(\Delta x)$. The forward upward formula is explicit so that one can write
$$u_j^{n+1} = -\frac{c\Delta t}{\Delta x}(u_j^n - u_{j-1}^n) + u_j^n.$$
Stepping in time happens from initial data $u_0^0, \ldots u_{j-1}^0, u_j^0, u_{j+1}^0, \ldots, u_J^0$. Boundary conditions may be given on u_0^n and u_J^n for all n. By rewriting the discretization to
$$u_j^{n+1} = \left(1 - \frac{c\Delta t}{\Delta x}\right) u_j^n + \frac{c\Delta t}{\Delta x} u_{j-1}^n$$
one can make things more convenient by shaping the computation using a matrix form.

Other possible discretizations are the *forward central scheme*
$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + c\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} + \mathcal{O}(\Delta t) + \mathcal{O}(\Delta x)^2 = 0$$

the *backward central scheme*

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}+c\frac{u_{j+1}^{n+1}-u_{j-1}^{n+1}}{2\Delta x}+\mathcal{O}(\Delta t)+\mathcal{O}(\Delta x)^2=0,$$

and more famously the *Crank-Nicolson central scheme*

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}+\frac{c}{2}\left(\frac{u_{j+1}^{n+1}-u_{j-1}^{n+1}}{2\Delta x}+\frac{u_{j+1}^{n}-u_{j-1}^{n}}{2\Delta x}\right)+\mathcal{O}(\Delta t)^2+\mathcal{O}(\Delta x)^2=0.$$

The $\mathcal{O}$ symbols express the error on the formulas. The stability of these methods turns out to be very different, as we will see later on.

4. Heat Equation Basics

The heat equation offers a similar if not bigger range of possibilities. The specific scheme we will look at here is the explicit centered difference scheme

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}-\kappa\frac{u_{j+1}^{n}-2u_j^n+u_{j-1}^{n}}{(\Delta x)^2}=0.$$

The error is $\mathcal{O}(\Delta t)+\mathcal{O}(\Delta x)^2$. Written explicitly we have

$$u_j^{n+1}=\frac{\kappa\Delta t}{(\Delta x)^2}\left(u_{j+1}^n-2u_j^n+u_{j-1}^n\right)+u_j^n.$$

Say $d=\kappa\Delta t/(\Delta x)^2$ to simplify notation. Then

$$u_j^{n+1}=du_{j+1}^n+(1-2d)u_j^n+du_{j-1}^n.$$

Assume for a minute that the boundary conditions given are homogeneous $u_0^n=u_J^n=0$. The finite difference scheme in matrix form is a tridiagonal matrix system that looks like

$$\begin{pmatrix} 1-2d & d & & & & & \\ & & \ddots & & & & \\ & & d & 1-2d & d & & \\ & & & & \ddots & & \\ & & & & & d & 1-2d \end{pmatrix}\begin{pmatrix} u_1^n \\ u_2^n \\ \vdots \\ u_{j-1}^n \\ u_j^n \\ u_{j+1}^n \\ \vdots \\ u_{J-1}^n \\ u_J^n \end{pmatrix}=\begin{pmatrix} u_1^{n+1} \\ \vdots \\ u_j^{n+1} \\ \vdots \\ u_J^{n+1} \end{pmatrix}.$$

In symbols $AU^n = U^{n+1}$ with $A \in \mathbb{R}^{J \times J}$. Stepping in time simply comes down to multiplying with the matrix A. It turns out that the error behaves similarly,

$$AE^n = E^{n+1}.$$

For the error to remain bounded in time we need $\rho(A) < 1$. Again, ρ is the spectral radius. From linear algebra the eigenvalues of the matrix A are

$$\lambda_k = (1 - 2d) + 2d \cos\left(\frac{\pi k}{J+1}\right).$$

One guarantees the biggest absolute value to be bounded by 1 by demanding $2d < 1$. The *matrix form stability criterion* is thus

$$\kappa \Delta t \leq \frac{(\Delta x)^2}{2}.$$

5. Von Neumann Stability

The most important notion of stability for a PDE is without a doubt *Von Neumann stability*. Assume we have a Fourier expansion in space of our function

