UNIVERSITY OF LUXEMBOURG
Physics and Materials Science
Research Unit (PHYMS)

04 – Numerical Integration

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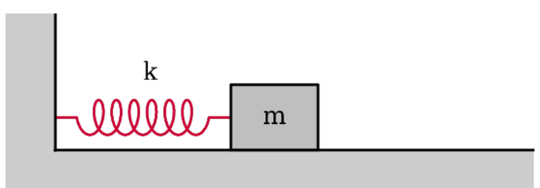
AA 2021/2022 Computational Methods for MSc in Physics

Why Should We Care?

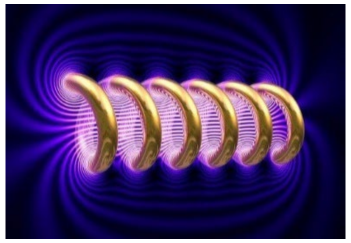
- There are plenty of physically important functions that cannot be integrated analytically (*e.g.*, a Gaussian)

$$\frac{d\boldsymbol{p}}{dt} = \boldsymbol{F}$$



$$\mathrm{div}\,\boldsymbol{D} = 4\pi\rho$$

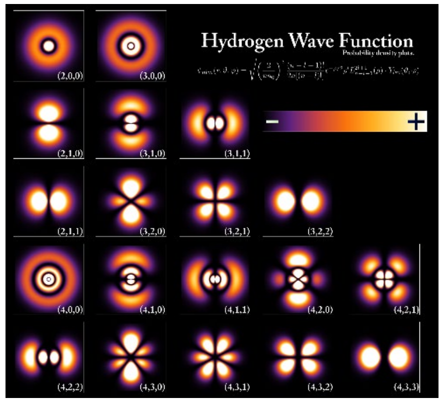
$$\mathrm{div}\,\boldsymbol{B} = 0$$



$$\mathrm{rot}\,\boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{B}}{\partial t}$$

$$\mathrm{rot}\,\boldsymbol{H} = \frac{4\pi}{c}\boldsymbol{j} + \frac{1}{c}\frac{\partial \boldsymbol{D}}{\partial t}$$

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$$



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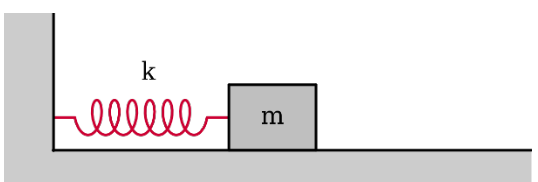

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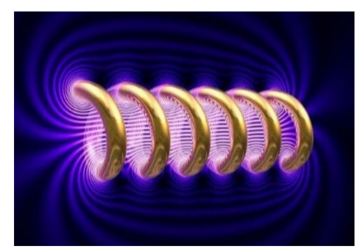

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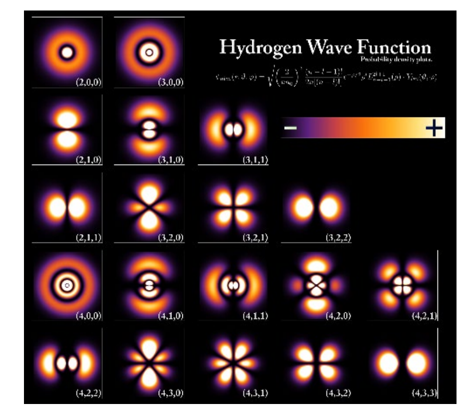


