Computational Physics

Lecture-09

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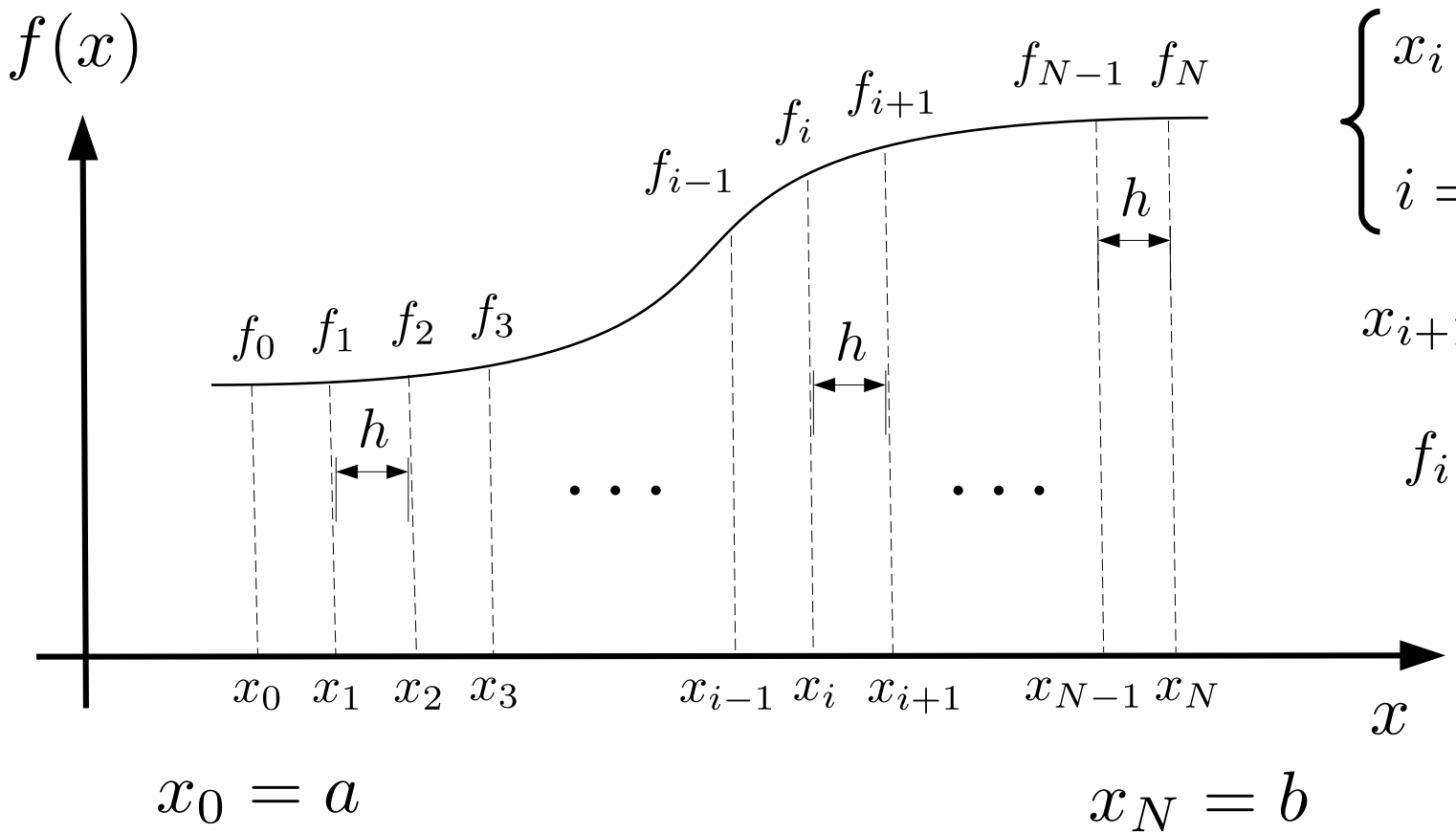
Contents

- Basis Concepts
- Numerical Differentiation
- Numerical Integration

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

- Rectangular Rule

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

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

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

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

Numerical Integration

- Simpson's 1/3-Rule $\quad S \approx \frac{h}{3}(f_i + 4f_{i+1} + f_{i+2})$

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

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

$$\int_a^b f(x)\mathrm{d}x \approx \frac{3h}{8}\sum_i^N w_i f_i$$

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

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

- Gaussian Quadrature Rule

  Two-point

$$\int_{x_i}^{x_{i+1}} f(x)\mathrm{d}x \approx \frac{x_{i+1}-x_i}{2}\left(C_1 f(x_1) + C_2 f(x_2)\right)$$

$$x_1 = \frac{x_{i+1}+x_i}{2} - \frac{1}{\sqrt{3}}\frac{x_{i+1}-x_i}{2}$$

$$x_2 = \frac{x_{i+1}+x_i}{2} + \frac{1}{\sqrt{3}}\frac{x_{i+1}-x_i}{2}$$

$$C_1 = C_2 = 1$$