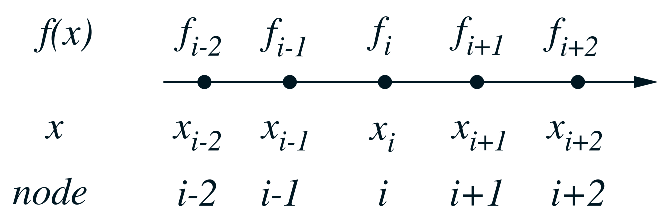
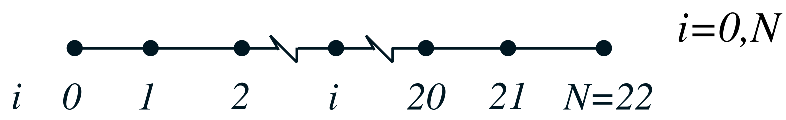
LECTURE 6

NUMERICAL DIFFERENTIATION

- To find ***discrete approximations*** to differentiation (since computers can only deal with functional values at discrete points)
- Uses of numerical differentiation
  - To represent the terms in o.d.e.'s and p.d.e.'s in a discrete manner
  - Many error estimates include derivatives of a function. This function is typically not available, but values of the function at discrete points are.
- Notation
  - Nodes are data points at which functional values are available or at which you wish to compute functional values
  - At the nodes $f(x_i) \equiv f_i$



• Node index $\rightarrow i \rightarrow$ indicates which node or point in space-time we are considering (here only one spatial or temporal direction)



• For equi-spaced nodal points, $h = x_{i+1} - x_i$

<u>Taylor Series Expansion for *f(x)* About a Typical Node *i*</u>

$$f(x) = f(x_i) + (x - x_i)f^{(1)}(x_i) + \frac{(x-x_i)^2}{2!}f^{(2)}(x_i) + \frac{(x-x_i)^3}{3!}f^{(3)}(x_i)$$

$$+ \frac{(x-x_i)^4}{4!}f^{(4)}(x_i) + \ + \frac{(x-x_i)^5}{5!}f^{(5)}(x_i) + \frac{(x-x_i)^6}{6!}f^{(6)}(x_i) + \ldots$$

- For the ***present*** analysis we will consider only the first four terms of the T.S. expansion (may have to consider more)

$$f(x) = f(x_i) + (x - x_i)f^{(1)}(x_i) + \frac{(x - x_i)^2}{2!}f^{(2)}(x_i) + \frac{(x - x_i)^3}{3!}f^{(3)}(x_i) + E$$

where

$$E = \frac{(x - x_i)^4}{4!}f^{(4)}(x_i) + \frac{(x - x_i)^5}{5!}f^{(5)}(x_i) + \frac{(x - x_i)^6}{6!}f^{(6)}(x_i) + \ldots \quad \Rightarrow$$

$$E = \frac{(x - x_i)^4}{4!}f^{(4)}(\xi) \qquad x_i \le \xi \le x \quad \Rightarrow$$

$$E \cong \frac{(x - x_i)^4}{4!}f^{(4)}(x_i) \quad \Rightarrow$$

$$E \cong O(x - x_i)^4$$

- If the Taylor series is convergent, each subsequent term in the error series should be becoming smaller.

- The terms in the error series may be expressed
  - Exactly as $E = \frac{(x-x_i)^4}{4!} f^{(4)}(\xi)$
    - We note that the value of ξ is not known
    - This single term exactly represents all the truncated terms in the Taylor series
  - Approximately as $E \cong \frac{(x-x_i)^4}{4!} f^{(4)}(x_i)$
    - This is the leading order truncated term in the series
    - This approximation for the error can also be thought of as being derived from the exact single term representation of the error with the approximation $f^{(4)}(\xi) \approx f^{(4)}(x_i)$
  - In terms of an ***order*** of magnitude only as $E \cong O(x-x_i)^4$
    - This term is often carried simply to ensure that ***all*** terms of the correct order have been carried in the derivations.
    - This error term is indicative of how the error ***relatively*** depends on the size of the interval!

