Computational Physics

Lecture-06

M. Reza Mozaffari

Physics Group, University of Qom

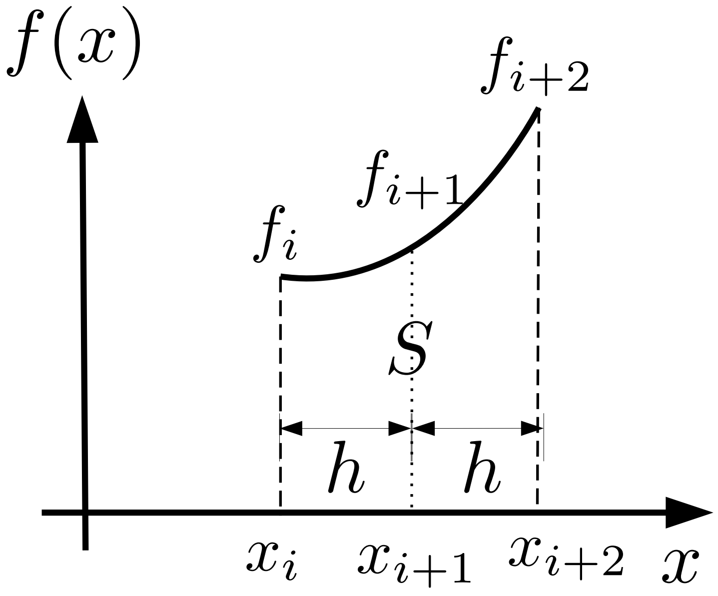
Contents

Numerical Integration

- Simpson's Rule (Simpson's 1/3-Rule)

Quadratic function:

$$f(x) = \frac{(x - x_{i+1})(x - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})} f_i + \frac{(x - x_{i+2})(x - x_i)}{(x_{i+1} - x_{i+2})(x_{i+1} - x_i)} f_{i+1} + \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} f_{i+2}$$



$$S = \int_{x_i}^{x_{i+2}} f(x) \mathrm{d}x$$

$$S \approx \frac{h}{3}(f_i + 4f_{i+1} + f_{i+2})$$

Numerical Integration

- Simpson's Rule (Simpson's 1/3-Rule)

$$S = \int_{x_i}^{x_{i+2}} f(x)\mathrm{d}x$$

$$f(x) = \frac{(x - x_{i+1})(x - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})} f_i \quad \Rightarrow \quad = \frac{(x - x_i - h)(x - x_i - 2h)}{(-h)(-2h)} f_i$$

$$+ \frac{(x - x_{i+2})(x - x_i)}{(x_{i+1} - x_{i+2})(x_{i+1} - x_i)} f_{i+1} \quad \Rightarrow \quad + \frac{(x - x_i - 2h)(x - x_i)}{(-h)(2h)} f_{i+1}$$

$$+ \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} f_{i+2} \quad \Rightarrow \quad + \frac{(x - x_i)(x - x_i - h)}{(2h)(h)} f_{i+2}$$

Numerical Integration

$$u = x - x_i \Rightarrow \mathrm{d}x = \mathrm{d}u$$

- Simpson's Rule (Simpson's 1/3-Rule)

$$S = \int_{x_i}^{x_{i+2}} f(x)\mathrm{d}x = \int_0^{2h} f(u)\mathrm{d}u$$

$$f(x) = \frac{(x - x_i - h)(x - x_i - 2h)}{(-h)(-2h)} f_i \Rightarrow = \frac{f_i}{2h^2}(u-h)(u-2h)$$

$$+ \frac{(x - x_i - 2h)(x - x_i)}{(-h)(h)} f_{i+1} \Rightarrow - \frac{f_{i+1}}{h^2}(u-2h)u$$

$$+ \frac{(x - x_i)(x - x_i - h)}{(2h)(h)} f_{i+2} \Rightarrow + \frac{f_{i+2}}{2h^2}u(u-h)$$

