Numerical Integration

Computational Physics, Landau et al.
Chap. 5 & Chap. 11.4

BCCP, B.A. Stickler et al. Chap 3. & 14.2

Numerical Integration

- Riemann Sums
- Composite Trapezoid Method
- Composite Simpson's Method
- Monte Carlo Method
  捉放法 (Random Number Generator)

Riemann Sums

Recall fundamental calculus

- Derivative

$$F'(x) = \lim_{h \to 0} \frac{F(x+h) - F(x)}{h} = f(x)$$

- Numerical Derivative

$$F'(x) \approx \frac{F(x+h) - F(x)}{h}$$

- Anti-Derivative

$$F(x+h) - F(x) = \int_{x}^{x+h} f(x)dx \approx f(x) \cdot h$$

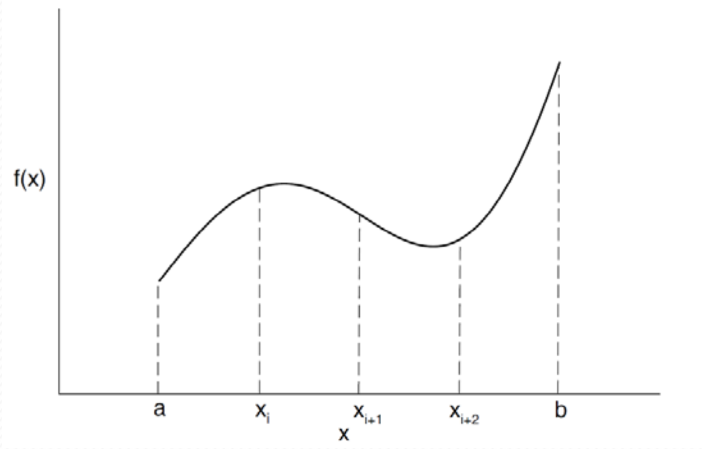
Recall fundamental calculus

- Approximation of definite integral

$$\int_{x}^{x+h} f(x)\,dx \approx f(x)\cdot h$$

Composite Method

- Divide the entire integrand into several segments
- Evaluate each segment by the given rule
  - Riemann Sum
  - Composite Trapezoid Method
  - Composite Simpson Rule