- Numerical solution of differential equations implies their integration

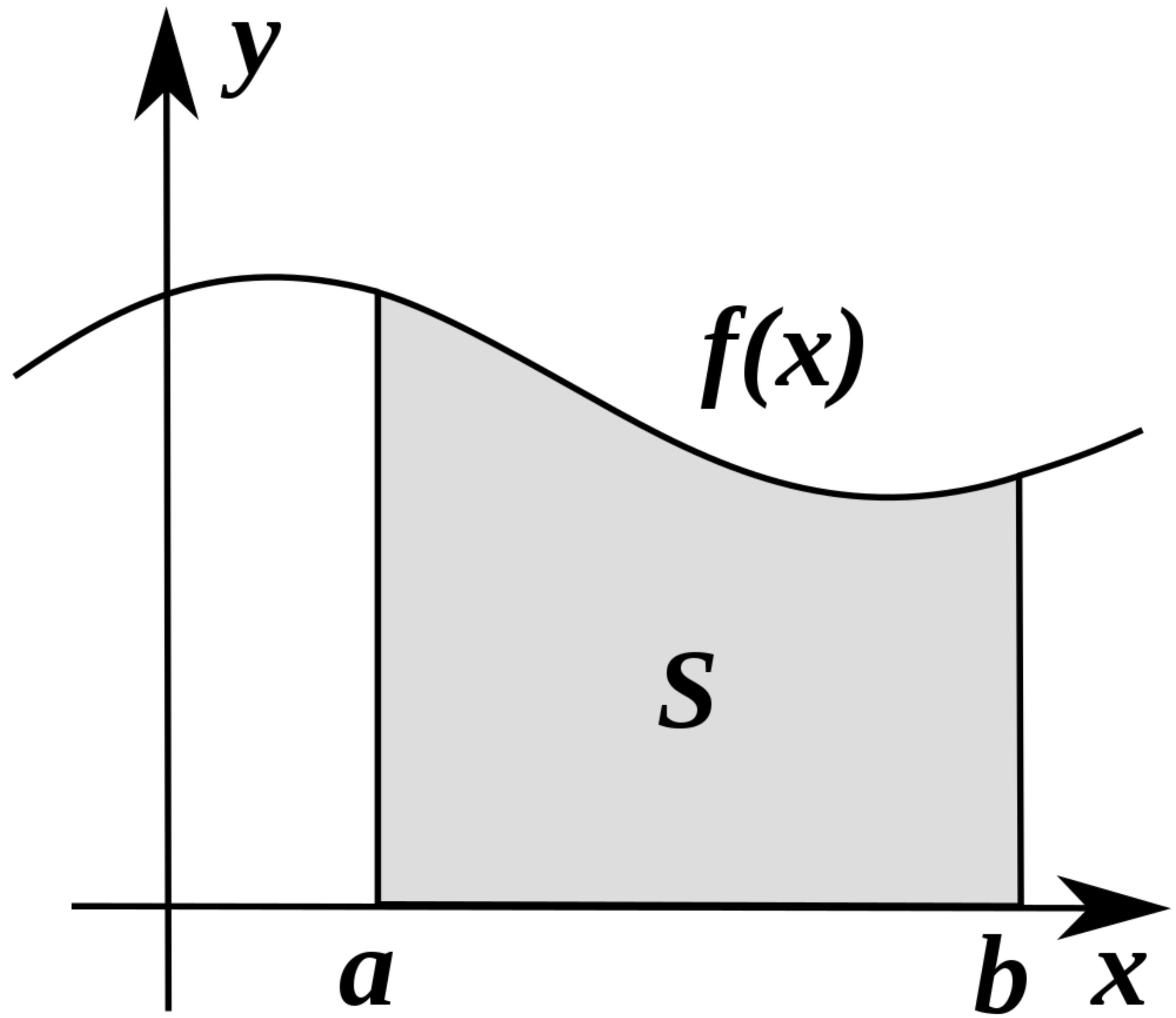
We should learn how to integrate numerically

