Computational Physics

Lecture-05

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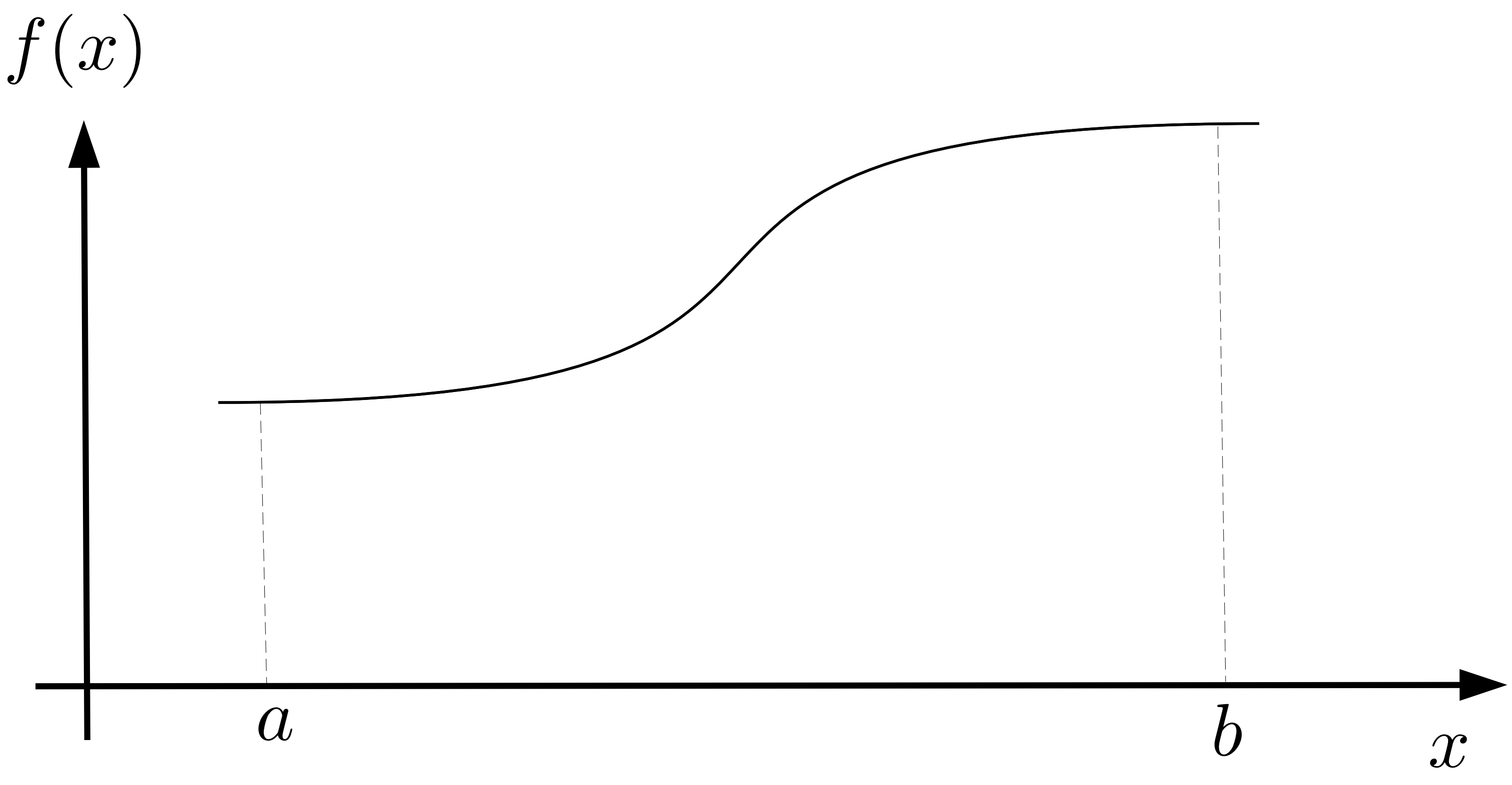
Contents

