Métodos Computacionais em Física

Aula 08

Cálculo de Integrais

O problema

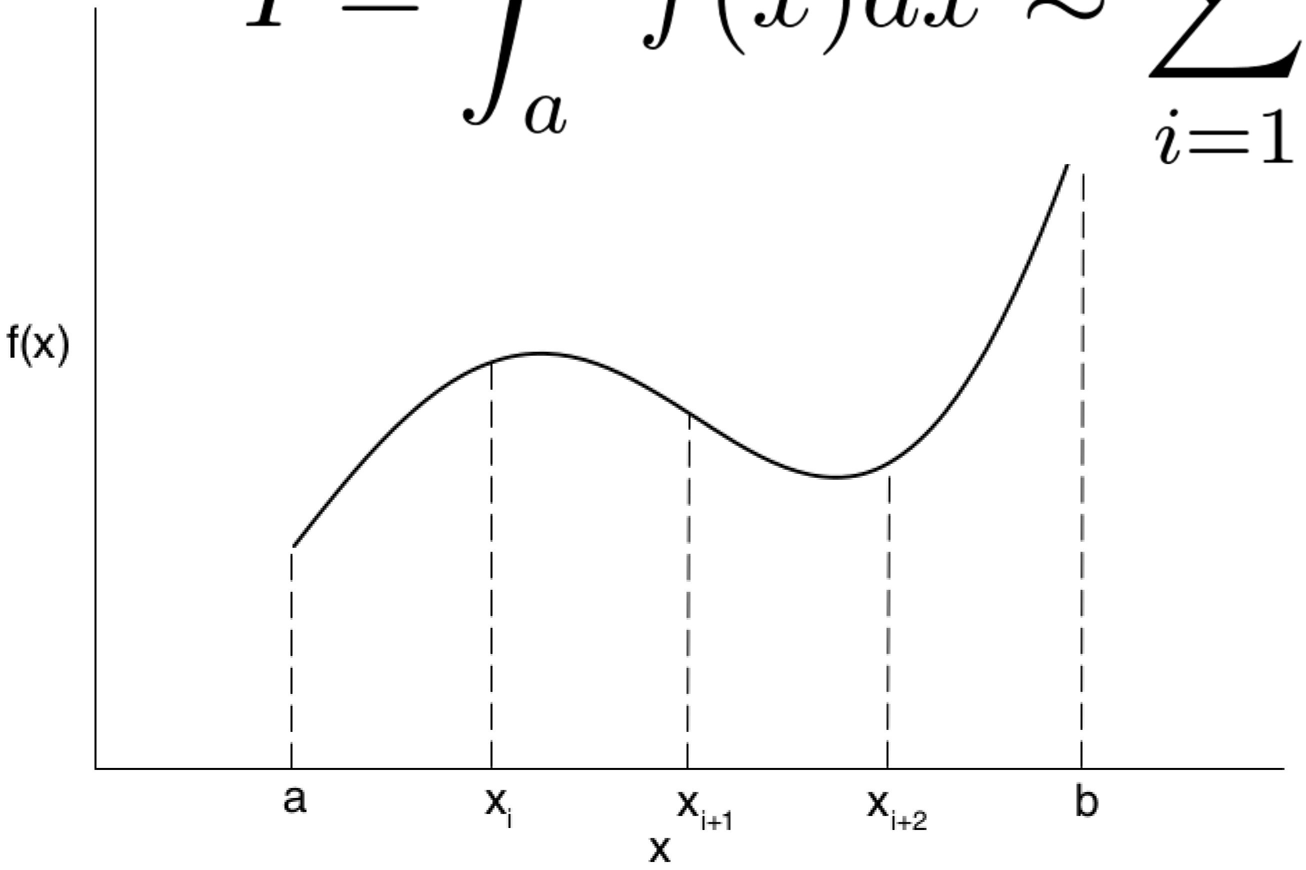
$$I = \int_a^b f(x)dx = \lim_{\Delta x_i \to 0} \sum_{i=1}^{N} f(x_i)\Delta x_i$$