Geometrical Meaning of the Integral

The integral evaluates the area under the graph of function $f(x)$

$$S = \int_a^b \color{red}{f(x)}\color{black}\, dx$$

the integrand function



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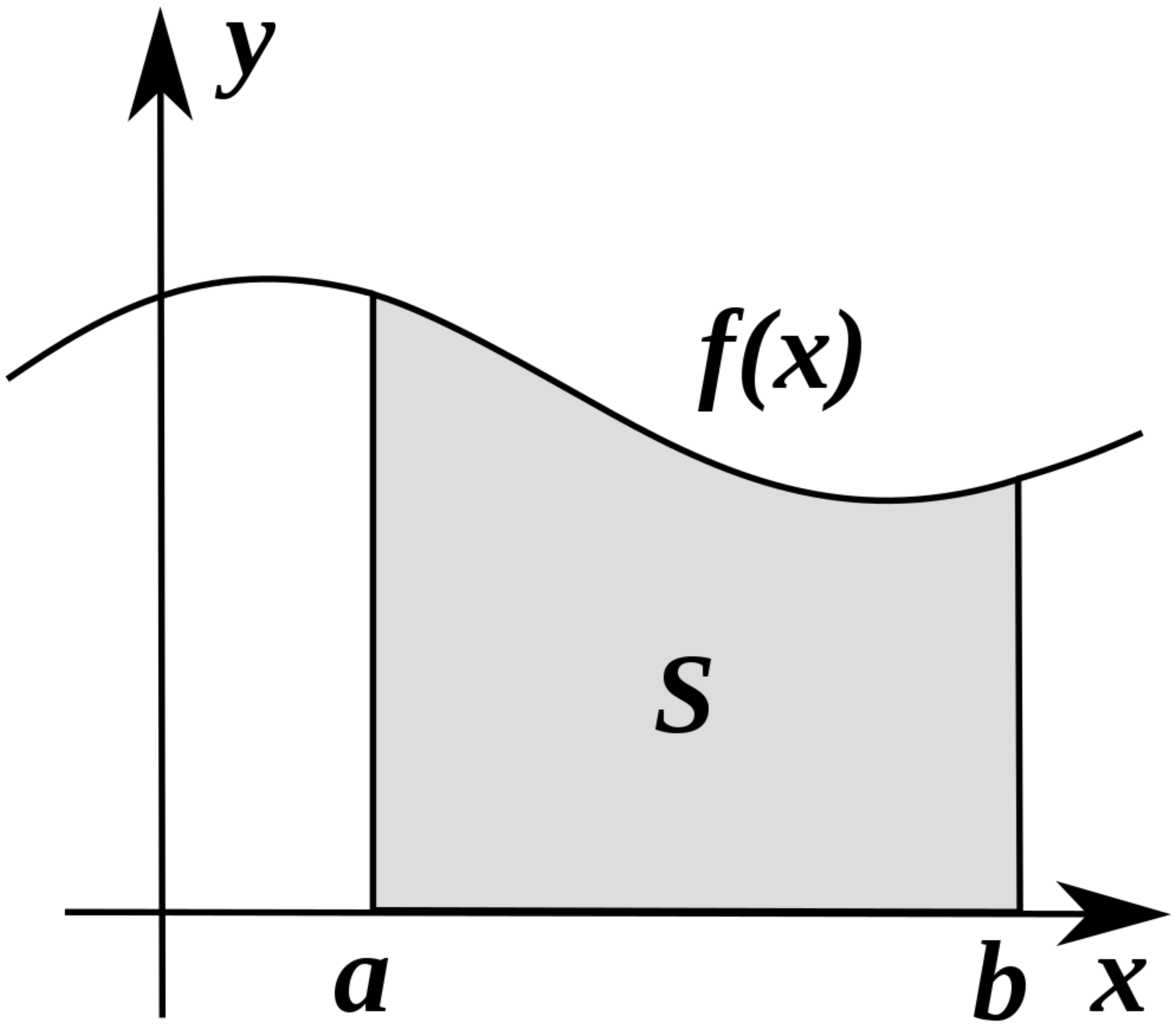

If there exists a function $F(x)$ such that $F'(x) = f(x)$, then Newton-Leibnitz rule holds:

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

$F(x)$ is called the *antiderivative* of the function $f(x)$

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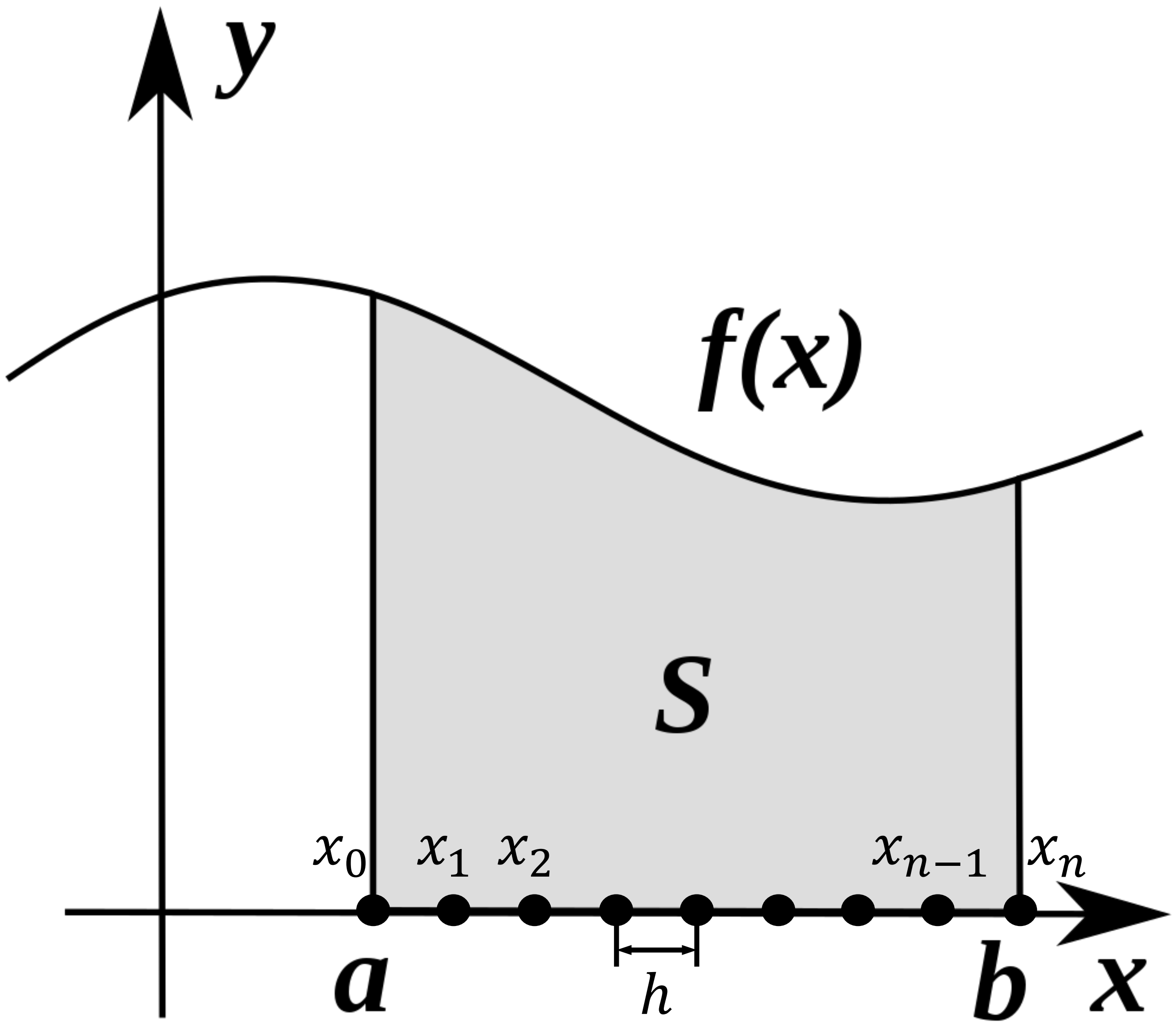


