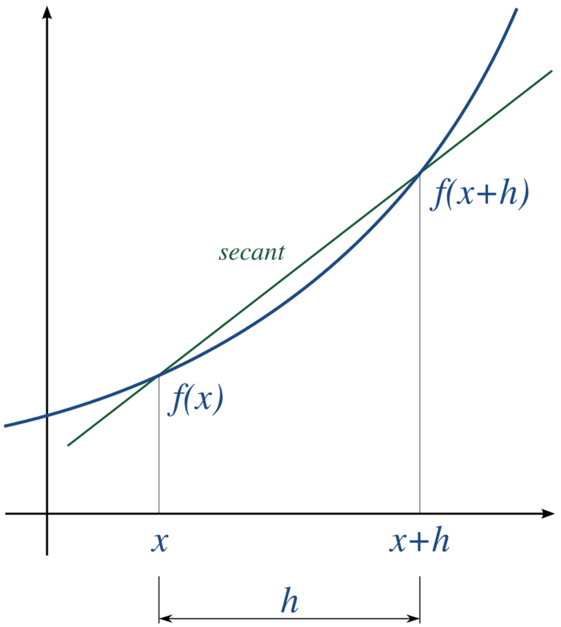
Numerical Differentiation

Numerical Differentiation

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

- Discretize a differential equation to solve it numerically

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



Taylor Series

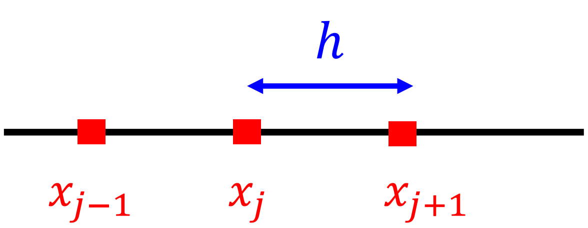
Taylor series of a function *f* at x=a

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

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

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

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

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

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

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

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

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

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

Second order accurate central difference formula:

Fourth order accurate central difference formula:

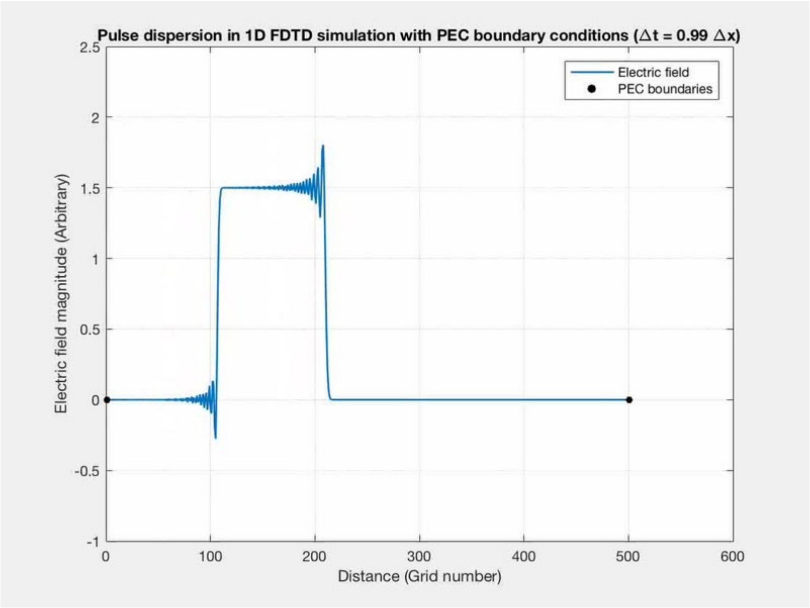
What about higher order derivatives?

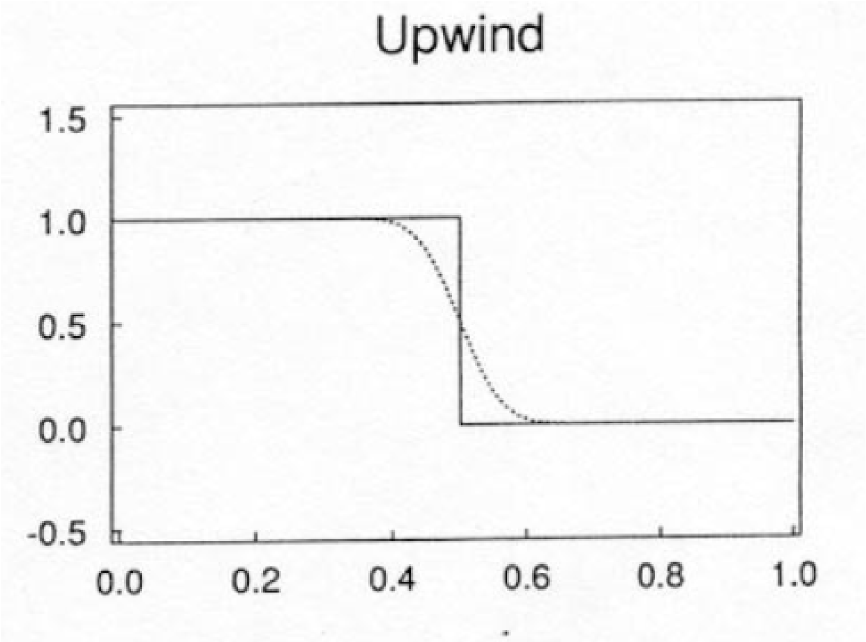
Add Taylor series expansions of $f(x_{j+1})$ and $f(x_{j-1})$