$$I = \int_a^b f(x)dx = F(b) - F(a)$$

$$F'(x) = f(x)$$

O que podemos fazer

$$I = \int_a^b f(x)dx \approx \sum_{i=1}^{N} f(x_i)\Delta x_i$$



$$x_1 = a$$

$$x_N = b$$

$$x_i = a + (i-1)h$$

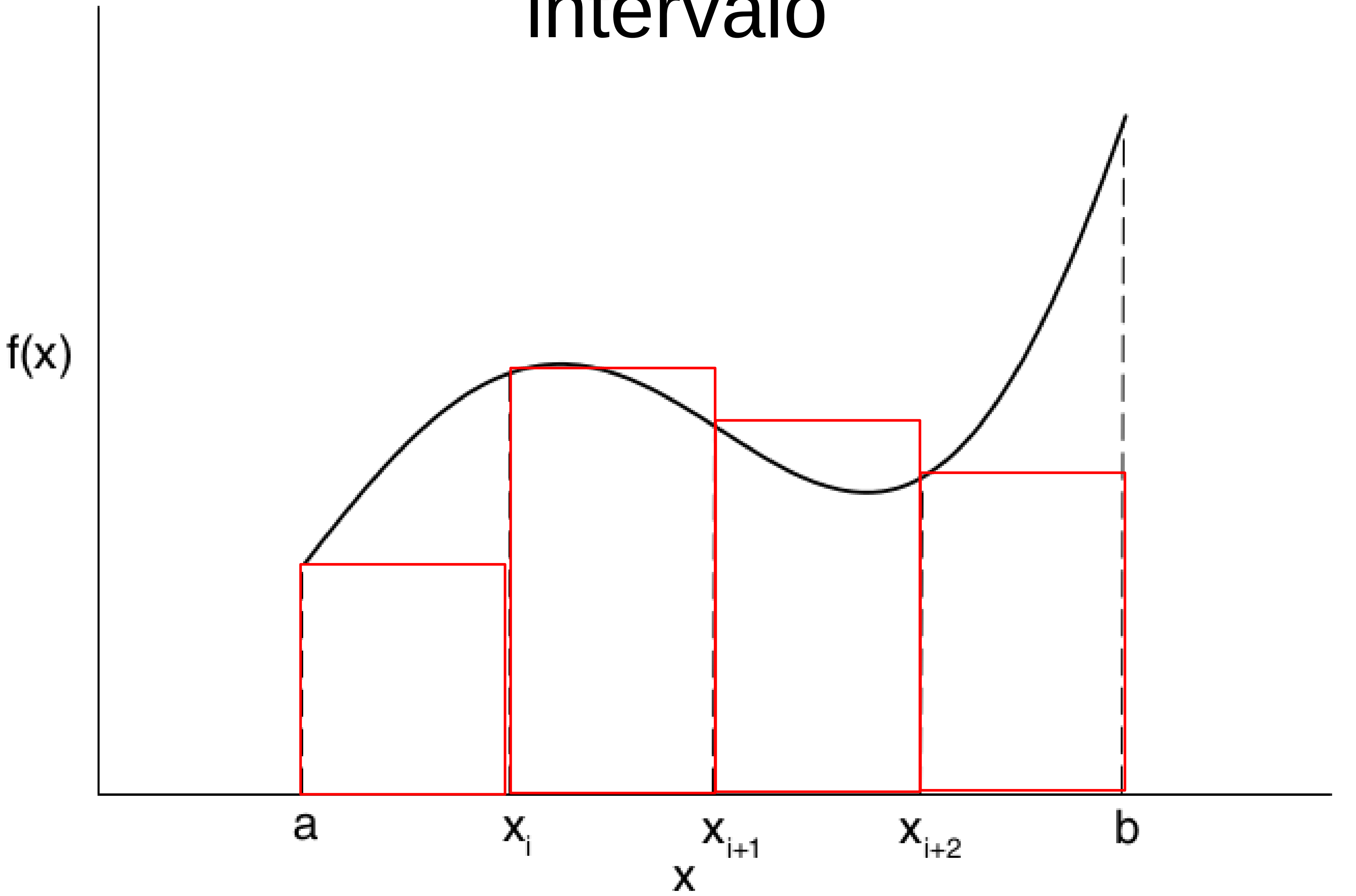
$$h = \frac{b-a}{N-1}$$

Em geral

$$I = \int_a^b f(x)dx \approx \sum_{i=1}^{N} f(x_i)w_i$$

Pesos que dependem da escolha do método

Tomando a função à esquerda do intervalo

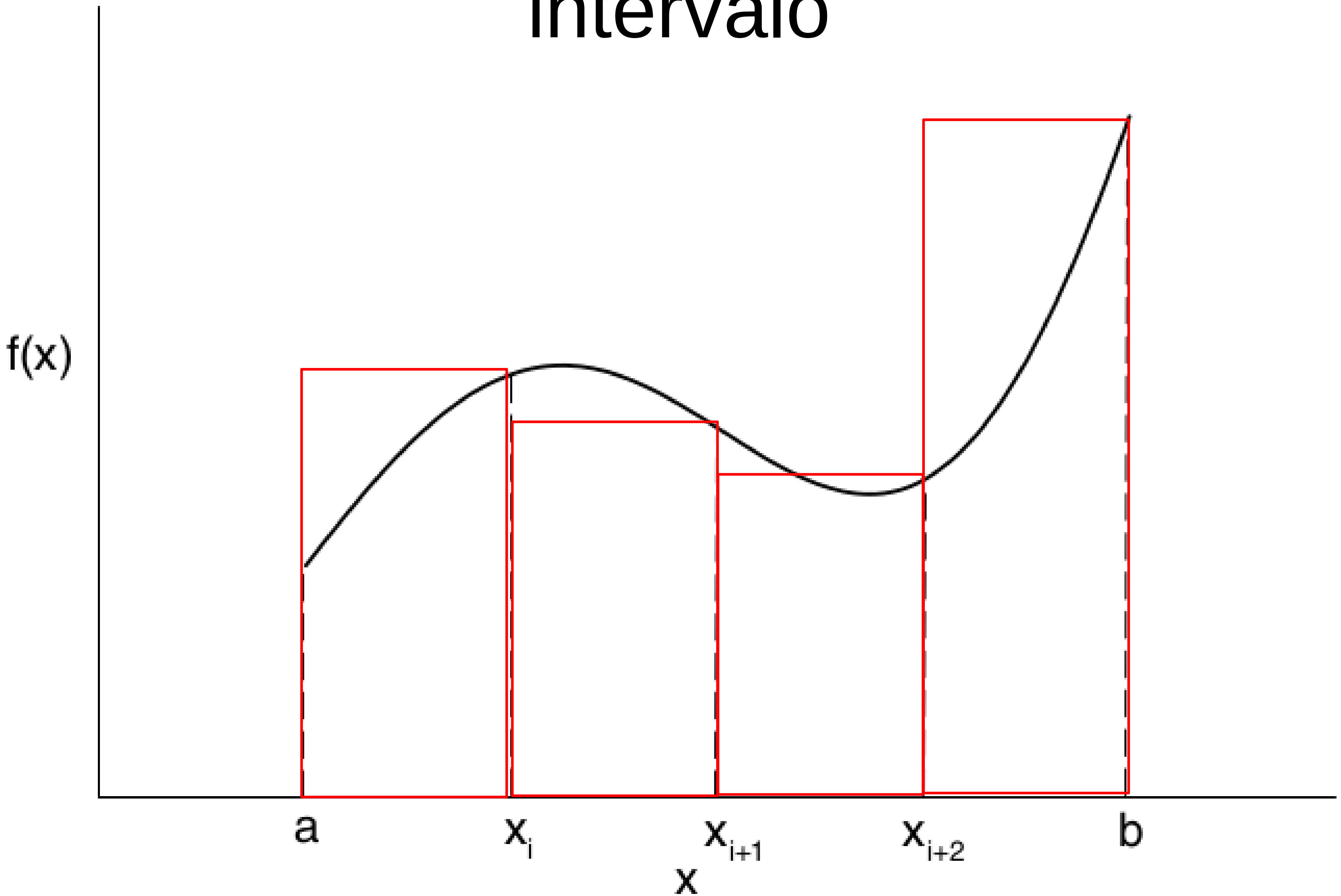


$$I = \sum_{i=1}^{N} f(x_i) w_i$$

$$w_i = h \quad \Rightarrow \quad i = 1, 2, 3, ..., N-1$$

$$w_N = 0$$

Tomando a função à direita do intervalo

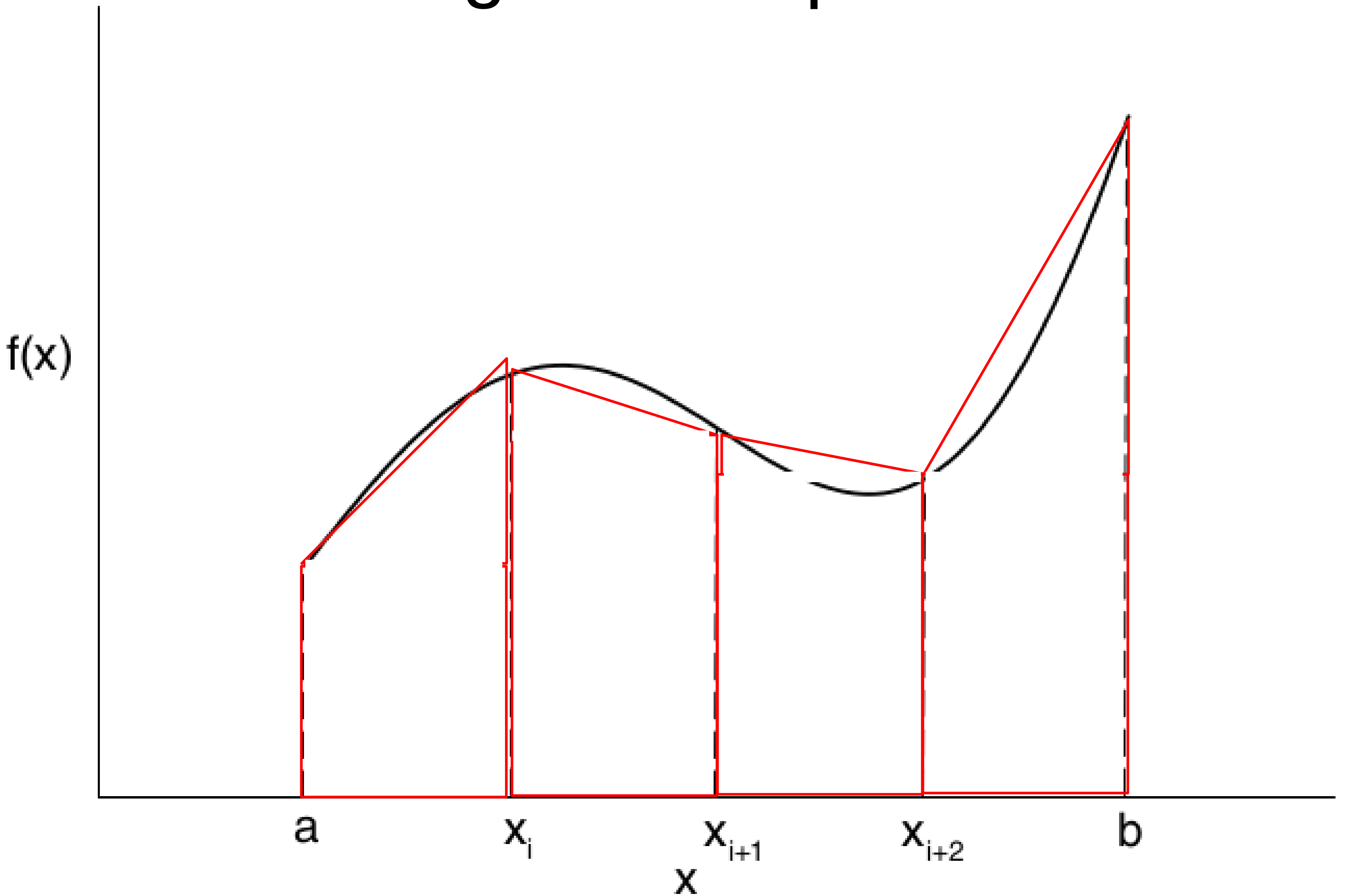