Numerical Integration

$$u = x - x_i \Rightarrow \mathrm{d}x = \mathrm{d}u$$

- Simpson's Rule (Simpson's 1/3-Rule)

$$S = \int_{x_i}^{x_{i+2}} f(x)\mathrm{d}x = \int_0^{2h} f(u)\mathrm{d}u$$

$$\int_0^{2h} f(u)\mathrm{d}u = \frac{f_i}{2h^2}\int_0^{2h}(u-h)(u-2h)\mathrm{d}u - \frac{f_{i+1}}{h^2}\int_0^{2h}(u-2h)u\mathrm{d}u + \frac{f_{i+2}}{2h^2}\int_0^{2h}u(u-h)\mathrm{d}u$$

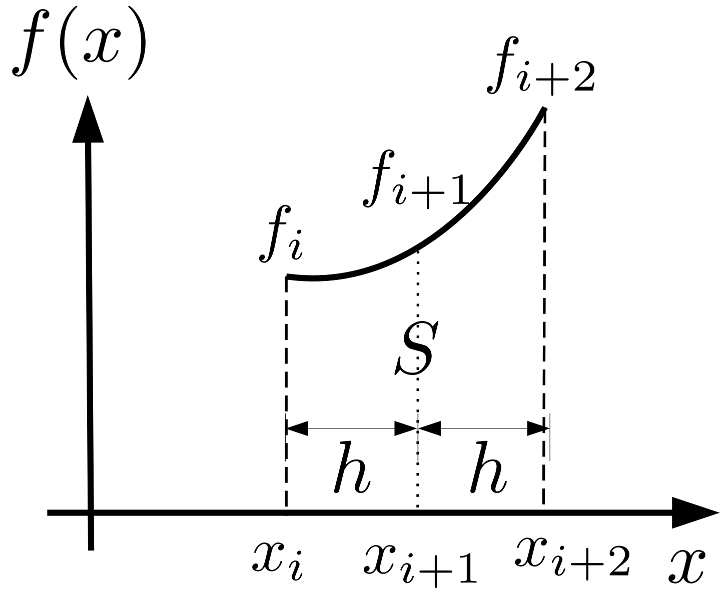
$$\int_0^{2h} f(u)\mathrm{d}u = \frac{f_i}{2h^2}\frac{2h^3}{3} - \frac{f_{i+1}}{h^2}\frac{-4h^3}{3} + \frac{f_{i+2}}{2h^2}\frac{2h^3}{3}$$

Numerical Integration

- Simpson's Rule (Simpson's 1/3-Rule)

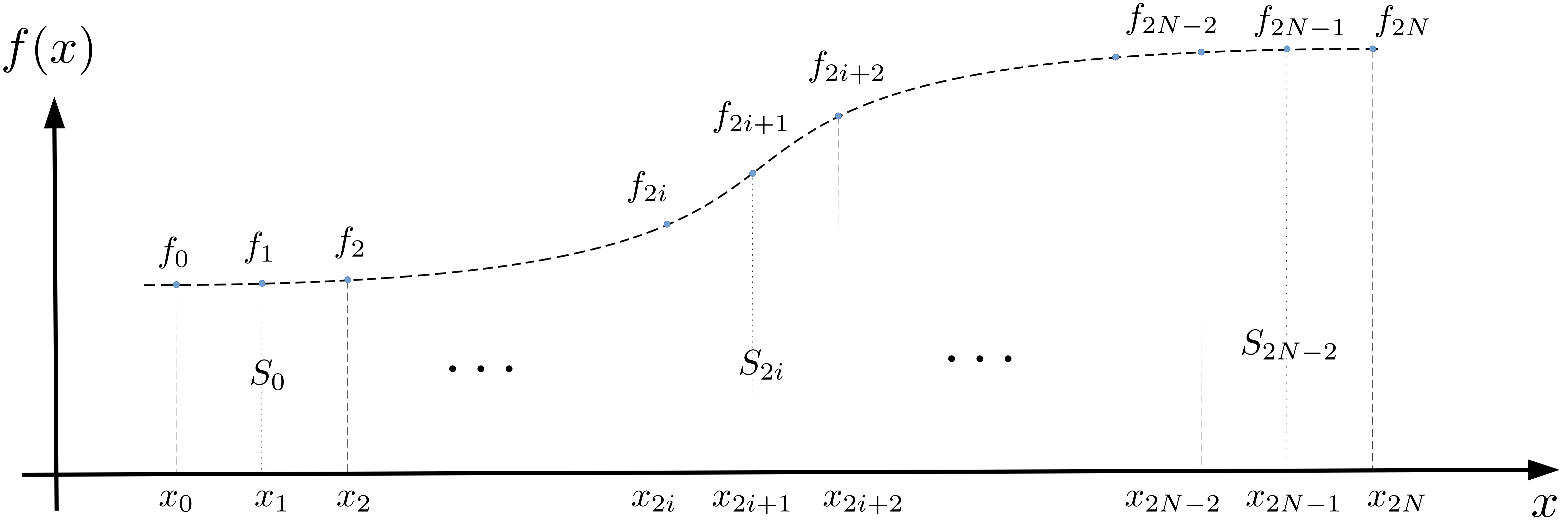
$$S = \int_{x_i}^{x_{i+2}} f(x)\mathrm{d}x = \int_0^{2h} f(u)\mathrm{d}u = \frac{f_i}{2h^2}\frac{2h^3}{3} + \frac{f_{i+1}}{h^2}\frac{4h^3}{3} + \frac{f_{i+2}}{2h^2}\frac{2h^3}{3}$$

