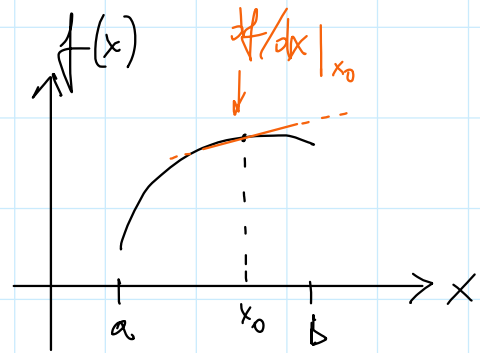


# Numerical differentiation

GOAL:  $f(x) \in [a, b]$   
 compute  $\frac{df}{dx} \Big|_{x_0}$



ANALYTICALLY:  $\frac{df}{dx} \Big|_{x_0} = \lim_{\Delta x \rightarrow 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$

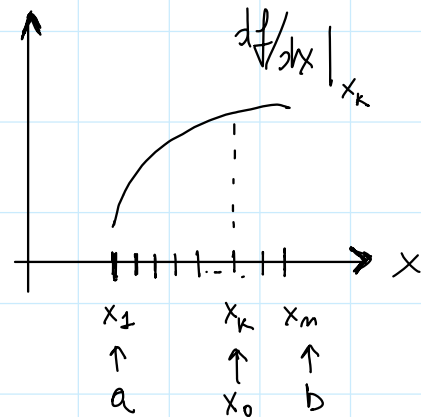
NUMERICALLY:

→ SUBDIVISION  $[a, b]$   $n$ -nodes  $\left( \begin{matrix} n-1 \\ \text{INTERVALS} \end{matrix} \right)$   
 ↓  
 points

$[x_1, x_2, \dots, x_k, \dots, x_n]$

$f(x_1) = f(a) ; f(x_k) = f(x_0) \dots$

↓  
 $f_1 \quad \dots \quad f_k \quad \dots \quad f_n$



IDEA: ESTIMATE  $df/dx$  from NODAL VALUES of  $f(x)$   
 $f_1, f_2, \dots, f_k, \dots, f_n$

→ TAYLOR EXPANSION  
 of  $f(x)$  around  $f(x_0)$   
 ↓  
 $f_k$

$$f(x) = \left[ f(x_0) + \frac{df}{dx} \Big|_{x_0} (x - x_0) + \frac{1}{2} \frac{d^2 f}{dx^2} \Big|_{x_0} (x - x_0)^2 \right] + O(x - x_0)^3$$

↑  
"BIG-O NOTATION"

$$\exists M \in \mathbb{R}^+ : |E(x)| \leq M (x - x_0)^3 \quad \text{for } (x - x_0) \rightarrow 0$$

↑  
 "there exist a  
 constant  $M$ "

↑  
 ERROR introduced by truncating TAYLOR

"there exist a positive real number ..."

ERROR introduced by truncating Taylor series to third-order

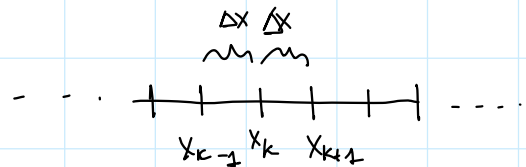
$$|E(x)| = \left| f(x) - \left[ f(x_0) + \frac{df}{dx} \Big|_{x_0} (x-x_0) + \frac{1}{2} \frac{d^2f}{dx^2} \Big|_{x_0} (x-x_0)^2 \right] \right|$$

→ If Taylor series is truncated to order  $N$ , the error goes to zero as  $(x-x_0)^N$  when  $(x-x_0) \rightarrow 0$

if  $N=2$  if  $(x-x_0) \Rightarrow E(x)$

$$(x' - x_0) = \frac{1}{2}(x - x_0) \Rightarrow E'(x) = \left(\frac{1}{2}\right)^N E(x) = \frac{1}{4} E(x)$$

HP: **UNIFORM SPACING**  
between  $x_1, x_2, \dots, x_n$



$$\begin{aligned} \rightarrow x_{k+1} - x_k &= \Delta x \\ x_k - x_{k-1} &= \Delta x \end{aligned}$$

Taylor Exp. around  $x_0$ :

$$f(x) = f_k + \frac{df}{dx} \Big|_k \Delta x + \frac{1}{2} \frac{d^2f}{dx^2} \Delta x^2 + \mathcal{O}(\Delta x^3) \quad [1]$$

$\uparrow$   $\uparrow$   
 $f(x_0)$   $(x-x_0)$

Taylor Exp  
from  $k$  to  $k+1$

truncated to third-order

$$f_{k+1} \stackrel{v}{=} f_k + \frac{df}{dx} \Big|_k \Delta x + \frac{1}{2} \frac{d^2f}{dx^2} \Big|_k \Delta x^2 + \mathcal{O}(\Delta x^3)$$

TRUNCATE TO SECOND-ORDER.

