Finite Difference

What is a finite difference?

Common definitions of the derivative of f(x):

$$\partial_x f = \lim_{dx \to 0} \frac{f(x+dx) - f(x)}{dx}$$

$$\partial_x f = \lim_{dx \to 0} \frac{f(x) - f(x-dx)}{dx}$$

$$\partial_x f = \lim_{dx \to 0} \frac{f(x+dx) - f(x-dx)}{2dx}$$

These are all correct definitions in the limit dx->0.

But we want dx to remain **FINITE**

What is a finite difference?

The equivalent ***approximations*** of the derivatives are:

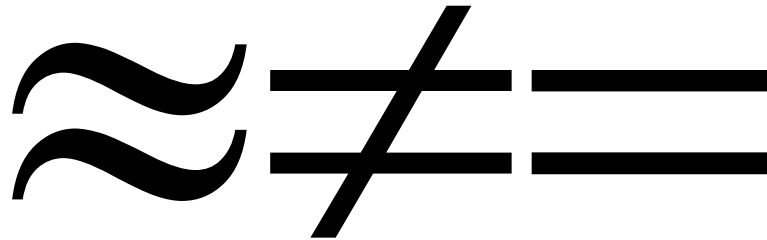$$\partial_x f^+ \approx \frac{f(x+dx) - f(x)}{dx}$$ forward difference

$$\partial_x f^- \approx \frac{f(x) - f(x-dx)}{dx}$$ backward difference

$$\partial_x f \approx \frac{f(x+dx) - f(x-dx)}{2dx}$$ centered difference

How good are the FD approximations?

$$\approx \neq =$$

This leads us to Taylor series....

Taylor series are expansions of a function f(x) for some finite distance dx to f(x+dx)

$$f(x \pm dx) = f(x) \pm \mathrm{dx} f^{'}(x) + \frac{dx^2}{2!} f^{"}(x) \pm \frac{dx^3}{3!} f^{'''}(x) + \frac{dx^4}{4!} f^{''''}(x) \pm ...$$

What happens, if we use this expression for

$$\partial_x f^+ \approx \frac{f(x+dx) - f(x)}{dx} \qquad ?$$

... that leads to :

$$\frac{f(x+dx)-f(x)}{dx} = \frac{1}{dx}\left[dx f'(x) + \frac{dx^2}{2!}f''(x) + \frac{dx^3}{3!}f'''(x) + ... \right]$$

$$= f'(x) + O(dx)$$

The error of the first derivative using the *forward* formulation is *of order dx*.

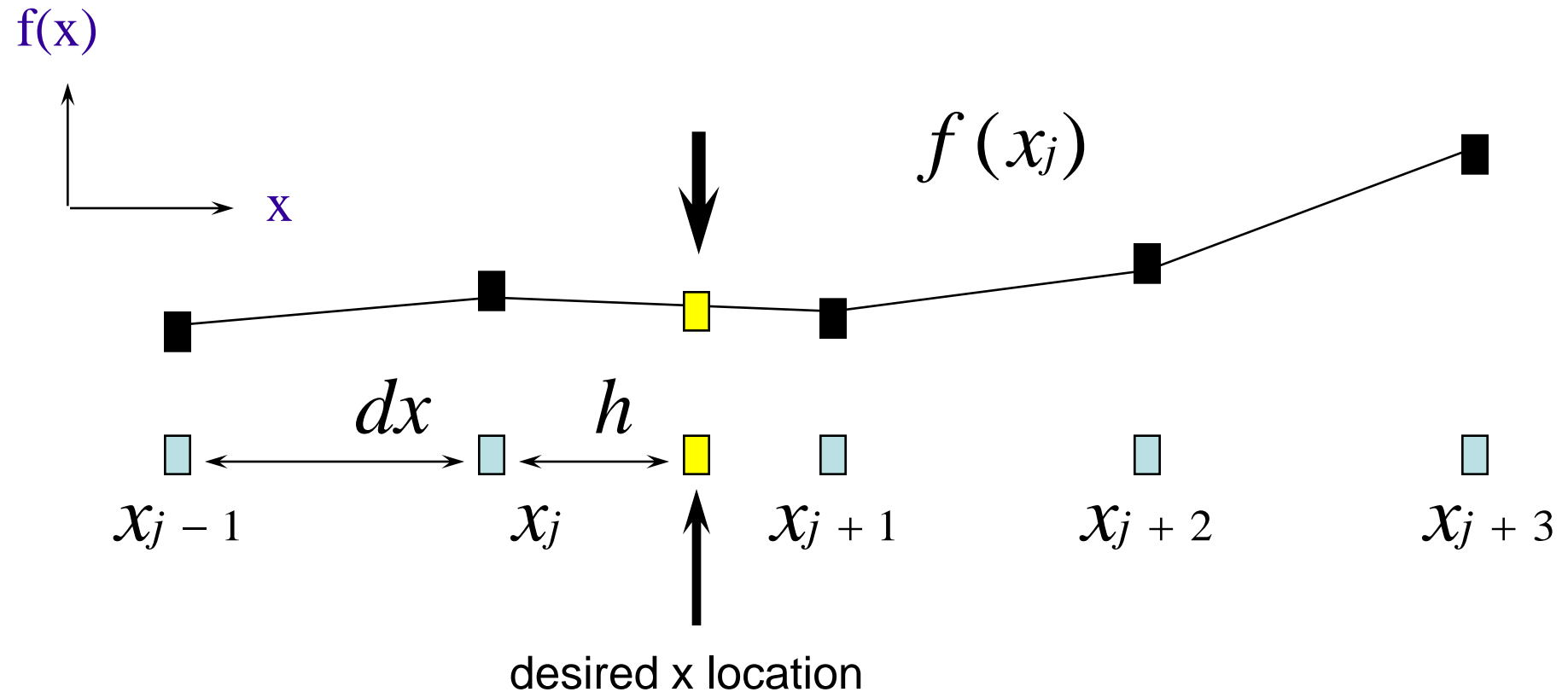Is this the case for other formulations of the derivative? Let's check!