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

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

Dispersive vs. Diffusive Formulas

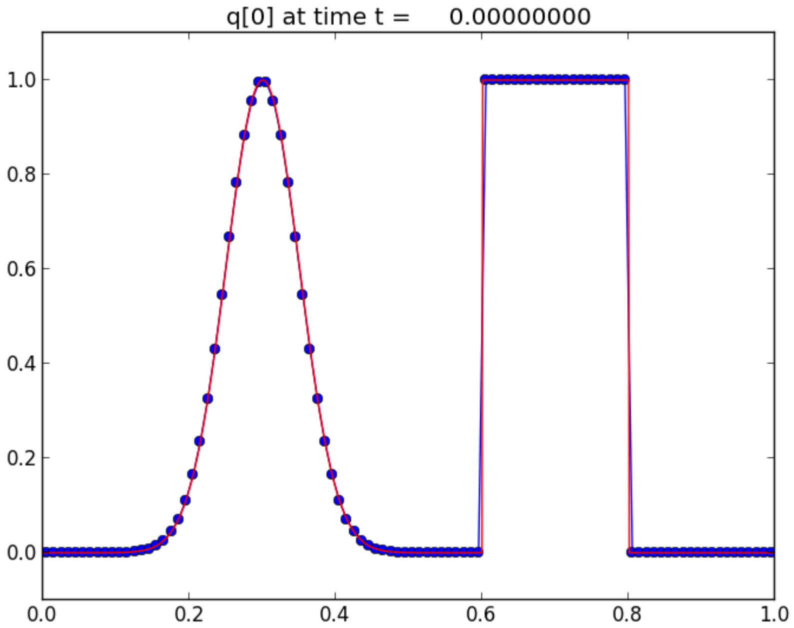


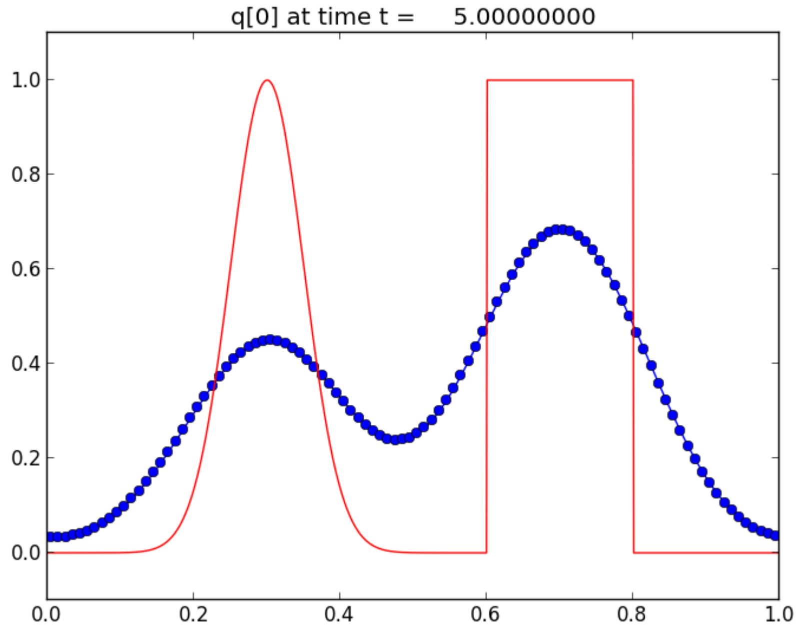


https://en.wikipedia.org/wiki/Numerical_dispersion

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

Illustration of Numerical diffusion





Use Richardson Extrapolation

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

Error Estimation

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				
f_j				
f_{j+1}				
f_{j+2}				

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 $a_0, \dots a_4$

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

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 $\frac{df}{d\xi}, \frac{d^2 f}{d\xi^2}$