$$u(x,t) = \sum_f \hat{u}(t) \exp{(ifx)}.$$

The sum is over f, the Fourier frequencies. Now take for u just one Fourier term

$$u(x,t) = \hat{u}(t) \exp{(ifx)}$$

and evaluate it at (x_j, t_n) to get

$$u_j^n = \hat{u}(t_n) \exp{(ifj\Delta x)}.$$

To simplify notation we can write $\hat{u}_n = \hat{u}(t_n)$. Then

$$\begin{aligned}
u_j^n &= \hat{u}_n \exp{(ifj\Delta x)}, \\
u_{j-1}^n &= \hat{u}_n \exp{(if(j-1)\Delta x)}, \\
u_{j+1}^n &= \hat{u}_n \exp{(if(j+1)\Delta x)}, \\
u_j^{n+1} &= \hat{u}_{n+1} \exp{(ifj\Delta x)}.
\end{aligned}$$

These expressions can be plugged directly into any finite difference scheme to check for stability. The *growth rate* G is defined as

$$G = \left| \frac{\hat{u}_{n+1}}{\hat{u}_n} \right|.$$

For stability we need $G < 1$ for all frequencies f. Conditional stability means we only have stability on a certain condition. Usually the condition limits Δt in function of Δx.

It is important to note that we are checking the stability for a method, not for an equation. The four methods discussed in the chapter on the one-way wave equation all solve the same equation, but have very different stability properties. We will not derive these here but it turns out that the forward central scheme is unstable, both the backward central scheme and Crank-Nicolson are unconditionally stable and the forward upwind method is conditionally stable. The condition for forward upwind is that $c\Delta t \leq \Delta x$.

6. Von Neumann for the Heat Equation

Let us do one rigorous stability analysis. The equation we will be looking at is the heat equation. The method is the one presented earlier,

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} - \kappa \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} = 0.$$

Start by plugging in the Fourier term expressions. One then obtains

$$\frac{\hat{u}_{n+1} e^{ifj\Delta x} - \hat{u}_n e^{ifj\Delta x}}{\Delta t} - \kappa \frac{\hat{u}_n e^{if(j+1)\Delta x} - 2\hat{u}_n e^{ifj\Delta x} + \hat{u}_n e^{if(j-1)\Delta x}}{(\Delta x)^2} = 0.$$

Secondly let us divide the result by $\hat{u}_n e^{ifj\Delta x}$. One obtains

$$\frac{\frac{\hat{u}_{n+1}}{\hat{u}_n} - 1}{\Delta t} - \kappa \frac{e^{if\Delta x} - 2 \ + e^{-if\Delta x}}{(\Delta x)^2} = 0.$$

There's some clear need for rearranging the terms. The result is

$$\frac{\hat{u}_{n+1}}{\hat{u}_n} = \frac{\kappa \Delta t}{(\Delta x)^2} \left(e^{if\Delta x} - 2 \ + e^{-if\Delta x} \right) + 1.$$

On the left hand side we have the growth rate. On the right hand side we can use the expression from complex analysis

$$e^{if\Delta x} + e^{-if\Delta x} = 2\cos(f\Delta x).$$

It follows that

$$G = \left| 1 + \frac{\kappa \Delta t}{(\Delta x)^2} (2\cos(f\Delta x) - 2) \right|.$$

Trigonometry saves us via the identity

$$\cos(f\Delta x) - 1 = -2\sin^2(f\Delta x/2).$$

The final result is that

$$G = \left| 1 - 4\frac{\kappa \Delta t}{(\Delta x)^2} \sin^2(f\Delta x/2) \right|.$$

For stability we need $G < 1$ so

$$-1 < 1 - 4\frac{\kappa \Delta t}{(\Delta x)^2}\sin^2(f\Delta x/2) < 1.$$

Elementary algebra leads to

$$2 > 4\frac{\kappa \Delta t}{(\Delta x)^2}\sin^2(f\Delta x/2) > 0.$$

The square of the sine is always a positive number so the right inequality is trivially satisfied. The left however might not be if $\sin^2(f\Delta x/2) = 1$. To ensure a bounded growth rate we need to require

$$\frac{\kappa \Delta t}{(\Delta x)^2} < \frac{1}{2}.$$

The criterion we just discovered is important in practical numerical calculations: it says that for the numerics to stay under control a much more fine time step is required. In fact, the time step should be less than the square of the spatial step.