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

The big question

How good are the FD approximations?

$$\approx \neq =$$

This leads us to Taylor series....

Taylor Series

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

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

What happens, if we use this expression for

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

?

Taylor Series

... that leads to :

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

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

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!

Taylor Series

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

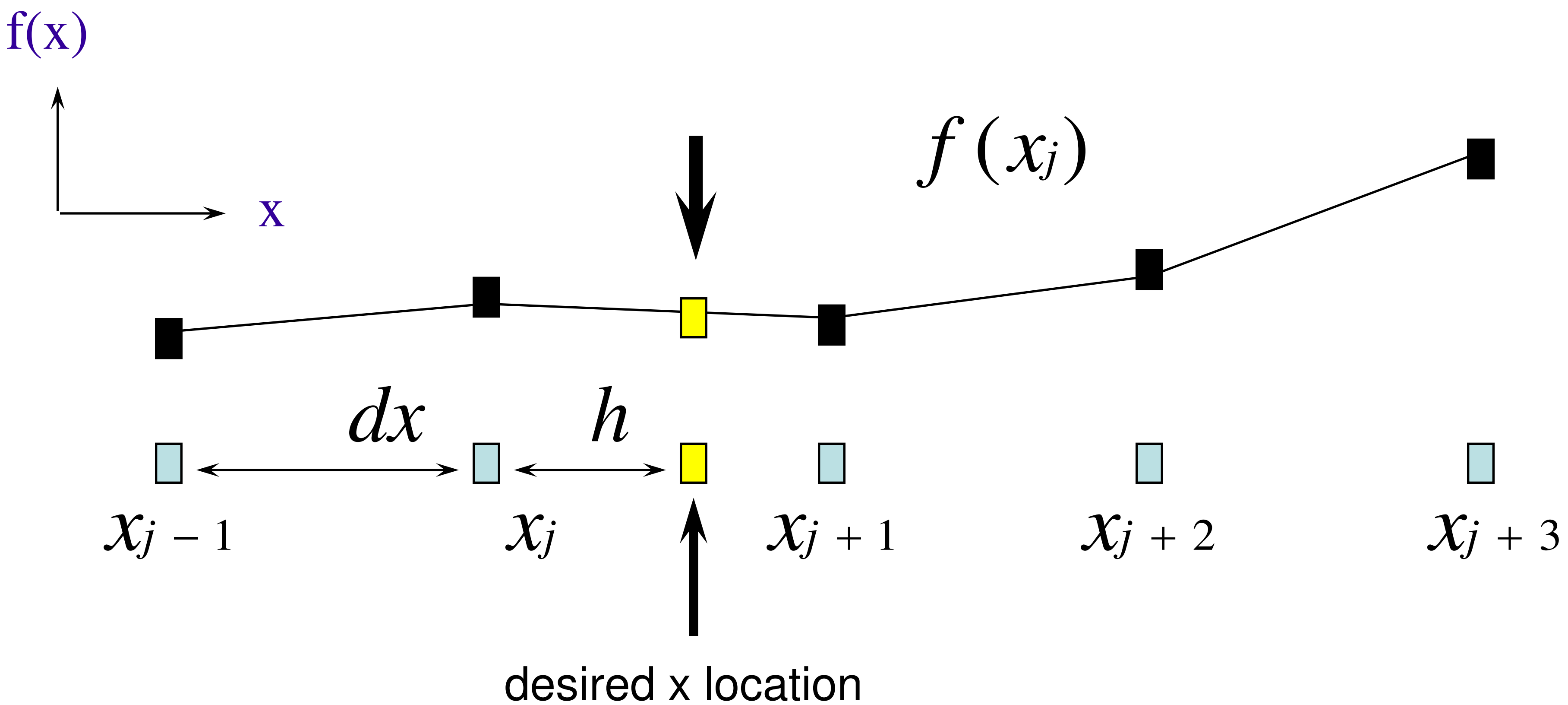
$$\frac{f(x+dx/2)-f(x-dx/2)}{dx}=\frac{1}{dx}\left[\mathrm{dx}f^{'}(x)+\frac{dx^3}{3!}f^{'''}(x)+\ldots\right]$$

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

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!

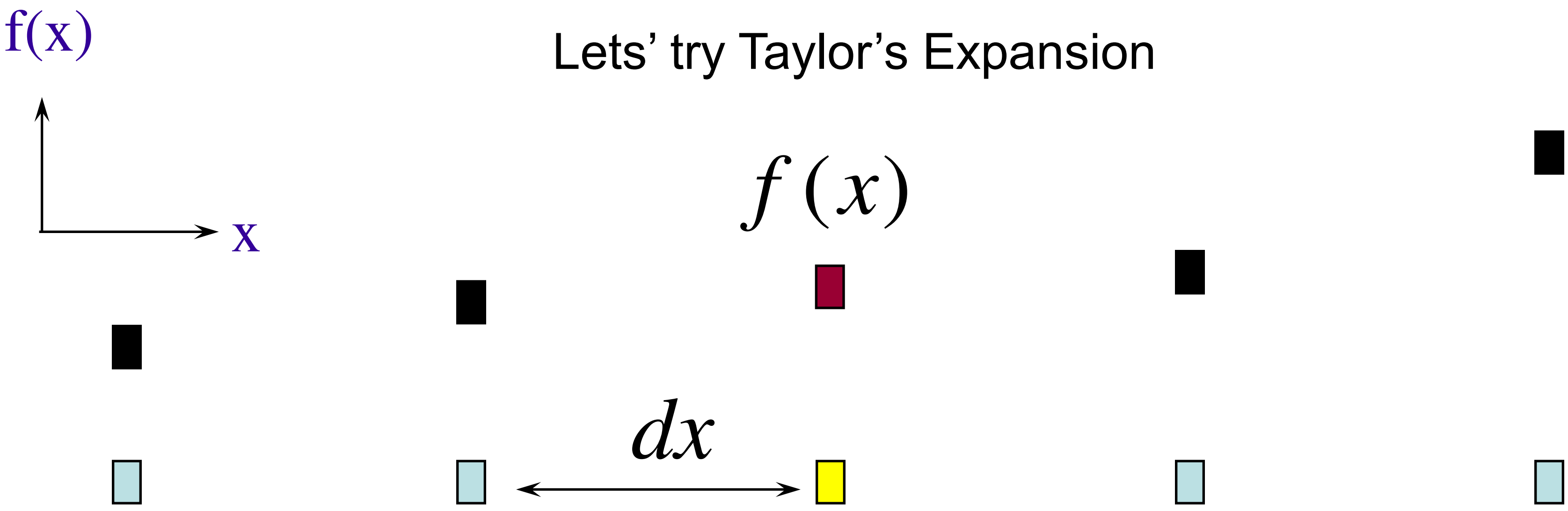
Alternative Derivation



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?

Lets' try Taylor's Expansion



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

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

we are looking for something like

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

2nd order weights

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	Derivative
$a+b=1$	$a+b=0$
$a-b=0$	$a-b=1/dx$

Taylor Operators

... 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 ...

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

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

Interpolation and difference weights

... and the result ...

Interpolation

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

Derivative

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

Can we generalise this idea to longer operators?

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

Higher order operators

*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 ...

Higher order operators

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

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

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

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

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

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

Linear system

... 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 ...

High-order interpolation

... 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

... 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 ...

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