Day. 16

Numerical Analysis.

[redacted]

A. Polynomial Interp
B. Undetermined Coef.

TODAY

We start: NUMERICAL DIFFERENTIATION.

- taking a derivative is pretty easy ... why would we do it numerically?

1. Approximating derivatives when solving ODE's or PDE's

2. Forming the derivative of a function which known only as empirical data.

The most straight forward way ...

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Using the definition of the derivative.

so $D_h f(x) \equiv \dfrac{f(x+h) - f(x)}{h}$

numerical derivative with stepsize h.

Ex Your data $(1, \frac{1}{2})(2, \frac{1}{6})(3, \frac{1}{10})$

we can approximate the derivative... here $h = 1$

$(1, \frac{1}{2})(2, \frac{1}{6}) \longrightarrow \dfrac{\frac{1}{6} - \frac{1}{2}}{1} = -\frac{1}{3}$ this is literally the slope.

What is the error in this approximation.

Expand $f(x)$ plug in $x = a + h$ replace $a = x$.

$$f(x+h) = f(x) + hf'(x) + \tfrac{1}{2}h^2 f''(c)$$

c is between x and $x+h$

plug this in ...

$$f'(x) - D_h f(x) = f'(x) - \frac{1}{h}\left[f(x) - hf'(x) + \frac{1}{2}h^2 f''(c) - f(x)\right]$$
$$= -\tfrac{1}{2} h f''(c)$$

If we took the next term in the taylor series we would find

$$f'(x) - D_h f(x) = -\tfrac{1}{2} h f''(x) - \tfrac{1}{6} h^2 f'''(c)$$

↳ higher remainder

if h is small then

$$f'(x) - D_h f(x) \approx -\tfrac{1}{2} h f''(x)$$

we can approximate the error of the derivative at a point by the curvature.

FORWARD DIFFERENCE

$$\boxed{f'(x) \approx \frac{f(x+h) - f(x)}{h}}$$

BACKWARD DIFFERENCE

$$\boxed{f'(x) \approx \frac{f(x) - f(x-h)}{h}}$$

IN applications ... sometimes one is better than the other ... for example calculating the derivative at the RIGHT BOUNDARY.

These are FIRST ORDER approximations the error decreases linearly as h decreases.

EX. Given n datapoints each Δx apart. $\Delta x = h = \frac{b-a}{n}$

$$f = \text{Data} = [f_1, f_2, f_3 \ldots, f_n]$$

How would I calculate the derivative at EACH point.

PSUEDO CODE

```
for i = 1:n-1
        fprime(i) = (f(i+1) - f(i)) / Δx
end

fprime(n) = (f(n) - f(n-1)) / Δx
```

Now that we have basic formulas ... how can we do better?

HIGHER ORDER METHODS.

Lets use polynomial interpolation and see if we can do a better job.

Let $P_n(x)$ be the degree n polynomial that interpolates $f(x)$ at $n+1$ node points $x_0, x_1, \dots, x_n$. To calculate $f'(x)$ at some point $x=t$ use

$$f'(t) \approx P_n'(t)$$

- We can actually come up with lots of different methods by varying n and the placement of the nodes.

Consider $n=2$ with evenly spaced nodes $x_0,\ x_0+h,\ x_0+2h$
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad x_0,\ \ x_1,\ \ x_2$

$$P_2 = f(x_0)L_0(x) + f(x_1)L_1(x) + f(x_2)L_2(x)$$

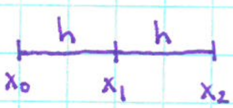
take the derivative of this ...

$$P_2'(x) = f(x_0)L_0'(x) + f(x_1)L_1'(x) + f(x_2)L_2'(x)$$

so we need to take the derivative of the Lagrange Basis Functions.

