Computational Physics

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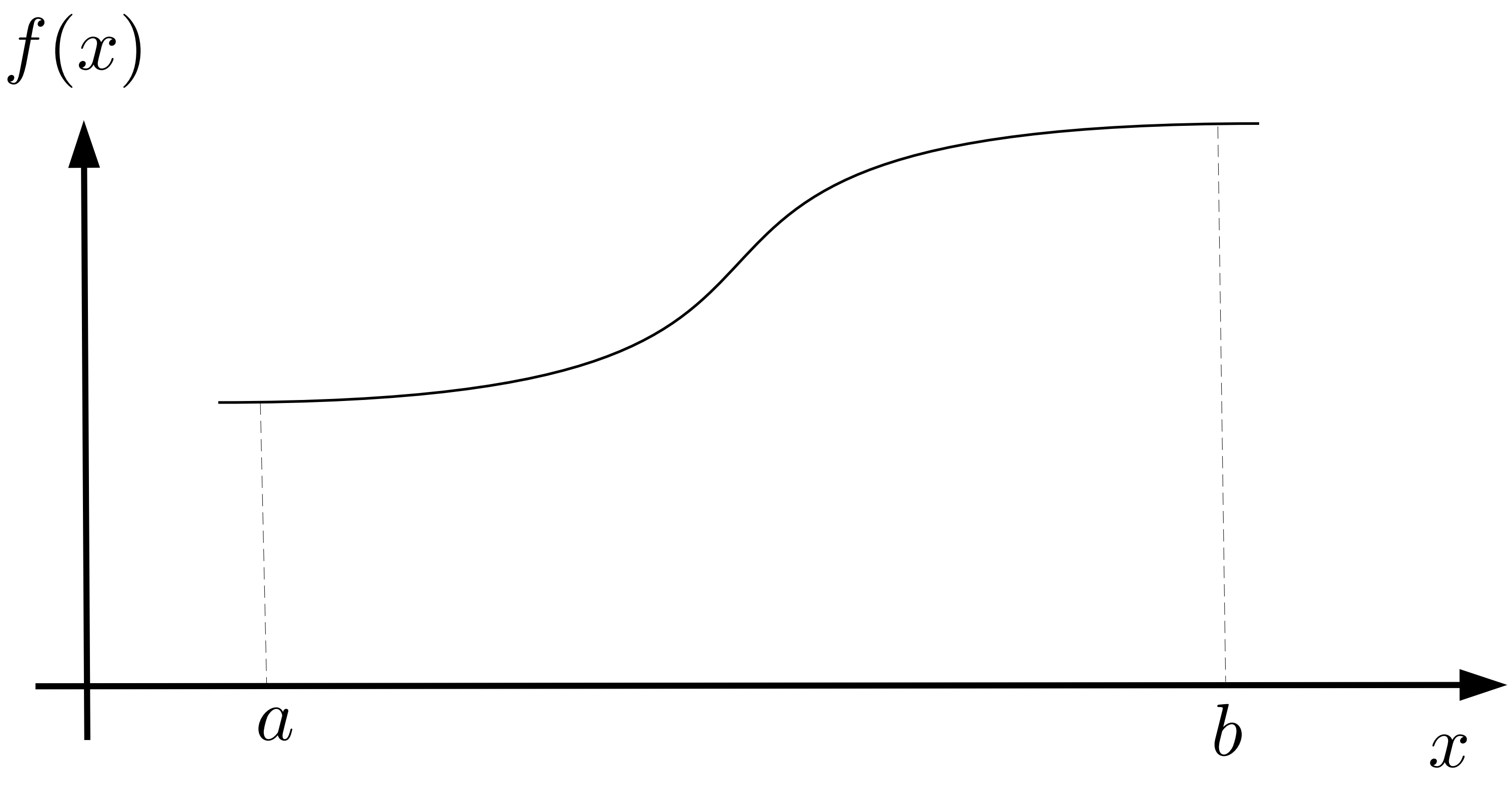
Physics Group, University of Qom