$$S = \int_{x_i}^{x_{i+2}} f(x)\mathrm{d}x = \frac{h}{3}(f_i + 4f_{i+1} + f_{i+2})$$



Numerical Integration

- Simpson's Rule (Simpson's 1/3-Rule)



$$S = S_0 + S_2 + S_4 + \cdots + S_{2i} + \cdots + S_{2N-2}$$

Numerical Integration

- Simpson's Rule (Simpson's 1/3-Rule)

$$S = S_0 + S_2 \cdots + S_{2i} + S_{2i+2} + \cdots + S_{2N-2}$$

$$S_0 \approx \frac{h}{3}(f_0 + 4f_1 + f_2), \quad S_2 \approx \frac{h}{3}(f_2 + 4f_1 + f_4), \quad S_4 \approx \frac{h}{3}(f_4 + 4f_5 + f_6)$$

$$\cdots, \quad S_{2i} \approx \frac{h}{3}(f_{2i} + 4f_{2i+1} + f_{2i+2}), \quad S_{2i+2} \approx \frac{h}{3}(f_{2i+2} + 4f_{2i+3} + f_{2i+4}), \quad \cdots$$

$$S_{2N-4} \approx \frac{h}{3}(f_{2N-4} + 4f_{2N-3} + f_{2N-2}), \quad S_{2N-2} \approx \frac{h}{3}(f_{2N-2} + 4f_{2N-1} + f_{2N})$$

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

Numerical Integration

- Simpson's Rule (Simpson's 1/3-Rule)

$$S = S_0 + S_2 \cdots + S_{2i} + S_{2i+2} + \cdots + S_{2N-2}$$

$$S = \frac{h}{3}\left(\underbrace{f_0 + 4f_1 + f_2}_{S_0} + \underbrace{f_2 + 4f_3 + f_4}_{S_2} + \right.$$

$$\cdots + \underbrace{f_{2i} + 4f_{2i+1} + f_{2i+2}}_{S_{2i}} +$$

$$\left. \cdots + \underbrace{f_{2N-2} + 4f_{2N-1}h + f_{2N}}_{S_{2N-2}}\right)$$

$$S = \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 2f_{2i} + 4f_{2i+1} + 2f_{2i+2} + \cdots + 2f_{2N-2} + 4f_{2N-1}h + f_{2N}\right)$$

Numerical Integration

- Simpson’s Rule (Simpson’s 1/3-Rule)

$$S = S_0 + S_2 \cdots + S_{2i} + S_{2i+2} + \cdots + S_{2N-2}$$

$$S = \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots\right.$$

$$\cdots + 2f_{2i} + 4f_{2i+1} + 2f_{2i+2} + \cdots$$

$$\left.\cdots + 2f_{2N-2} + 4f_{2N-1}h + f_{2N}\right)$$

$$\int_a^b f(x)\mathrm{d}x \approx S = \frac{h}{3}\left(f_0 + 4\sum_{i=0}^{N-1} f_{2i+1} + 2\sum_{i=0}^{N-2} f_{2i+2} + f_{2N}\right)$$