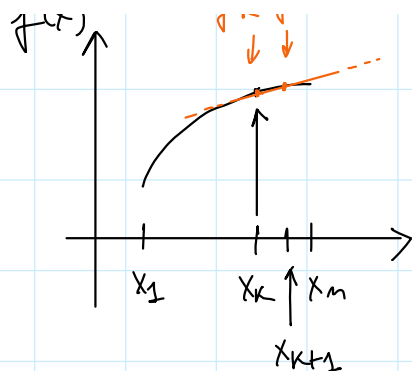
$$\Rightarrow f_{k+1} = f_k + \frac{df}{dx} \Big|_k \Delta x + \mathcal{O}(\Delta x^2)$$

FORWARD  
finite difference

$f(x)$   
 $\uparrow$

$$\frac{df}{dx} \Big|_k = \frac{f_{k+1} - f_k}{\Delta x} + \underbrace{\frac{\mathcal{O}(\Delta x^2)}{\Delta x}}_{\mathcal{O}(\Delta x)}$$

FIRST-ORDER  
DERIVATIVE  
FINITE difference  
formula



$O(\Delta x)$

FIRST-ORDER accurate

$$+ \frac{df}{dx} (x_{k+1} - x_k) = - \frac{df}{dx} \Delta x$$

TAYLOR EXPANSION from  $x_k$  to  $x_{k-1}$

$$f_{k-1} = f_k - \frac{df}{dx} \Big|_k \Delta x + \frac{1}{2} \frac{d^2 f}{dx^2} \Delta x^2 + O(\Delta x^3) \quad [2]$$

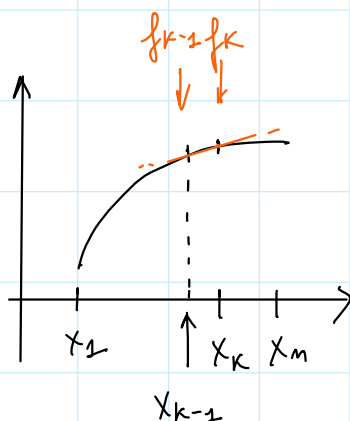
TRUNCATION to second-order

$$f_{k-1} = f_k - \frac{df}{dx} \Big|_k \Delta x + O(\Delta x^2)$$

BACKWARD  
Finite difference  
formula

$$\frac{df}{dx} \Big|_k = \frac{f_k - f_{k-1}}{\Delta x} + O(\Delta x)$$

First-order  
accuracy



$$\frac{df}{dx} \Big|_k \approx \frac{f_k - f_{k-1}}{\Delta x}$$

THIRD-ORDER

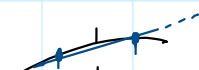
Combining [1] - [2]

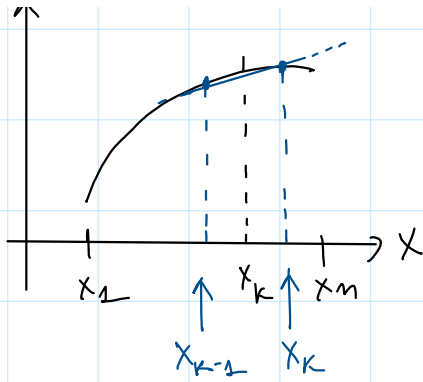
$$f_{k+1} - f_{k-1} = \cancel{0} f_k + 2 \frac{df}{dx} \Big|_k \Delta x + \cancel{0} \frac{d^2 f}{dx^2} \Delta x^2 + O(\Delta x^3)$$

$$\Rightarrow \frac{df}{dx} \Big|_k = \frac{f_{k+1} - f_{k-1}}{2\Delta x} + O(\Delta x^2)$$

CENTERED finite  
difference formula  
for first-order derivative

ACCURACY: SECOND-ORDER





ROUNDoff errors  
(finite amount of digits)  
 $\neq$

ERRORS. FW / BW  $\rightarrow$   $\Delta x \rightarrow E(x)$   
 $\frac{\Delta x}{2} \rightarrow \frac{E(x)}{2}$   
 C  $\rightarrow$   $\Delta x \rightarrow E(x)$   
 (centered)  $\frac{\Delta x}{2} \rightarrow \frac{E(x)}{4}$

TRUNCATION  
errors  
(finite amount of  
terms in TAYLOR  
series to express  
derivatives in terms  
of algebraic expressions)