Lecture-02

Contents

Numerical Differentiation

- Finite Differences

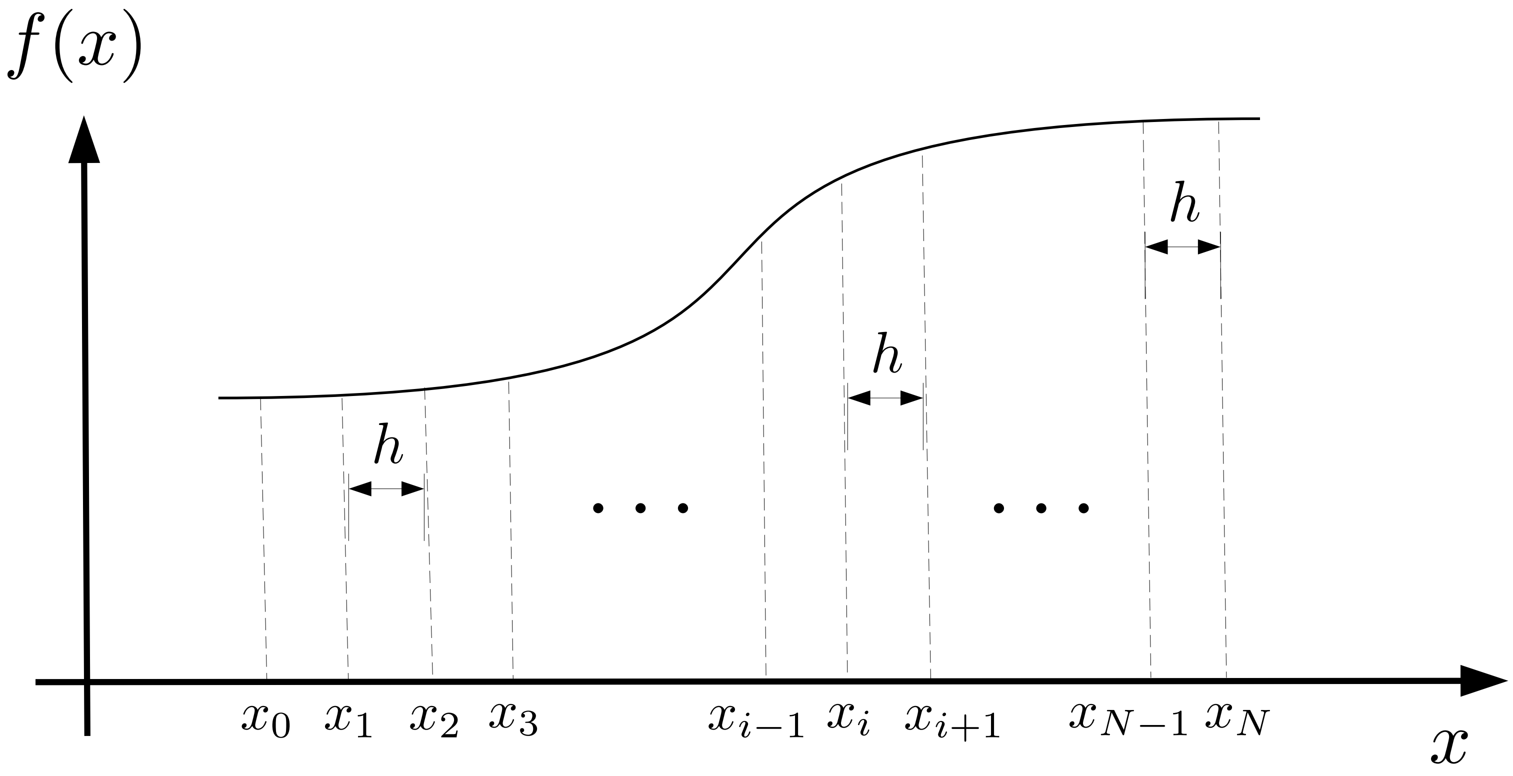


Smooth function $f(x)$

$$x \in [a,\, b]$$

Numerical Differentiation

- Finite Differences



$x_0 = a$ $\qquad$ $x_N = b$

Smooth function $f(x)$

$$x \in [a,\, b]$$

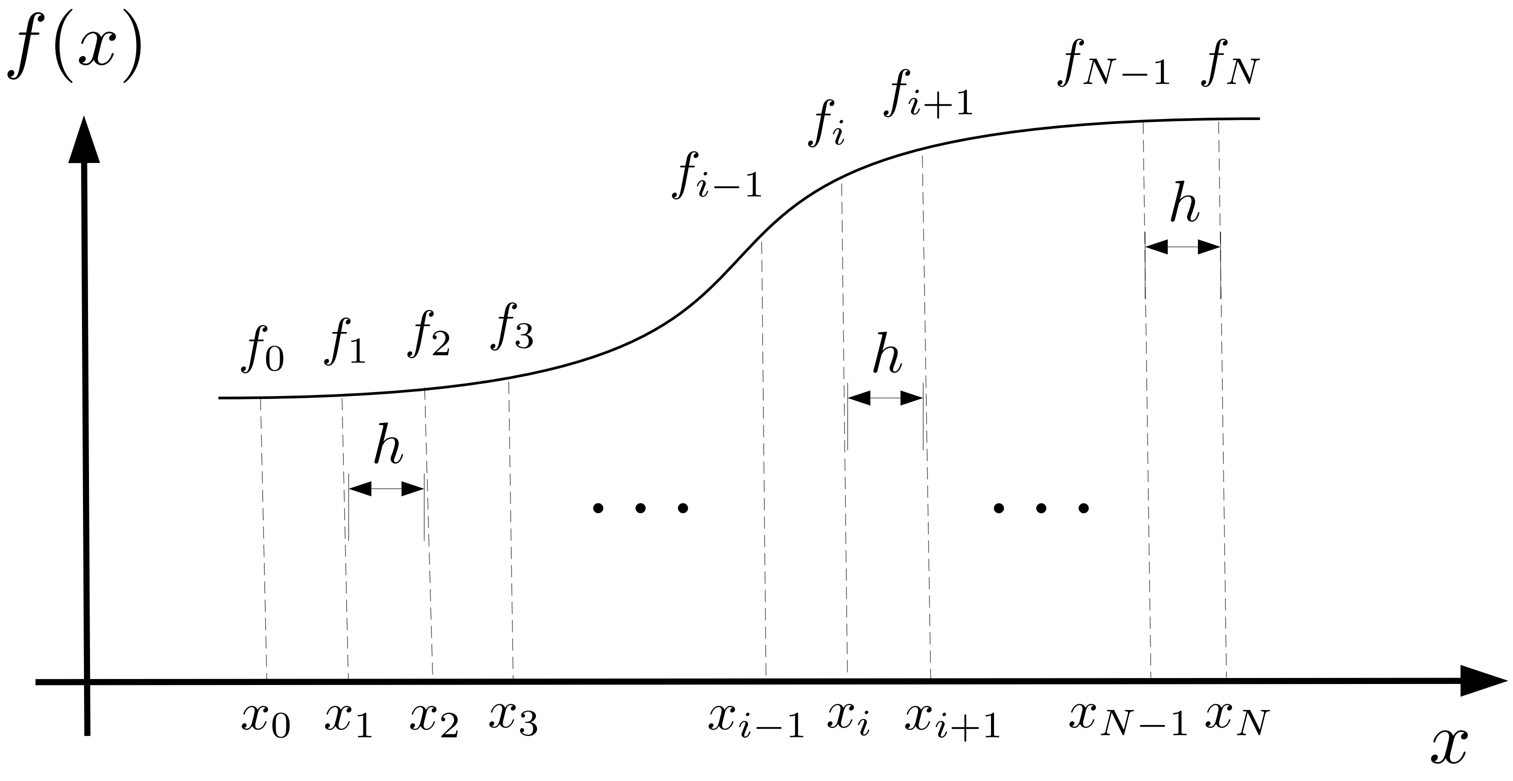
$$h = \frac{b-a}{N}$$

$$\begin{cases} x_i = a + h\, i \\ i = 0, 1, 2, \cdots, N \end{cases}$$

$$x_{i+1} = x_i + h$$

Numerical Differentiation

- Finite Differences



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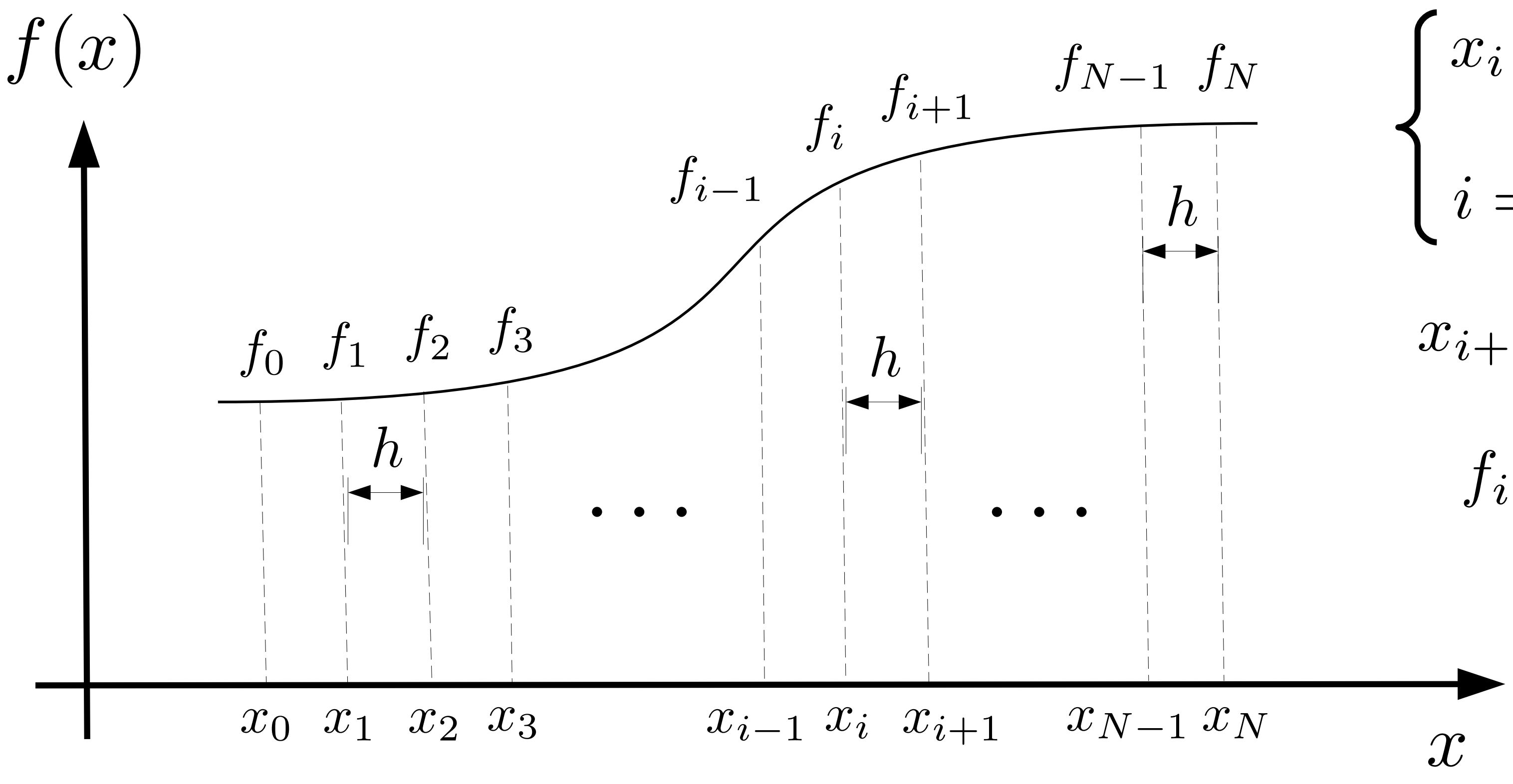
Numerical Differentiation

- Finite Differences



$$x_0 = a \qquad x_N = b$$

$$h = \frac{b-a}{N}$$

$$\begin{cases} x_i = a + h\,i \\ i = 0, 1, 2, \cdots, N \end{cases}$$

$$x_{i+1} = x_i + h$$

$$f_i = f(x_i)$$

x	$f(x)$
x_0	f_0
x_1	f_1
x_2	f_2
$\vdots$	$\vdots$
x_{i-1}	f_{i-1}
x_i	f_i
x_{i+1}	f_{i+1}
$\vdots$	$\vdots$
x_{N-1}	f_{N-1}
x_N	f_N

Numerical Differentiation

- Taylor expansion

$$f(x_i + h) = f(x_i) + \frac{f^{(1)}(x_i)}{1!}h + \frac{f^{(2)}(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots$$

x	x_0	x_1	x_2	$\cdots$	x_{i-1}	x_i	x_{i+1}	$\cdots$	x_{N-1}	x_N
$f(x)$	f_0	f_1	f_2	$\cdots$	f_{i-1}	f_i	f_{i+1}	$\cdots$	f_{N-1}	f_N
$f^{(1)}(x)$	$f_0^{(1)}$	$f_1^{(1)}$	$f_2^{(1)}$	$\cdots$	$f_{i-1}^{(1)}$	$f_i^{(1)}$	$f_{i+1}^{(1)}$	$\cdots$	$f_{N-1}^{(1)}$	$f_N^{(1)}$