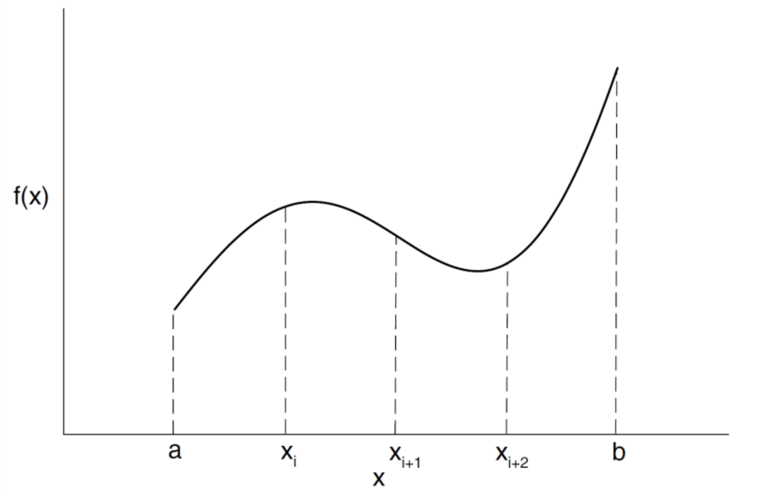


Box Counting

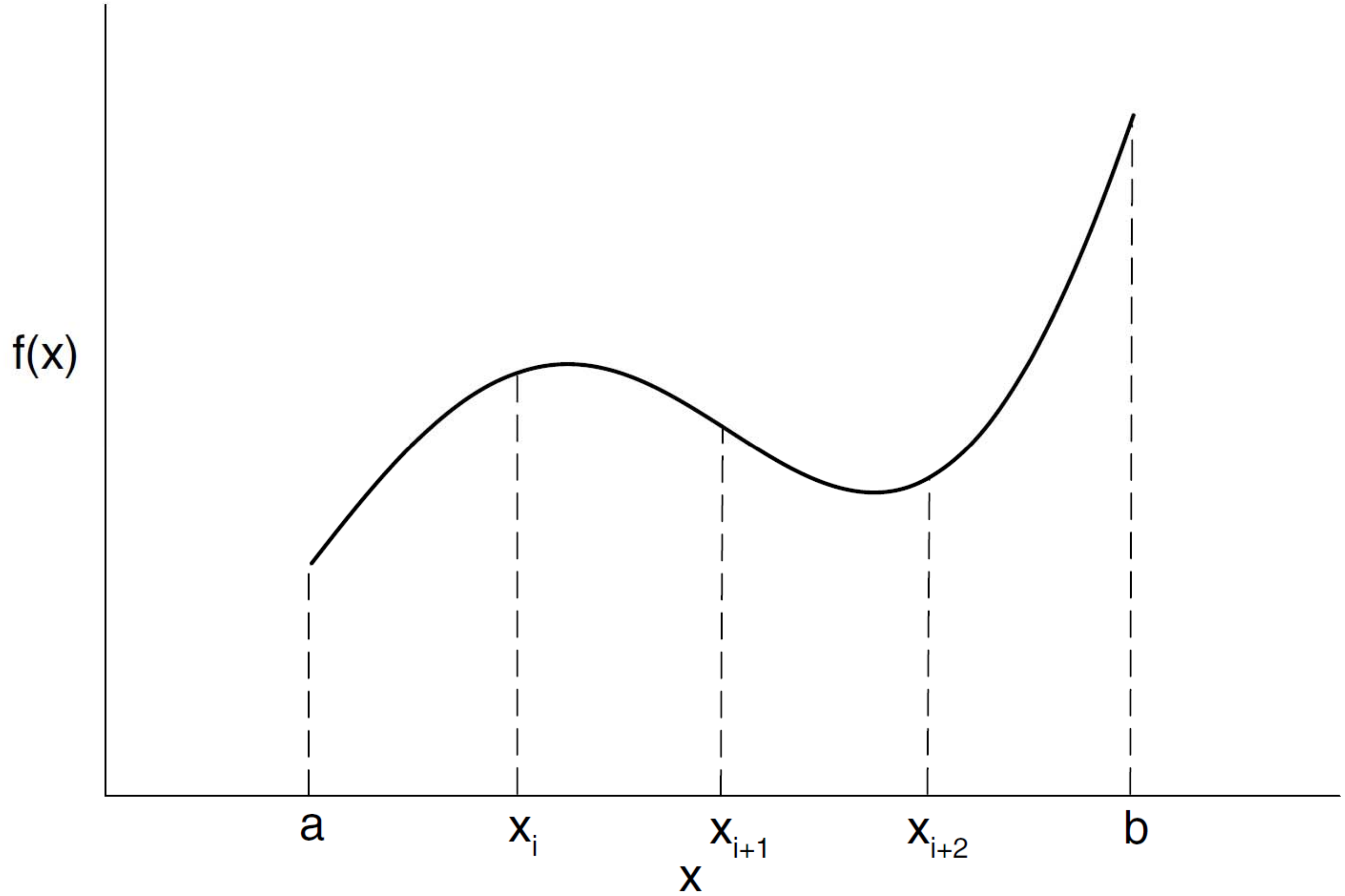
- Riemann Integral

$$\int_a^b f(x)\,dx = \lim_{n->\infty} \sum_{i=0}^{n} f(a + i(\frac{b-a}{n}))(\frac{b-a}{n})$$

