Finite Difference Approximations

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1 Finite Difference Setup

Previously we looked at spectral discretizations: discretizations of the Laplacian into a basis where each element is global. But in many cases it might make sense to look at a local basis, i.e. a basis where a function is represented by local values. The easiest of which is to simply represent a function by an array of its values.

Look at the Poisson Equation $\Delta u = f(x)$. Let's take our domain to be $\Omega = [0, 1]$. In this case, let's discretize the equation by taking values at $x + j\Delta x$ for some fixed Δx. Now the basis for our functions is $\{x + j\Delta x\}$ and our representation for the function is $[u(x + j\Delta x)]$. Let's denote this array representation of $u(x)$ as U, and $u_i = u(x + i\Delta x)$. The idea is that, if Δx is sufficiently small, the error will go to zero and this is then the same as solving the full continuous PDE.

1.1 Discretization of the Derivative Operators: Forward and Backward Differences

One again, the interesting mathematics is how the derivative operator is discretized. In this case, we will use what's known as finite differences. The simplest finite difference approximation is known as the first order forward difference. This is commonly denoted as

$$\delta_+ u = \frac{u(x + \Delta x) - u(x)}{\Delta x}$$

This looks like a derivative, and we think it's a derivative as $\Delta x \to 0$, but let's show that this approximation is meaningful. Assume that u is sufficiently nice. Then from a Taylor series we have that

$$u(x + \Delta x) = u(x) + \Delta x u'(x) + \mathcal{O}(\Delta x^2)$$

(here I write $(\Delta x)^2$ as Δx^2 out of convenience, note that those two terms are not necessarily the same). That term on the end is called "Big-O Notation". What is means is that those terms are asymtopically like Δx^2. If Δx is small, then $\Delta x^2 \ll \Delta x$ and so we can think of those terms as smaller than any of the terms we show in the expansion. By simplification notice that we get

$$\frac{u(x+\Delta x)-u(x)}{\Delta x} = u'(x) + \mathcal{O}(\Delta x)$$

This means that δ_+ is correct up to first order, where the $\mathcal{O}(\Delta x)$ portion that we dropped is the error. Thus δ_+ is a first order approximation.

Notice that the same proof shows that the backwards difference,

$$\delta_- u = \frac{u(x)-u(x-\Delta x)}{\Delta x}$$

is first order.

1.2 First Order Central Differences

Now let's look at

$$\delta_0 u = \frac{u(x+\Delta x)-u(x-\Delta x)}{2\Delta x}.$$

The claim is this differencing scheme is second order. To show this, we once again turn to Taylor Series. Let's do this for both terms:

$$\begin{aligned} u(x+\Delta x) &= u(x) + \Delta x u'(x) + \frac{\Delta x^2}{2}u''(x) + \mathcal{O}(\Delta x^3) \\ u(x-\Delta x) &= u(x) - \Delta x u'(x) + \frac{\Delta x^2}{2}u''(x) + \mathcal{O}(\Delta x^3) \end{aligned}$$

Now we subtract the two:

$$u(x+\Delta x) - u(x-\Delta x) = 2\Delta x u'(x) + \mathcal{O}(\Delta x^3)$$

and thus we move tems around to get

$$\delta_0 u = \frac{u(x+\Delta x)-u(x-\Delta x)}{2\Delta x} = u'(x) + \mathcal{O}\left(\Delta x^2\right)$$

What does this improvement mean? Let's say we go from Δx to $\frac{\Delta x}{2}$. Then while the error from the first order method is around $\frac{1}{2}$ the original error, the error from the central differencing method is $\frac{1}{4}$ the original error! When trying to get an accurate solution, this quadratic reduction can make quite a difference in the number of required points.