- Evaluate $f(x_{i+1})$

$$f(x_{i+1}) = f(x_i) + (x_{i+1} - x_i)f^{(1)}(x_i) + \frac{(x_{i+1} - x_i)^2}{2!}f^{(2)}(x_i)$$

$$+ \frac{(x_{i+1} - x_i)^3}{3!}f^{(3)}(x_i) + O(x_{i+1} - x_i)^4 \quad \Rightarrow$$

$$f_{i+1} = f_i + hf_i^{(1)} + \frac{h^2}{2}f_i^{(2)} + \frac{h^3}{6}f_i^{(3)} + O(h)^4$$

- Evaluate $f(x_{i+2})$

$$f(x_{i+2}) = f(x_i) + (x_{i+2} - x_i)f^{(1)}(x_i) + \frac{(x_{i+2} - x_i)^2}{2!}f^{(2)}(x_i)$$

$$+ \frac{(x_{i+2} - x_i)^3}{3!}f^{(3)}(x_i) + O(x_{i+2} - x_i)^4 \quad \Rightarrow$$

$$f_{i+2} = f_i + 2h\,f_i^{(1)} + 2h^2f_i^{(2)} + \frac{4}{3}h^3f_i^{(3)} + O(h)^4$$

- Evaluate $f(x_{i-1})$

$$f(x_{i-1}) = f(x_i) + (x_{i-1} - x_i)f^{(1)}(x_i) + \frac{(x_{i-1} - x_i)^2}{2!}f^{(2)}(x_i)$$

$$+ \frac{(x_{i-1} - x_i)^3}{3!}f^3(x_i) + O(x_{i-1} - x_i)^4 \qquad \Rightarrow$$

$$f_{i-1} = f_i - hf_i^{(1)} + \frac{h^2}{2}f_i^{(2)} - \frac{h^3}{6}f_i^{(3)} + O(h)^4$$

- Similarly we can evaluate $f(x_{i-2})$

$$f_{i-2} = f_i - 2hf_i^{(1)} + 2h^2 f_i^{(2)} - \frac{4}{3}h^3 f_i^{(3)} + O(h)^4$$

Approximating Derivatives by Linearly Combining Functional Values at Nodes

Forward first order accurate approximation to the first derivative

- Consider 2 nodes, i and $i+1$

- Combine the difference of the functional values at these two nodes

$$f_{i+1} - f_i = f_i + hf_i^{(1)} + \frac{h^2}{2}f_i^{(2)} + \frac{h^3}{6}f_i^{(3)} + O(h)^4 - f_i \qquad \Rightarrow$$

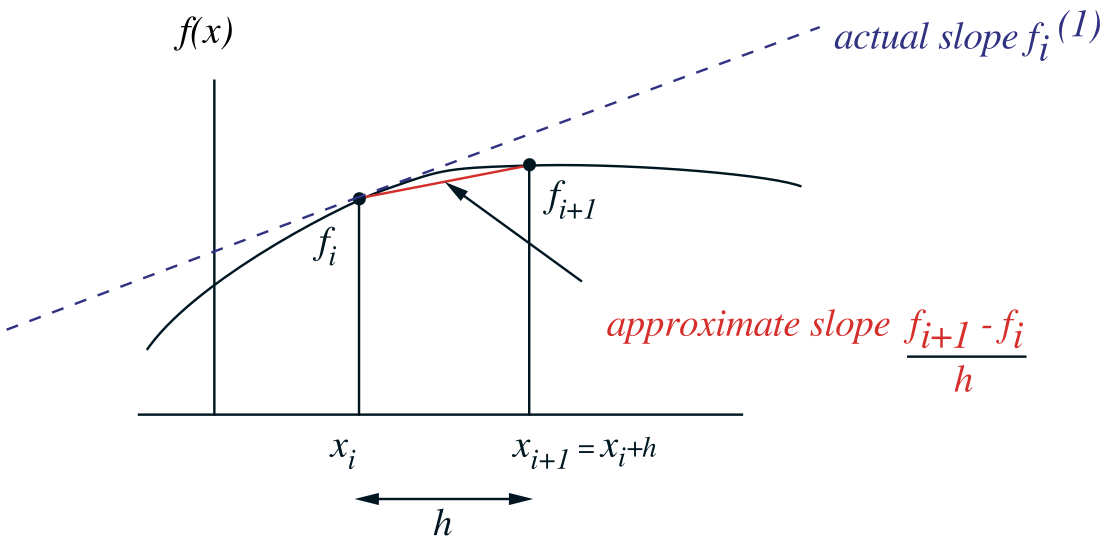
$$hf_i^{(1)} = f_{i+1} - f_i - \frac{h^2}{2}f_i^{(2)} - \frac{h^3}{6}f_i^{(3)} + O(h)^4 \qquad \Rightarrow$$