$$= \lim_{h->0} \sum_{i=0}^{n} f(a + ih)(h)$$

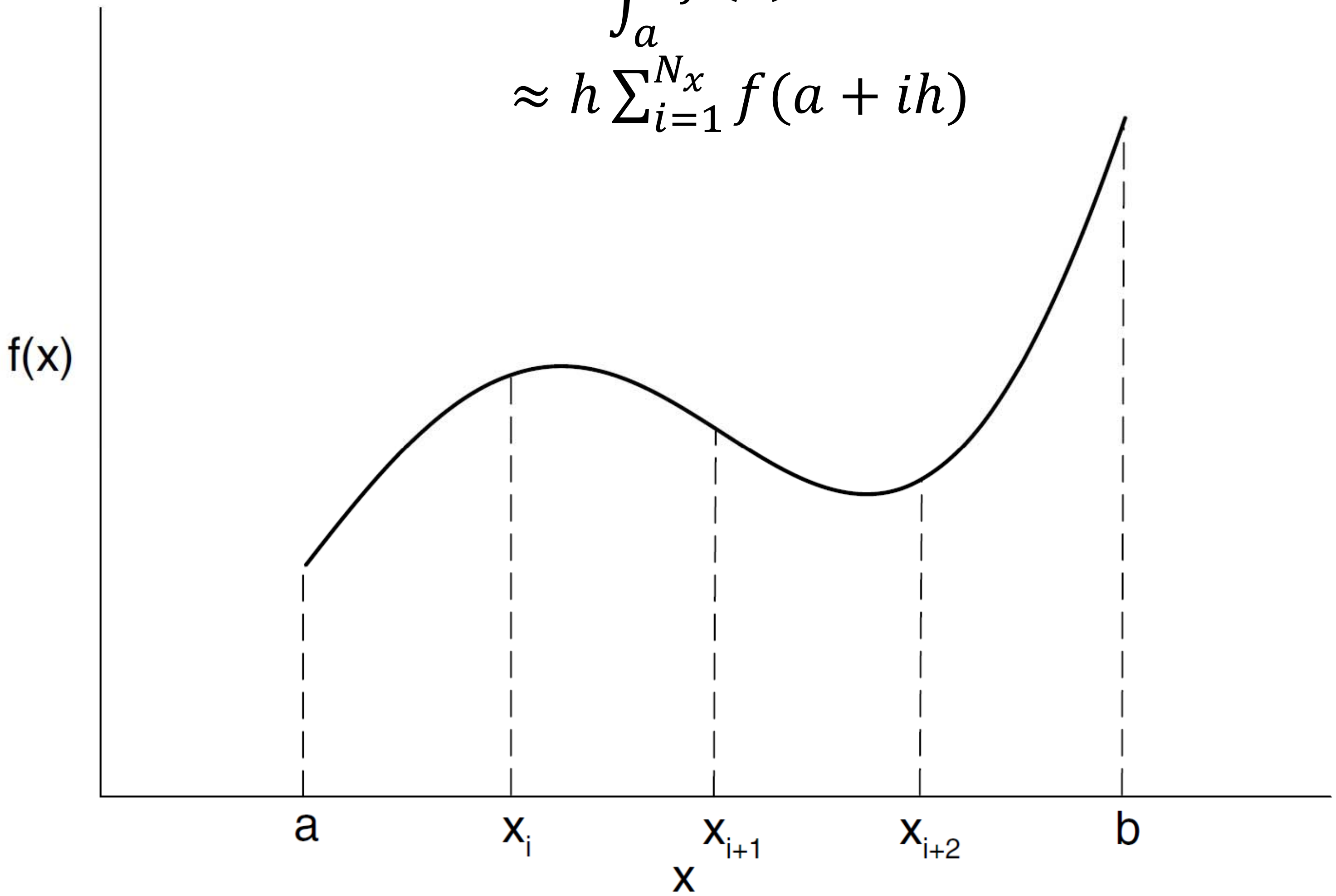


Box Counting



Box Counting

$$\int_a^b f(x)dx \approx h\sum_{i=1}^{N_x} f(a+ih)$$



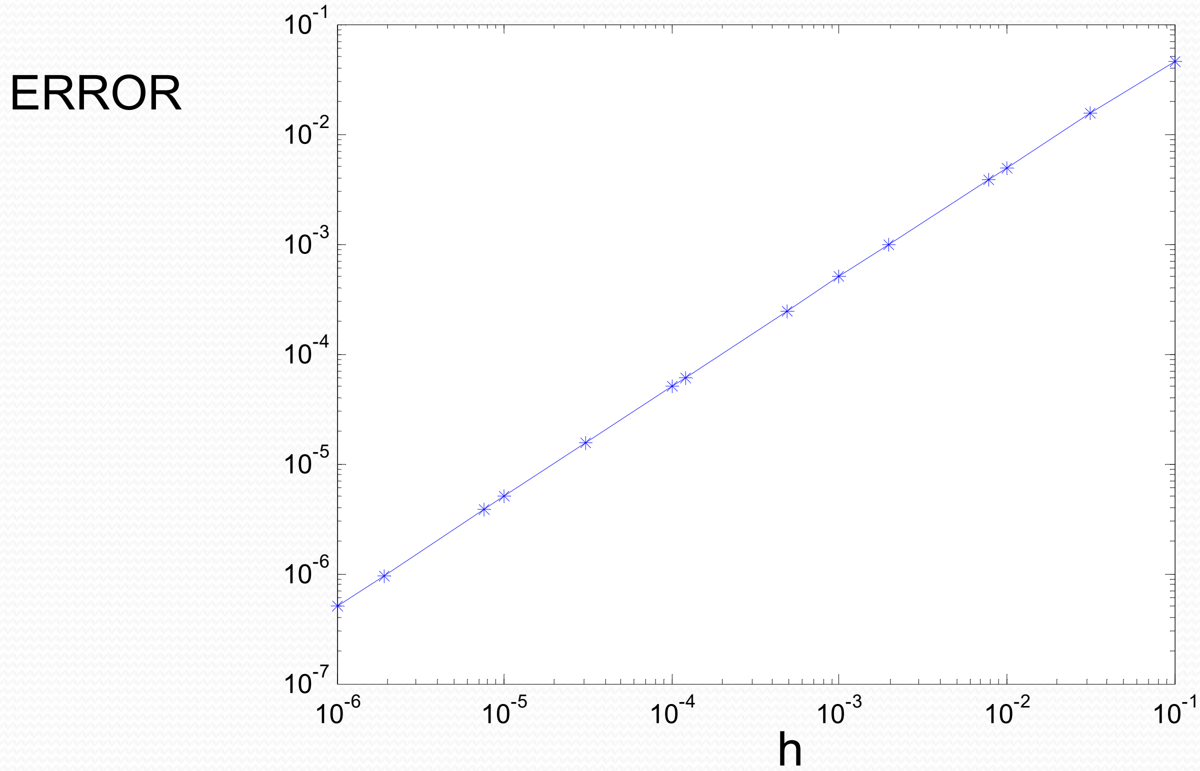
Error of finite Riemann Sum

- Integrate a known function

- Set h = 0.1, 0.01, 0.001,…
- or set N = 10,100,1000, ….

- Plot the absolute error of the approximation and the known integral

Error of finite Riemann Sum



Numerical Integration

- Approximate integral by finite Riemann Sum

$$\int_a^b f(x)\,dx \approx h\sum_{i=1}^{n} f(a+ih) \approx h\sum_{i=1}^{n} f(a+(i-1)h)$$

- Error is roughly proportional to h (not good)
- Intuitive and fast

Goal in Numerical Integration

- In most cases integration doesn't guarantee a close form $\int_a^b f(x)\,dx$
- In the numerical integration, algorithms aim at approximation integration by the following form

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} f(a+ih)(h) = \sum_{i=0}^{n} h \cdot f_i$$

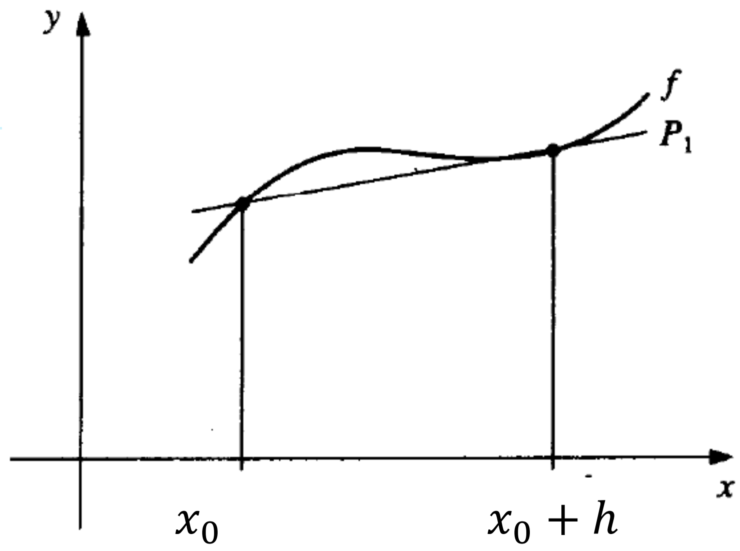
$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} w_i f(x_i) = \sum_{i=0}^{n} w_i \cdot f_i$$