1.3 Second Derivative Central Difference

Now we want a second derivative approximation. Let's show the classic central difference formula for the second derivative:

$$\delta_0^2 u = \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{\Delta x^2}$$

is second order. To do so, we expand out the two terms:6

$$
\begin{aligned}
u(x+\Delta x) &= u(x) + \Delta x u'(x) + \frac{\Delta x^2}{2} u''(x) + \frac{\Delta x^3}{6} u'''(x) + \mathcal{O}\left(\Delta x^4\right) \\
u(x-\Delta x) &= u(x) - \Delta x u'(x) + \frac{\Delta x^2}{2} u''(x) - \frac{\Delta x^3}{6} u'''(x) + \mathcal{O}\left(\Delta x^4\right)
\end{aligned}
$$

and now plug it in. It's clear the $u(x)$ cancels out. The opposite signs makes $u'(x)$ cancel out, and then the same signs and cancellation makes the u'' term have a coefficient of 1. But, the opposite signs makes the u''' term cancel out. Thus when we simplify and divide by Δx^2 we get

$$
\frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{\Delta x^2} = u''(x) + \mathcal{O}\left(\Delta x^2\right).
$$

2 Finite Differencing from Polynomial Interpolation

Finite differencing can also be derived from polynomial interpolation. Draw a line between two points. What is the approximation for the first derivative?

$$
\delta_+ u = \frac{u(x+\Delta x) - u(x)}{\Delta x}
$$

Now draw a quadratic through three points. i.e., given u_1, u_2, and u_3 at $x = 0$, Δx,$2\Delta x$, we want to find the interpolating polynomial

$$
g(x) = a_1 x^2 + a_2 x + a_3.
$$

Setting $g(0) = u_1$, $g(\Delta x) = u_2$, and $g(2\Delta x) = u_3$, we getthe following relations:

$$
\begin{aligned}
u_1 &= g(0) = a_3 \\
u_2 &= g(\Delta x) = a_1 \Delta x^2 + a_2 \Delta x + a_3 \\
u_3 &= g(2\Delta x) = 4a_1 \Delta x^2 + 2a_2 \Delta x + a_3
\end{aligned}
$$

which when we write in matrix form is:

$$
\begin{pmatrix} 0 & 0 & 1 \\ \Delta x^2 & \Delta x & 1 \\ 4\Delta x^2 & 2\Delta x & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}
$$

and thus we can invert the matrix to get the a's:

$$
\begin{aligned}
a_1 &= \frac{u_3 - 2u_2 - u_1}{2\Delta x^2} \\
a_2 &= \frac{-u_3 + 4u_2 - 3u_1}{2\Delta x} \\
a_3 &= u_1
\end{aligned}
$$

or

$$g(x) = \frac{u_3 - 2u_2 - u_1}{2\Delta x^2}x^2 + \frac{-u_3 + 4u_2 - 3u_1}{2\Delta x}x + u_1$$

Now we can get derivative approximations from this. Notice for example that

$$g'(x) = \frac{u_3 - 2u_2 - u_1}{\Delta x^2}x + \frac{-u_3 + 4u_2 - 3u_1}{2\Delta x}$$

Now what's the derivative at the middle point?

$$g'(\Delta x) = \frac{u_3 - 2u_2 - u_1}{\Delta x} + \frac{-u_3 + 4u_2 - 3u_1}{2\Delta x} = \frac{u_3 - u_1}{2\Delta x}.$$

And now check

$$g''(\Delta x) = \frac{u_3 - 2u_2 - u_1}{\Delta x^2}$$

which is the central derivative formula. This gives a systematic way of deriving higher order finite differencing formulas. In fact, this formulation allows one to derive finite difference formulae for non-evenly spaced grids as well! The algorithm which automatically generates stencils from the interpolating polynomial forms is the Fornberg algorithm.

3 Finite Differencing Operators

Now we write these operators as matrices. Notice that for the vector $U = \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix}$, we have that

$$\delta_+ U = \begin{pmatrix} u_2 - u_1 \\ \vdots \\ u_n - u_{n-1} \end{pmatrix}$$

and so

$$\delta_+ = \begin{pmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{pmatrix}$$

We can do the same to understand the other operators. But notice something: this operator isn't square! In order for this to be square, in order to know what happens at the endpoint, we need to know the boundary conditions. I.e., an assumption on the value or derivative at $u(0)$ or $u(1)$ is required in order to get the first/last rows of the matrix!