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \longrightarrow L_0'(x) = \frac{2x-(x_1+x_2)}{(x_0-x_1)(x_0-x_2)}$$

similarly $\quad L_1'(x) = \dfrac{2x-(x_0+x_2)}{(x_1-x_0)(x_1-x_2)}$ and $L_2'(x) = \dfrac{2x-(x_0+x_1)}{(x_2-x_0)(x_2-x_1)}$

evenly spaced nodes 

$$L_0'(x) = \frac{2x-(x_1+x_2)}{2h^2} \qquad L_1'(x) = \frac{2x-(x_0+x_2)}{-h^2} \qquad L_2'(x) = \frac{2x-(x_0+x_1)}{2h^2}$$

Now say we want $f'(x_1)$ plug this in and define

$$x_0 = x_1 - h$$
$$x_2 = x_1 + h$$

$$P_2'(x_1) = f(x_0)\left[\frac{2x_1 - x_1 - x_2}{2h^2}\right] + f(x_1)\left[\frac{2x_1 - x_0 - x_2}{-h^2}\right] + f(x_2)\left[\frac{2x_1 - x_0 - x_1}{2h^2}\right]$$

$$= f(x_1 - h)\left[\frac{-h}{2h^2}\right] + f(x_1)\left[\frac{\overbrace{x_1 - x_2}^{-h} + \overbrace{x_1 - x_0}^{h}}{-h^2}\right] + f(x_1+h)\left[\frac{h}{2h^2}\right]$$

$$\boxed{f'(x_1) = \frac{f(x_1+h) - f(x_1-h)}{2h}}$$

Centered Difference Formula.

What is the order of convergence?

We must start by considering the error in $P_2(x)$

$$f(x) - P_2(x) = \underbrace{\psi_2(x)\, f[x_0, x_1, x_2, x]}_{\text{remainder – error term}}$$

$$\frac{(x-x_0)(x-x_1)(x-x_2)f^{(3)}(c_x)}{3!}$$

Recall... $P_2 = f(x_0) + (x-x_0)f[x_0,x_1] + (x-x_0)(x-x_1) f[x_0,x_1,x_2]$

where $\psi_2(x) = (x-x_0)(x-x_1)(x-x_2)$

we derived this from the NEWTON DIVIDED DIFFERENCE FORMULA.

Take the derivative.

$$E = f'(x) - P_2'(x) = \psi_2'(x)\, f[x_0\, x_1\, x_2\, x] + \psi_2 \frac{d}{dx} f[x_0\, x_1\, x_2, x]$$

RECALL $f[x_0, x_1, \ldots, x_n, x] = \frac{1}{(n+1)!} f^{(n+1)}(c_x)$

the divided difference is related to the derivative.

where c_x is between the largest and smallest x_n's

then $E = \psi_2'(x)\,\frac{1}{3!} f^{(3)}(c_x) + \psi_2(x)\,\frac{1}{4!} f^{4}(c_x)$

$\psi_2'(x_1) = (x_1 - x_0)(x_1 - x_2)$ or $-h^2$

$\psi_2(x_1) = 0$

If we are evaluating at $x = x_1$ then

$$E = f'(x_1) - P_2'(x_1) = \frac{\psi_2'(x_1)}{6} f'''(c_2) = \boxed{-\frac{h^2}{6} f'''(c_2)}$$

THE ERROR decreases as the square of h.

SECOND ORDER METHOD.

- We often need approximations to higher derivatives.

For Example ... Derive an approximation for $f''(x)$ at $x = t$.

- USE Taylor Polynomials and UNDETERMINED COEFFICIENTS.

Say I want to use the points $t+h$, t, $t-h$ to approximate $f''(x)$.

1. write down your wish.

$$f''(t) \approx D_h^2 f(t) \equiv A f(t+h) + B f(t) + C f(t-h)$$

2. now write out taylor polynomials:

$$f(t+h) \sim f(t) + h f'(t) + \frac{h^2}{2} f''(t) + \dots$$

$$f(t-h) \sim f(t) - h f'(t) + \frac{h^2}{2} f''(t) - \dots$$

3. plug these in

$$D_h^2 f(t) \cong A\left[f(t) + hf'(t) + h^2/_2 f''(t) + \cdots\right] + Bf(t) + C\left[f(t) - hf'(t) + h^2/_2 f''(t) - \cdots\right]$$

4. gather like derivatives.

$$D_h^2 f(t) \approx (A+B+C) f(t) + h(A-C) f'(t) + h^2/_2 (A+C) f''(t) + \cdots$$

so to have $D_h^2 f(t) \cong f''(t)$

we need

5. Solve for Coeff.

$$\left.\begin{aligned} A + B + C &= 0 \\ h(A-C) &= 0 \\ \frac{h^2}{2}(A+C) &= 1 \end{aligned}\right\} \quad \begin{aligned} A = C &= 1/h^2 \\ B &= -2/h^2 \end{aligned}$$

So

$$D_h^2 f(t) = \frac{f(t+h) - 2f(t) + f(t-h)}{h^2}$$

What about the error?

$$f''(t) - D_h^2(t) \approx -\frac{h^2}{12} f^{(4)}(\xi)$$

how do we know this ...

