Partial Differential Equations

1 More on Numerical Derivatives

The central difference formula approximates the derivative of a function $f(x)$ as

$$f'(x) = \frac{f(x+h/2) - f(x-h/2)}{h} \tag{1}$$

The second derivative could therefore be calculated based on the first derivative as

$$f''(x) = \frac{f'(x+h/2) - f'(x-h/2)}{h} \tag{2}$$

Using the central difference to approximate the first derivatives that appear in the second derivative formula (let $x \to x \pm h/2$) gives

$$\begin{aligned} f''(x) &= \frac{f'(x+h/2) - f'(x-h/2)}{h} \\ &= \frac{\frac{f[(x+h/2)+h/2]-f[(x+h/2)-h/2]}{h} - \frac{f[(x-h/2)+h/2]-f[(x-h/2)-h/2]}{h}}{h} \\ &= \frac{f(x+h) - f(x) - (f(x) - f(x-h))}{h^2} \\ &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \end{aligned} \tag{3}$$

Section 8, Exercise 1

Now let's consider partial derivatives of a function of two variables, $f(x, y)$. The first derivaties with respect to x or y are straightforward based on the central difference formula:

$$\frac{\partial f}{\partial x} = \frac{f(x+h/2, y) - f(x-h/2, y)}{h} \tag{4}$$

$$\frac{\partial f}{\partial y} = \frac{f(x, y+h/2) - f(x, y-h/2)}{h} \tag{5}$$

The second derivatives with respect to each variable individually are (based on the second derivate formula above):

$$\frac{\partial^2 f}{\partial x^2} = \frac{f(x+h, y) - 2f(x, y) + f(x-h, y)}{h^2} \tag{6}$$

$$\frac{\partial^2 f}{\partial y^2} = \frac{f(x, y+h) - 2f(x, y) + f(x, y-h)}{h^2} \tag{7}$$

The mixed second derivative (with respect to both variables) is:

$$\begin{aligned}
\frac{\partial^2 f}{\partial x \partial y} &= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right) \\
&= \frac{\partial}{\partial x}\left(\frac{f(x, y+h/2) - f(x, y-h/2)}{h}\right) \\
&= \frac{\frac{\partial f(x,y+h/2)}{\partial x} - \frac{\partial f(x,y-h/2)}{\partial x}}{h} \\
&= \frac{\frac{f(x+h/2,y+h/2)-f(x-h/2,y+h/2)}{h} - \frac{f(x+h/2,y-h/2)-f(x-h/2,y-h/2)}{h}}{h} \\
&= \frac{f(x+h/2, y+h/2) - f(x-h/2, y+h/2) - f(x+h/2, y-h/2) + f(x-h/2, y-h/2)}{h^2}
\end{aligned} \tag{8}$$

2 Boundary Value Problems

2.1 Relaxation Method

We're going to study methods for solving partial differential equations. First, we will consider boundary value problems, in which we have a partial differential equation describing the behavior of a function in some region of space, and we are given a constraint on the value of the function at the boundary of the region. We will use the *method of finite differences*, which involves dividing space into a grid of discrete points. The grid should include points on the boundary where the value of the function is known as well as interior points where we want to calculate the solution.

Our example is Laplace's equation for the electrostatic potential in the absence of any electric charges. Recall Gauss's Law, which is one of Maxwell's equations:

$$\nabla \cdot \vec{E} = \rho/\epsilon_0 \tag{9}$$

where $\vec{E}$ is the electric field, ρ is the charge density, and ϵ_0 is a constant. With no electric charges present in the region of interest, $\rho = 0$ and we have

$$\nabla \cdot \vec{E} = 0 \tag{10}$$

In electrostatics (which means problems with no time dependence), we can define the electric field to be the gradient of a scalar electrostatic potential Φ (because $\nabla \times \vec{E} = 0$ in statics and the curl of a gradient is always zero):

$$\vec{E} = -\nabla\Phi \tag{11}$$

Taking the divergence of both sides gives us Laplace's equation:

$$\begin{aligned}
-\nabla \cdot \nabla\Phi &= \nabla \cdot \vec{E} \\
-\nabla^2\Phi &= 0 \\
\nabla^2\Phi &= 0
\end{aligned} \tag{12}$$

where ∇^2 is the Laplacian, given by

$$\nabla^2\Phi = \frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} + \frac{\partial^2\Phi}{\partial z^2} \tag{13}$$