Numerical Integration

- Finite Differences

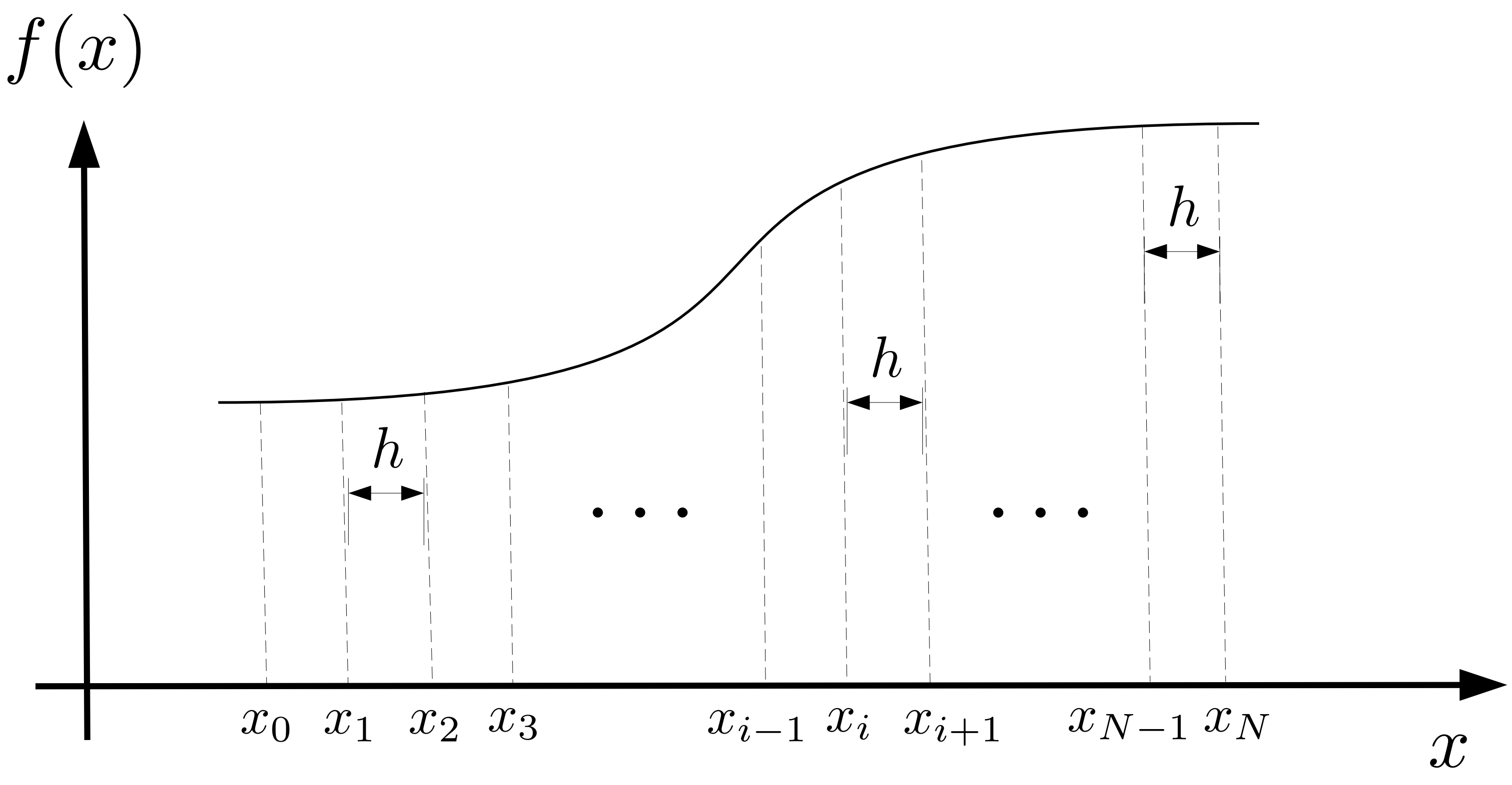


Smooth function $f(x)$

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

Numerical Integration

- Finite Differences



$x_0 = a$

$x_N = b$

Smooth function $f(x)$

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