$f^{(2)}(x)$	$f_0^{(2)}$	$f_1^{(2)}$	$f_2^{(2)}$	$\cdots$	$f_{i-1}^{(2)}$	$f_i^{(2)}$	$f_{i+1}^{(2)}$	$\cdots$	$f_{N-1}^{(2)}$	$f_N^{(2)}$
$\vdots$		$\vdots$				$\vdots$			$\vdots$	

Numerical Differentiation

- Taylor expansion

$$f(x_i+h) = f(x_i) + \frac{f^{(1)}(x_i)}{1!}h + \frac{f^{(2)}(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots$$

x	x_0	x_1	x_2	$\cdots$	x_{i-1}	x_i	x_{i+1}	$\cdots$	x_{N-1}	x_N
$f(x)$	f_0	f_1	f_2	$\cdots$	f_{i-1}	f_i	f_{i+1}	$\cdots$	f_{N-1}	f_N
$f^{(1)}(x)$	$f_0^{(1)}$	$f_1^{(1)}$	$f_2^{(1)}$	$\cdots$	$f_{i-1}^{(1)}$	$f_i^{(1)}$	$f_{i+1}^{(1)}$	$\cdots$	$f_{N-1}^{(1)}$	$f_N^{(1)}$
$f^{(2)}(x)$	$f_0^{(2)}$	$f_1^{(2)}$	$f_2^{(2)}$	$\cdots$	$f_{i-1}^{(2)}$	$f_i^{(2)}$	$f_{i+1}^{(2)}$	$\cdots$	$f_{N-1}^{(2)}$	$f_N^{(2)}$
$\vdots$	$\vdots$					$\vdots$			$\vdots$	

$$x_{i+1} = x_i + h$$

$$f_{i+1} = f_i + \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 + \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

Numerical Differentiation

- Taylor expansion

$$f(x+h) = f_{i+1} = f_i + \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 + \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

$$f(x-h) = f_{i-1} = f_i - \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 - \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