Numerical Integration

- Simpson's Rule (Simpson's 1/3-Rule)

$$
\begin{cases}
\int_a^b f(x)\mathrm{d}x \approx \frac{h}{3}\sum_i^N w_i f_i \\
\int_a^b f(x)\mathrm{d}x \approx \frac{h}{3}\left(f_0 + 4\sum_{i=0}^{N-1} f_{2i+1} + 2\sum_{i=0}^{N-2} f_{2i+2} + f_{2N}\right)
\end{cases}
$$

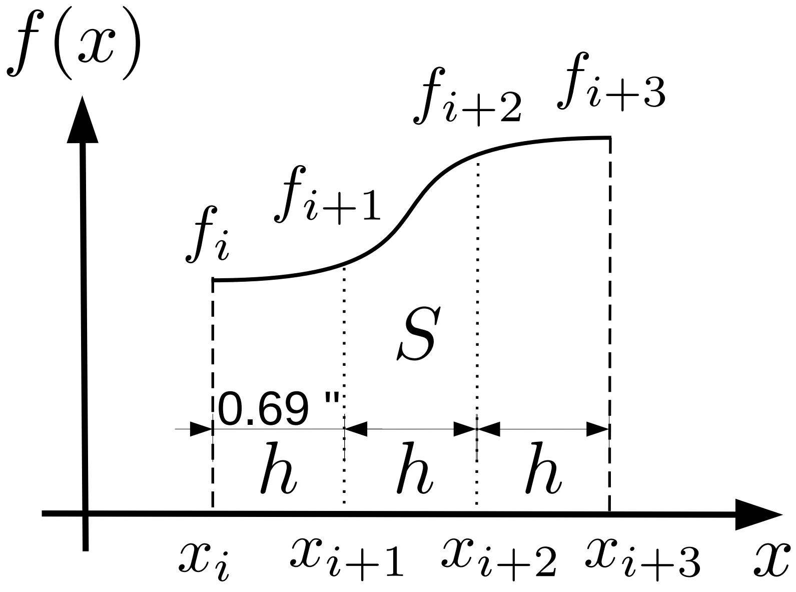
x	$f(x)$	$w(x)$
x_0	f_0	1
x_1	f_1	4
x_2	f_2	2
$\vdots$	$\vdots$	$\vdots$
x_{2i}	f_{2i}	2
x_{2i+1}	f_{2i+1}	4
x_{2i+2}	f_{2i+2}	2
$\vdots$	$\vdots$	$\vdots$
x_{2N-1}	f_{2N-1}	4
x_{2N}	f_{2N}	1

Numerical Integration

- Simpson's 3/8-Rule

Third order function:

$$f(x) = \frac{(x-x_{i+1})(x-x_{i+2})(x-x_{i+3})}{(x_i-x_{i+1})(x_i-x_{i+2})(x_i-x_{i+3})}f_i$$
$$+\frac{(x-x_{i+2})(x-x_{i+3})(x-x_i)}{(x_{i+1}-x_{i+2})(x_{i+1}-x_{i+3})(x_{i+1}-x_i)}f_{i+1}$$
$$+\frac{(x-x_{i+3})(x-x_i)(x-x_{i+1})}{(x_{i+2}-x_{i+3})(x_{i+2}-x_i)(x_{i+2}-x_{i+1})}f_{i+2}$$
$$+\frac{(x-x_i)(x-x_{i+1})(x-x_{i+2})}{(x_{i+3}-x_i)(x_{i+3}-x_{i+1})(x_{i+3}-x_{i+2})}f_{i+3}$$