$$I = \sum_{i=1}^{N} f(x_i) w_i$$

$$w_i = h \quad \Rightarrow \quad i = 2, 3, 4, ..., N$$

$$w_1 = 0$$

Regra do trapézio



$$I = \sum_{i=1}^{N} \frac{1}{2}\Big(f(x_i) + f(x_{i+1})\Big) w_i$$

$$w_i = h \quad \Rightarrow \quad i = 1, 2, 3, ..., N-1$$

$$w_N = 0$$

$$I = \sum_{i=1}^{N} f(x_i) w'_i$$

$$w'_i = h \quad \Rightarrow \quad i = 2, 3, 4, ..., N-1$$

$$w'_i = h/2 \quad \Rightarrow \quad i = 1, N$$

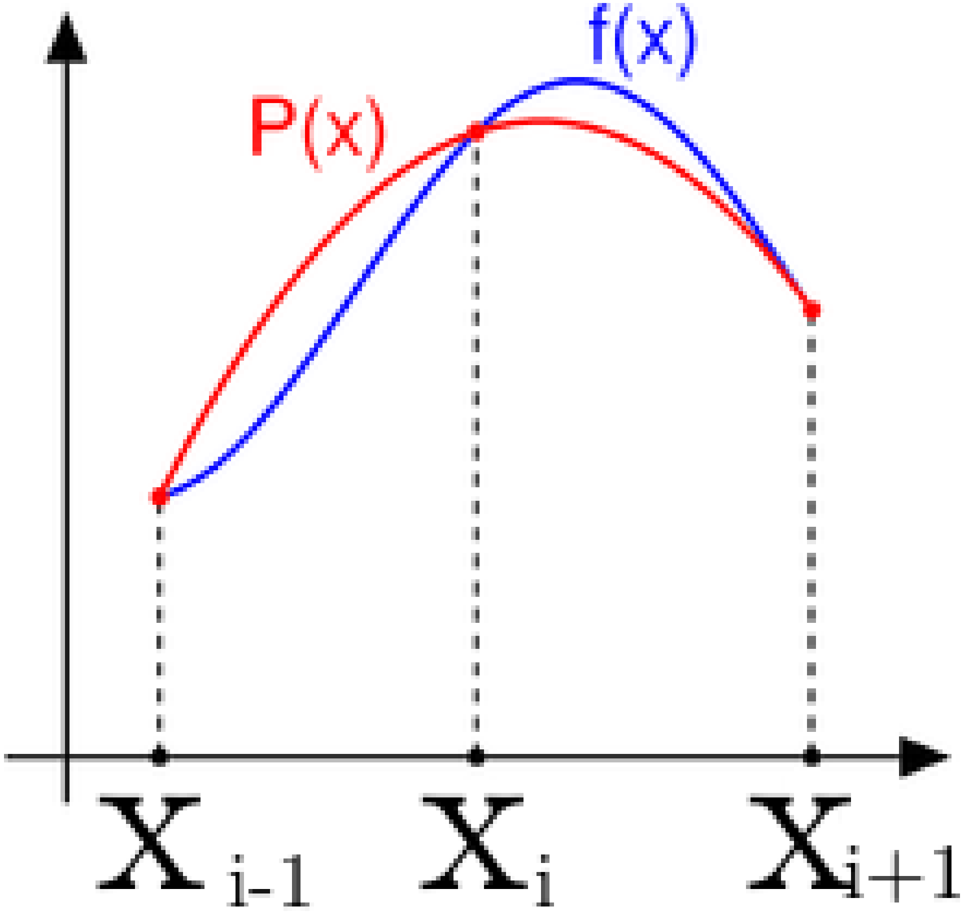
Hands on

- Escreva programas para o cálculo das funções:

$$f(x) = x^n, n = 1, 2, 3, 4, 5, ...$$

$$f(x) = e^{\pm x}$$

Método de Simpson



$$P(x) = \alpha x^2 + \beta x + \gamma$$