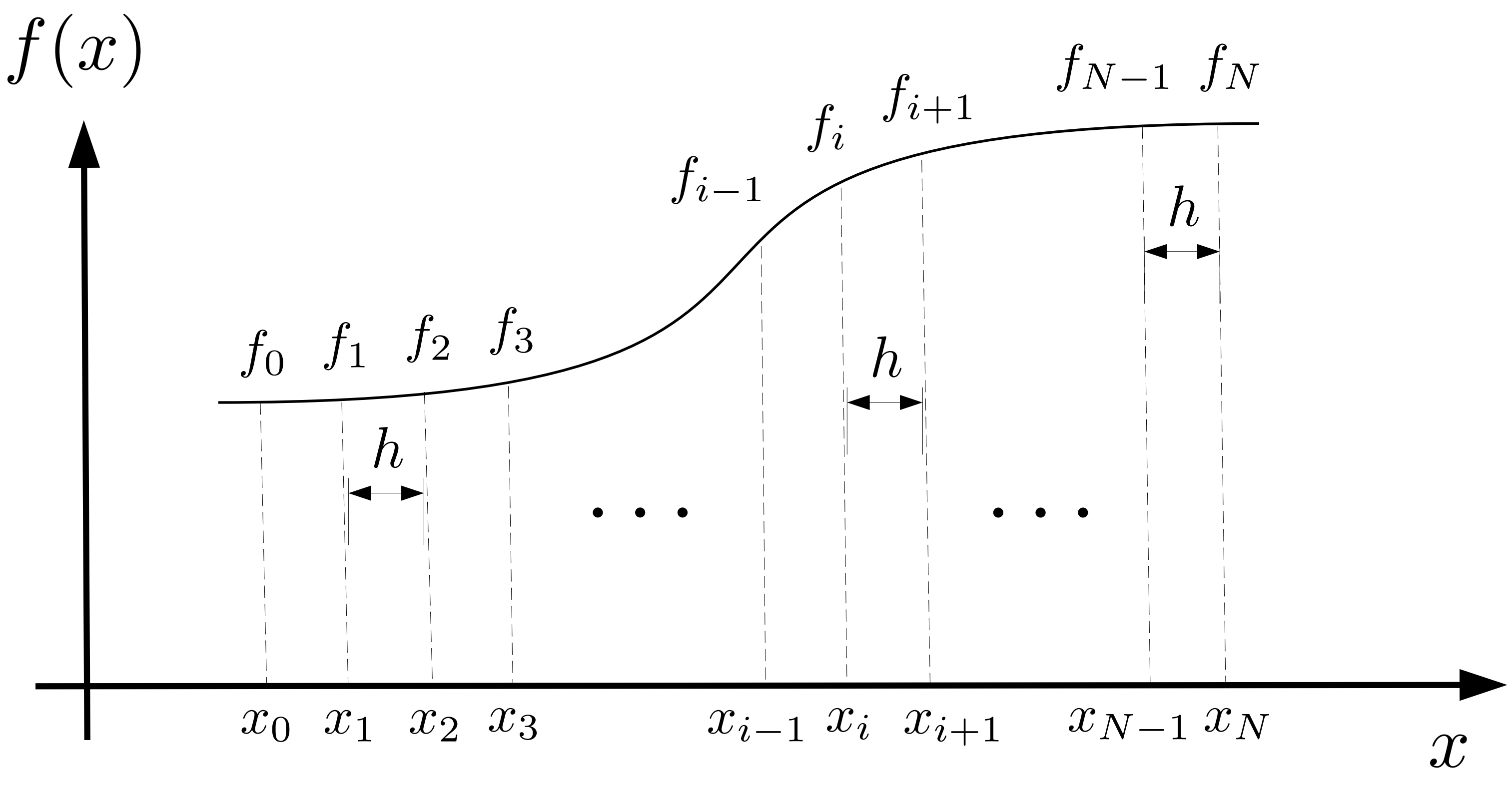
$$h = \frac{b-a}{N}$$

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

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

Numerical Integration

- Finite Differences



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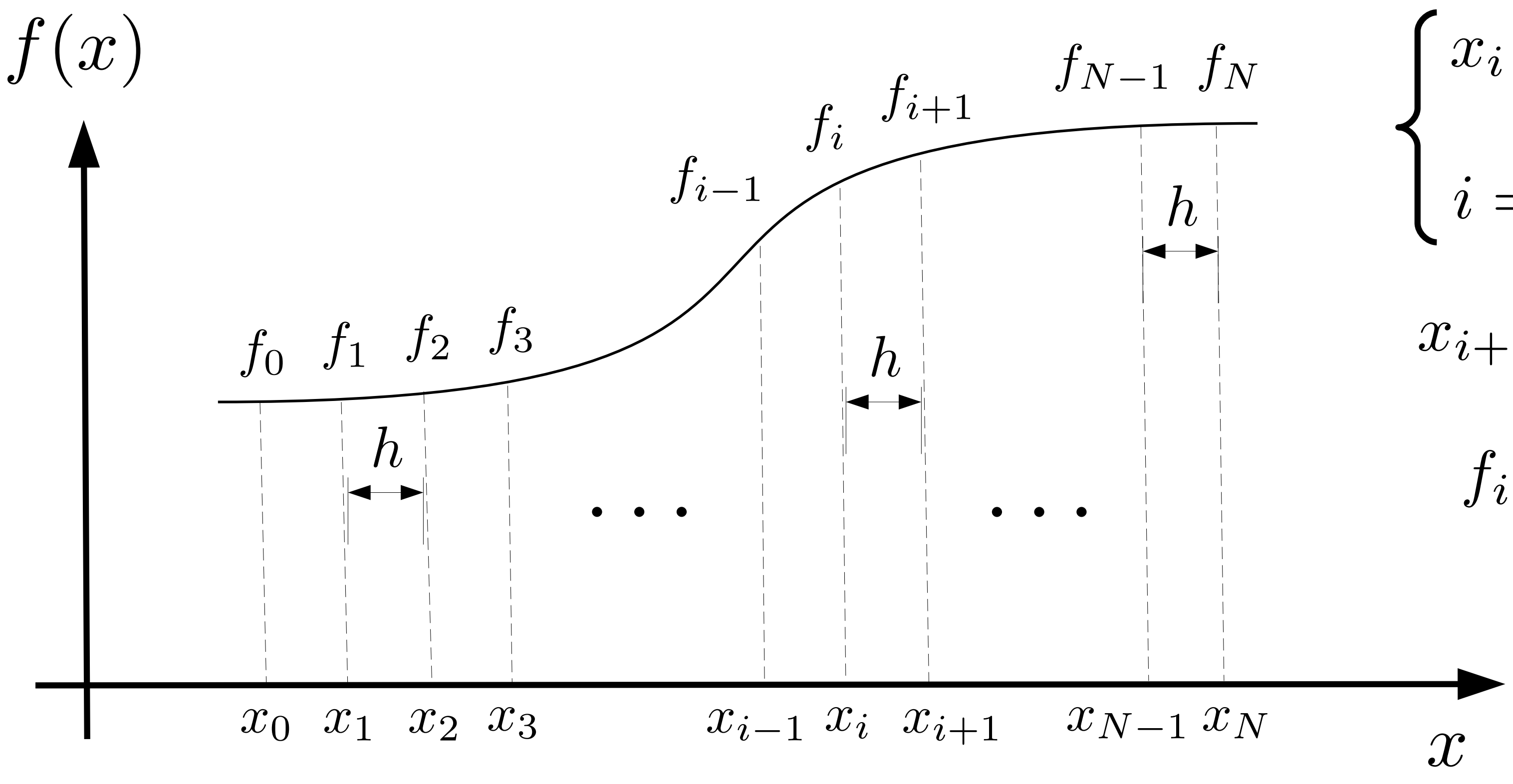
Numerical Integration