This is in general three-dimensional, but we will limit ourselves to two dimensions, so here is the equation we wish to solve:

$$\frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} = 0 \tag{14}$$

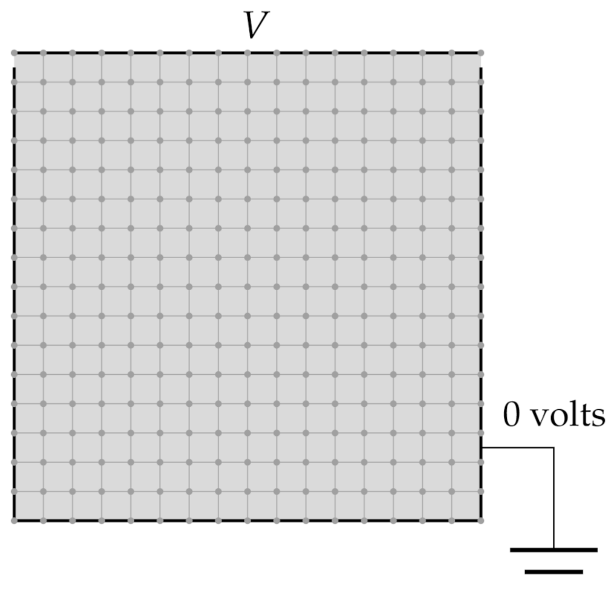

Figure 1:

Our region of interest is a 2D box. The boundary conditions are that one wall has a fixed potential V and the other walls have fixed potentials of zero, see Figure 1. The figure shows the grid of points we will use for the finite difference method. Assume the distance between grid points is a. The second derivatives, with points evaluated only the grid, can be written as

$$\frac{\partial^2\Phi}{\partial x^2} = \frac{\Phi(x+a,y) - 2\Phi(x,y) + \Phi(x-a,y)}{a^2} \tag{15}$$

$$\frac{\partial^2\Phi}{\partial y^2} = \frac{\Phi(x,y+a) - 2\Phi(x,y) + \Phi(x,y-a)}{a^2} \tag{16}$$

and therefore the Laplacian is

$$\frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} = \frac{\Phi(x+a,y) + \Phi(x-a,y) + \Phi(x,y+a) + \Phi(x,y-a) - 4\Phi(x,y)}{a^2} \tag{17}$$

Setting this to zero, and canceling the factor of a^2, we have

$$\Phi(x+a,y)+\Phi(x-a,y)+\Phi(x,y+a)+\Phi(x,y-a)-4\Phi(x,y)=0 \tag{18}$$

We have an equation of this form for every point (x, y) on our grid. The solution to this set of equations gives us the value of Φ at every grid point. Our partial differential equation has been transformed into a set of simultaneous linear equations.

Section 8, Exercise 2

We could use Gaussian elimination or LU decomposition to solve these equations, but actually the relaxation method works quite well. We previously studied the relaxation method to solve nonlinear equations, but it can be used in this case as well. Let's rearrange the equation above:

$$\Phi(x,y)=\frac{1}{4}\left(\Phi(x+a,y)+\Phi(x-a,y)+\Phi(x,y+a)+\Phi(x,y-a)\right) \tag{19}$$

It's clear from this that the function value at point (x, y) is being calculated as the average of surrounding points. We fix the value of Φ along the boundary of the grid according to the boundary conditions, and then make guesses for the interior points on the right-hand-side of the equation. Then we calculate the left-hand-side of the equation. Then we take the new values for all the grid points and feed them back in to the right-hand-side. We continue this until we see convergence. This method for solving Laplace's equation is called the *Jacobi method*.

In the example, we'll assume the box has a side length of 1 m, with a grid spacing of 1 cm. (Notice, however, that the grid spacing or size of the region never comes into the calculation.) We'll let V, the potential on the top of the box be 1 V.

Example: Laplace's equation

To increase the accuracy of this approximation, we could increase the number of grid points (at the expense of running time) or make higher-order approximations to the derivatives. This method would be difficult to apply in the case that the boundaries of the region were not rectangular. There are other finite difference methods thatuse grids with variable spacing or with non-rectangular regions. In these cases, the simple average we used above for the derivative approximation would not apply, and a more complicated calculation would be necessary.

