Numerical Differentiation

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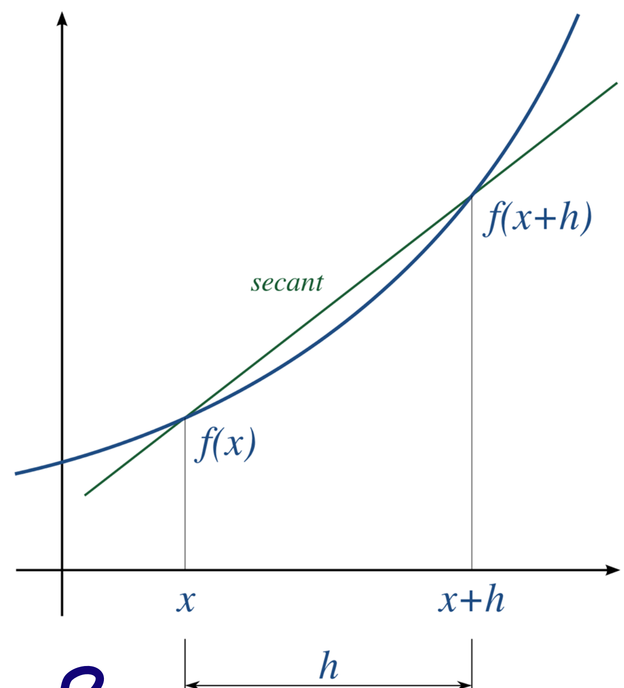
- Calculate the derivative of a given function represented by a data set

- Discretize a differential equation to solve it numerically



$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \Gamma \nabla^2 \phi + q$$

$$u \frac{\partial \phi}{\partial x} + v \frac{\partial \phi}{\partial y} \qquad \Gamma \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right)$$

Taylor Series

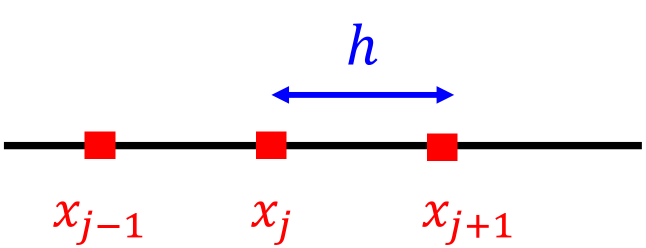
Taylor series of a function *f* at x=a

$$\boxed{f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n}$$

$$\boxed{f(x) = f(a) + \frac{f'(a)(x-a)}{1!} + \frac{f''(a)(x-a)^2}{2!} + \frac{f'''(a)(x-a)^3}{3!} + \cdots}$$

Taylor series of $f(x)$ at x_j (i.e. $a = x_j$)

$$\boxed{f(x) = f(x_j) + \frac{f'(x_j)(x-x_j)}{1!} + \frac{f''(x_j)(x-x_j)^2}{2!} + \frac{f'''(x_j)(x-x_j)^3}{3!} + \cdots}$$



Now substitute $x = x_{j+1}$

Note $(x_{j+1} - x_j) = +h$

$$f(x_{j+1}) = f(x_j) + \frac{f'(x_j)\overbrace{(x_{j+1} - x_j)}^{h}}{1!} + \frac{f''(x_j)\overbrace{(x_{j+1} - x_j)^2}^{h^2}}{2!} + \frac{f'''(x_j)\overbrace{(x_{j+1} - x_j)^3}^{h^3}}{3!} + \cdots$$

First order accurate ***forward*** difference formula:

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{h} + \frac{h}{2} f''(x_j)$$

Now substitute $x = x_{j-1}$

Note $(x_{j-1} - x_j) = -h$

$$f(x_{j-1}) = f(x_j) + \frac{f'(x_j)(x_{j-1} - x_j)}{1!} + \frac{f''(x_j)(x_{j-1} - x_j)^2}{2!} + \frac{f'''(x_j)(x_{j-1} - x_j)^3}{3!} + \cdots$$

First order accurate ***backward*** difference formula:

$$f'(x_j) = \frac{f(x_j) - f(x_{j-1})}{h} + O(h)$$

Subtract Taylor series expansion of $f(x_{j+1})$ from $f(x_{j-1})$

Second order accurate central difference formula:

$$f'(x_j) = \frac{f(x_{j+1}) - f(j-1)}{2h} + O(h^2)f'''$$

stencil

Fourth order accurate central difference formula:

$$f_j' = \frac{f_{j-2} - 8f_{j-1} + 8f_{j+1} - f_{j+2}}{12h} + O(h^4)f^{v}$$

What about higher order derivatives?