... with the *centered* formulation we get:

$$\frac{f(x+dx/2) - f(x-dx/2)}{dx} = \frac{1}{dx}\left[\mathrm{dx}f^{'}(x) + \frac{dx^3}{3!}f^{'''}(x) + ... \right]$$

$$= f^{'}(x) + O(dx^2)$$

The error of the first derivative using the centered approximation is *of order dx^2*.

This is an **important** results: it DOES matter which formulation we use. The centered scheme is more accurate!
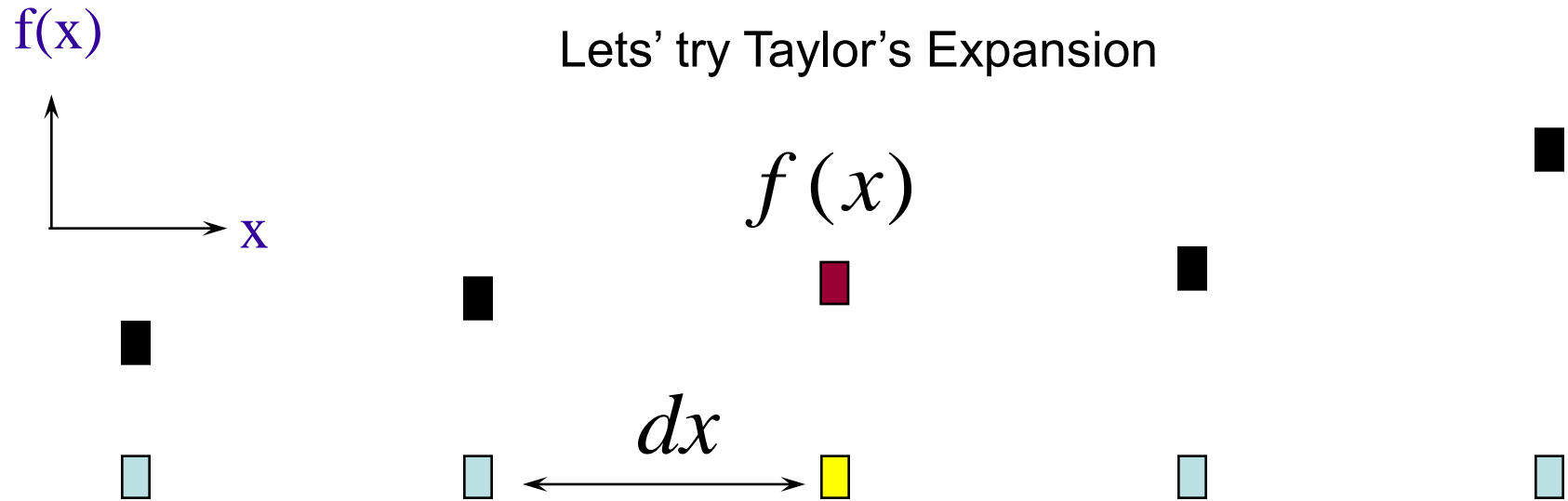
f(x)

x

$f(x_j)$

dx h

x_{j-1} x_j x_{j+1} x_{j+2} x_{j+3}

desired x location

What is the (approximate) value of the function or its (first, second ..) derivative at the desired location ?