Composite Trapezoid Method

Trapezoid Rules

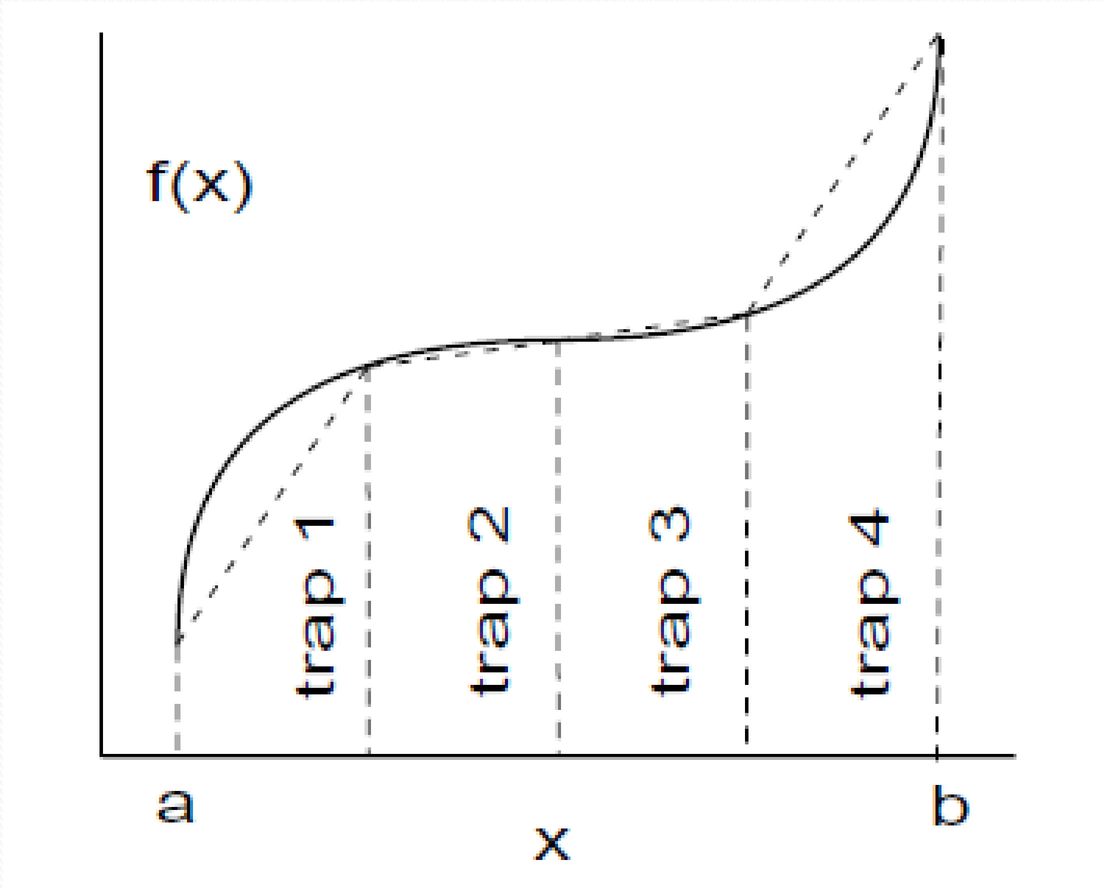
- Linear approximation of a function

$$\int_{x_i}^{x_i+h} f(x)dx \simeq \frac{h(f_i + f_{i+1})}{2} = \tfrac{1}{2}hf_i + \tfrac{1}{2}hf_{i+1}$$