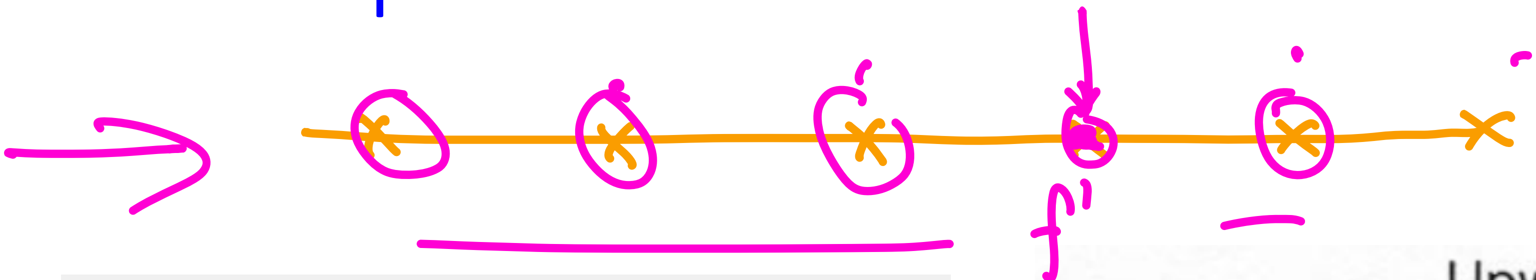
Add Taylor series expansions of $f(x_{j+1})$ and $f(x_{j-1})$

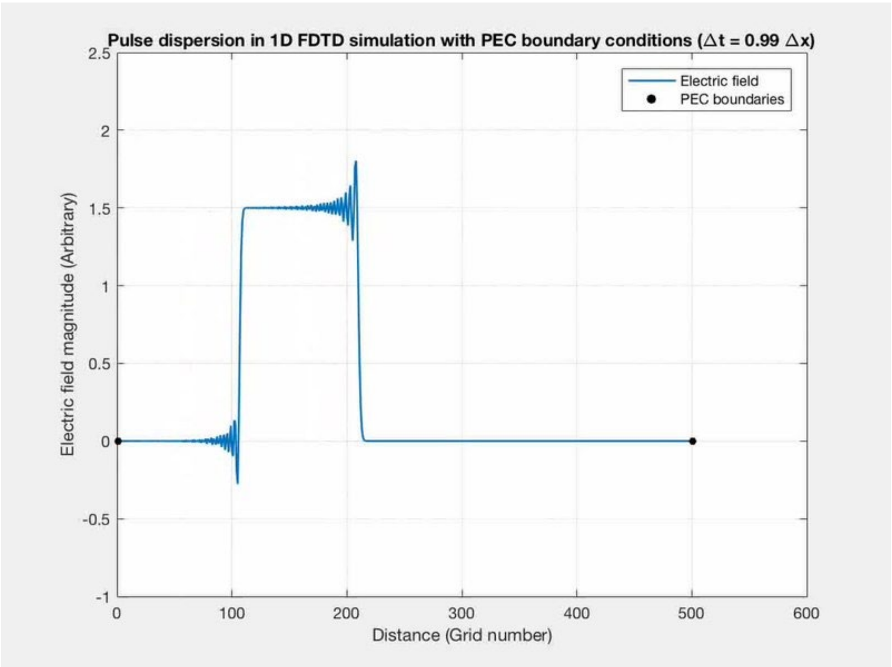
Second order accurate central difference formula for $f''(x_j)$:

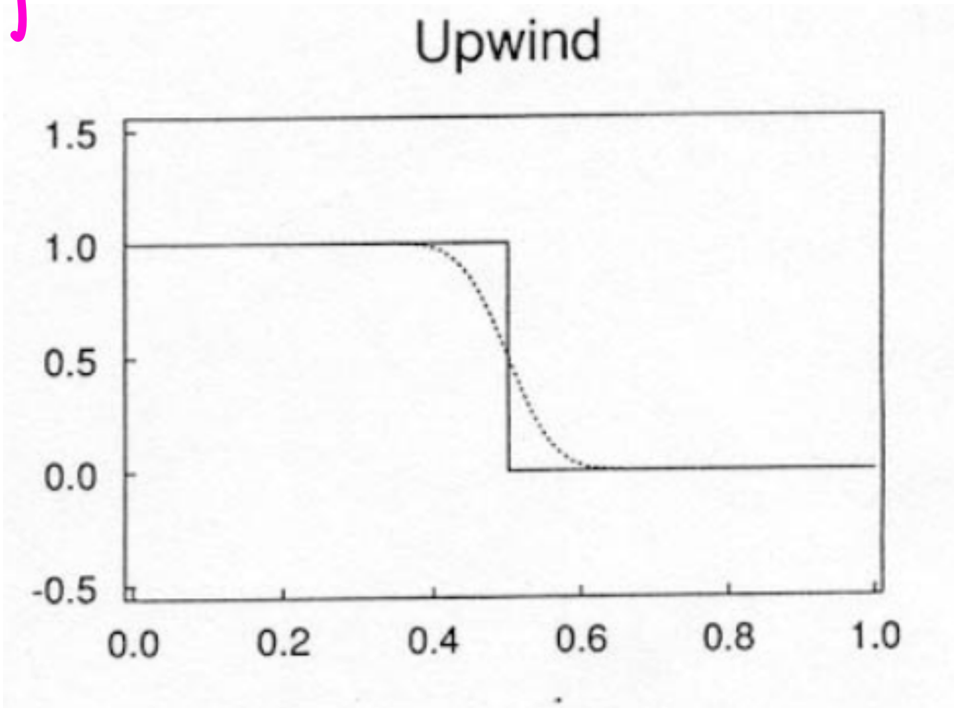
$$\boxed{f_j'' = \frac{f_{j+1} - 2f_j + f_{j-1}}{h^2} + \mathcal{O}(\mathrm{h}^2)}$$

f'''