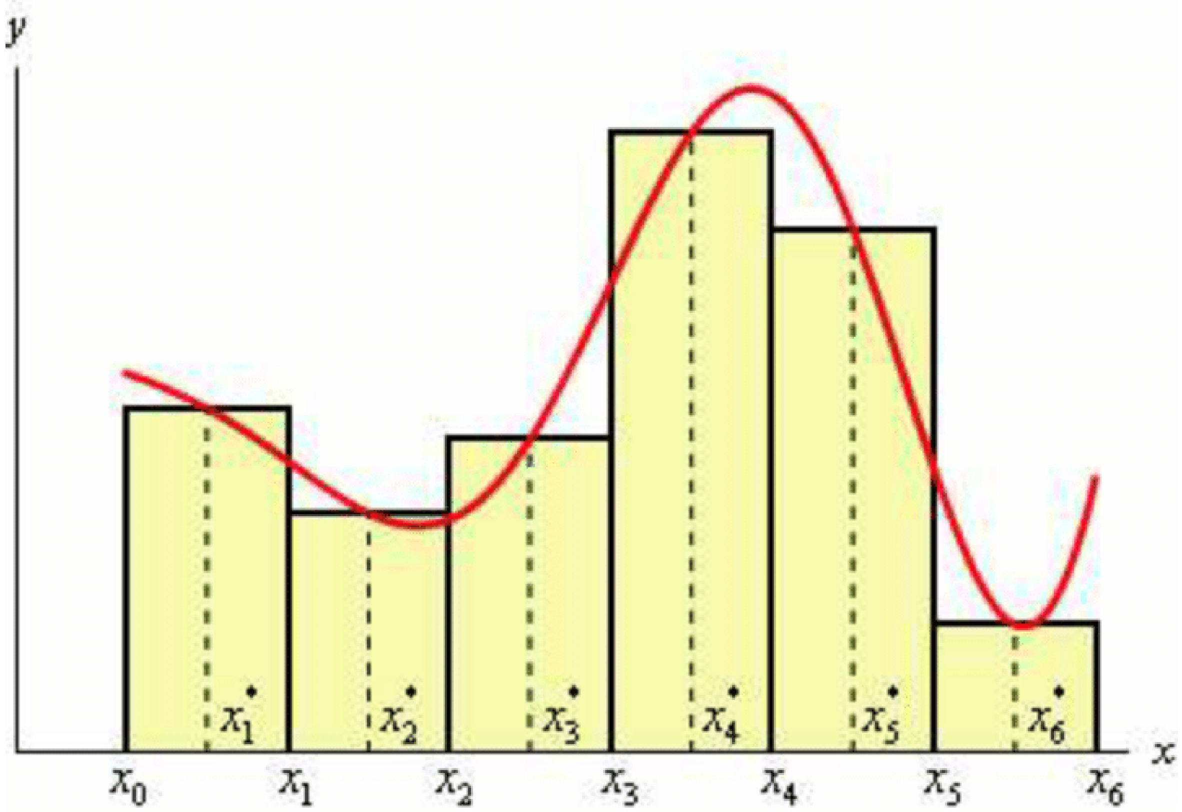
A uniform partition of $[a, b]$:

$a = x_0 < x_1 < x_2 \dots < x_{n-1} < x_n = b,$ $\quad x_i - x_{i-1} = h = (b-a)/n$, for $i = 1, \dots, n$

Midpoint Rule

$$S = \int_a^b f(x)\,dx \approx S_{mid} = \sum_{i=0}^{n-1} f\left(\frac{x_i + x_{i+1}}{2}\right) \cdot h$$

