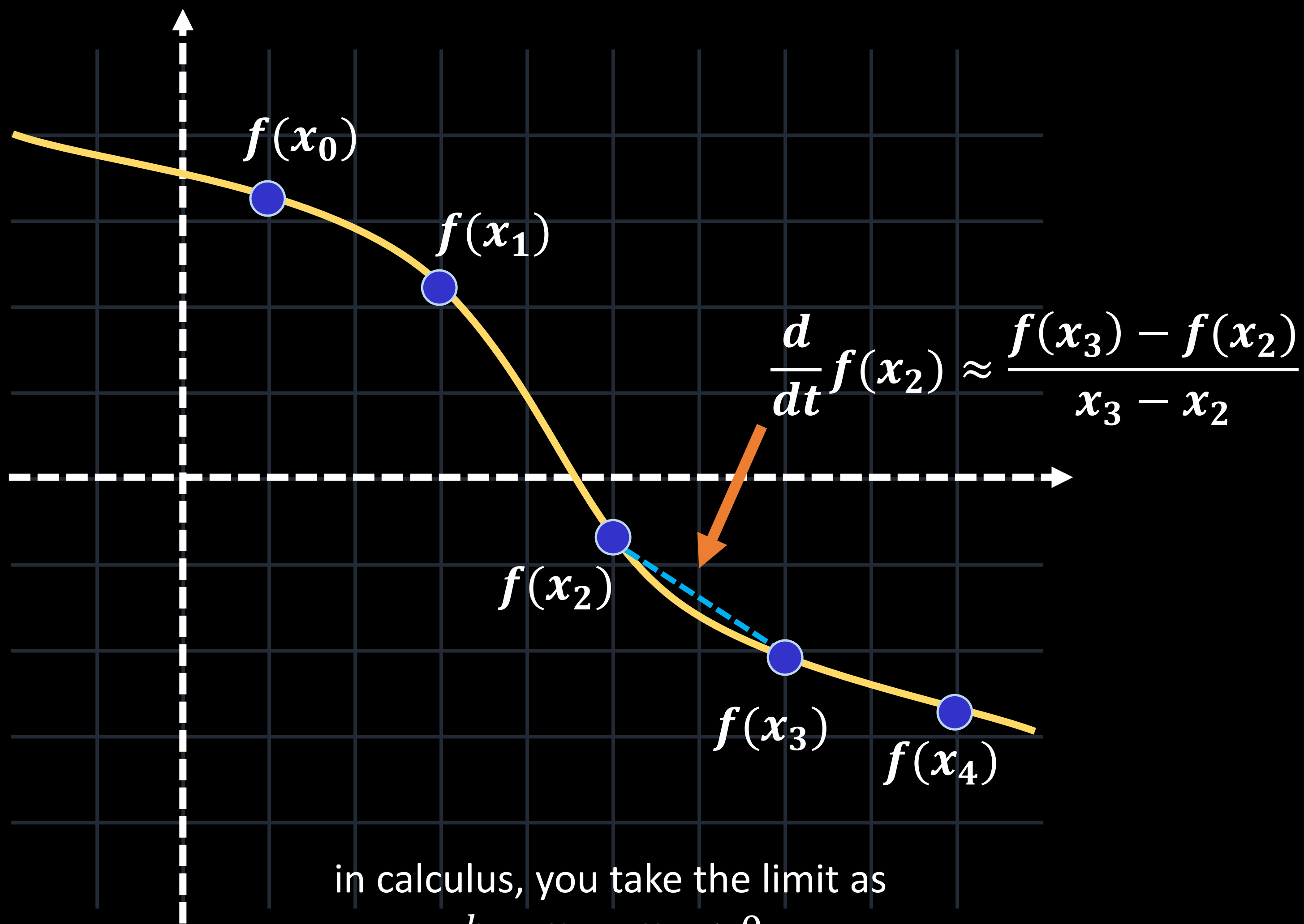
Finite Difference Calculus

Finite difference calculus

- Calculations must be done on discrete (often equally-spaced) values representing functions
  - ex. $3.0, 3.5, 4.0, 5.0, 7.0, 10, \cdots$
  - measurements of physical systems
    - speed, temperature, etc.
  - simulations of complex systems
  - Roots or extrema of these functions must be found
    - rely on knowing the derivative – ex. Newton's method

- Estimating a derivative based on discrete samples:
  - Finite difference methods

Finite differences



in calculus, you take the limit as
$h = x_3 - x_2 \to 0$

Finite differences

- Computers don't allow $h \to 0$
  - can't solve analytically if we don't know the function

- Rely on finite differences and bounding the error
- Forward difference:

$$\frac{d}{dt} f(x_2) \approx \Delta f(x_2) = \frac{f(x_3) - f(x_2)}{x_3 - x_2}$$