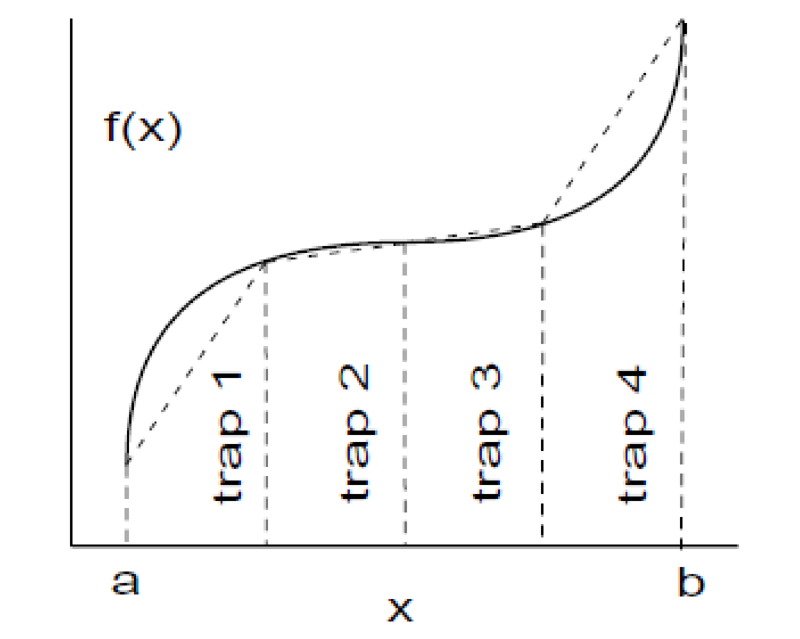


(Composite)Trapezoid Method

- Expand Trapezoid Rule for each segment



(Composite)Trapezoid Method

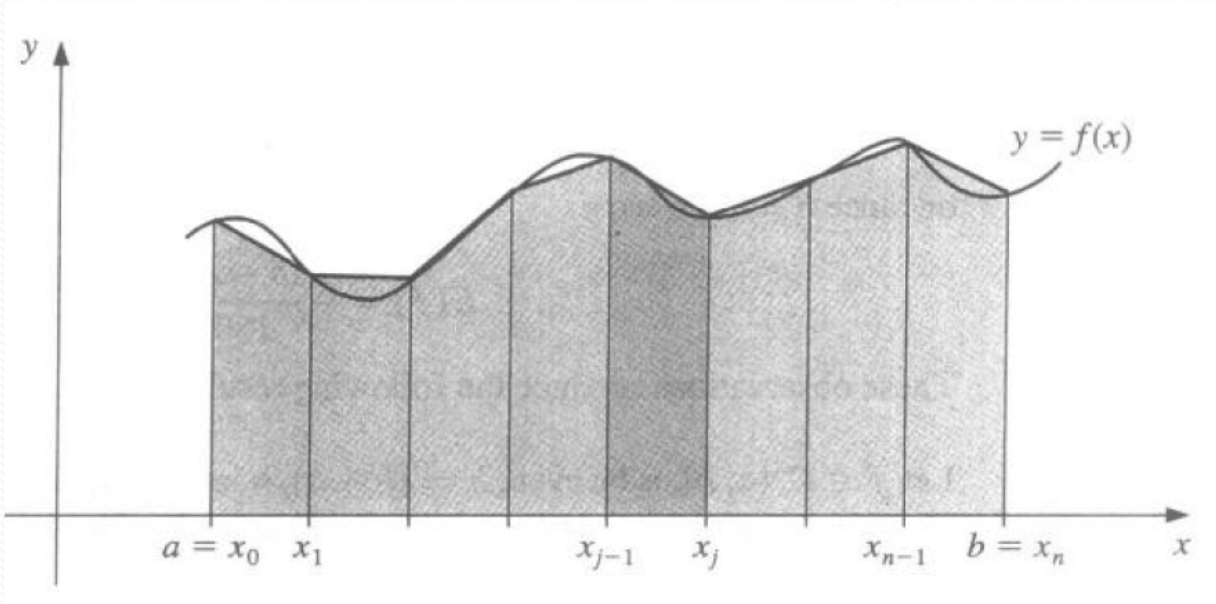


Composite Trapezoid Method

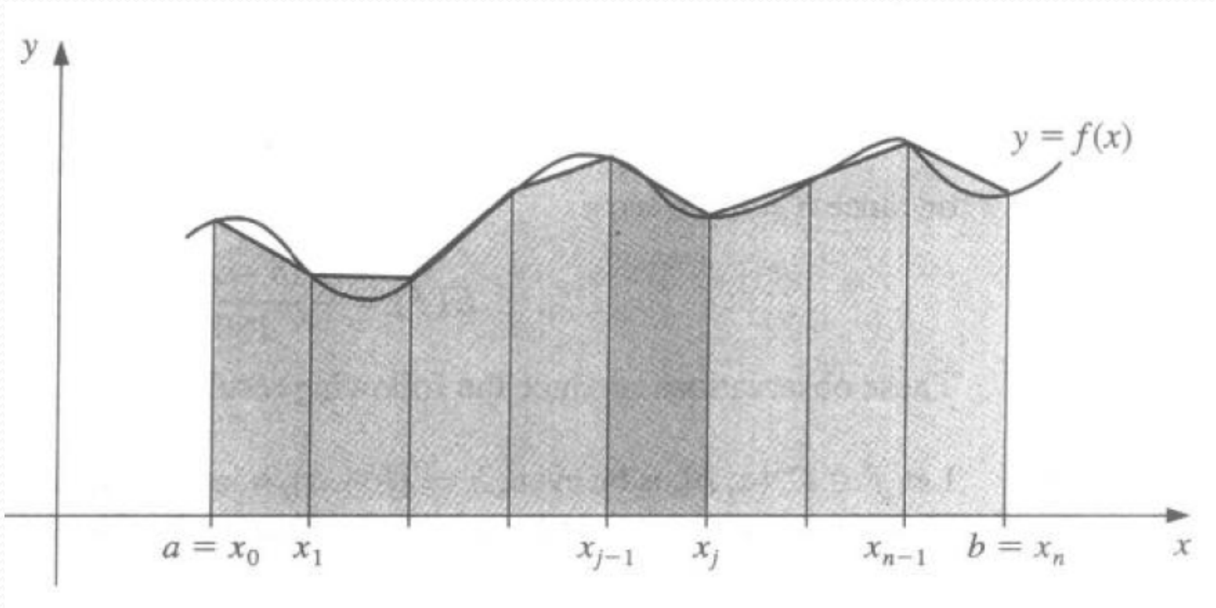
- Expand Trapezoid Rule for each segment