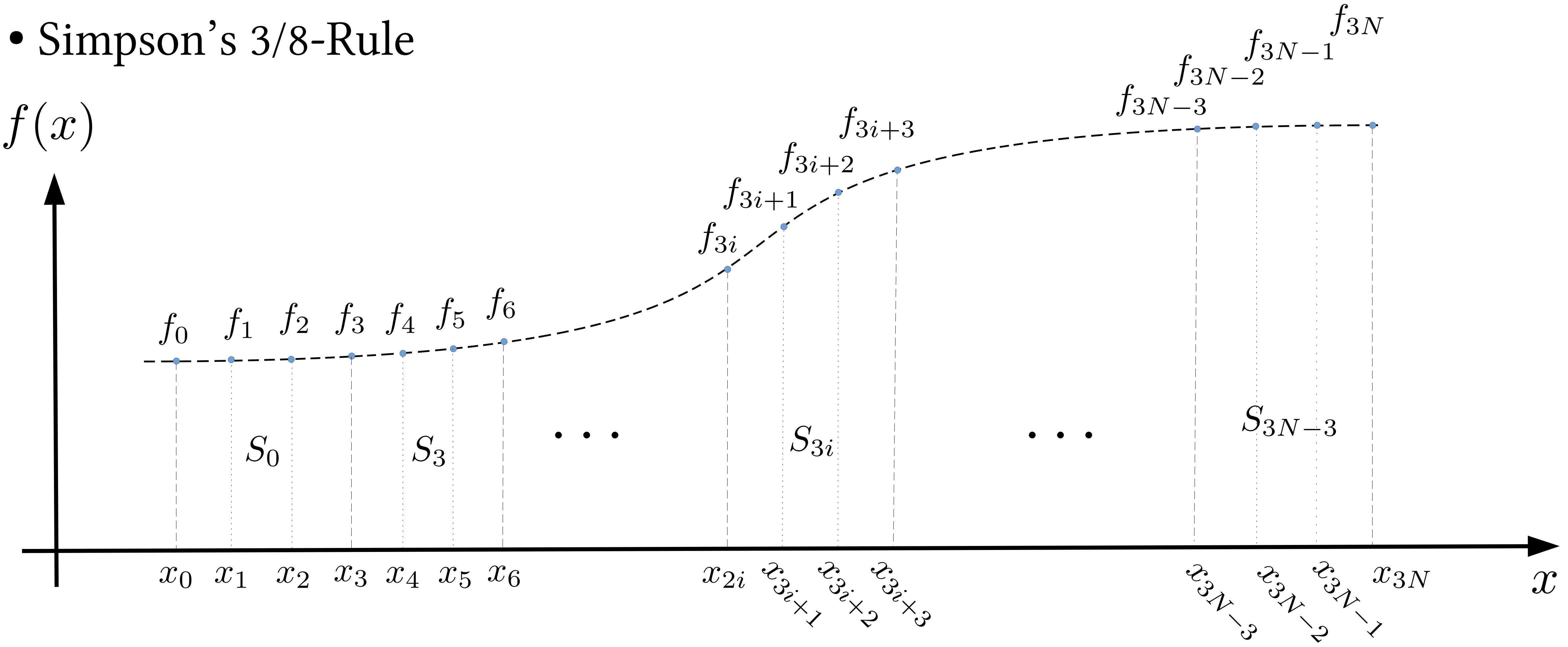


$$S = \int_{x_i}^{x_{i+3}} f(x)\mathrm{d}x$$

$$S \approx \frac{3h}{8}(f_i + 3f_{i+1} + 3f_{i+2} + f_{i+3})$$

Numerical Integration

- Simpson’s 3/8-Rule



$$S = S_0 + S_3 + \cdots + S_{3i} + \cdots + S_{3N-3}$$

Numerical Integration

- Simpson's 3/8-Rule

$$S = S_0 + S_3 + \cdots + S_{3i} + \cdots + S_{3N-3}$$

$$S_0 \approx \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3), \quad S_3 \approx \frac{3h}{8}(f_3 + 3f_4 + 3f_5 + f_6)$$

$$\cdots, \quad S_{3i} \approx \frac{8h}{3}(f_{3i} + 3f_{3i+1} + 3f_{3i+2} + f_{3i+3}), \quad \cdots$$