Within every subinterval the function $f(x)$ is approximated by the **constant value**



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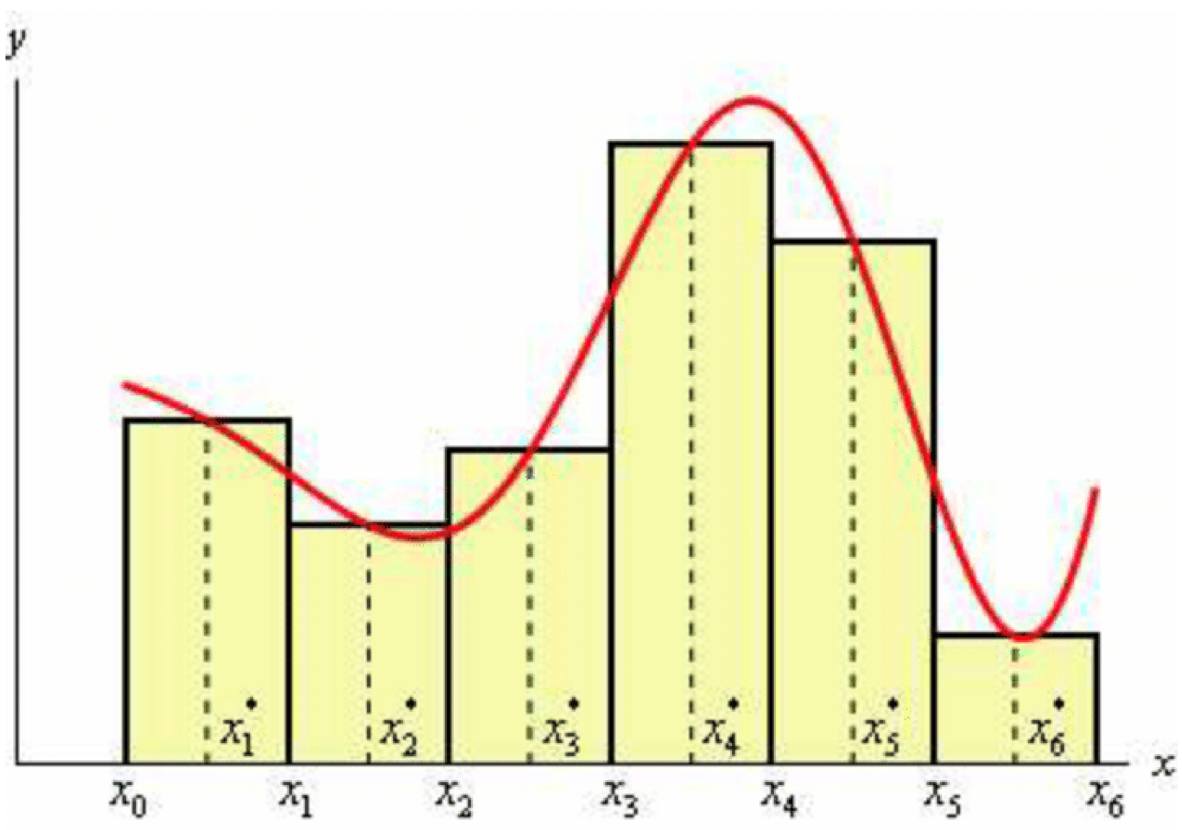
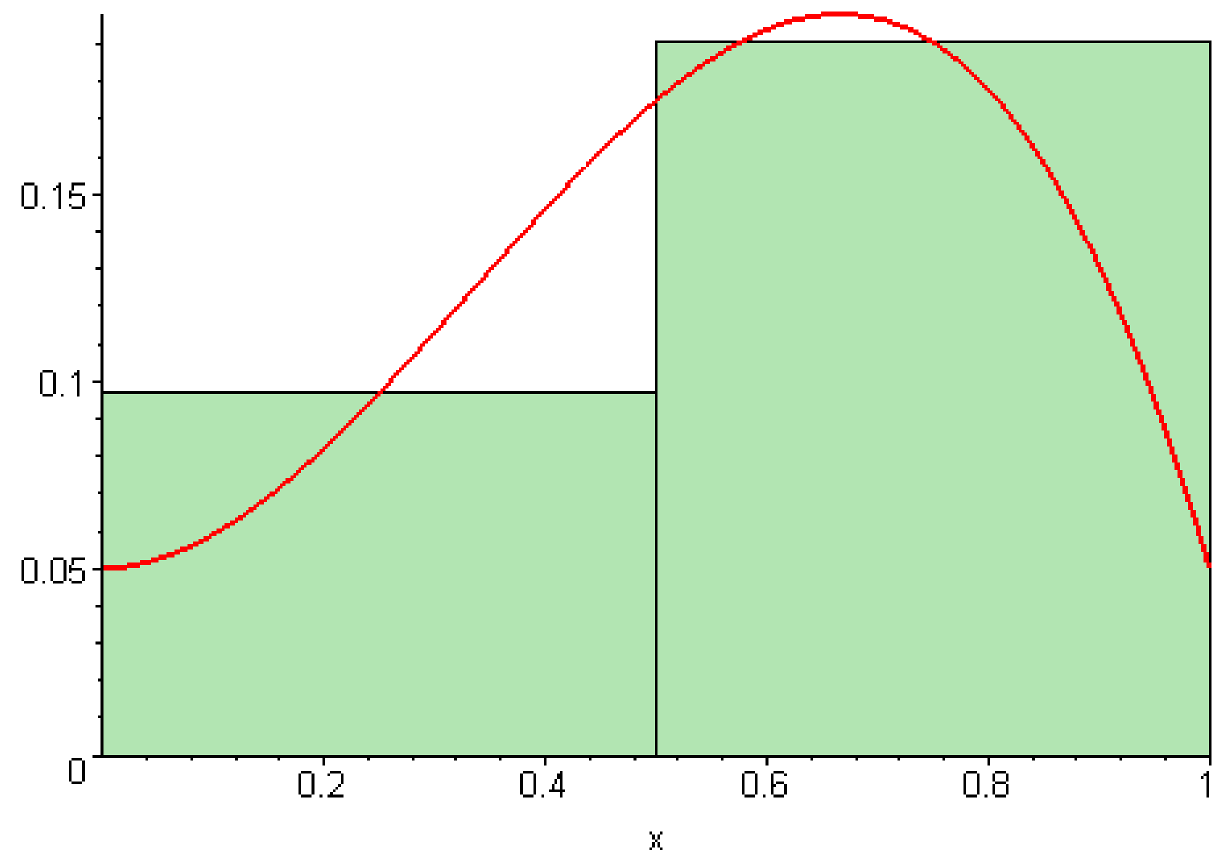
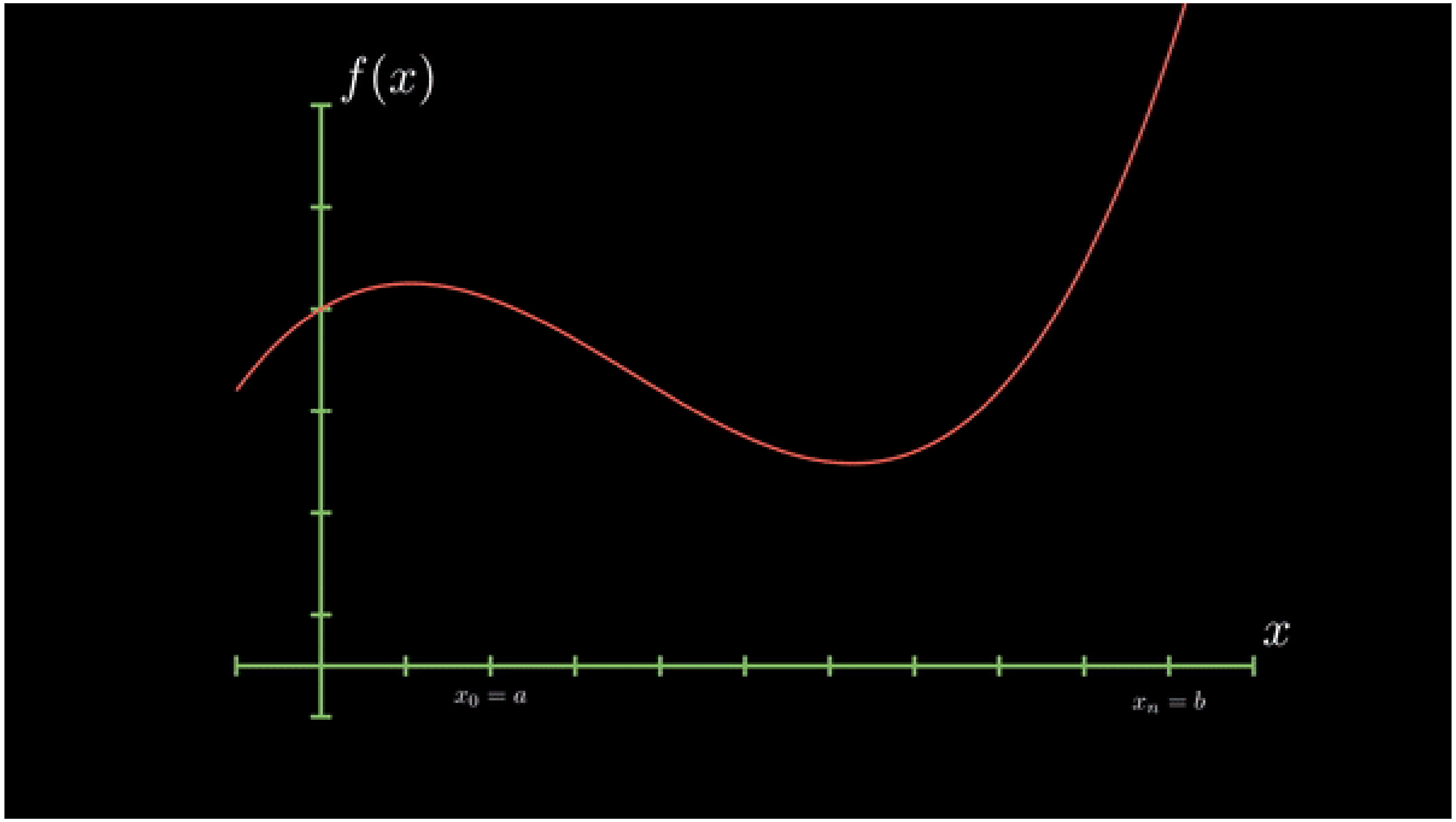




