

Numerically Computed Derivatives:

- Exact formulas can be very complicated ~ easier to approximate functions

Starting with first order derivatives

Approximations:

- $f'(x) \approx \frac{f(x+h)-f(x)}{h}$
- Assuming $h > 0$
- This is the exact value for linear functions ($y = 2x$)
- Other functions introduce error ($y = x^2 + 9 * x^3$)

Taylor Series EQ

- $f(x) \approx f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \frac{f'''(x_0)}{3!}(x - x_0)^3 + \dots$
- $f(x) \approx \sum_{n=0}^n \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$

Computing Error of Approximation

- $f(x+h) \approx f(x) + f'(x)(x+h-x) + \frac{f''(x)}{2!}(x+h-x)^2 + \dots$
- (AKA) $f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \dots$
- $f(x) \approx \sum_{n=0}^n \frac{f^{(n)}(x)}{n!}(h)^n$
- So actually....
 - We Approximated $f'(x) \approx \frac{f(x+h)-f(x)}{h}$
 - Actually (Order 2 Sol) $f'(x) = \frac{f(x+h)-f(x)}{h} - \frac{h}{2}f''(x)$, where $-\frac{h}{2}f''(x)$ is the error in the previous assumption and removing this is called a "truncation error"

Forward/Backward Differencing

- Forward: $f'(x) \approx \frac{f(x+h)-f(x)}{h}$
- Backward: $f'(x) \approx \frac{f(x)-f(x-h)}{h}$

Explaining the Equations:

The derivative is effectively a measure of some rate of change. Here we have x which can be a scalar or an array. To approximate the derivative using continuous values, the rate of change must be computed at each point on the function with respect to x . $f(x)$ or y is what is being derived with respect. As such, we measure $f(x)$ and difference it to a point behind ($f(x-h)$) or in front ($f(x+h)$) with respect the change in $x = (x+h-x = h)$. The best solution is for $h \rightarrow 0$. We see this is the second order error term $-\frac{h^2}{2}f''(x)$ where a lower h significantly reduces error (rate of convergence).

Truncation error is measured in terms of error. Nth order derivatives have error of the order of $O(h^n)$

To reduce error, we combine back and forward differencing into central differencing.

- **Center:** $f'(x) \approx \frac{f(x+h)-f(x-h)}{2h}$

Showing the lesser Error (2nd order case)

- $f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x)$
- $f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x)$

Therefore...

- $f'(x) = \frac{f(x+h)-f(x-h)}{h^2} - \frac{h^2}{12}f''(x)$, with a truncation error $= -\frac{h^2}{12}f''(x)$

Moving to 2nd Order Derivative...

Looking at the Taylor expansions of $f(x \pm h)$ we can derive

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

And 3rd Order Derivative...

Looking at the Taylor expansions of $f(x \pm h)$ we can derive

- $f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x)$
- $f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x)$

Remember Taylor EQ:

- $f(x) \approx f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2!}(x-x_0)^2 + \frac{f'''(x_0)}{3!}(x-x_0)^3 + \dots$

Applying to +2h

- $f(x+2h) \approx f(x) + f'(x)(x-x+2h) + \frac{f''(x)}{2!}(x-x+2h)^2 + \frac{f'''(x)}{3!}(x-x+2h)^3 + \dots$
- $f(x+2h) \approx f(x) + 2hf'(x) + \frac{f''(x)}{2!}(2h)^2 + \frac{f'''(x)}{3!}(2h)^3 + \dots$
- $f(x+2h) \approx f(x) + 2hf'(x) + \frac{f''(x)}{2!}(2h)^2 + \frac{f'''(x)}{3!}(2h)^3 + \dots$
- $f(x+2h) = f(x) + 2hf'(x) + 2h^2f''(x) + \frac{4h^3}{3}f'''(x)$
- $f(x-2h) = f(x) - 2hf'(x) + 2h^2f''(x) - \frac{4h^3}{3}f'''(x)$

- $f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f'''(x)$
- $f(x+2h) - f(x-2h) = 4hf'(x) + \frac{8h^3}{3}f'''(x)$
- $f(x+2h) - f(x-2h) - 2(f(x+h) - f(x-h)) = 4hf'(x) + \frac{8h^3}{3}f'''(x) - 4hf'(x) - 2\frac{h^3}{3}f'''(x)$
- $f(x+2h) - f(x-2h) - 2(f(x+h) - f(x-h)) = 2h^3f'''(x)$
- $f'''(x) = \frac{f(x+2h)-f(x-2h)-2(f(x+h)-f(x-h))}{2h^3}$

And 4th Order Derivative...

$$\bullet f^4(x) = \frac{f(x+2h)+f(x-2h)+6f(x)-4(f(x+h)+f(x-h))}{h^4}$$

Looking at all Approx

$$\begin{aligned}\bullet f^1(x) &\approx \frac{f(x+h)-f(x-h)}{2h} \\ \bullet f^2(x) &\approx \frac{f(x+h)-2f(x)+f(x-h)}{h^2} \\ \bullet f^3(x) &\approx \frac{f(x+2h)-f(x-2h)-2(f(x+h)-f(x-h))}{2h^3} \\ \bullet f^4(x) &\approx \frac{f(x+2h)+f(x-2h)+6f(x)-4(f(x+h)+f(x-h))}{h^4}\end{aligned}$$

<http://www2.math.umd.edu/~dlevy/classes/amsc466/lecture-notes/differentiation-chap.pdf>
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Differentiation Via Interpolation

Generate differentiation formulas by differentiating interpolant

How Can this be reduced in complexity?

As mentioned before, a change in the function is defined as $\Delta f = f^1(x)$ Therefore logically we can say

$$\begin{aligned}\bullet f^1(x) &\approx \Delta f \\ \bullet f^2(x) &\approx \Delta \Delta f = \Delta f^1 \\ \bullet f^3(x) &\approx \Delta \Delta \Delta f = \Delta f^2 \\ \bullet f^4(x) &\approx \Delta \Delta \Delta \Delta f = \Delta f^3\end{aligned}$$

Δ = change or more specifically a shift operator Shift Operator $\rightarrow T_h = e^{h \frac{d}{dx}}$

$$\Delta = \frac{T_h - T_{-h}}{2h} = \frac{e^{h \frac{d}{dx}} - e^{-h \frac{d}{dx}}}{2h}$$

Review of Binomial Theorem

$$(x+y)^n = \sum_{k=0}^n \binom{n}{k} x^{n-k} y^k$$

$$(x+y)^n = \sum_{k=0}^n \frac{n!}{k!(n-k)!} x^{n-k} y^k$$

Where $\binom{n}{k}$ is the number of k combinations from a total of n

This formula makes it easy to explain binomials ie two summed or subtracted variables

Back to Complexity Reduction

We have a binomial expansion problem

$$\Delta^{2k} = \left(\frac{T_h - T_{-h}}{2h}\right)^{2k}$$

$$= \frac{1}{h^{2k}} \sum_{m=-k}^k \frac{2k!}{(k+m)!(2k-k-m)!} (-1)^{m+k} f(x + mh)$$

with vars k=order/2,m=,h=1e-2