Taylor Series.

The next term in the series would be $\frac{h^3}{3!}(\cancel{A-C})^{0} f'''(t)$

and then $\frac{h^4}{4!}(A+C) f''''(t)$

Similar to analysis of Forward Difference error $\longrightarrow$ $A+C = \frac{1}{h^2} + \frac{1}{h^2} = \frac{2}{h^2}$ $\Rightarrow \frac{h^2}{12} f^{(4)}(t)$

see p. 7.

Ex

What if instead I wanted to use t $t+h$ and $t+2h$

1. Goal $D_h^2 f(t) \equiv Af(t) + Bf(t+h) + Cf(t+2h)$

2. Taylor Polynomials

YOU TRY

$$f(t+h) = f(t) + hf'(t) + \frac{h^2}{2} f''(t) + \cdots$$

$$f(t+2h) = f(t) + 2hf'(t) + 2h^2 f''(t) + \cdots$$

3. Plug in $D_h^2 f(t) \equiv Af(t) + B\left[f(t) + hf'(t) + \frac{h^2}{2} f''(t) + \cdots\right] + C\left[f(t) + 2hf'(t) + 2h^2 f''(t) + \cdots\right]$

4. Gather Like derivatives.

$$D_h^2 f(t) \cong (A+B+C)f(t) + (B+2C)hf'(t) + (B+4C)\frac{h^2}{2} f''(t)$$

$$\left.\begin{aligned} A+B+C &= 0 \\ h(B+2C) &= 0 \\ \frac{h^2}{2}(B+4C) &= 1 \end{aligned}\right\}$$

$h^2C - 2h^2C = -1$

$h^2C = 1$ $\boxed{C = 1/h^2}$

$h(B + 2/h^2) = 0$ $hB = -2/h$ $\boxed{B = -2/h^2}$

$A = -B - C = 2/h^2 - 1/h^2 = \boxed{1/h^2}$

$$\boxed{D_h^2 f(t) = f(t+2h) - 2f(t+h) + f(t)}$$

1. Write out the error term...

$$f''(x) - D_h^2(x) = f''(x) - \frac{1}{h^2}\left[f(x+h) - 2f(x) + f(x-h)\right]$$

expand $f(x)$ near α $\sim f(\alpha) + (x-\alpha)f'(\alpha) + \frac{(x-\alpha)^2}{2}f''(\alpha) + \frac{(x-\alpha)^3}{6}f'''(\alpha) + \frac{(x-\alpha)^4}{24}f^{(4)}(c_x)$

2. Expand for $f(x+h)$ and $f(x-h)$...

when $x = \alpha - h$ or $x = \alpha + h$

$$f(\alpha+h) = f(\alpha) + hf'(\alpha) + \frac{h^2}{2}f''(\alpha) + \frac{h^3}{6}f'''(\alpha) + \frac{h^4}{24}f^{(4)}(c_x)$$

$$f(\alpha-h) = f(\alpha) - hf'(\alpha) + \frac{h^2}{2}f''(\alpha) - \frac{h^3}{6}f'''(\alpha) + \frac{h^4}{24}f^{(4)}(c_x)$$

3. Plug into formula

plug these in... lots of stuf cancels letting $\underline{\alpha = x}$

$$f(x+h) - 2f(x) + f(x-h) = h^2 f''(x) + \frac{h^4}{12}f^{(4)}(c_x).$$

then

$$f''(x) - D_h^2(x) = f''(x) - \frac{1}{h^2}\left[h^2 f''(x) + \frac{h^4}{12}f^{(4)}(c_x)\right]$$

$$= -\frac{h^2}{12}f^{(4)}(c_x).$$

This is our error term!

I needed to go to $f^{(4)}(c_x)$ because I saw that the $\frac{h^3}{6}f'''(\alpha)$ terms would cancel when I add $f(x+h) + f(x-h)$.