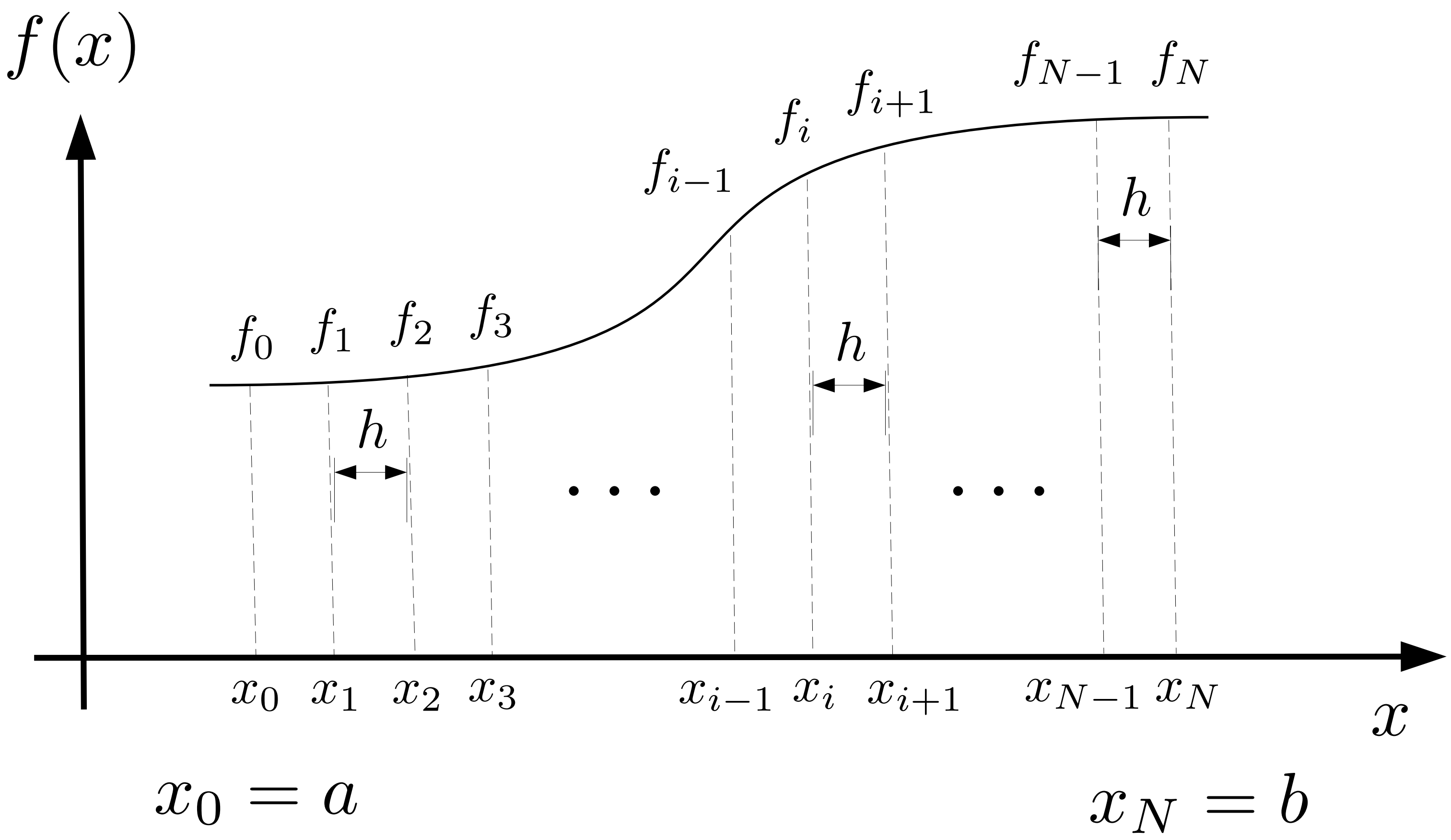
$$f(x+2h) = f_{i+2} = f_i + \frac{f_i^{(1)}}{1!}(2h) + \frac{f_i^{(2)}}{2!}(2h)^2 + \frac{f_i^{(3)}}{3!}(2h)^3 + \cdots$$

$$f(x-2h) = f_{i-2} = f_i - \frac{f_i^{(1)}}{1!}(2h) + \frac{f_i^{(2)}}{2!}(2h)^2 - \frac{f_i^{(3)}}{3!}(2h)^3 + \cdots$$