Dispersive vs. Diffusive Formulas



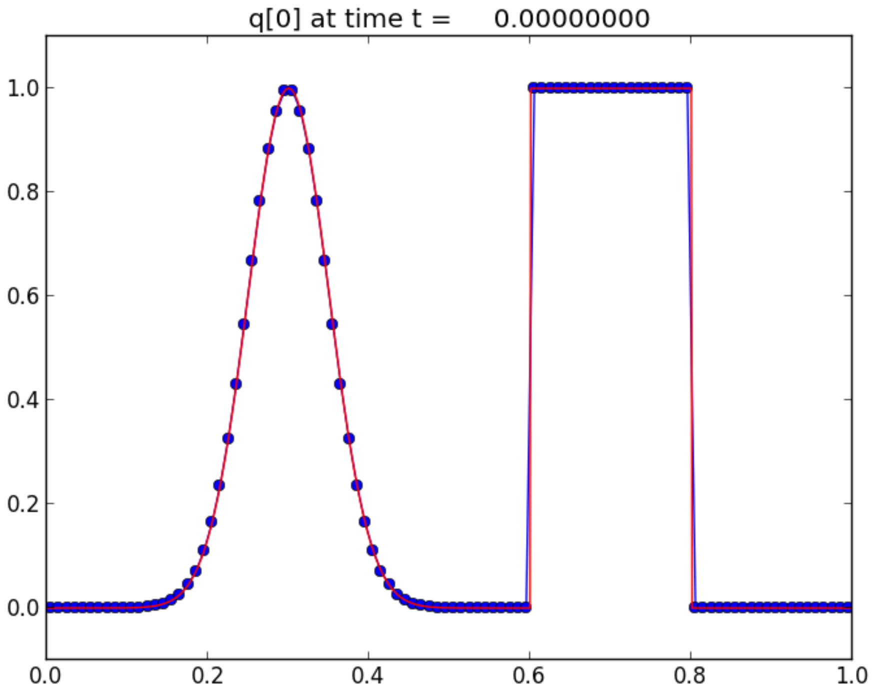


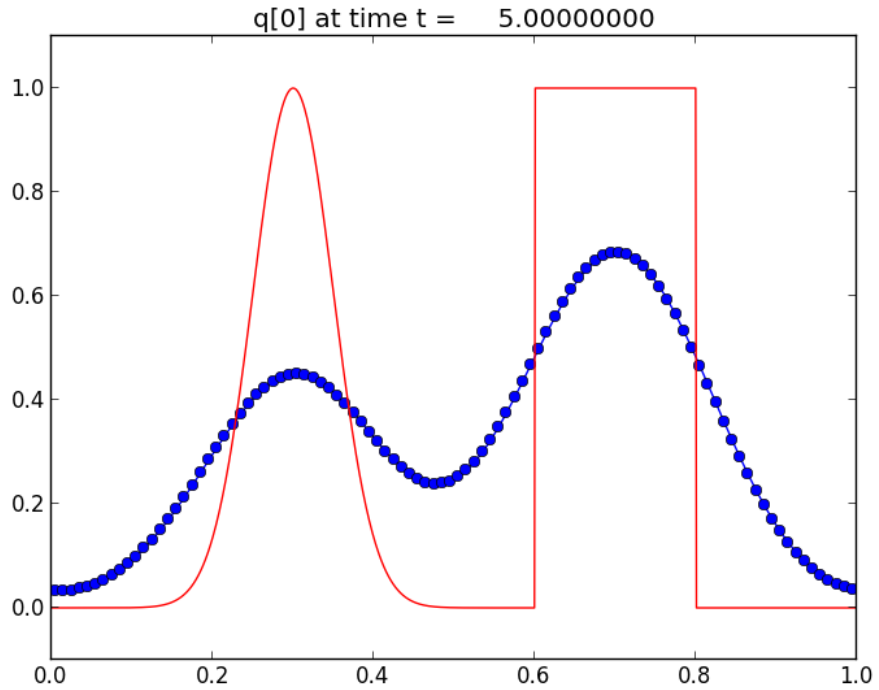


https://en.wikipedia.org/wiki/Numerical_dispersion

Source: LeVeque, R. J., Numerical Methods for Conservation Laws

Illustration of Numerical diffusion





Use Richardson Extrapolation

Find a 4th order accurate formula for $f''(x_j)$

$$4\left(f''(x_0) = \frac{1}{h^2}\left[f(x_0-h) - 2f(x_0) + f(x_0+h) \right] - \frac{h^2}{12} f^{v}(x_0) - \frac{h^4}{360} f^{vi}(x_0) \right)$$

$h \to 2h$

$$f''(x_0) = \frac{1}{4h^2}\left[f(x_0-2h) - 2f(x_0) + f(x_0+2h) \right] - \frac{4h^2}{12} f^{v}(x_0) - \frac{16h^4}{360} f^{vi}(x_0)$$

Error Estimation

Richardson extrapolation

$$e(h) \approx \frac{1}{3}\left[f''_{2h} - f''_{h} \right]$$

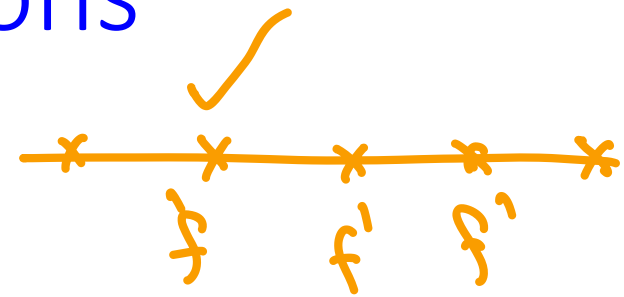
Construction of Finite Difference Formulas

$$f_j' + \sum_{k=0}^{N} a_k f_{j+k} = \mathcal{O}(?)$$

	f_j	f_j'	f_j''	f'''_j
f'_j	0	1	0	0
a_0 f_j	a_0	0	0	0
a_1 $\underline{f_{j+1}}$	a_1	$a_1 h$	$a_1 h^2/2$	$a_1 h^3/6$
a_2 f_{j+2}	a_2	$a_2\, 2h$	$a_2 \frac{(2h)^2}{2}$	$a_2 \frac{(2h)^3}{6}$

Padé Approximations

Use first order derivatives in the neighboring points



$$f_j' + a_0 f_j + a_1 f_{j+1} + a_2 f_{j-1} + a_3 f'_{j+1} + a_4 f_{j-1}' = \mathcal{O}(?)$$

Use Taylor Tables to determine $a_0, \ldots a_4$

$$f_{j+1}' + f_{j-1}' + 4 f_j' = \frac{3}{h}\left(f_{j+1} - f_{j-1}\right) + \frac{h^4}{30} f_j^{v}$$