$$f_i^{(1)} = \frac{f_{i+1} - f_i}{h} - \frac{h}{2}f_i^{(2)} - \frac{h^2}{6}f_i^{(3)} + O(h)^3$$

- First derivative of f ***at node*** i is approximated as

$$f_i^{(1)} = \frac{f_{i+1} - f_i}{h} + E \quad \text{where} \quad E \cong -\frac{h}{2} f_i^{(2)}$$

- This is the first forward difference and the error is called first order in h (i.e. $E \cong O(h)$)



- Notes:
    - There is a clear dependence of the error on h
    - The first forward difference approximation is ***exact*** for 1st degree polynomials

Backward first order accurate approximation to the first derivative

- Consider nodes $i-1$ and i and define $f_i - f_{i-1}$

$$f_i - f_{i-1} = f_i - \left(f_i - hf_i^{(1)} + \frac{h^2}{2}f_i^{(2)} - \frac{h^3}{6}f_i^{(3)} + O(h)^4\right)$$

$$\Rightarrow$$

$$f_i - f_{i-1} = hf_i^{(1)} - \frac{h^2}{2}f_i^{(2)} + \frac{h^3}{6}f_i^{(3)} + O(h)^4$$

- First backward difference of f is then defined as:

$$f_i^{(1)} = \frac{f_i - f_{i-1}}{h} + E$$

- Error is again ***first order*** in h

$$E = \frac{1}{2}hf_i^{(2)} \cong O(h)$$

Central second order accurate approximation to the first derivative

- Consider nodes i, $i-1$ and $i+1$ and examine $f_{i+1} - f_{i-1}$

$$f_{i+1} - f_{i-1} = \left(f_i + hf_i^{(1)} + \frac{h^2}{2}f_i^{(2)} + \frac{h^3}{6}f_i^{(3)} + O(h)^4\right) \quad -\left(f_i - hf_i^{(1)} + \frac{h^2}{2}f_i^{(2)} - \frac{h^3}{6}f_i^{(3)} + O(h)^4\right)$$

