Estimating Derivatives

In the accompanying Mathematica notebook I showed a general technique that can be used to estimate various derivatives of a function $f(x)$ at a point $x = x_0$ by using nearby function values. We developed two key formulas. These *centered difference* formulas use nearby values of $f(x)$ to estimate $f'(x_0)$ and $f''(x_0)$:

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0 + h)}{2\ h}$$

$$f''(x_0) \approx \frac{f(x_0 - h) - 2\ f(x_0) + f(x_0 + h)}{h^2}$$

These approximation formulas can also be applied to partial derivatives. If $g(x,t)$ is a function of two variables, we can approximate both its t partial derivatives and its x partial derivatives by similar formulas:

$$\frac{\partial g}{\partial t}(x_0,t_0) \approx \frac{g(x_0,t_0+k) - g(x_0,t_0-k)}{2\ k}$$

$$\frac{\partial^2 g}{\partial t^2}(x_0,t_0) \approx \frac{g(x_0,t_0-k) - 2\ g(x_0,t_0) + g(x_0,t_0+k)}{k^2}$$

$$\frac{\partial g}{\partial x}(x_0,t_0) \approx \frac{g(x_0+h,t_0) - g(x_0-h,t_0)}{2\ h}$$

$$\frac{\partial^2 g}{\partial x^2}(x_0,t_0) \approx \frac{g(x_0 - h,t_0) - 2\ g(x_0,t_0) + g(x_0+h,t_0)}{h^2}$$

The Method of Finite Differences

We can use the approximation formulas above to rewrite a PDE by replacing its partial derivatives with estimates. For example, we can rewrite the wave equation

$$\frac{\partial^2 u}{\partial t^2} - c^2\ \frac{\partial^2 u}{\partial x^2} = f(x,t)$$

in the vicinity of a point (x_0,t_0) as

$$\frac{u(x_0,t_0-k) - 2\ u(x_0,t_0) + u(x_0,t_0+k)}{k^2} - c^2\ \frac{u(x_0 - h,t_0) - 2\ u(x_0,t_0) + u(x_0+h,t_0)}{h^2} \approx f(x_0,t_0)$$

Here I am assuming that the size of the step in the t direction, k, is not necessarily the same size as the step in the x direction, h. This is quite common in practice, so we have to be be careful to keep these step sizes distinct.

One application of this approximation is that it can be used to express $u(x_0,t_0+k)$ in terms of values with earlier values of t. Solving the equation above for $u(x_0,t_0+k)$ turns this approximation into an *evolution formula* that shows how the solution evolves in time.

$$u(x_0,t_0+k) = k^2\, f(x_0,t_0)+c^2\, k^2\, \frac{u(x_0 - h,t_0) - 2\, u(x_0,t_0) + u(x_0+h,t_0)}{h^2} - u(x_0,t_0-k)+2\, u(x_0,t_0)$$

This allows us to drive the solution forward in time using values that we have already computed.

Part of the information we will need to go forward in time will come from one of the boundary conditions:

$$u(x_0,0) = \psi(x_0)$$

The only complication is that to go forward from t_0 to $t_0 + k$ we will also need to know what happened at t_0-k. The boundary condition at $t = 0$ tells us what $u(x_0,0)$ should be, but it does not tell us what $u(x_0,-k)$ is. To deal with that complication we will introduce a trick.

The trick is to use the centered difference formula for $\frac{\partial u}{\partial t}$ at $(x_0,0)$ in combination with the second boundary condition:

$$\gamma(x_0) = \frac{\partial u}{\partial t}(x_0,0) \approx \frac{u(x_0,k) - u(x_0,-k)}{2\, k}$$

The evolution formula itself gives us a second equation involving both $u(x_0,k)$ and $u(x_0,-k)$:

$$u(x_0,k) = k^2\, f(x_0,0)+c^2\, k^2\, \frac{u(x_0 - h,0) - 2\, u(x_0,0) + u(x_0+h,0)}{h^2} - u(x_0,-k)+2\, u(x_0,0)$$

We can combine these equations to eliminate the $u(x_0,-k)$ term and express $u(x_0,k)$ in terms of known quantities:

$$u(x_0,k) = \frac{k^2}{2}\, f(x_0,0)+c^2\, k^2\, \frac{\psi(x_0 - h) - 2\, \psi(x_0) + \psi(x_0+h)}{2\, h^2} + k\, \gamma(x_0) + \psi(x_0)$$

Once $u(x_n,0)$ and $u(x_n,k)$ are known for a grid of sample points running from $0+h$ to l-h we can use the evolution rule to drive us forward in time. The accompanying Mathematica notebook will show how this works in practice.