$$S_{3N-3} \approx \frac{8h}{3}(f_{3N-3} + 3f_{3N-2} + 3f_{3N-1} + f_{3N})$$

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

Numerical Integration

- Simpson's 3/8-Rule

$$S = S_0 + S_3 + \cdots + S_{3i} + \cdots + S_{3N-3}$$

$$S = \frac{3h}{8}\big(\underbrace{f_0 + 3f_1 + 3f_2 + f_3}_{S_0} + \underbrace{f_3 + 3f_4 + 3f_5 + f_6}_{S_3} + \cdots$$

$$\cdots + \underbrace{f_{3i} + 3f_{3i+1} + 3f_{3i+2} + f_{3i+3}}_{S_{3i}} + \cdots$$

$$\cdots + \underbrace{f_{3N-3} + 3f_{3N-2} + 3f_{3N-1} + f_{3N}}_{S_{3N-3}}\big)$$

$$S = \frac{3h}{8}\left(f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + \cdots + 2f_{3i} + 3f_{3i+1} + 3f_{3i+2} + 2f_{3i+3} + \cdots + 2f_{3N-3} + 3f_{3N-2} + 3f_{3N-1} + f_{3N}\right)$$

Numerical Integration

- Simpson's 3/8-Rule

$$S = S_0 + S_3 + \cdots + S_{3i} + \cdots + S_{3N-3}$$

$$S = \frac{3h}{8}\left(f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + \right.$$

$$\cdots + 2f_{3i} + 3f_{3i+1} + 3f_{3i+2} + 2f_{3i+3} + \cdots$$

$$\left. \cdots + 2f_{3N-3} + 3f_{3N-2} + 3f_{3N-1} + f_{3N}\right)$$

$$\int_a^b f(x)\mathrm{d}x \approx S = \frac{3h}{8}\left(f_0 + 3\sum_{i=0}^{N-1} f_{3i+1} + 3\sum_{i=0}^{N-1} f_{3i+2} + 2\sum_{i=0}^{N-2} f_{3i+3} + f_{3N}\right)$$

Numerical Integration

- Simpson's 3/8-Rule

$$\begin{cases} \int_a^b f(x)\mathrm{d}x \approx \frac{3h}{8} \sum_i^N w_i f_i \\ \int_a^b f(x)\mathrm{d}x \approx \frac{3h}{8} \left(f_0 + 3\sum_{i=0}^{N-1} f_{3i+1} + 3\sum_{i=0}^{N-1} f_{3i+2} \right. \end{cases}$$

$$\left. +2\sum_{i=0}^{N-2} f_{3i+3} + f_{3N} \right)$$

x	$f(x)$	$w(x)$
x_0	f_0	1
x_1	f_1	3
x_2	f_2	3
x_3	f_3	2
$\vdots$	$\vdots$	$\vdots$
x_{3N-3}	f_{3N-3}	2
x_{3N-2}	f_{3N-2}	3
x_{3N-1}	f_{3N-1}	3
x_{3N}	f_{3N}	1

Numerical Integration

- Trapezoidal Rule

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

- Simpson's Rule (Simpson's 1/3-Rule)