- Finite Differences



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

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

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

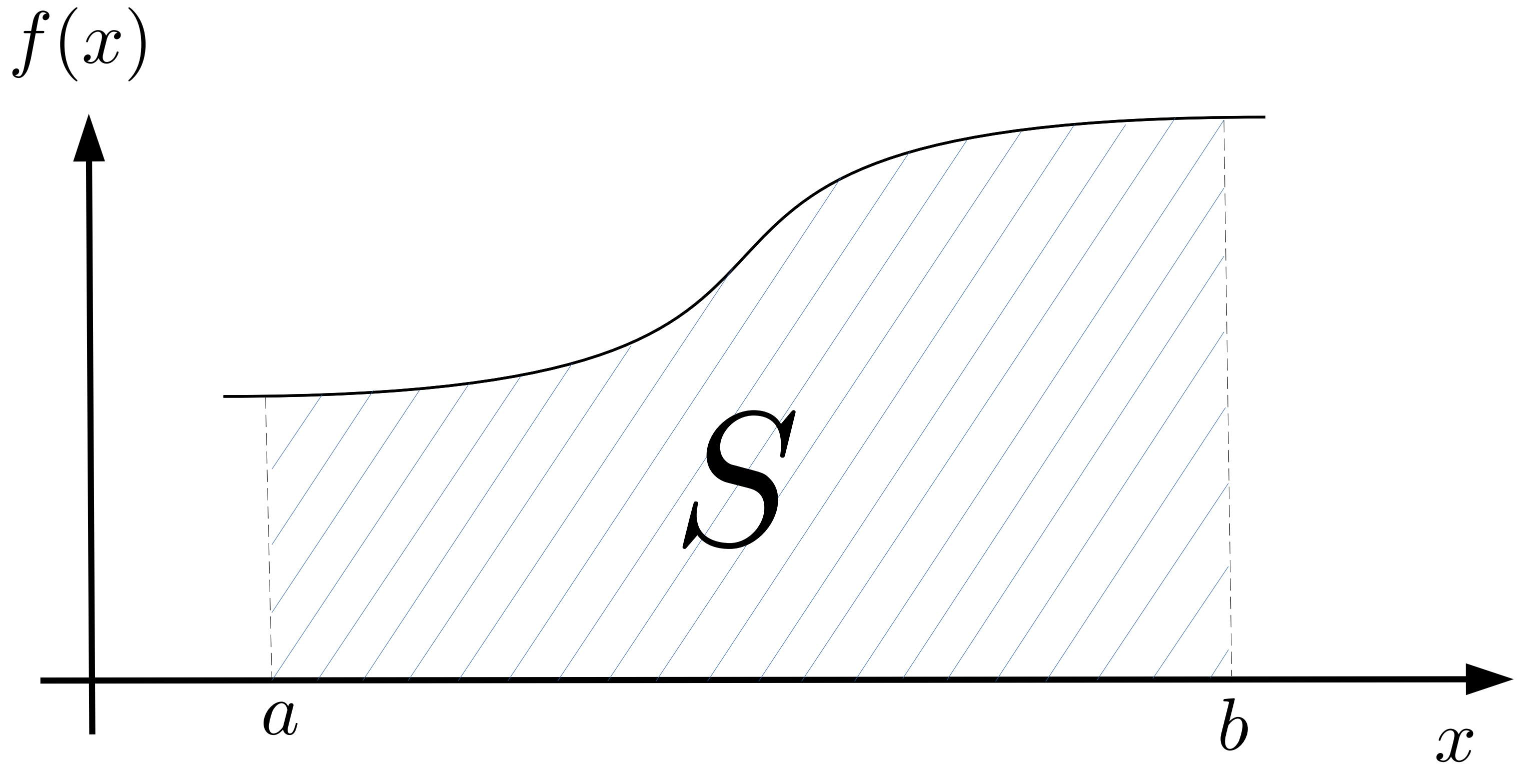
$$x_{i+1} = x_i + h$$

$$f_i = f(x_i)$$

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 Integration

- Approximate integral $$\int_a^b f(x)\mathrm{d}x \approx h\sum_i^N w_i f_i$$



Smooth function $f(x)$

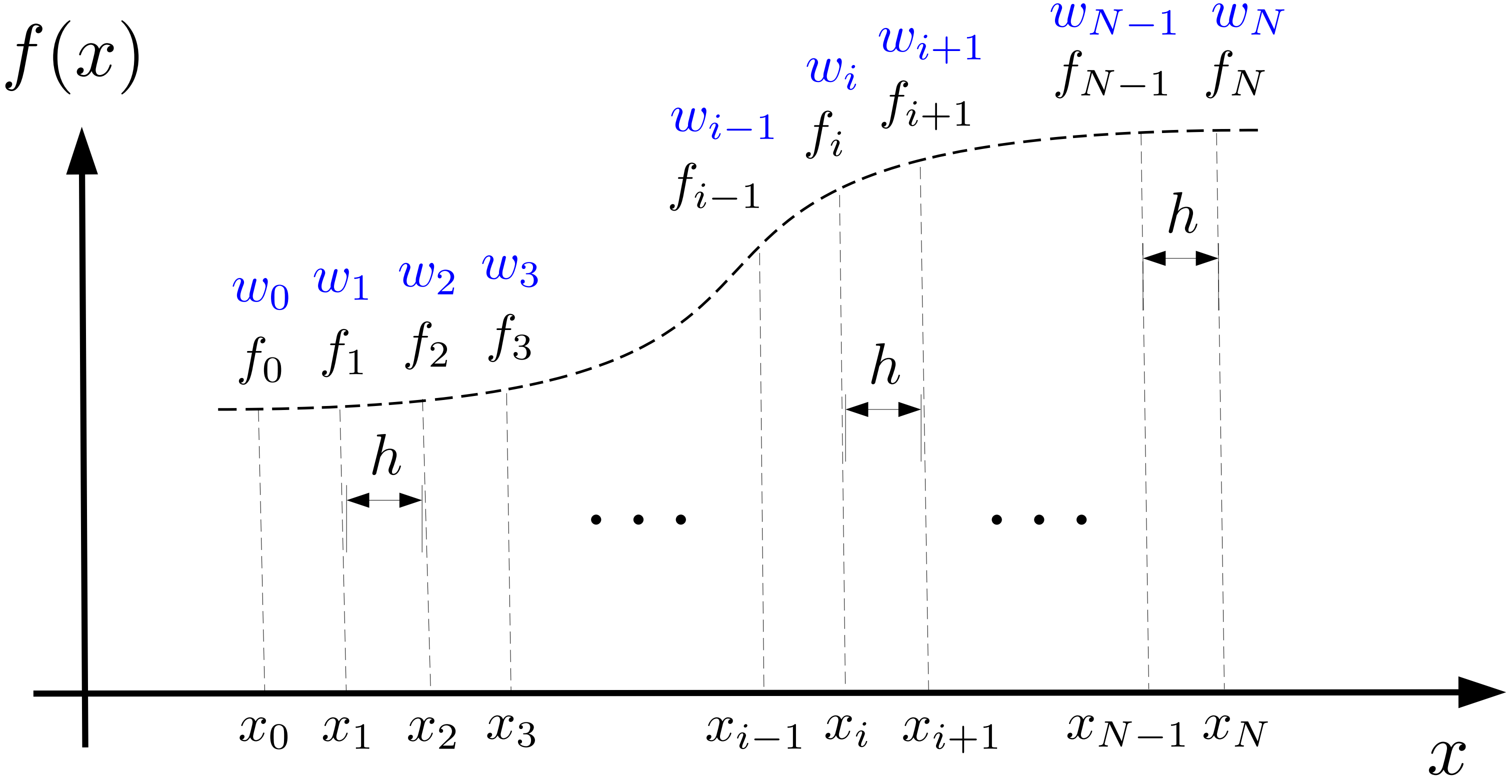
$$x \in [a,\, b]$$

$$S = \int_a^b f(x)\mathrm{d}x$$

Numerical Integration

