MAT 228A Notes

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1 Finite Difference Methods

Big idea is to approximate derivatives using function values at discrete points, i.e. approximating derivatives using differences.

1.1 How to approximate a derivative with a difference

Define the forward difference operator D_+ by

$$D_+(u(x)) \coloneqq \frac{u(x+h)-u(x)}{h}$$

where h is fixed. We can also define the backward difference operator D_- by

$$D_-(u(x)) \coloneqq \frac{u(x)-u(x-h)}{h}.$$

How accurately do these approximate $\dfrac{\mathrm{d}}{\mathrm{d}x}$? Define ε as the error of the apprimation, i.e.

$$\varepsilon \coloneqq D_+(u(x)) - u'(x)$$

Use a Taylor expansion as $h \to 0$:

$$\begin{aligned} u(x+h) &= u(x) + hu'(x) + \frac{h^2}{2}u''(x) + \frac{h^3}{6}u'''(x) + \dots \\ D_+(u(x)) &= u'(x) + \frac{h}{2}u''(x) + \frac{h^2}{6}u'''(x) + \dots \end{aligned}$$

so

$$\varepsilon = \frac{h}{2}u''(x) + \frac{h^2}{6}u'''(x)$$

Assuming $h \ll 1$ and u'' is bounded, then we can say $\varepsilon = \mathcal{O}(h)$. The same idea holds for D_-.

$$u(x-h) = u(x) - hu'(x) + \frac{h^2}{2}u''(X) - \dots$$

So,

$$D_-(u(x)) = u'(x) \underbrace{- \frac{h}{2}u''(x) + \frac{h^2}{6}u'''(x) + \dots}_{=\varepsilon}$$

and thus $\varepsilon = \mathcal{O}(h)$.

Now define the "centered difference operator" D_0 by

$$\begin{aligned} D_0(u(x)) \coloneqq \frac{1}{2}(D_+ + D_-)u(x) &= \frac{u(x+h)-u(x-h)}{2h} \\ &= u'(x) + \frac{h^2}{6}u'''(x) + \dots \qquad \text{by Taylor expansion} \end{aligned}$$

So $\varepsilon = \mathcal{O}\big(h^2\big)$ when ε is the error term for D_0.

Terminology:

- D_+ and D_- provide first order accurate approximations to the derivative
- D_0 provides second order accurate appoximations to the derivative

In practice, halving h should result in halving of the absolute error of first-order approximations and quartering the absolute error of second-order approximations (passed-out sheet). In this problem,

$$\text{Absolute Error} = D_+(u(2)) - u'(2)$$

$$\text{Relative Error} = \frac{D_+(u(2)) - u'(2)}{u'(2)} \qquad \text{how many digits of accuracy do we expect}$$

1.2 In General...

For a fixed h, $D_+(u(x))$ can be evaluated everywhere. For finite difference methods, we start on a discrete domain. For example, an infinite equally-spaced lattice on the real line, points separated by a distance of h. The points are labeled x_j where $x_j := jh$ for $j \in \mathbb{Z}$.

So $u_j \approx u(x_j)$ and we define $(D_+u)_j$ by

$$(D_+u)_j := \frac{u_{j+1} - u_j}{h}$$

1.3 Approximating Higher Derivatives

We can apply the difference operators multiple times. For second derivatives. We could use

$$D_+^2 \qquad D_-^2 \qquad D_0^2 \qquad D_+D_- \qquad D_0D_+ \qquad \dots$$

All of these are approximations to the second derivative. Two good ones are D_0^2 and D_+D_- (or D_-D_+).

$$\begin{aligned} (D_0u)_j &= \frac{u_{j+1} - u_{j-1}}{2h} \\ \implies (D_0^2u)_j &= \frac{u_{j+2} - 2u_h + u_{j-2}}{4h^2} \end{aligned}$$

and

$$\begin{aligned} (D_-u)_j &= \frac{u_j - u_{j-1}}{h} \\ \implies (D_+D_-u)_j &= \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} \end{aligned}$$

So we see D_0^2 is the exact same operator as D_+D_- but with a coarser mesh.

Another way we derive an approximation to the second derivative is by seeing that for second derivatives, we must use at least three points. So at x_j we should also use x_{j-1} and x_{j+1} since they are the closest to x_j. What linear combination should we use?

$$(D^2u)_j = au_{j-1} + bu_j + cu_{j+1} \tag{1}$$

where a, b, and c are constants to be determined. Assume this should be equivalent to

$$\begin{aligned} (D^2u)_j = au_{j-1} + bu_j + cu_{j+1} &= au(x-h) + bu(x) + cu(x-h) \quad (2) \\ &= a\left(u(x) - hu'(x) + \frac{h^2}{2}u''(x) - \frac{h^3}{6}u'''(x) + \frac{h^4}{24}u^{(4)}(x) + \dots\right) + bu(x) \quad (3) \\ &\quad + c\left(u(x) + hu'(x) + \frac{h^2}{2}u''(x) + \frac{h^3}{6}u'''(x) + \frac{h^4}{24}u^{(4)}(x) + \dots\right) \quad (4) \\ &= (a+b+c)u(x) + (c-a)hu'(x) + (a+c)\frac{h^2}{2}u''(x) + \dots \quad (5) \end{aligned}$$

We require

$$\begin{aligned} a + b + c &= 0 \quad (6) \\ -ha + hc &= 0 \quad (7) \\ \frac{h^2}{2}a + \frac{h^2}{2}c &= 1 \quad (8) \end{aligned}$$

The solution is

$$a = c = \frac{1}{h^2} \qquad \text{and} \qquad b = \frac{-2}{h^2} \tag{9}$$

which coincides with D_+D_-. Next we need to show the higher order terms are small...

$$(D_+D_-u)_j = u''(x_j) + \cancelto{0}{\frac{h^3}{6}(c-a)u'''(x)} + \frac{h^4}{24}(a+c)u^{(4)}(x) + \dots \tag{10}$$

$$= u''(x_j) + \frac{h^2}{12}u^{(4)}(x) + \dots \tag{11}$$

and so this is a second-order approximation.

If we pick x_{j+1} and x_{j+2} we lose symmetry, so we will lose the free second-order approximation. D_+D_+ is first-order accurate. Similarly, if we have unequal grid spacing, we lose the symmetry of D_+D_-. We would expect three-point operators to give first-order accuracy in general.

1.4 Derivation of approximation of n^{th} derivative of p^{th} order accuracy

How many points do we need assuming no symmetry? Say we have m points.

$$w_1u_1 + w_2u_2 + \dots + w_mu_m \tag{12}$$

Taylor series..

$$A_0u(x) + A_1u'(x) + \dots + A_{n-1}u^{(n-1)}(x) + A_nu^{(n)}(x) + A_{n+1}u^{(n+1)}(x) + \dots \tag{13}$$

So we want $A_0 = A_1 = \dots = A_{n-1} = 0$ and $A + n = 1$. This means we have $n+1$ constraints, so generically we need $n+1$ points. To get the accuracy, we expect $w \sim \frac{1}{h^n}$, i.e. $A_{n+1}u^{(n+1)}(x)$ has size h. So we need

$$m = \underbrace{(n+1)}_{\text{for } n^{\text{th}} \text{ derivative}} + \underbrace{(p-1)}_{\text{for } p^{\text{th}} \text{ order accuracy}} \tag{14}$$