How can we calculate the weights for the neighboring points?

f(x)

Lets' try Taylor's Expansion

$$f(x)$$

$$dx$$

$$f(x+dx) \approx f(x) + f'(x)dx \qquad (1)$$

$$f(x-dx) \approx f(x) - f'(x)dx \qquad (2)$$

we are looking for something like

$$f^{(i)}(x) \approx \sum_{j=1,L} w_j^{(i)} f(x_{index(j)})$$

deriving the second-order scheme …

$$af^{+} \approx af + af'dx$$

$$bf^{-} \approx bf - bf'dx$$

$$\Rightarrow af^{+} + bf^{-} \approx (a+b)f + (a-b)f'dx$$

the solution to this equation for a and b leads to
a system of equations which can be cast in matrix form

Interpolation

$$a + b = 1$$

$$a - b = 0$$

Derivative

$$a + b = 0$$

$$a - b = 1/dx$$

... in matrix form ...

Interpolation

$$\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Derivative

$$\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 1/dx \end{pmatrix}$$

... so that the solution for the *weights* is ...

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ 1/dx \end{pmatrix}$$

... and the result ...

Interpolation

Derivative

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix}$$

$$\begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{2dx} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Can we generalise this idea to longer operators?

Let us start by extending the Taylor expansion beyond f(x±dx):

$*a\ |$ $$f(x-2dx) \approx f - (2dx)f' + \frac{(2dx)^2}{2!}f'' - \frac{(2dx)^3}{3!}f'''$$

$*b\ |$ $$f(x-dx) \approx f - (dx)f' + \frac{(dx)^2}{2!}f'' - \frac{(dx)^3}{3!}f'''$$

$*c\ |$ $$f(x+dx) \approx f + (dx)f' + \frac{(dx)^2}{2!}f'' + \frac{(dx)^3}{3!}f'''$$

$*d\ |$ $$f(x+2dx) \approx f + (2dx)f' + \frac{(2dx)^2}{2!}f'' + \frac{(2dx)^3}{3!}f'''$$

... again we are looking for the coefficients a,b,c,d with which
the function values at x±(2)dx have to be multiplied in order
to obtain the interpolated value or the first (or second) derivative!

... Let us add up all these equations like in the previous case ...

$$af^{--} + bf^{-} + cf^{+} + df^{++} \approx$$

$$f(a+b+c+d)+$$

$$dxf'(-2a-b+c+2d)+$$

$$dx^2 f''(2a + \frac{b}{2} + \frac{c}{2} + 2d)+$$

$$dx^3 f'''(-\frac{8}{6}a - \frac{1}{6}b + \frac{1}{6}c + \frac{8}{6}d)$$

... we can now ask for the coefficients a,b,c,d, so that the left-hand-side yields either f,f',f'',f''' ...

... if you want the interpolated value ...

$$a + b + c + d = 1$$

$$-2a - b + c + 2d = 0$$

$$2a + \frac{b}{2} + \frac{c}{2} + 2d = 0$$

$$-\frac{8}{6}a - \frac{1}{6}b + \frac{1}{6}c + \frac{8}{6}d = 0$$

... you need to solve the matrix system ...

... Interpolation ...

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ -2 & -1 & 1 & 2 \\ 2 & 1/2 & 1/2 & 2 \\ -8/6 & -1/6 & 1/6 & 8/6 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

... with the result after inverting the matrix on the lhs ...

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} -1/6 \\ 2/3 \\ 2/3 \\ -1/6 \end{pmatrix}$$

... first derivative ...

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ -2 & -1 & 1 & 2 \\ 2 & 1/2 & 1/2 & 2 \\ -8/6 & -1/6 & 1/6 & 8/6 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} 0 \\ 1/dx \\ 0 \\ 0 \end{pmatrix}$$

... with the result ...

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \frac{1}{2dx} \begin{pmatrix} 1/6 \\ -4/3 \\ 4/3 \\ -1/6 \end{pmatrix}$$