$$\int_a^b f(x)dx = \frac{h}{2}\{[f(a)+f(x_1)]+[f(x_1)+f(x_2)]$$

$$+\ldots+[f(x_{n-1})+f(b)]$$

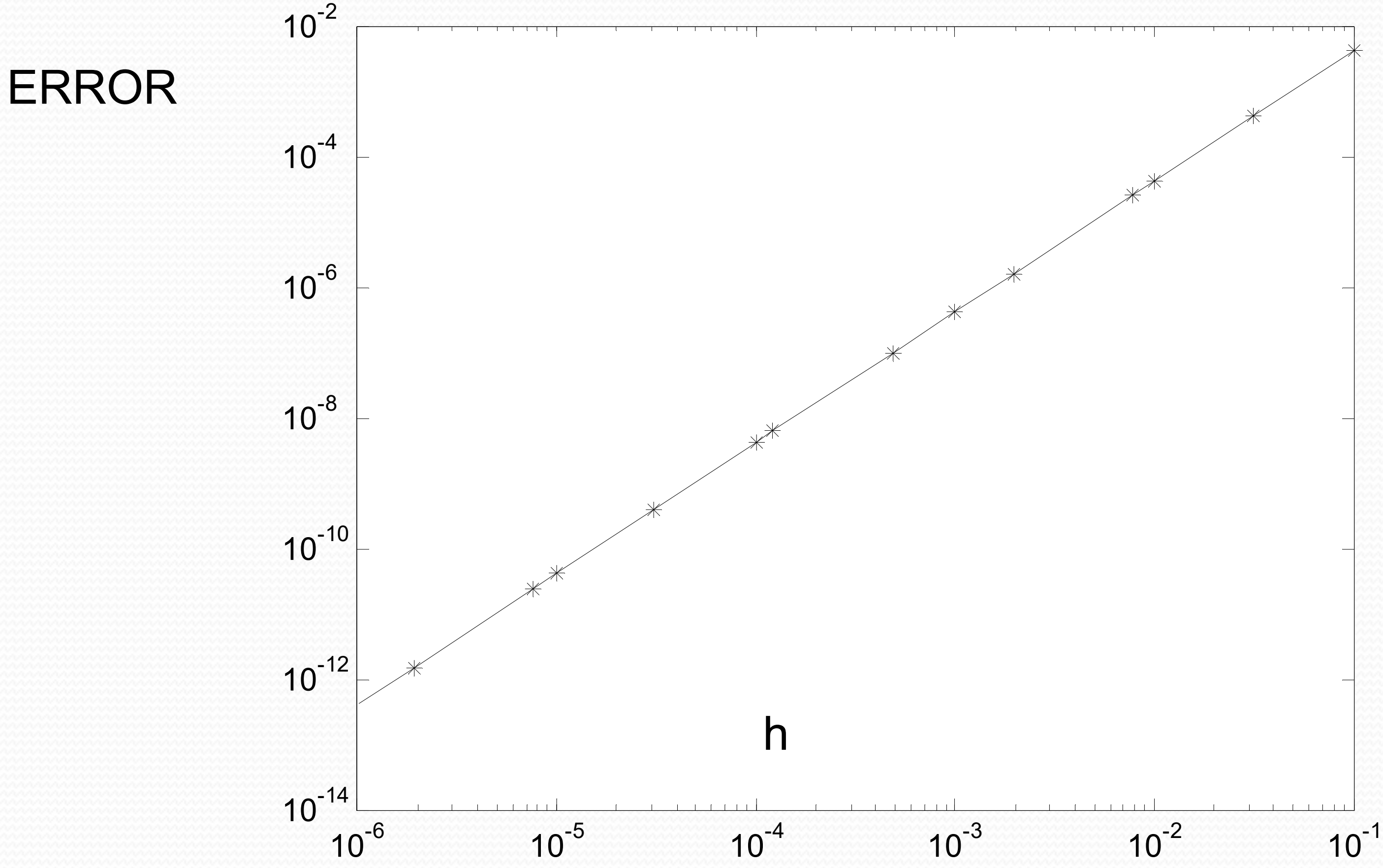


Composite Trapezoid Method



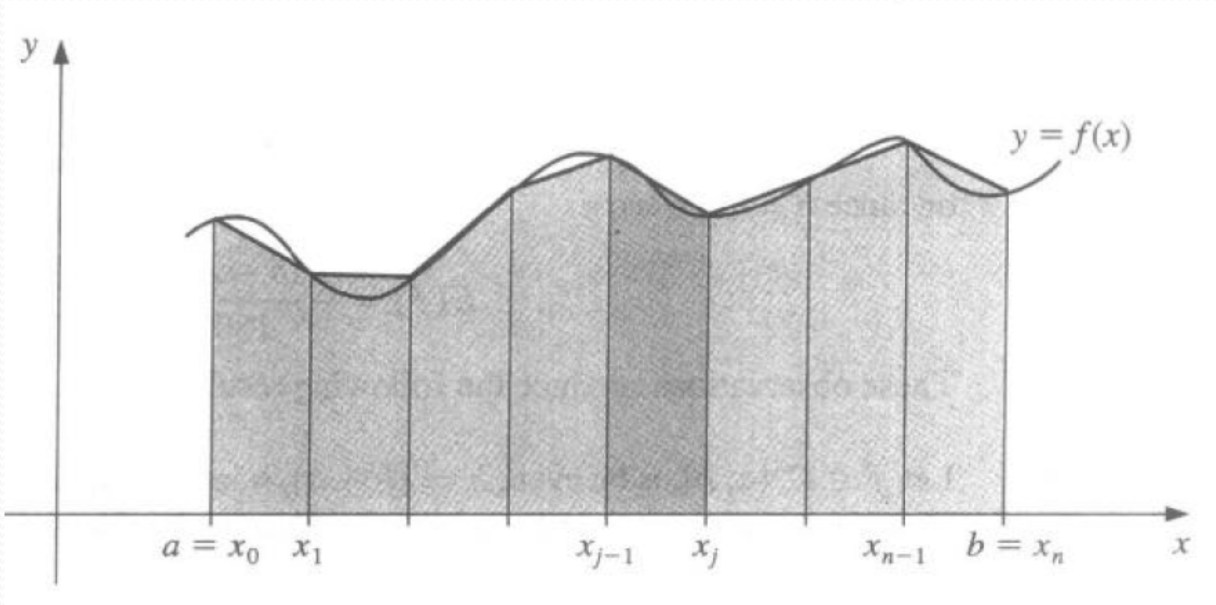
$$\int_{x_0}^{x_n} f(x)dx \approx \frac{h}{2}[f(x_0) + 2\sum_{j=1}^{n-1} f(x_j) + f(x_n)]$$