$$\vdots \qquad\qquad \vdots \qquad\qquad \vdots$$

Numerical Differentiation

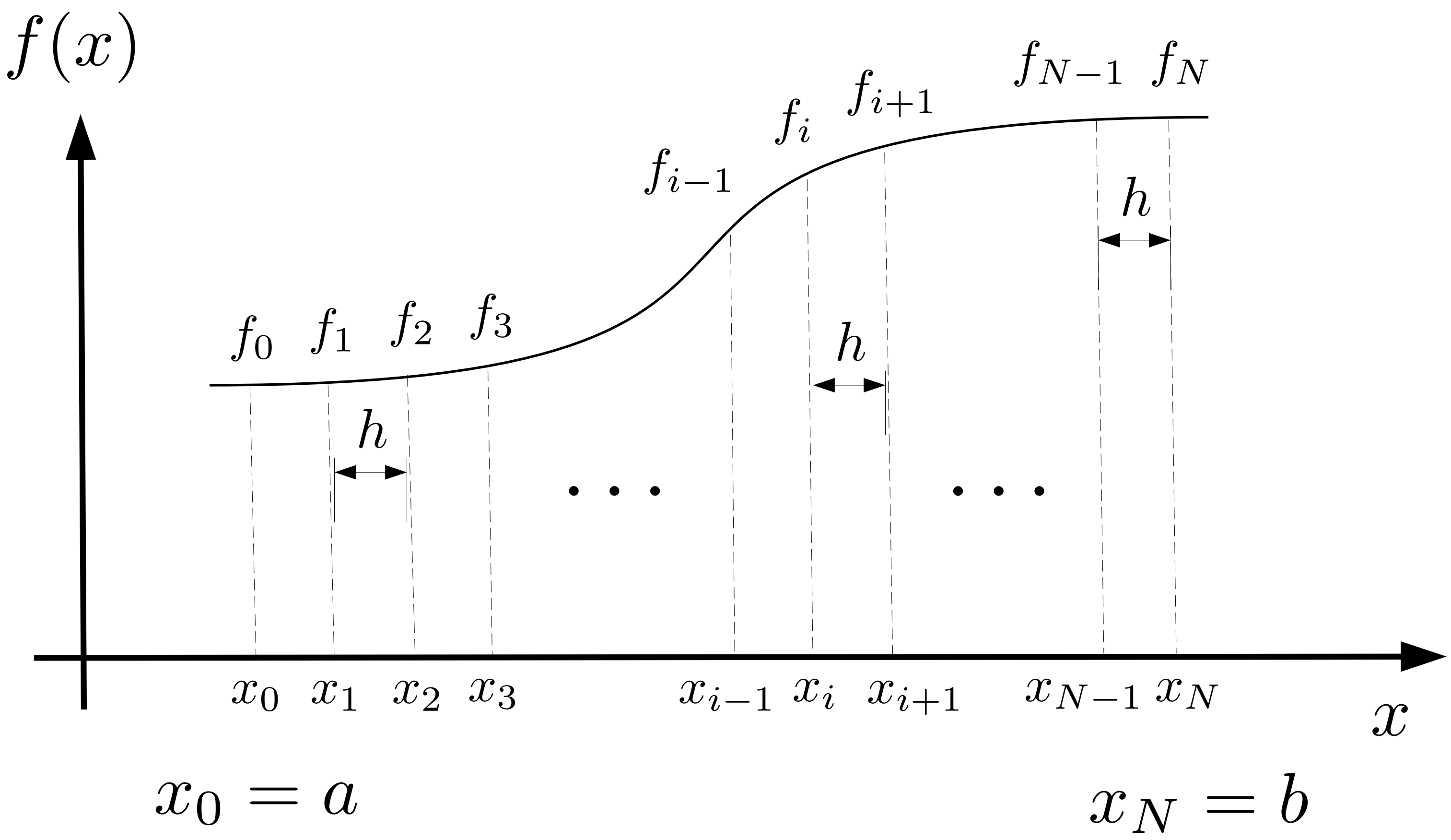
- First order derivative



x	$f(x)$
x_0	f_0
x_1	f_1
x_2	f_2
$\vdots$	$\vdots$
x_{i-1}	f_{i-1}
x_i	f_i
x_{i+1}	f_{i+1}
$\vdots$	$\vdots$
x_{N-1}	f_{N-1}
x_N	f_N

Numerical Differentiation

- First order derivative



x	$f(x)$	$f^{(1)}(x)$
x_0	f_0	$f_0^{(1)}$
x_1	f_1	$f_1^{(1)}$
x_2	f_2	$f_2^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(1)}$
x_i	f_i	$f_i^{(1)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(1)}$
x_N	f_N	$f_N^{(1)}$

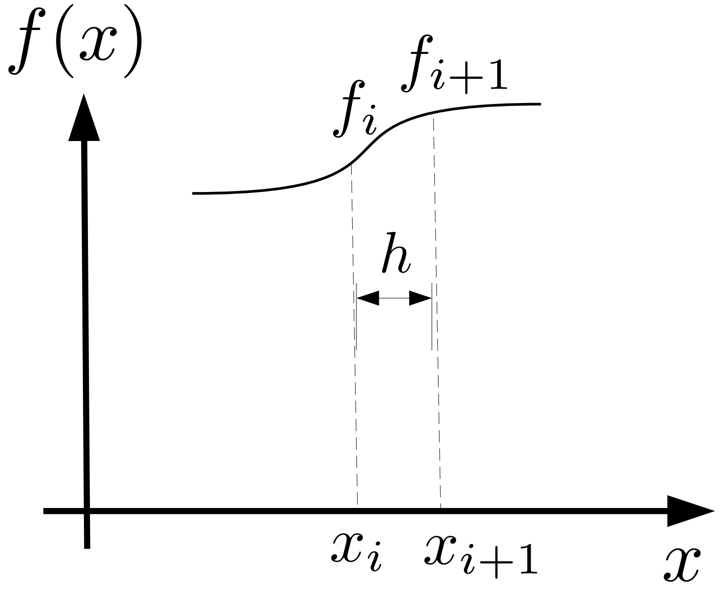
Numerical Differentiation

- First order derivative

$$f_{i+1} = f_i + \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 + \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

Truncate: $$f_{i+1} \approx f_i + f_i^{(1)}h + \mathrm{O}(h^2)$$

$$f_i^{(1)} \approx \frac{f_{i+1} - f_i}{h} + \mathrm{O}(h)$$



Forward difference derivative(two-point)

Numerical Differentiation

- First order derivative

$$f_{i+1} = f_i + \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 + \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

Truncate: $f_{i+1} \approx f_i + f_i^{(1)} h + \mathrm{O}(h^2)$

$$f_i^{(1)} \approx \frac{f_{i+1} - f_i}{h} + \mathrm{O}(h)$$

Forward difference derivative(two-point)

x	$f(x)$	$f^{(1)}(x)$
x_0	f_0	$f_0^{(1)}$
x_1	f_1	$f_1^{(1)}$
x_2	f_2	$f_2^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(1)}$
x_i	f_i	$f_i^{(1)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(1)}$
x_N	f_N	$f_N^{(1)}$

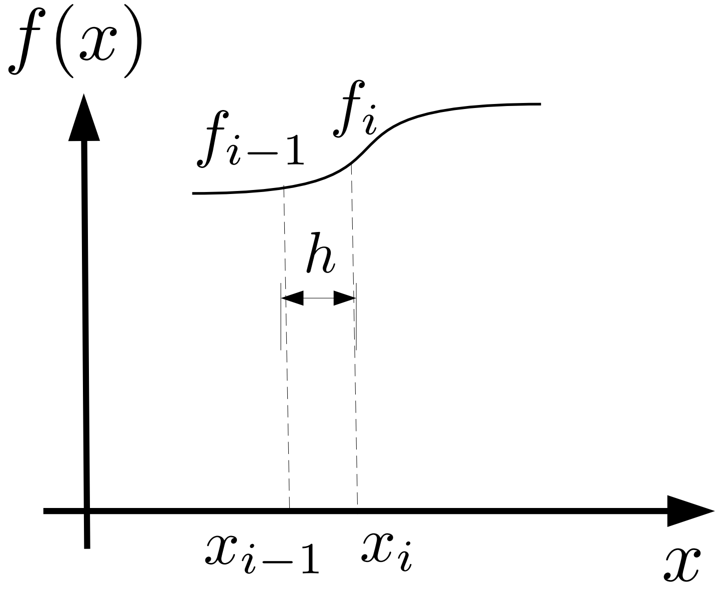
Numerical Differentiation

- First order derivative

$$f_{i-1} = f_i - \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 - \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

Truncate: $f_{i-1} \approx f_i - f_i^{(1)}h + \mathrm{O}(h^2)$

$$f_i^{(1)} \approx \frac{f_i - f_{i-1}}{h} + \mathrm{O}(h)$$



Backward difference derivative(two-point)

Numerical Differentiation

- First order derivative

$$f_{i-1} = f_i - \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 - \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

Truncate: $f_{i-1} \approx f_i - f_i^{(1)}h + \mathrm{O}(h^2)$

$$f_i^{(1)} \approx \frac{f_i - f_{i-1}}{h} + \mathrm{O}(h)$$

Backward difference derivative(two-point)