Trapezoidal Rule

$$S = \int_a^b f(x)\,dx \approx S_{trap} = \sum_{i=0}^{n-1} \frac{f(x_i) + f(x_{i+1})}{2} \cdot h = \frac{f(a) + f(b)}{2} \cdot h + \sum_{i=1}^{n-1} f(x_i) \cdot h$$

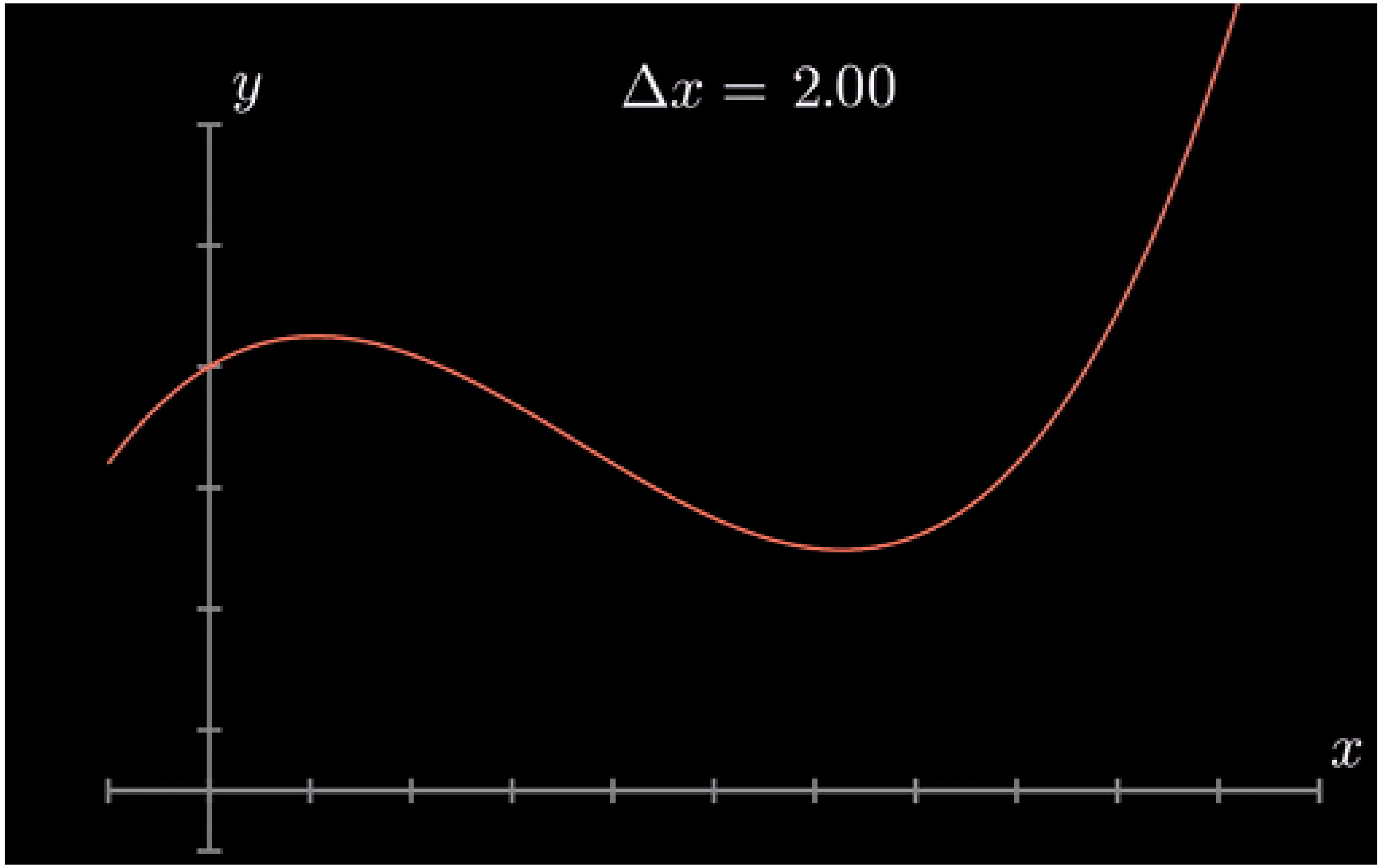
Within every subinterval the function $f(x)$ is approximated by a **linear function**