2.2 Faster Methods

One way to make the Jacobi method converge faster is to use a variant of the Jacobi method called the *Gauss-Seidel* method. In the Jacobi method, we had a grid of values for Φ_{ij}, and we used these values to calculate new values for the grid Φ'_{ij}. We always use the Φ grid in the calculation, and then update Φ to be the new Φ' once we have cycled over all the points on the grid. In the Gauss-Seidel method, we don't store the old values. Once a new value is calculated at a particular ij point, we overwrite the old value with the new value and never use the old value again. We update as we go, instead of saving two copies of Φ until we have looped over the entire grid. This method is not only faster, it also uses less memory since less information is being stored.

Example: Gauss-Seidel

So we see that this alone did not make much of a difference in the convergence time.

Another way to speed up convergence is to use *overrelaxation*, which involves changing the function value by a little more than is called for by our equation. Starting with the equation for $\Phi(x,y)$ above, we include a small parameter ω as:

$$\Phi(x,y) = \frac{1+\omega}{4}\left(\Phi(x+a,y)+\Phi(x-a,y)+\Phi(x,y+a)+\Phi(x,y-a)\right) - \omega\Phi(x,y) \tag{20}$$

We will implement this in combination with the Gauss-Seidel method. First we need to pick a value of ω. In general larger values of ω lead to faster calculations, but if we use a value that is too large, the calculation can become numerically unstable. It has been proven that values of ω less than 1 lead to stable calculations, so we will restrict ω accordingly.

Example: Overrelaxation

2.3 Poisson's Equation

To derive Laplace's equation, we assumed the charge density $\rho = 0$. If we return to Gauss's Law with ρ non-zero, we can derive Poisson's equation:

$$\begin{aligned} \nabla\cdot\vec{E} &= \frac{\rho}{\epsilon_0} \\ \nabla\cdot(-\nabla\Phi) &= \frac{\rho}{\epsilon_0} \\ \nabla^2\Phi &= -\frac{\rho}{\epsilon_0} \end{aligned} \tag{21}$$

This changes our equation for the relaxation method as:

$$\Phi(x,y) = \frac{1}{4}\left(\Phi(x+a,y)+\Phi(x-a,y)+\Phi(x,y+a)+\Phi(x,y-a)\right) + \frac{a^2}{4\epsilon_0}\rho(x,y) \tag{22}$$

This can be solved in the same way as Laplace's equation, provided that the charge density ρ is given at each grid point.

3 Initial Value Problems

Now we will consider initial value problems, in which we have a partial differential equation describing the behavior of a function in space and time, and we are given the starting conditions. As an example, we will consider the diffusion equation:

$$\frac{\partial \Phi}{\partial t} = D\frac{\partial^2 \Phi}{\partial x^2} \tag{23}$$

where D is the diffusion coefficient. This equation is used to calculation the motion of diffusing gases and liquids, as well as the flow of heat in thermal conductors (often called the heat equation in heat flow problems). We will use what's called a *forward integration method.*

3.1 FTCS Method

First we divide the spatial dimensions into an evenly spaced grid. In this case, we only have one spatial dimension, x, so it's really just a line of evenly spaced points in x. Assuming the spacing is a, we can approximate the second derivative on the right-hand side as

$$\frac{\partial^2 \Phi}{\partial x^2} = \frac{\Phi(x+a,t) - 2\Phi(x,t) + \Phi(x-a,t)}{a^2} \tag{24}$$

$$\tag{25}$$

With this, the diffusion equation becomes

$$\frac{\partial \Phi}{\partial t} = \frac{D}{a^2}\left(\Phi(x+a,t) - 2\Phi(x,t) + \Phi(x-a,t)\right) \tag{26}$$

Now we have a differential equation which we can solve using Euler's method. (If you're wondering why we don't use the higher-order Runge-Kutta methods, it's because it's not worth it to use a more precise method since we've already introduced a second-order error by approximating the second derivative.) Using Euler's method, we have

$$\begin{aligned}\Phi(x,t+h) &= \Phi(x,t) + h\frac{\partial \Phi}{\partial t}\\ \Phi(x,t+h) &= \Phi(x,t) + \frac{hD}{a^2}\left(\Phi(x+a,t) - 2\Phi(x,t) + \Phi(x-a,t)\right) \qquad (27)\end{aligned}$$

If we use this equation repeatly at every grid point in x, we can get the time evolution of Φ at those values of x. This is called the *forward-time centered-space method* (FTCS method).