- Derive the forward difference and error using a Taylor series approximation. Bound the error.

$$v(x_{i+1}) = v(x_i) + v'(x_i)(x_{i+1} - x_i) + O[(x_{i+1} - x_i)^2]$$

  - Solve for $v'(x_i)$

$$v'(x_i) = \frac{v(x_{i+1}) - v(x_i) - O[(x_{i+1} - x_i)^2]}{(x_{i+1} - x_i)}$$

$$v'(x_i) = \frac{v(x_{i+1}) - v(x_i)}{(x_{i+1} - x_i)} + O(x_{i+1} - x_i)$$

$$v'(x) = \frac{v(x + h) - v(x)}{h} + O(h)$$

Forward + backward differences

- First forward finite difference approximation:

$$v'(x) = \frac{v(x+h)-v(x)}{h}$$

- First backward finite difference approximation.

$$v'(x) = \frac{v(x)-v(x-h)}{h}$$

based on the Taylor expansion

$$v(x-h) = v(x) - v'(x)h + O(h^2)$$

- Both methods exhibit linear error: $O(h)$

Central difference approximation

- Can we create a more accurate estimate?
- Expansions out to the second derivative:
  - Forward expansion:

$$v(x+h) = v(x) + v'(x)h + \frac{v''(x)}{2}h^2 + O(h^3)$$

  - Backward expansion:

$$v(x-h) = v(x) - v'(x)h + \frac{v''(x)}{2}h^2 + O(h^3)$$

- Calculate $v(x+h) - v(x-h)$:

$$v(x+h) - v(x-h) = 2v'(x)h + O(h^3)$$

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

Finite differences (summary)

- First forward finite difference approximation:

$$v'(x) = \frac{v(x+h) - v(x)}{h} \quad \text{at } O(h) \text{ error}$$

- First backward finite difference approximation:

$$v'(x) = \frac{v(x) - v(x-h)}{h} \quad \text{at } O(h) \text{ error}$$

- First central finite difference approximation:

$$v'(x) = \frac{v(x+h) - v(x-h)}{2h} \quad \text{at } O(h^2) \text{ error}$$

Problems

- Discretization error
  - Analytically we take $h \to 0$, but this isn't possible
  - Small h improves accuracy at the cost of speed
  - Large h introduces artifacts (like aliasing)

- Loss of precision
  - As h gets smaller, discretization error drops but $x \approx x + h$
  - If $f(x)$ is computed with n digits of precision, it is difficult to compute $f'(x)$ with n digits of precision.

- Noise
  - As h gets smaller, noise is amplified
  - If $f(x)$ or $f(x+h)$ are in error by d, then $f'(x)$ is in error by ${}^{d}/_{h}$

- All errors are cumulative for higher order derivatives.

Examples

- Algorithm depends on usage (ex. boundary value problems)

Calculate $f'(x)$, for $f(x) = |x|$ for $x = 0.5$ and $h = 0.75$

exact = 1

forward = $\frac{1.25-0.5}{0.75} = 1$

backward = $\frac{0.5-0.25}{0.75} = \frac{1}{3}$

central = $\frac{1.25-0.25}{1.5} = \frac{2}{3}$

Examples

- Compute the derivative of $\log x$ using **forward** and **central** differences with 3 significant figures, $x = 100$, and $h = 10$. How many bits are lost?
  - exact = .00434
  - forward:

$$\frac{\log(110) - \log(100)}{10} \approx \frac{2.04 - 2}{10} = \frac{.02}{10} = .004$$

$$\frac{-\log\left(1 - \frac{\log 100}{\log 110}\right)}{\log 2} \approx 5.62$$

  - central:

$$\frac{\log(110) - \log(90)}{20} \approx \frac{2.04 - 1.95}{20} = \frac{.09}{20} = .0045$$

$$\frac{-\log\left(1 - \frac{\log 90}{\log 110}\right)}{\log 2} \approx 4.55$$

Examples

- Compute the derivative using central differences and 3 significant figures.

$$f(x) = e^x \qquad \text{for } x = 1 \text{ and } h = 0.5$$

$$\frac{e^{1.5} - e^{0.5}}{2 \cdot 0.5} \approx \frac{4.48 - 1.65}{1} = 2.83$$

- What is the relative error?

$$\text{exact} = 2.72$$

$$e_r = \frac{|2.83 - 2.72|}{|2.72|} \approx 4\%$$

- How many bits are lost if $h = 0.01$?

$$\frac{-\log\left(1 - \frac{e^{0.99}}{e^{1.01}}\right)}{\log 2} \approx \frac{-\log\left(1 - \frac{2.69}{2.74}\right)}{\log 2} \approx \frac{-\log(1 - 0.98)}{\log 2} \approx 5.66$$

between 5 and 6 bits are lost