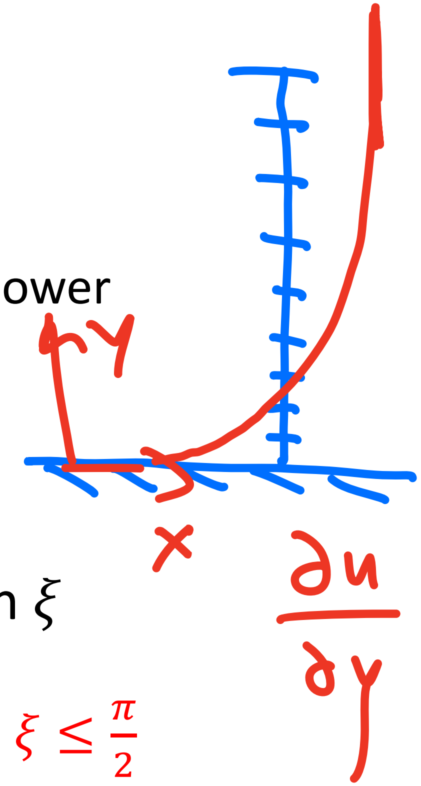
A tridiagonal system of equations for f_j'

$$\boxed{\mathbf{A} f_j' = \frac{1}{h} f_j}$$

For this reason Padé schemes are **global** schemes

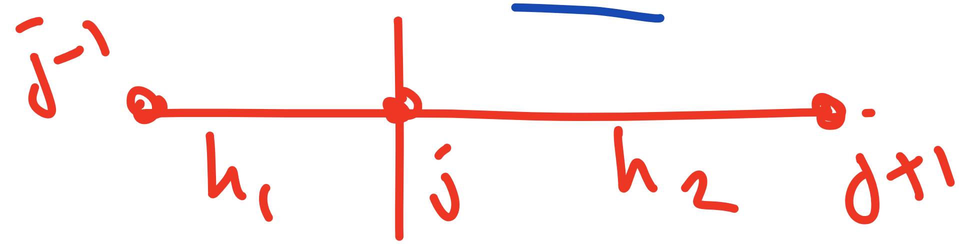
Non-uniform Mesh

- Finite difference formula on a non-uniform mesh generally has lower order of accuracy than their counterparts on a uniform mesh
  - Difficult to eliminate the terms in a Taylor series expansion



Use a transformation $\xi = g(x)$ to create a uniform mesh in ξ

Example: $\xi = \cos^{-1} x \ \ transforms \ 0 \leq x \leq 1 \quad to \quad 0 \leq \xi \leq \frac{\pi}{2}$

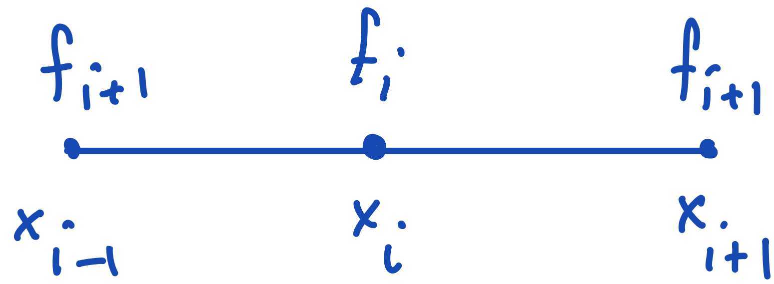


$$\frac{df}{dx} = \frac{d\xi}{dx}\frac{df}{d\xi} = g'\frac{df}{d\xi}$$

$$\frac{d^2 f}{dx^2} = \frac{d}{dx}\left[g'\frac{df}{d\xi}\right] = g''\frac{df}{d\xi} + (g')^2\frac{d^2 f}{d\xi^2}$$

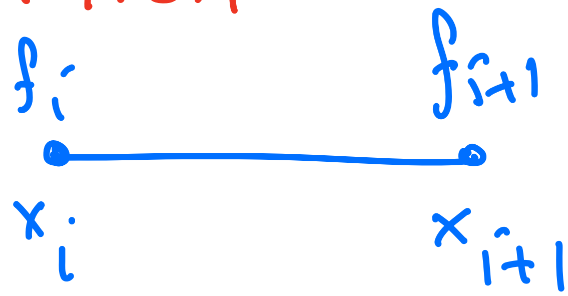
Apply FD formulas for $\frac{df}{d\xi}, \frac{d^2 f}{d\xi^2}$

Interpolation $\quad x_i, \; f_i \quad i = 0, 1, \ldots, n$



Lagrange Interpolation

for two points



$$p(x) = f_i \frac{(x - x_{i+1})}{\underbrace{x_i - x_{i+1}}_{-h}} + f_{i+1} \frac{(x - x_i)}{\underbrace{x_{i+1} - x_i}_{h}}$$

$$p(x) = -\frac{f_i (x - x_{i+1})}{h} + f_{i+1} \frac{(x - x_i)}{h}$$

$$p'(x) = \frac{f_{i+1} - f_i}{h}$$

1st order forward difference