$$\Rightarrow$$

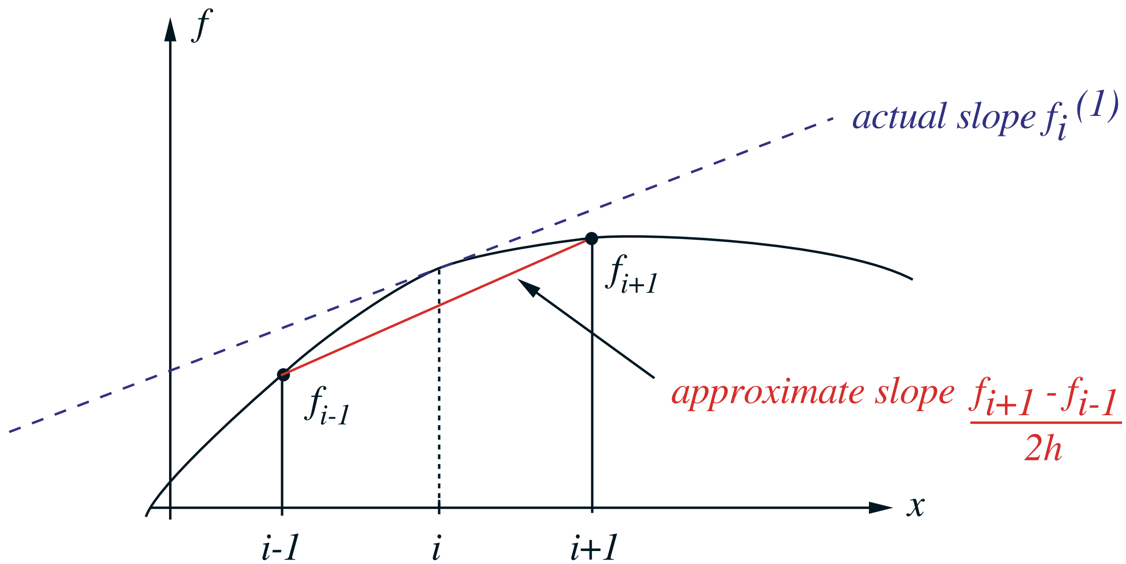
$$f_{i+1} - f_{i-1} = 2hf_i^{(1)} + \frac{h^3}{3}f_i^{(3)} + O(h)^4$$

- Central difference approximation to the first derivative is

$$f_i^{(1)} = \frac{f_{i+1} - f_{i-1}}{2h} + E$$

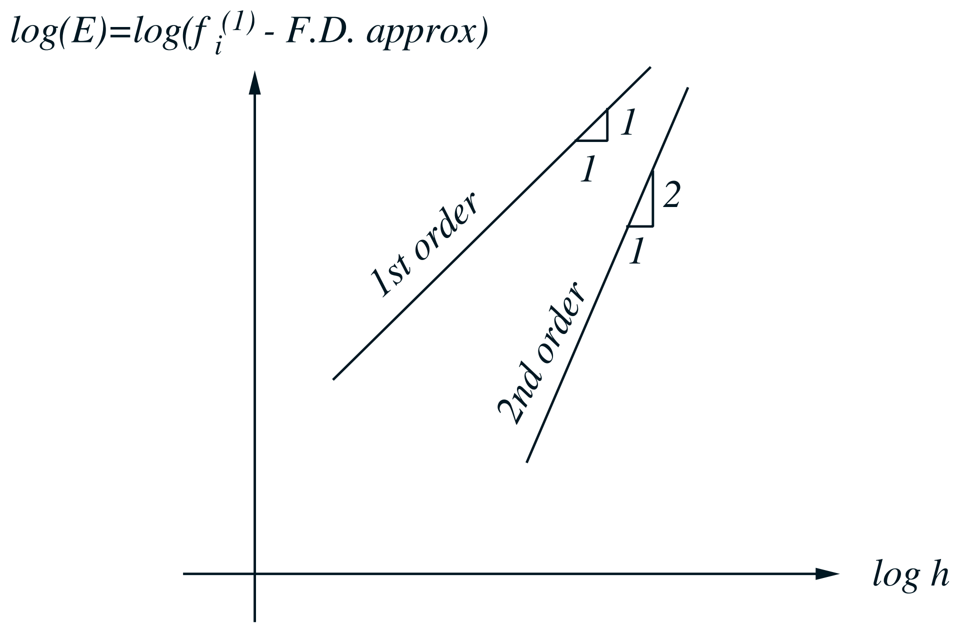
- Formula has an error which is ***second order*** in h

$$E = \frac{h^2}{6}f_i^{(3)} \cong O(h)^2$$



- The smaller h, the smaller the error
- Error is obviously generally better for the central $O(h)^2$ formula than the forward or backward $O(h)$ formulae!
- Expression is exact for 2nd degree polynomials due to the third derivative in the expression for E

- Strictly the order of the error is indicative of the rate of convergence as opposed to the absolute error