- Approximate integral

$$\int_a^b f(x)\mathrm{d}x \approx h\sum_i^N w_i f_i$$



x	$f(x)$	$w(x)$
x_0	f_0	w_0
x_1	f_1	w_1
x_2	f_2	w_2
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	w_{i-1}
x_i	f_i	w_i
x_{i+1}	f_{i+1}	w_{i+1}
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	w_{N-1}
x_N	f_N	w_N

Numerical Integration

- Rectangular Rule

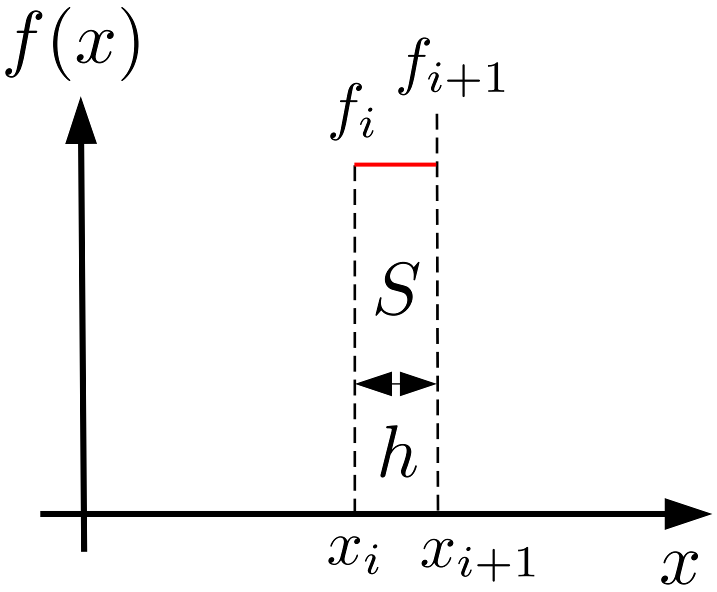
Constant Equation:

$f(x) = f_i = \text{cont.}$

$$S = \int_{x_i}^{x_{i+1}} f(x)\mathrm{d}x \approx f_i \int_{x_i}^{x_{i+1}} \mathrm{d}x \approx f_i(x_{i+1} - x_i)$$