Error of Trapezoid method



Composite Trapezoid Method

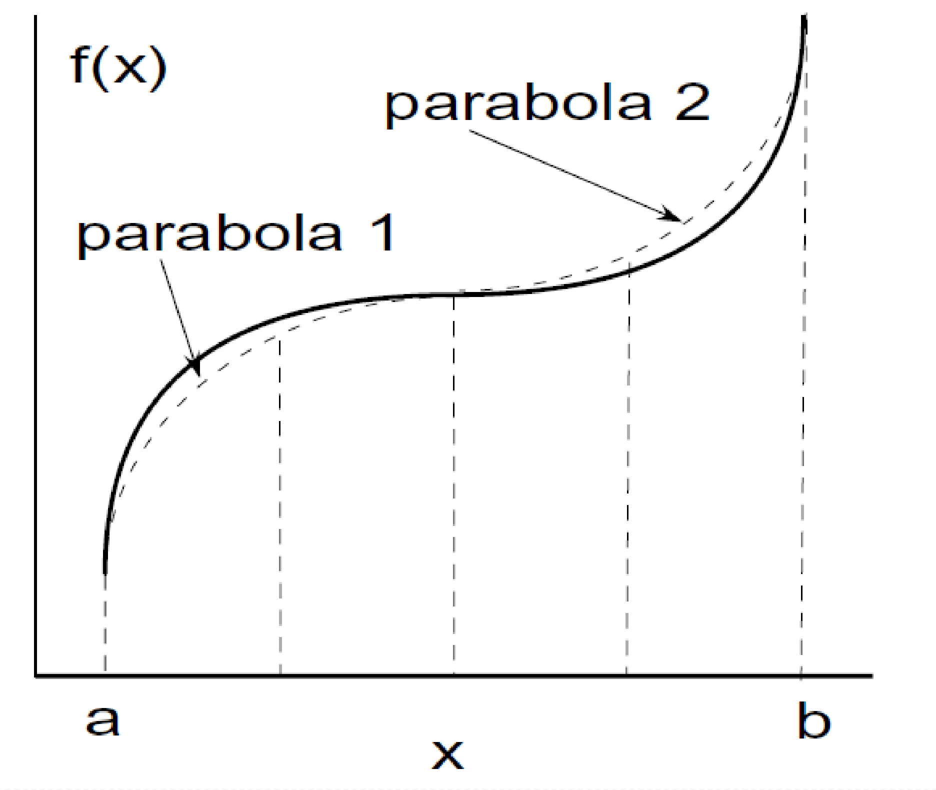
- 以分段線性函數(Piecewise linear function)近似原函數
- 則各個分段線性函數積分也會近似於原函數



Composite Simpson's Method

Composite Simpson's Method

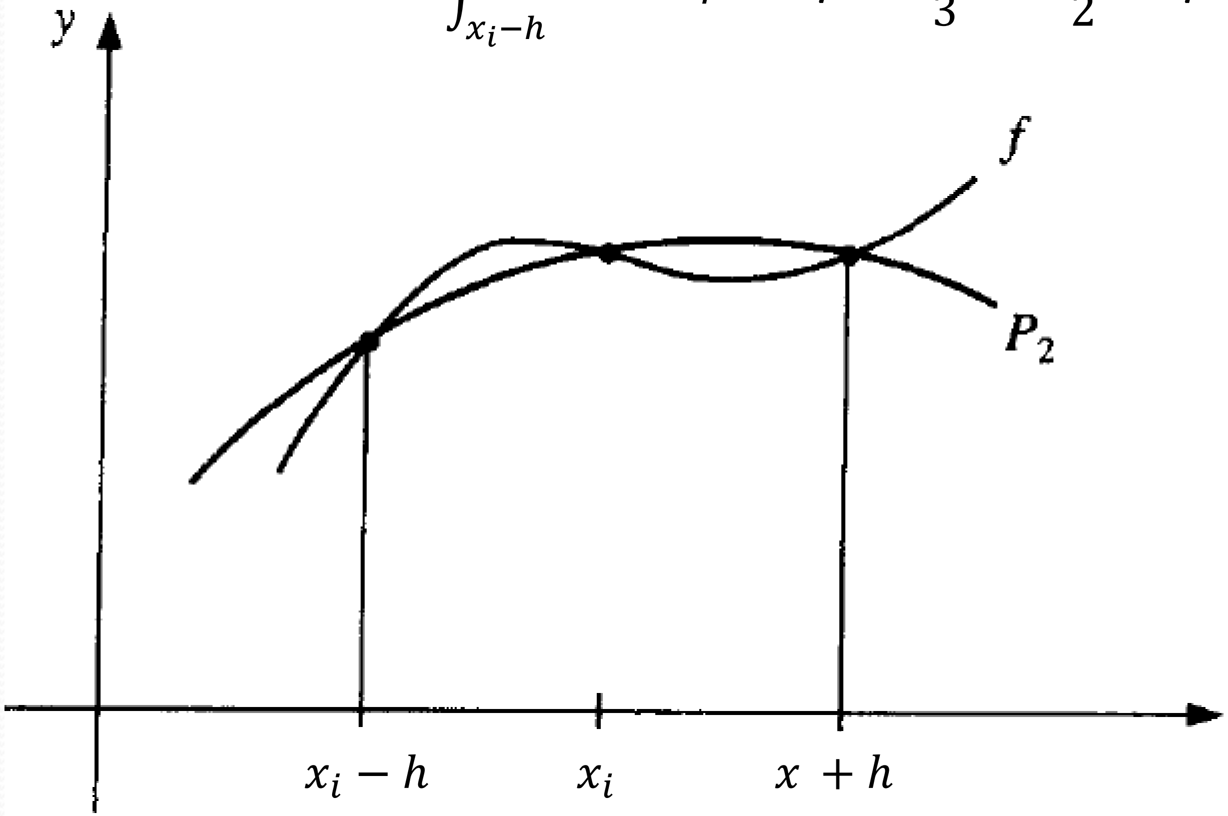
- 以分段二次性函數(Piecewise qudratic function)近似原函數
- 則各個分段線性函數積分也會近似於原函數