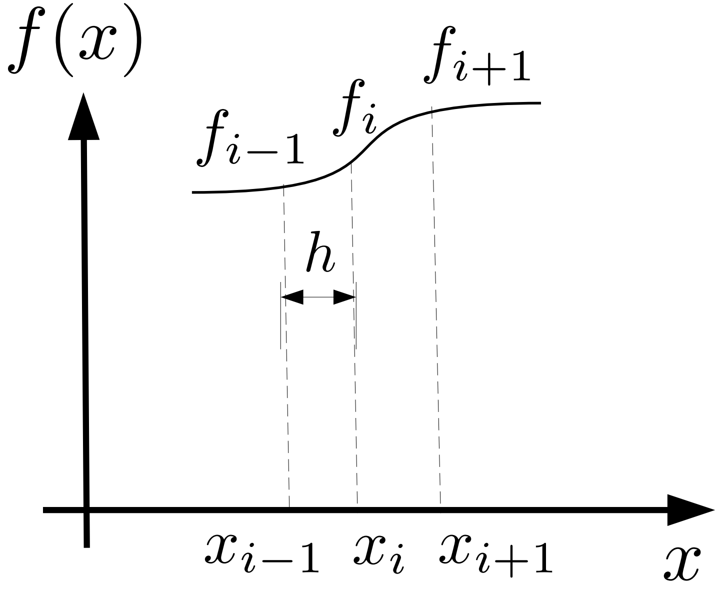
x	$f(x)$	$f^{(1)}(x)$
x_0	f_0	$f_0^{(1)}$
x_1	f_1	$f_1^{(1)}$
x_2	f_2	$f_2^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(1)}$
x_i	f_i	$f_i^{(1)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(1)}$
x_N	f_N	$f_N^{(1)}$

Numerical Differentiation

- First order derivative

$$f_{i+1} = f_i + \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 + \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

$$f_{i-1} = f_i - \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 - \frac{f_i^{(3)}}{3!}h^3 + \cdots \qquad -$$



$$f_{i+1} - f_{i-1} = 2f_i^{(1)}h + 2\frac{f_i^{(3)}}{3!}h^3 + \cdots$$

Truncate: $$f_{i+1} - f_{i-1} \approx 2f_i^{(1)}h + \mathrm{O}(h^3)$$

Numerical Differentiation

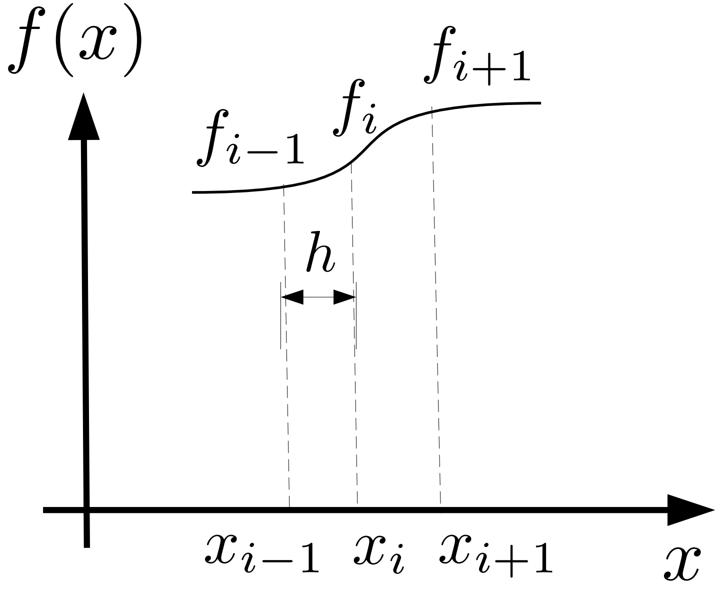
- First order derivative

$$f_{i+1} = f_i + \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 + \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

$$f_{i-1} = f_i - \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 - \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

Truncate: $$f_{i+1} - f_{i-1} \approx 2f_i^{(1)}h + \mathrm{O}(h^3)$$

$$f_i^{(1)} \approx \frac{f_{i+1} - f_{i-1}}{2h} + \mathrm{O}(h^2)$$



Central difference derivative(three-point)

Numerical Differentiation

- First order derivative

$$f_{i+1} = f_i + \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 + \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

$$f_{i-1} = f_i - \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 - \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

Truncate: $f_{i+1} - f_{i-1} \approx 2f_i^{(1)}h + \mathrm{O}(h^3)$

$$f_i^{(1)} \approx \frac{f_{i+1} - f_{i-1}}{2h} + \mathrm{O}(h^2)$$

Central difference derivative(three-point)

x	$f(x)$	$f^{(1)}(x)$
x_0	f_0	$f_0^{(1)}$
x_1	f_1	$f_1^{(1)}$
x_2	f_2	$f_2^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(1)}$
x_i	f_i	$f_i^{(1)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(1)}$
x_N	f_N	$f_N^{(1)}$

Numerical Differentiation

- First order derivative

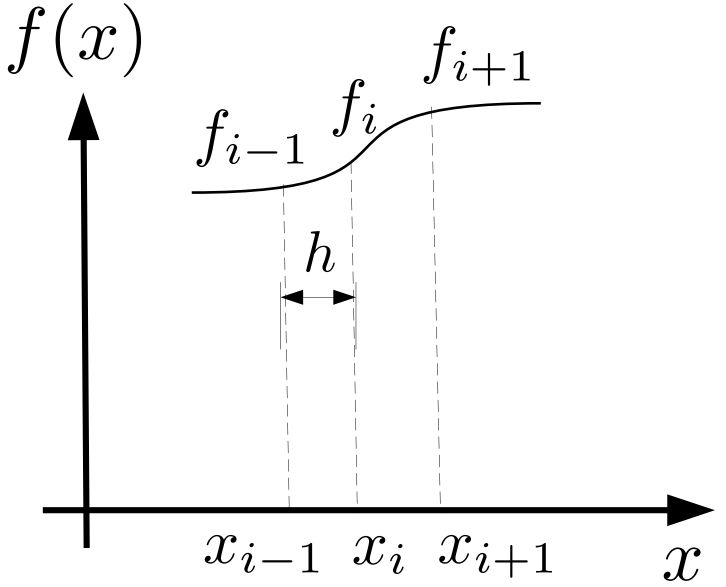
Asymmetry

$$f_i^{(1)} \approx \frac{f_{i+1} - f_i}{h} + \underline{\underline{O(h)}}$$ Forward

$$f_i^{(1)} \approx \frac{f_i - f_{i-1}}{h} + \underline{\underline{O(h)}}$$ Backward

Symmetry

$$f_i^{(1)} \approx \frac{f_{i+1} - f_{i-1}}{2h} + \underline{\underline{O(h^2)}}$$ Central