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

$$S = \int_{x_i}^{x_{i+1}} f(x)\mathrm{d}x \approx f_i h$$

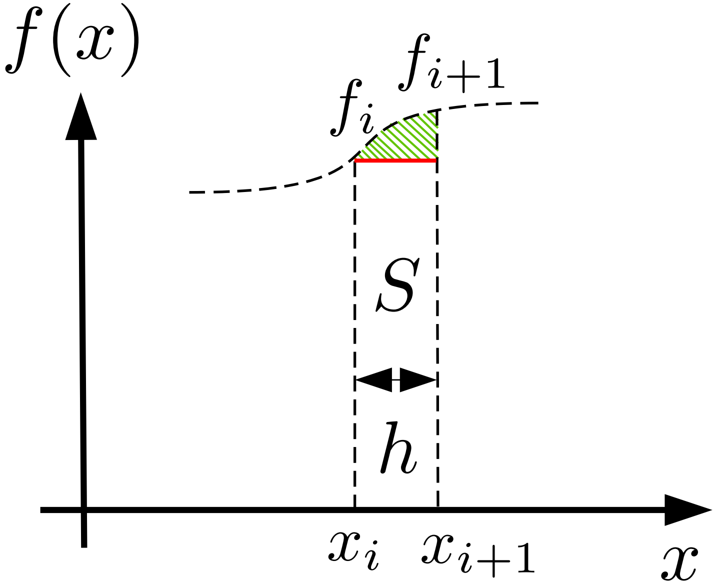


Numerical Integration

- Rectangular Rule

Constant function:

$f(x) = f_i = \text{cont.}$



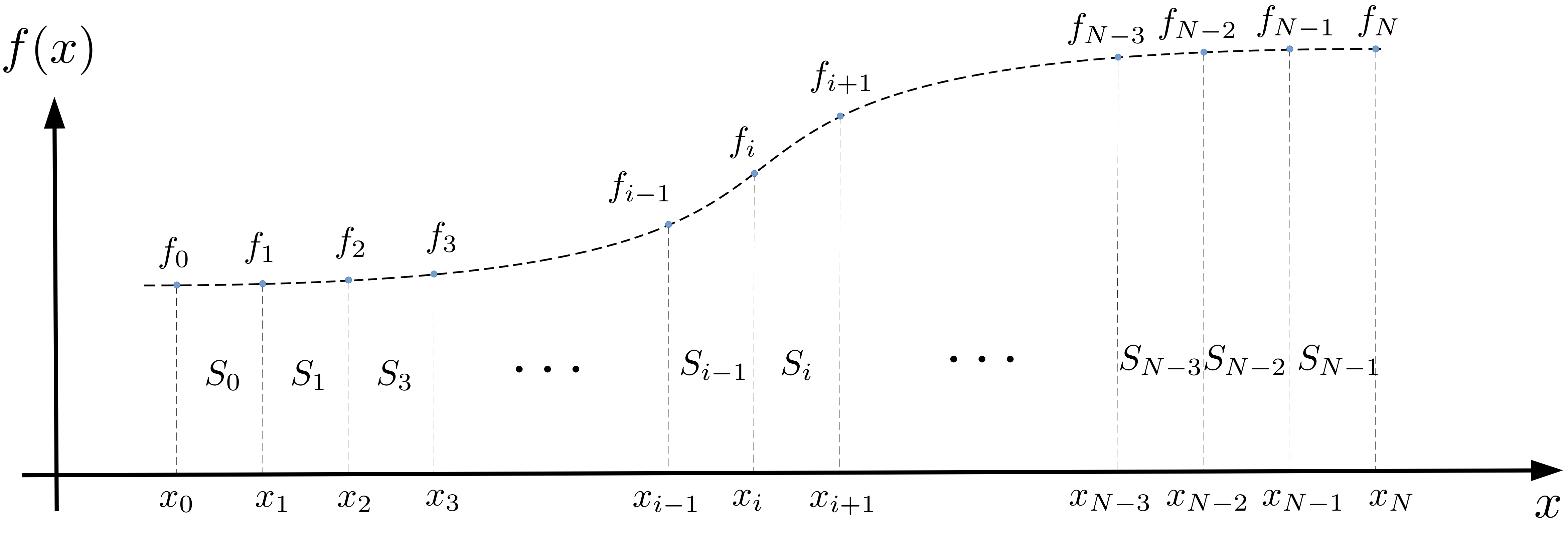
$$S = \int_{x_i}^{x_{i+1}} f(x)\mathrm{d}x \approx f_i \int_{x_i}^{x_{i+1}} \mathrm{d}x \approx f_i(x_{i+1} - x_i)$$

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

$$S = \int_{x_i}^{x_{i+1}} f(x)\mathrm{d}x \approx f_i h$$

Numerical Integration

- Rectangular Rule



$$S = S_0 + S_1 + S_3 + \cdots + S_{i-1} + S_i + \cdots + S_{N-3} + S_{N-2} + S_{N-1}$$

Numerical Integration

- Rectangular Rule

$$S = S_0 + S_1 + S_3 + \cdots + S_{i-1} + S_i + \cdots + S_{N-2} + S_{N-1}$$

$$S_0 \approx f_0 h, \quad S_1 \approx f_1 h, \quad S_2 \approx f_2 h$$

$$\cdots, \quad S_{i-1} \approx f_{i-1} h, \quad S_i \approx f_i h, \quad \cdots$$

$$S_{N-2} \approx f_{N-2} h, \quad S_{N-1} \approx f_{N-1} h$$

$$x_1 - x_0 = x_2 - x_1 = x_3 - x_2 = \cdots = x_{N-1} - x_{N-2} = x_N - x_{N-1} = h$$