As an example, we will solve the following version of the diffusion equation, called the heat equation in this context:

$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T}{\partial x^2} \tag{28}$$

where T is the temperature profile of a 1 cm think stainless steel container. The container is initially at a uniform temperature of 20°C. Then it is placed in a bath of cold water at 0°C and filled with hot water at 50°C. We'll only concern ourselves with the bottom of the container, where the bottom side is in contact with the cold water and the top side is in contact with the hot water. The variable x will measure the distance from bottom to top in the steel, up to 1 cm. We have the boundary conditions in x: $T = 0°\text{C}$ at $x = 0$ cm and $T = 50°\text{C}$ at $x = 1$ cm. The intial condition in the interior is that $T = 20°\text{C}$ at $t = 0$ s. The diffusion constant is the thermal diffusivity of steel, $D = 4.25 \times 10^{-6}$ m^2/s. Furthermore, we'll assume that the temperature of the hot and cold water is not affected, so that the boundary conditions stay the same Applying the solution above to this equation we have

$$T(x, t+h) = T(x, t) + \frac{hD}{a^2}\left(T(x+a, t) - 2T(x, t) + T(x-a, t)\right) \tag{29}$$

Example: Heat Equation

3.2 The Wave Equation

Another important partial differential equation in physics is the wave equation, which is given in one dimension by

$$\frac{\partial^2 \Phi}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2 \Phi}{\partial t^2} = 0 \tag{30}$$

For our purposes, we'll write it this way:

$$\frac{\partial^2 \Phi}{\partial t^2} = v^2 \frac{\partial^2 \Phi}{\partial x^2} \tag{31}$$

If we were to use the FTCS method, we would approximate the second derivative on the right-hand side, leading to

$$\frac{\partial^2 \Phi}{\partial t^2} = \frac{v^2}{a^2}\left(\Phi(x+a, t) - 2\Phi(x, t) + \Phi(x-a, t)\right) \tag{32}$$

Then, like we did with ordinary differential equations, we could turn this second order equation into two first order equations as:

$$\frac{\partial \Phi}{\partial t} = \beta \tag{33}$$

$$\frac{\partial \beta}{\partial t} = \frac{v^2}{a^2}\left(\Phi(x+a, t) - 2\Phi(x, t) + \Phi(x-a, t)\right) \tag{34}$$

Then applying Euler's method we have

$$\Phi(x, t+h) = \Phi(x, t) + h\beta(x, t) \tag{35}$$

$$\beta(x, t+h) = \beta(x, t) + \frac{hv^2}{a^2}\left(\Phi(x+a, t) - 2\Phi(x, t) + \Phi(x-a, t)\right) \tag{36}$$

Let's look at a solution to the wave equation. We'll consider a wave on a string. The string has length L, and is held fixed at both ends.

Section 8, Exercise 3

With the ends fixed, we have $\Phi = 0$ at $x = 0$ and $x = L$. For the initial condition ($t = 0$), let's assume the string forms a perfect sine wave, with $\Phi(x, 0) = A \sin\left(\frac{2\pi x}{L}\right)$. Note we will also need an initial condition for $\beta = \partial\Phi/\partial t$. Let's assume $\beta(x, 0) = 0$. Let $L = 10$ cm, $A = 10$ cm, $v = 50$ cm/s.

Example: Wave Equation

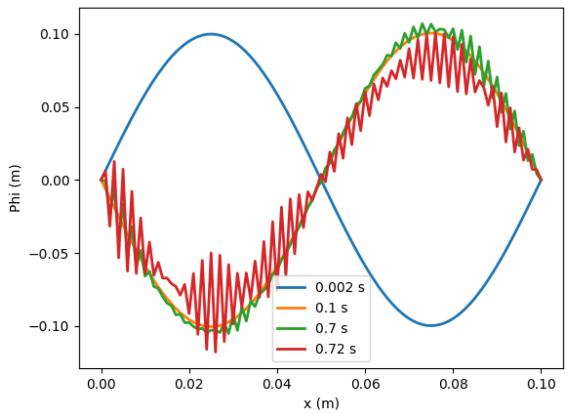

Figure 2:

The results are shown in Figure 2. At early times, our solution behaves as we expect. At later times, we start to see some instability, which grows quickly. The solution is numerically unstable. The time at which the solution becomes unstable is highly dependent upon the initial conditions and parameters of the problem, but it will always become unstable with this method.

