Finite Differences: Partial Derivatives and Boundary Value Problems

Suppose we now have $f(x, y)$, a function of two or more variables.

Question 1. What is the definition of the partial derivative with respect to x?

$$\lim_{h \to 0} \frac{f(x+h, y) - f(x, y)}{h}$$

Question 2. Find a first order formula to approximate the partial derivative with respect to x.

$$\frac{\partial f}{\partial x}(a, b) \approx \frac{f(a+h, b) - f(a, b)}{h}$$

The previous work on functions of one variable immediately imply that the error is $\frac{h}{2} g''(c)$ where $g(x) = f(x, b)$, and c is a number between a and $a + h$.

The previous work gives approximations for second derivatives as well, especially when they are not mixed. For instance,

$$\frac{\partial^2 f}{\partial x^2}(a, b) \approx \frac{f(a-h, b) - 2f(a, b) + f(a+h, b)}{h^2}.$$

Question 3. Find an approximation formula for the mixed derivative $\frac{\partial^2 f}{\partial x \partial y}(a, b)$.

Set $g(x) = \frac{\partial f}{\partial y}(x, b)$. Then we can use the approximation

$$\begin{aligned}
g'(a) &\approx \frac{g(a+h) - g(a-h)}{2h} \\
&= \frac{\frac{\partial f}{\partial y}(a+h, b) - \frac{\partial f}{\partial y}(a-h, b)}{2h} \\
&= \frac{\frac{f(a+h,b+h) - f(a+h,b-h)}{2h} - \frac{f(a-h,b+h) - f(a-h,b-h)}{2h}}{2h} \\
&= \frac{f(a+h, b+h) - f(a+h, b-h) - f(a-h, b+h) + f(a-h, b-h)}{4h^2}
\end{aligned}$$

Because the notation is getting bulky, we use the coefficients on h as subscripts on f to write this as:

$$\frac{\partial^2 f}{\partial x \partial y}(a, b) \approx \frac{f_{1,1} - f_{1,-1} - f_{-1,1} + f_{-1,-1}}{4h^2}$$

Example 1. For the function $f(x, y) = xy^2 + x$ and the point $(1, 2)$, approximate the partial derivatives and the mixed second derivative of f using $h = 0.1$.

$$\frac{\partial f}{\partial x}(1,2) = \frac{1.1(2^2)+1.1-5}{0.1} = \frac{5.5-5}{0.1} = 5$$

$$\frac{\partial f}{\partial y}(1,2) = \frac{1(2.1)^2+1-5}{0.1} = \frac{5.41-5}{0.1} = 4.1$$

$$\frac{\partial^2 f}{\partial x \partial y}(1,2) = \frac{5.951-5.071-4.869+4.149}{4(0.01)} = 4$$

Boundary Value Problem

One of the other common uses of finite differences is to solve boundary value problems. We return to functions of one variable and examine the second-order boundary value problem

$$\begin{cases} y'' = f(t,y,y') \\ f(a) = y_a \\ f(b) = y_b \end{cases}$$

on some interval $a \leq t \leq b$.

Question 4. What is the difference between an initial value problem and a boundary value problem?

We're looking at two values $y(a)$ and $y(b)$ instead of $y(a)$ and $y'(a)$.

Question 5. Verify that the boundary value problem

$$\begin{cases} y'' = -y \\ y(0) = 0 \\ y(\pi) = 0 \end{cases}$$

has infinitely many solutions of the form $y = k \sin t$.

Since $y'' = -k\sin t = -y$, $y(0) = k\sin(0) = 0$ and $y(\pi) = k\sin(0) = 0$, all functions that are scalar multiples of sine are solutions to this boundary value problem.

The finite difference method consists of replacing y'' with the finite difference formula using points between the boundary values a and b. That is, we take the interval $[a,b]$ and divide it up into an evenly spaced grid (particularly in in higher dimensions, its called a *mesh* grid).

We denote the new approximation variables using w_i for $i = 0, 1, \ldots, n, n+1$. The first approximation, w_0, is known, as it is y_a. Similarly, we know w_{n+1}, which is y_b. Then we are solving a system of equations for $w_1, \ldots, w_n$. The spacing of the grid is given by $h = \frac{1}{n+1}$.