Numerical Differentiation

- First order derivative

$$f_i^{(1)} \approx \frac{f_{i+1} - f_i}{h} + \mathrm{O}(h)$$

Forward

$$f_i^{(1)} \approx \frac{f_{i+1} - f_{i-1}}{2h} + \mathrm{O}(h^2)$$

Central

$$f_i^{(1)} \approx \frac{f_i - f_{i-1}}{h} + \mathrm{O}(h)$$

Backward

x	$f(x)$	$f^{(1)}(x)$
x_0	f_0	$f_0^{(1)}$
x_1	f_1	$f_1^{(1)}$
x_2	f_2	$f_2^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(1)}$
x_i	f_i	$f_i^{(1)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(1)}$
x_N	f_N	$f_N^{(1)}$

Numerical Differentiation

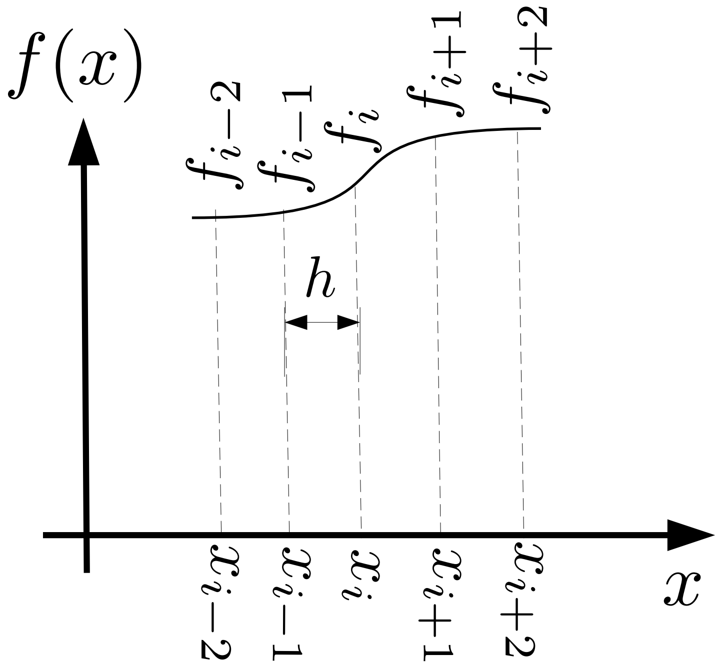
- First order derivative

$$f_{i-2} = f_i - \frac{f_i^{(1)}}{1!}(2h) + \frac{f_i^{(2)}}{2!}(2h)^2 - \frac{f_i^{(3)}}{3!}(2h)^3 + \cdots$$

$$f_{i-1} = f_i - \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 - \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

$$f_{i+1} = f_i + \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 + \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

$$f_{i+2} = f_i + \frac{f_i^{(1)}}{1!}(2h) + \frac{f_i^{(2)}}{2!}(2h)^2 + \frac{f_i^{(3)}}{3!}(2h)^3 + \cdots$$



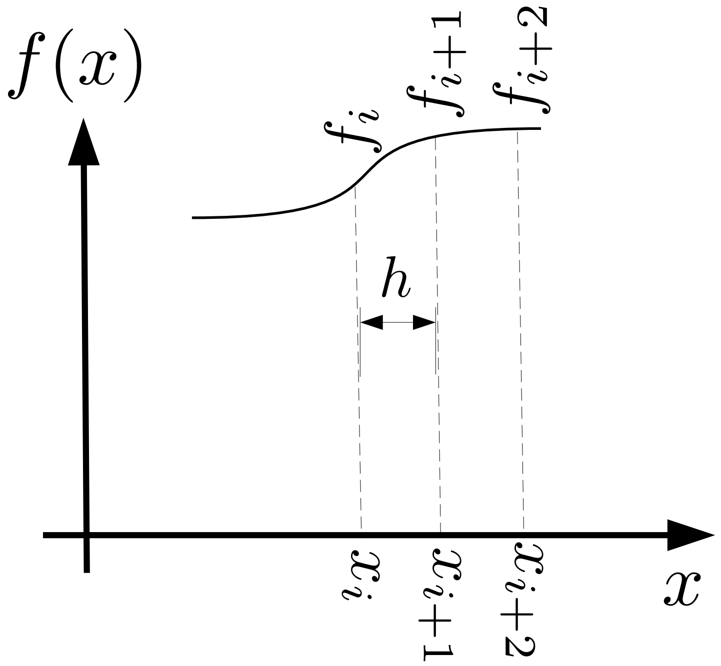
Numerical Differentiation

- First order derivative (3-points)

$$4f_{i+1} - f_{i+2} = 3f_i + 2f_i^{(1)}h - \frac{1}{3}f_i^{(3)}h^3 + \cdots$$

Truncate: $$4f_{i+1} - f_{i+2} \approx 3f_i + 2f_i^{(1)}h + \mathrm{O}(h^3)$$

$$f_i^{(1)} \approx \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + \mathrm{O}(h^2)$$



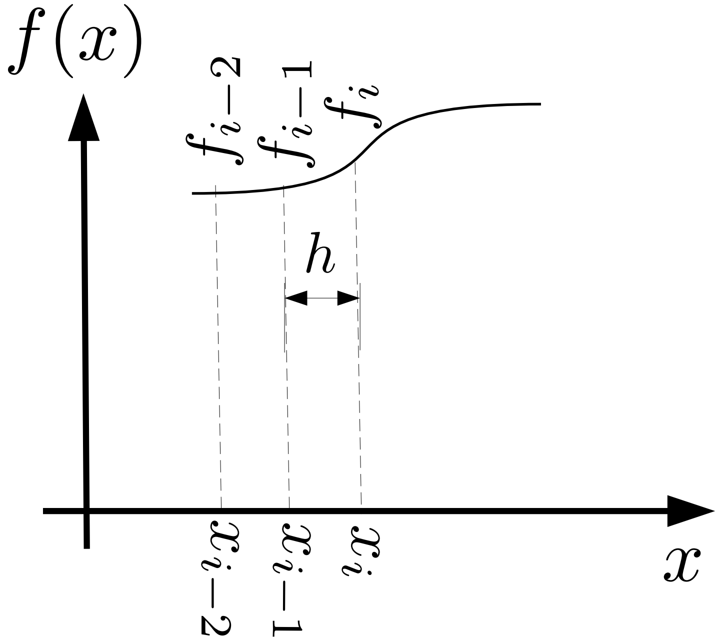
Numerical Differentiation

- First order derivative (3-points)

$$f_{i-2} - 4f_{i-1} = -3f_i + 2f_i^{(1)}h - \frac{1}{3}f_i^{(3)}h^3 + \cdots$$

Truncate: $-4f_{i-1} + f_{i-2} \approx -3f_i + 2f_i^{(1)}h + \mathrm{O}(h^3)$

$$f_i^{(1)} \approx \frac{f_{i-2} - 4f_{i-1} + 3f_i}{2h} + \mathrm{O}(h^2)$$



Numerical Differentiation

- First order derivative

Asymmetry

$$f_i^{(1)} \approx \frac{f_{i+1} - f_i}{h} + \underline{\underline{O(h)}} \qquad \text{2-point}$$