Simpson's Rule

$$S_{Simp} = \frac{h}{3} \cdot \sum_{i=1}^{n} \left(f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i}) \right) = \frac{h}{3} \cdot \left(f(a) + f(b) + 2 \sum_{i=1}^{n-1} f(x_{2i}) + 4 \sum_{i=1}^{n} f(x_{2i-1}) \right)$$

Within every subinterval the function $f(x)$ is approximated by a **parabola**



IMPORTANT! For this method, the grid should contain an **even** number of subintervals (*i.e.*, an **odd** number of points)

Midpoint Rule: The Error Analysis

By definition, we can express the integral over $[a, b]$ as a sum:

$$S = \int_a^b f(x)\,dx = \sum_{i=0}^{n-1} S_i = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)\,dx \qquad S_i = \int_{x_i}^{x_{i+1}} f(x)\,dx$$

For its numerical approximation, we have also:

$$S_{mid} = \sum_{i=0}^{n-1} S_i^{mid} = \sum_{i=0}^{n-1} f\left(\frac{x_i + x_{i+1}}{2}\right) \cdot h \qquad S_i^{mid} = f\left(\frac{x_i + x_{i+1}}{2}\right) \cdot h$$

The local error definition:

$$\delta_i = \left|S_i - S_i^{mid}\right| = \left|\int_{x_i}^{x_{i+1}} f(x)\,dx - f\left(\frac{x_i + x_{i+1}}{2}\right) \cdot h\right|$$

For the following derivation, it is useful to note that:

$$\frac{x_i + x_{i+1}}{2} = x_i + \frac{h}{2}$$

Midpoint Rule: The Error Analysis

Taylor expansions in the Lagrange form near the left end x_i:

$$f(x) = f(x_i) + f'(x_i)(x - x_i) + \frac{1}{2} f''(\xi_1)(x - x_i)^2$$

$$f\left(\frac{x_i + x_{i+1}}{2}\right) = f(x_i) + f'(x_i)\frac{h}{2} + \frac{1}{2} f''(\xi_2)\frac{h^2}{4}$$

Let's formally integrate the expansion for $f(x)$:

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = \left(f(x_i)\cdot x + \frac{f'(x_i)(x - x_i)^2}{2} + \frac{f''(\xi_1)(x - x_i)^3}{6}\right)\Bigg|_{x_i}^{x_{i+1}} = f(x_i)\cdot h + f'(x_i)\cdot\frac{h^2}{2} + f''(\xi_1)\cdot\frac{h^3}{6}$$

Then for the local error we have:

$$\delta_i = \left|S_i - S_i^{mid}\right| = \left|f''(\xi_1)\cdot\frac{h^3}{6} - f''(\xi_2)\cdot\frac{h^3}{8}\right| \le M\cdot h^3$$

The global error could be also easily estimated as:

$$\Delta = |S - S_{mid}| = \left|\sum_{i=0}^{n-1} S_i - \sum_{i=0}^{n-1} S_i^{mid}\right| = \left|\sum_{i=0}^{n-1}\delta_i\right| \le \sum_{i=0}^{n-1} Mh^3 \le nMh^3 = M(b-a)h^2$$

Summary

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-1} f\left(\frac{x_i + x_{i+1}}{2}\right) \cdot h + O(\boldsymbol{h^2})$$

Midpoint rule

$$\int_a^b f(x)\,dx = \frac{f(a)+f(b)}{2} \cdot h + \sum_{i=1}^{n-1} f(x_i) \cdot h + O(\boldsymbol{h^2})$$

Trapezoidal rule

$$\int_a^b f(x)\,dx = \frac{h}{3} \cdot \left(f(a) + f(b) + 2\sum_{i=1}^{n-1} f(x_{2i}) + 4\sum_{i=1}^{n} f(x_{2i-1}) \right) + O(\boldsymbol{h^4})$$

Simpson’s rule

In contrast to the numerical differentiation, round-off errors are not so important for the numerical integration. Most of the times, we can neglect them. Thus, the errors of numerical integration mainly arise due to the **truncation error**.