Since we are solving second-order problems, we replace y'' with the three point centered formula developed in the previous handout:

$$y'' = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2}$$

and also rewrite it in our new grid notation:

$$\frac{w_{i-1} - 2w_i + w_{i+1}}{h^2}$$

Example 2. Use finite differences to approximate solutions to the linear BVP for $n = 3$.

$$\begin{cases} y'' = 4y \\ y(0) = 1 \\ y(1) = 3 \end{cases}$$

First note that our interval is $[0, 1]$ and we have a step size of $\frac{1}{4}$. So $t_1 = 0.25, t_2 = 0.5, t_3 = 0.75$, and $t_4 = 1$ as expected.

For this differential equation we have

$$\frac{w_{i-1} - 2w_i + w_{i+1}}{h^2} = 4w_i$$

Grouping like terms and noting that $2 + 4h^2 = \frac{9}{4}$ we have

$$\begin{aligned} 1 - \frac{9}{4}w_1 + w_2 &= 0 \\ w_1 - \frac{9}{4}w_2 + w_3 &= 0 \\ w_2 - \frac{9}{4}w_3 + 3 &= 0 \end{aligned}$$

So in matrix form we have:

$$\begin{bmatrix} -\frac{9}{4} & 1 & 0 \\ 1 & -\frac{9}{4} & 1 \\ 0 & 1 & -\frac{9}{4} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ -3 \end{bmatrix}.$$

Then solving by Gaussian elimination (you can use linalg.solve() for instance) gives

$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} = \begin{bmatrix} 1.0249 \\ 1.3061 \\ 1.9138 \end{bmatrix}$$

With the endpoints, the approximation compared to y is

$$w = \begin{bmatrix} 1.0000 \\ 1.0249 \\ 1.3061 \\ 1.9138 \\ 3.0000 \end{bmatrix} \qquad y = \begin{bmatrix} 1.0000 \\ 1.0181 \\ 1.2961 \\ 1.9049 \\ 3.0000 \end{bmatrix}.$$

Example 3. Use finite difference to approximate solutions to the linear BVP for $n = 7$.

$$\begin{cases} y'' = (2 + 4t^2)y \\ y(0) = 1 \\ y(1) = e \end{cases}$$

Our interval is still $[0, 1]$ but the step size is now $\frac{1}{8}$. We also have that $t_i = \frac{i}{8}$. So a finite difference equation is

$$\frac{w_{i-1} - 2w_i + w_{i+1}}{h^2} = (2 + 4\frac{i^2}{64})w_i$$

The middle coefficient will be $-2 - (\frac{1}{64})(2 + \frac{i^2}{16})$ which gives the system of equations

$$\begin{bmatrix} -\frac{2081}{1024} & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -\frac{521}{256} & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -\frac{2089}{1024} & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -\frac{131}{64} & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -\frac{1034}{503}* & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -\frac{529}{256} & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -\frac{2129}{1024} \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \\ w_6 \\ w_7 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -e \end{bmatrix}$$

Solving by row reduction and back substitution gives:

$$\begin{bmatrix} 1.0173 \\ 1.0675 \\ 1.15514 \\ 1.2890 \\ 1.48338 \\ 1.7603 \\ 2.15409 \end{bmatrix}$$

With the end points, we're comparing

$$w = \begin{bmatrix} 1.000000000000000 \\ 1.017346037963531 \\ 1.067477641603622 \\ 1.155137756081340 \\ 1.289048503370908 \\ 1.483383399255987 \\ 1.760289441388713 \\ 2.154089704238659 \\ 2.718281828459046 \end{bmatrix} \qquad y = \begin{bmatrix} 1.000000000000000 \\ 1.015747708586686 \\ 1.064494458917860 \\ 1.150992944691176 \\ 1.284025416687741 \\ 1.477904195411738 \\ 1.755054656960298 \\ 2.150337915952300 \\ 2.718281828459046 \end{bmatrix}$$

*In the lecture, you'll see I noticed that this didn't seem quite right. All the denominators should have been powers of 2, so I assumed I had simply transposed some digits when typing.

But in fact, it was not a typo, but a result that was rounding-error influenced. Working this out by hand, the coefficient should be $-\frac{2105}{1024} = -2.055664062500000$. But when my calculator did this, it got closer to $-2.055666003976143 = -\frac{1034}{503}$.