Numerical Integration

- Rectangular Rule

$$S = S_0 + S_1 + S_3 + \cdots + S_{i-1} + S_i + \cdots + S_{N-3} + S_{N-2} + S_{N-1}$$

$$S = f_0 h + f_1 h + f_3 h + \cdots + f_{i-1} h + f_i h + \cdots + f_{N-3} h + f_{N-2} h + f_{N-1} h$$

$$S = h(f_0 + f_1 + f_3 + \cdots + f_{i-1} + f_i + \cdots + f_{N-3} + f_{N-2} + f_{N-1})$$

$$\int_a^b f(x)\mathrm{d}x \approx S = h\left(\sum_{i=0}^{N-1} f_i\right)$$

Numerical Integration

- Rectangular Rule

$$\begin{cases} \int_a^b f(x)\mathrm{d}x \approx h\sum_i^N w_i f_i \\ \int_a^b f(x)\mathrm{d}x \approx h\left(\sum_{i=0}^{N-1} f_i\right) \end{cases}$$

x	$f(x)$	$w(x)$
x_0	f_0	1
x_1	f_1	1
x_2	f_2	1
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	1
x_i	f_i	1
x_{i+1}	f_{i+1}	1
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	1
x_N	f_N	0

Numerical Integration

- Trapezoidal Rule

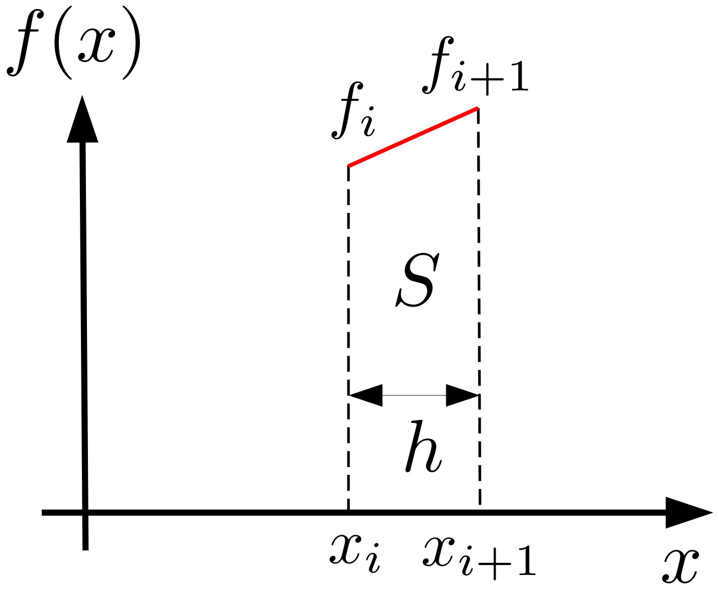
Linear function:

$$f(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}} f_i + \frac{x - x_i}{x_{i+1} - x_i} f_{i+1}$$

$$S = \int_{x_i}^{x_{i+1}} f(x)\mathrm{d}x \approx \frac{f_i + f_{i+1}}{2}(x_{i+1} - x_i)$$

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

$$S = \int_{x_i}^{x_{i+1}} f(x)\mathrm{d}x \approx \frac{f_i + f_{i+1}}{2} h$$



Numerical Integration

- Trapezoidal Rule

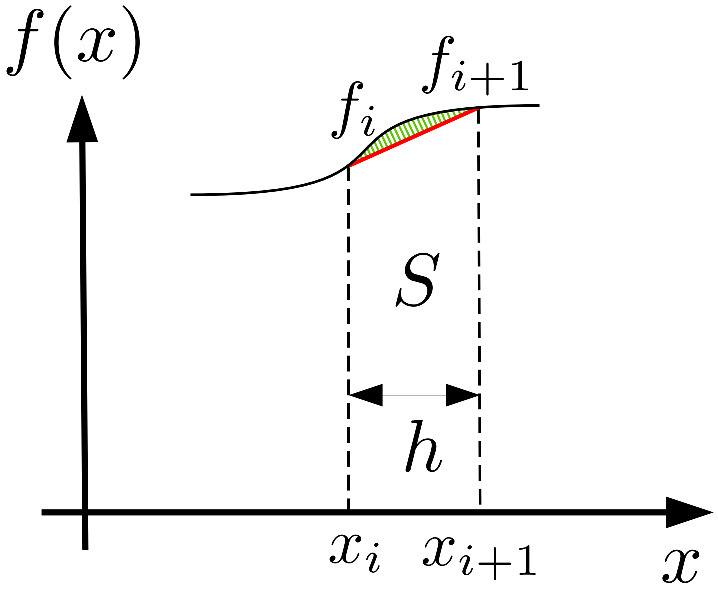
Linear function:

$$f(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}} f_i + \frac{x - x_i}{x_{i+1} - x_i} f_{i+1}$$

$$S = \int_{x_i}^{x_{i+1}} f(x)\mathrm{d}x \approx \frac{f_i + f_{i+1}}{2}(x_{i+1} - x_i)$$