Forward first order accurate approximation to the second derivative

- Now consider nodes i, $i+1$ and $i+2$ and the linear combination of functional values $f_{i+2} - 2f_{i+1} + f_i$

$$f_{i+2} - 2f_{i+1} + f_i = \left(f_i + 2hf_i^{(1)} + 2h^2 f_i^{(2)} + \frac{8}{6}h^3 f_i^{(3)} + O(h)^4\right)$$

$$-2\left(f_i + hf_i^{(1)} + \frac{h^2}{2}f_i^{(2)} + \frac{1}{6}h^3 f_i^{(3)} + O(h)^4\right) + (f_i)$$

$$\Rightarrow$$

$$f_{i+2} - 2f_{i+1} + f_i = h^2 f_i^{(2)} - h^3 f_i^{(3)} + O(h)^4$$

- Forward difference approximation to second derivative

$$\boldsymbol{f_i^{(2)} = \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} + E}$$

- Error ***first order*** in h

$$\boldsymbol{E = hf_i^{(3)} = O(h)}$$

TABLE OF DIFFERENCE APPROXIMATIONS

- First Derivative Approximations
  - Forward difference approximations:

$$f_i^{(1)} = \frac{f_{i+1} - f_i}{h} + E \quad , \quad E \cong -\frac{1}{2} h f_i^{(2)}$$

$$f_i^{(1)} = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h} + E \quad , \quad E \cong \frac{1}{3} h^2 f_i^{(3)}$$

$$f_i^{(1)} = \frac{2f_{i+3} - 9f_{i+2} + 18f_{i+1} - 11f_i}{6h} + E \quad , \quad E \cong -\frac{1}{4} h^3 f_i^{(4)}$$

  - Backward difference approximations:

$$f_i^{(1)} = \frac{f_i - f_{i-1}}{h} + E \quad , \quad E \cong \frac{1}{2} h f_i^{(2)}$$

$$f_i^{(1)} = \frac{3f_i - 4f_{i-1} + f_{i-2}}{2h} + E \quad , \quad E \cong \frac{1}{3} h^2 f_i^{(3)}$$

$$f_i^{(1)} = \frac{11f_i - 18f_{i-1} + 9f_{i-2} - 2f_{i-3}}{6h} + E \quad , \quad E \cong \frac{1}{4} h^3 f_i^{(4)}$$

- Central difference approximations:

$$f_i^{(1)} = \frac{f_{i+1} - f_{i-1}}{2h} + E \quad , \quad E \cong -\frac{1}{6} h^2 f_i^{(3)}$$

$$f_i^{(1)} = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} + E \quad , \quad E \cong \frac{1}{30} h^4 f_i^{(5)}$$

- Second Derivative Approximations
  - Forward difference approximations

$$f_i^{(2)} = \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} + E \quad , \quad E \cong -h f_i^{(3)}$$

$$f_i^{(2)} = \frac{-f_{i+3} + 4f_{i+2} - 5f_{i+1} + 2f_i}{h^2} + E \quad , \quad E \cong \frac{11}{12} h^2 f_i^{(4)}$$

- Backward difference approximations:

$$f_i^{(2)} = \frac{f_i - 2f_{i-1} + f_{i-2}}{h^2} + E \quad , \quad E \cong h f_i^{(3)}$$

$$f_i^{(2)} = \frac{2f_i - 5f_{i-1} + 4f_{i-2} - f_{i-3}}{h^2} + E \quad , \quad E \cong \frac{11}{12} h^2 f_i^{(4)}$$

- Central difference approximations:

$$f_i^{(2)} = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + E \quad , \quad E \cong -\frac{1}{12} h^2 f_i^{(4)}$$

$$f_i^{(2)} = \frac{-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2}}{12h^2} + E \quad , \quad E \cong \frac{1}{90} h^4 f_i^{(6)}$$

- ***All the derivative approximations we have examined are linear combinations of functional values at nodes!!***

- ***What is a general technique for finding the associated coefficients?***