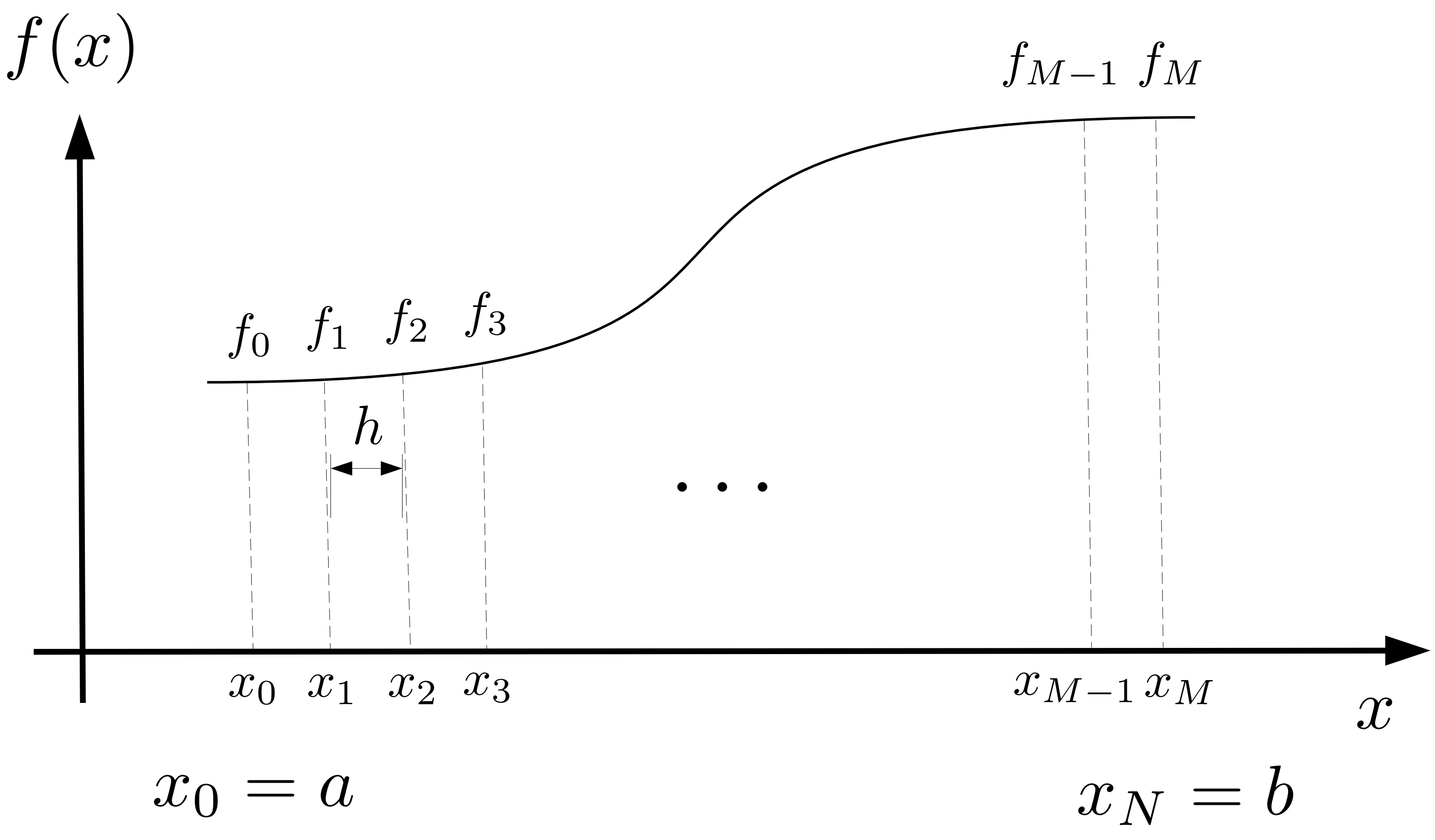
$$S = \int_{x_i}^{x_{i+2}} f(x)\mathrm{d}x \approx \frac{h}{3}(f_i + 4f_{i+1} + f_{i+2})$$

- Simpson's 3/8-Rule

$$S = \int_{x_i}^{x_{i+3}} f(x)\mathrm{d}x \approx \frac{3h}{8}(f_i + 3f_{i+1} + 3f_{i+2} + f_{i+3})$$

Numerical Integration

- Finite Differences



Smooth function $f(x)$

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

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

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

$$f_i = f(x_i)$$

Numerical Integration

- Trapezoidal Rule $M = N, \quad h = (b-a)/N$

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

- Simpson's Rule (Simpson's 1/3-Rule) $M = 2N, \quad h = (b-a)/2N$

$$\int_a^b f(x)\mathrm{d}x \approx \frac{h}{3}\left(f_0 + 4\sum_{i=0}^{N-1} f_{2i+1} + 2\sum_{i=0}^{N-2} f_{2i+2} + f_{2N}\right)$$

- Simpson's 3/8-Rule $M = 3N, \quad h = (b-a)/3N$

$$\int_a^b f(x)\mathrm{d}x \approx \frac{3h}{8}\left(f_0 + 3\sum_{i=0}^{N-1} f_{3i+1} + 3\sum_{i=0}^{N-1} f_{3i+2} + 2\sum_{i=0}^{N-2} f_{3i+3} + f_{3N}\right)$$