I'm not going to go into the mathematical details, but one can perform what's called a *von Neumann stability analysis*, which shows that for the diffusion (heat) equation, The FTCS method produces stable solutions so long as the time spacing h meets the condition

$$h \leq \frac{a^2}{2D} \tag{37}$$

The same analysis for the wave equation shows that no matter how small h is, the FTCS method is *never* stable for the wave equation.

The *implicit method* can be used for the wave equation to avoid the stability problems of the FTCS method. Consider Equations 35 and 36. If we take $h \to -h$, and then $t \to t + h$, we have

$$\begin{aligned}
\Phi(x, t+h) &= \Phi(x, t) + h\beta(x, t) \\
\Phi(x, (t+h) - h) &= \Phi(x, t+h) - h\beta(x, t+h) \\
\Phi(x, t) &= \Phi(x, t+h) - h\beta(x, t+h)
\end{aligned} \tag{38}$$

and

$$\begin{aligned}
\beta(x,t+h) &= \beta(x,t) + \frac{hv^2}{a^2}\left(\Phi(x+a,t) - 2\Phi(x,t) + \Phi(x-a,t)\right)\\
\beta(x,(t+h)-h) &= \beta(x,t+h) - \frac{hv^2}{a^2}\left(\Phi(x+a,t+h) - 2\Phi(x,t+h) + \Phi(x-a,t+h)\right)\\
\beta(x,t) &= \beta(x,t+h) - \frac{hv^2}{a^2}\left(\Phi(x+a,t+h) - 2\Phi(x,t+h) + \Phi(x-a,t+h)\right)
\end{aligned} \tag{39}$$

With Equations 38 and 39, we no longer have an explicit expression for $\Phi(x,t+h)$ in terms of $\Phi(x,t)$ and $\beta(x,t)$, but we can consider this as a set of simultaneous equations in the values of Φ and β at each grid point, which can be solved by standard methods like Gaussian elimination or LU decomposition. The von Neumann stability analysis shows that this solution is always numerically stable.

However, we have another problem with this solution (again, we won't go into the math), which is that the wave solution with this method will eventually decay away to zero, which is unphysical. With no friction (or other force with similar effects), the amplitude should stay constant. Roughly speaking, the Fourier components of the solution with the FTCS will grow exponentially, while they will decay exponentially with the implicit method.

The *Crank-Nicolson method* solves this problem by taking an average of the two (FTCS and implicit method) solutions. The resulting equations are:

$$\Phi(x,t+h) - \frac{1}{2}h\beta(x,t+h) = \Phi(x,t) + \frac{1}{2}h\beta(x,t) \tag{40}$$

$$\begin{aligned}
&\beta(x,t+h) - \frac{hv^2}{2a^2}\left[\Phi(x+a,t+h) + \Phi(x-a,t+h) - 2\Phi(x,t+h)\right]\\
&\quad= \beta(x,t) + \frac{hv^2}{2a^2}\left[\Phi(x+a,t) + \Phi(x-a,t) - 2\Phi(x,t)\right]
\end{aligned} \tag{41}$$

These have been arranged such that the $(t+h)$-dependent terms are on the left-hand side and the t-dependent terms are on the right as is usual for the Euler method.

Note that the functions Φ and β at each grid point only depend on the values of the points immediately to the left and right. When this is written up as a matrix problem, it involves tridiagonal matrices, and as we already saw, those can be solved quickly with Gaussian elimination.

The actual execution of the solution is complicated by the fact that we have two functions to solve for (Φ and β) at each of n grid points. It's done by making a two-element vector (Φ,β), and solving for the n vectors simultaneously. (This includes vectors and matrices of vectors...) So we'll end with just this sketch of how to do the problem.