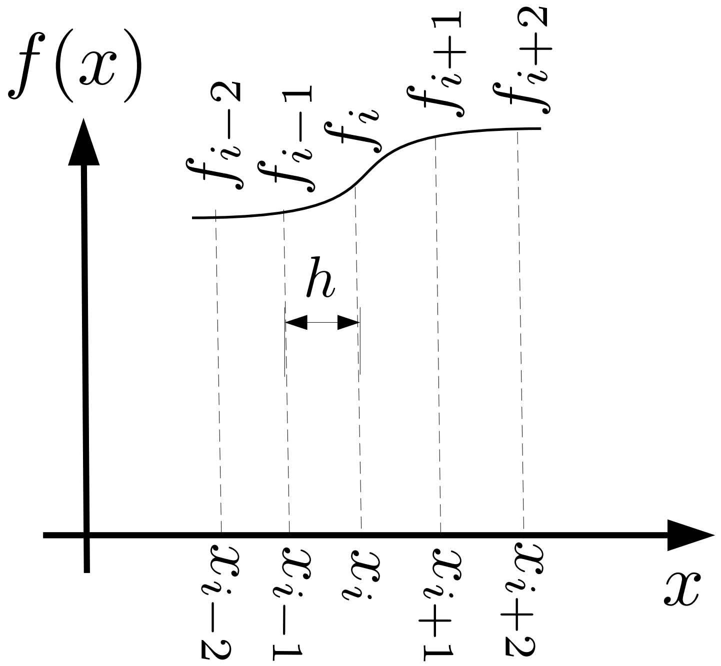
$$f_i^{(1)} \approx \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + \underline{\underline{O(h^2)}} \qquad \text{3-point}$$

$$\vdots$$

$$f_i^{(1)} \approx \frac{f_i - f_{i-1}}{h} + \underline{\underline{O(h)}} \qquad \text{2-point}$$

$$f_i^{(1)} \approx \frac{f_{i+2} - 4f_{i-1} + 3f_i}{2h} + \underline{\underline{O(h^2)}} \qquad \text{3-point}$$

$$\vdots$$



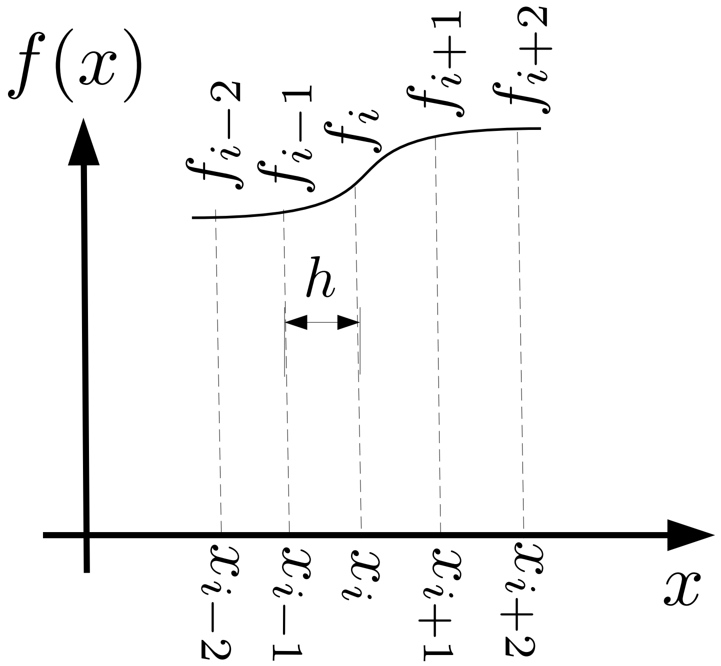
Numerical Differentiation

- First order derivative (5-points)

$$-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2} = 12f_i^{(1)}h - \frac{1}{30}f_i^{(5)}h^5 + \cdots$$

$$-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2} \approx 12f_i^{(1)}h + \mathrm{O}(h^5)$$

$$f_i^{(1)} \approx \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} + \mathrm{O}(h^4)$$



Numerical Differentiation

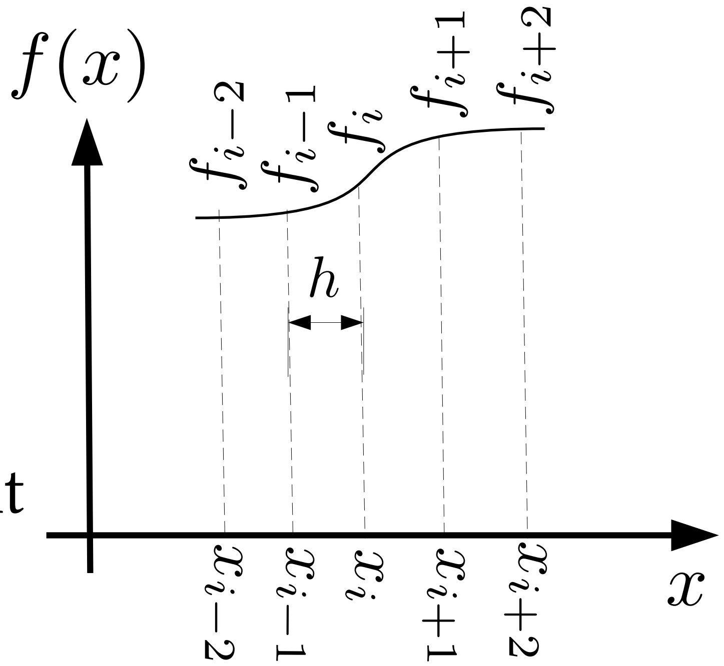
- First order derivative

Symmetry

$$f_i^{(1)} \approx \frac{f_{i+1} - f_{i-1}}{2h} + \mathrm{O}(h^2) \qquad \text{3-point}$$

$$f_i^{(1)} \approx \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} + \mathrm{O}(h^4) \qquad \text{5-point}$$

$$\vdots$$



Numerical Differentiation

- First order derivative

$$f_i^{(1)} \approx \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + \mathrm{O}(h^2)$$

$$f_i^{(1)} \approx \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} + \mathrm{O}(h^4)$$

$$f_i^{(1)} \approx \frac{f_{i-2} - 4f_{i-1} + 3f_i}{2h} + \mathrm{O}(h^2)$$

x	$f(x)$	$f^{(1)}(x)$
x_0	f_0	$f_0^{(1)}$
x_1	f_1	$f_1^{(1)}$
x_2	f_2	$f_2^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(1)}$
x_i	f_i	$f_i^{(1)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(1)}$
x_N	f_N	$f_N^{(1)}$