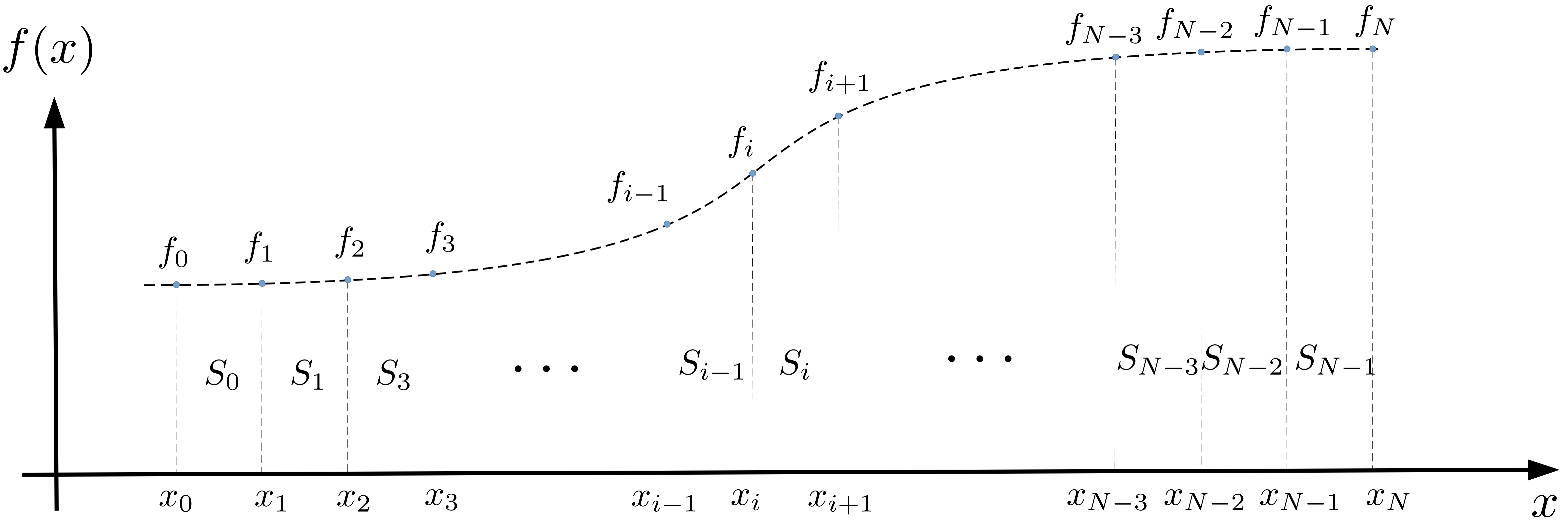
$$x_{i+1} = x_i + h$$

$$S = \int_{x_i}^{x_{i+1}} f(x)\mathrm{d}x \approx \frac{h}{2}(f_i + f_{i+1})$$



Numerical Integration

- Trapezoidal Rule



$$S = S_0 + S_1 + S_3 + \cdots + S_{i-1} + S_i + \cdots + S_{N-3} + S_{N-2} + S_{N-1}$$

Numerical Integration

- Trapezoidal Rule

$$S = S_0 + S_1 + S_3 + \cdots + S_{i-1} + S_i + \cdots + S_{N-2} + S_{N-1}$$

$$S_0 \approx \frac{f}{2}(f_0 + f_1), \quad S_1 \approx \frac{h}{2}(f_1 + f_2), \quad S_2 \approx \frac{h}{2}(f_2 + f_3), \quad S_3 \approx \frac{h}{2}(f_3 + f_4)$$

$$\cdots, \quad S_{i-1} \approx \frac{h}{2}(f_{i-1} + f_i), \quad S_i \approx \frac{h}{2}(f_i + f_{i+1}), \quad \cdots$$

$$S_{N-2} \approx \frac{h}{2}(f_{N-2} + f_{N-1}), \quad S_{N-1} \approx \frac{h}{2}(f_{N-1} + f_N)$$

$$x_1 - x_0 = x_2 - x_1 = x_3 - x_2 = \cdots = x_{N-1} - x_{N-2} = x_N - x_{N-1} = h$$

Numerical Integration

- Trapezoidal Rule

$$S = S_0 + S_1 + \cdots + S_{i-1} + S_i + \cdots + S_{N-3} + S_{N-2} + S_{N-1}$$

$$S = \frac{h}{2}(\underbrace{f_0 + f_1}_{S_0} + \underbrace{f_1 + f_2}_{S_1} + \underbrace{f_2 + f_3}_{S_2} + \cdots$$

$$+ \cdots + \underbrace{f_{i-1} + f_i}_{S_{i-1}} + \underbrace{f_i + f_{i+1}}_{S_i} + \cdots$$

$$\cdots + \underbrace{f_{N-2} + f_{N-1}}_{S_{N-2}} + \underbrace{f_{N-1} + f_N}_{S_{N-1}})$$

$$S = \frac{h}{2}(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{i-1} + 2f_i + \cdots + 2f_{N-2} + 2f_{N-1} + f_N)$$

Numerical Integration

- Trapezoidal Rule

$$S = S_0 + S_1 + \cdots + S_{i-1} + S_i + \cdots + S_{N-3} + S_{N-2} + S_{N-1}$$

$$S = \frac{h}{2}(f_0 + 2f_1 + 2f_2 + \cdots + 2f_{i-1} + 2f_i + \cdots + 2f_{N-2} + 2f_{N-1} + f_N)$$

$$\int_a^b f(x)\mathrm{d}x \approx S = \frac{h}{2}\left(f_0 + 2\sum_{i=1}^{N-1} f_i + f_N\right)$$

Numerical Integration

- Trapezoidal Rule

$$\begin{cases} \int_a^b f(x)\mathrm{d}x \approx \frac{h}{2}\sum_i^N w_i f_i \\ \int_a^b f(x)\mathrm{d}x \approx \frac{h}{2}(f_0 + 2\sum_{i=1}^{N-1} f_i + f_N) \end{cases}$$

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