$$P(x_{i-1}) = \alpha x_i^2 + \alpha h_i^2 - 2\alpha h x_i + \beta x_i - \beta h + \gamma = f(x_{i-1}) = f_{i-1}$$

$$P(x_i) = \alpha x_i^2 + \beta x_i + \gamma = f(x_i) = f_i$$

$$P(x_{i+1}) = \alpha x_i^2 + \alpha h_i^2 + 2\alpha h x_i + \beta x_i + \beta h + \gamma = f(x_{i+1}) = f_{i+1}$$

$$\int_{x_{i-1}}^{x_{i+1}} P(x)dx = \frac{1}{3}\alpha x^3\Big|_{x_{i-1}}^{x_{i+1}} + \frac{1}{2}\beta x\Big|_{x_{i-1}}^{x_{i+1}} x_{i+1}{}_{x_{i-1}} + 2\gamma h$$

$$\int_{x_{i-1}}^{x_{i+1}} P(x)dx = (2\alpha x_i^2 + \frac{2}{3}\alpha h^2 + 2\beta x_i + 2\gamma)h$$

$$\int_{x_{i-1}}^{x_{i+1}} P(x)dx = (f_{i-1} + 4f_i + f_{i+1})\frac{h}{3}$$

Dois intervalos:

$$x_{i-1} \rightarrow x_i$$

$$x_i \rightarrow x_{i+1}$$

Condição para a regra de Simpson

- N deve ser um número ímpar para termos un número par de intervalos

$$I = \sum_{i=2,4,6,\ldots}^{N-1} \left(f_{i-1} + 4f_i + f_{i+1} \right) \frac{h}{3} = \sum_{i=1}^{N} f_i w_i$$

$$w_i = h/3, \quad i = 1, N$$

$$w_i = 4h/3, \quad i = \text{par}$$

$$w_i = 2h/3, \quad i = \text{ímpar} \neq 1, N$$

Polinômios Superiores

$$\int_{x_{i-1}}^{x_{i+2}} P(x)dx = (f_{i-1} + 3f_i + 3f_{i+1} + f_{i+2})\frac{3h}{8}$$

$$\int_{x_{i-2}}^{x_{i+2}} P(x)dx = (7f_{i-1} + 32f_{i-1} + 12f_i + 32f_{i+1} + 7f_{i+2})\frac{2h}{45}$$