Simpson's Method

$$f(x) \approx \alpha x^2 + \beta x + \gamma$$

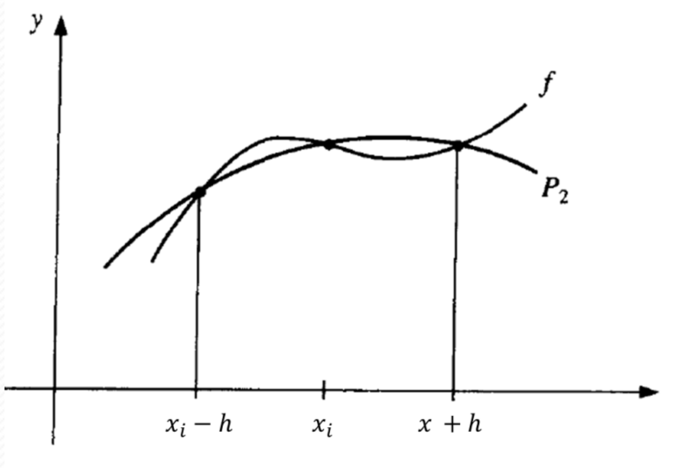
$$\int_{x_i-h}^{x_i+h} \alpha x^2 + \beta x + \gamma = \frac{\alpha x^3}{3} + \frac{\beta x^2}{2} + \gamma x \Big|_{x_i - h}^{x_i + h}$$



Simpson's Method

$$\left.\frac{\alpha x^3}{3} + \frac{\beta x^2}{2} + \gamma x \right|_{x_i - h}^{x_i + h} = Af(x_i + h) + Bf(x_i) + Cf(x_i - h)$$

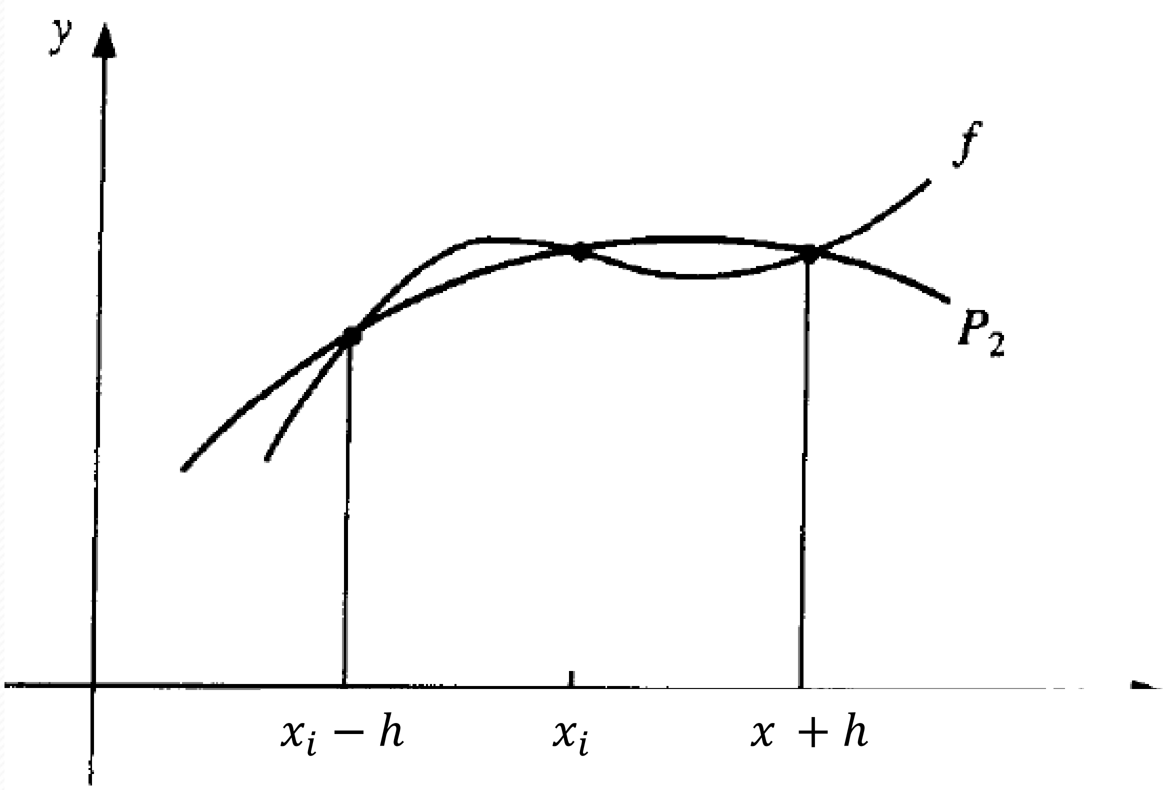
Find out A, B and C to approximate the integration
In terms of a linear combination of known function values.



Simpson's Method

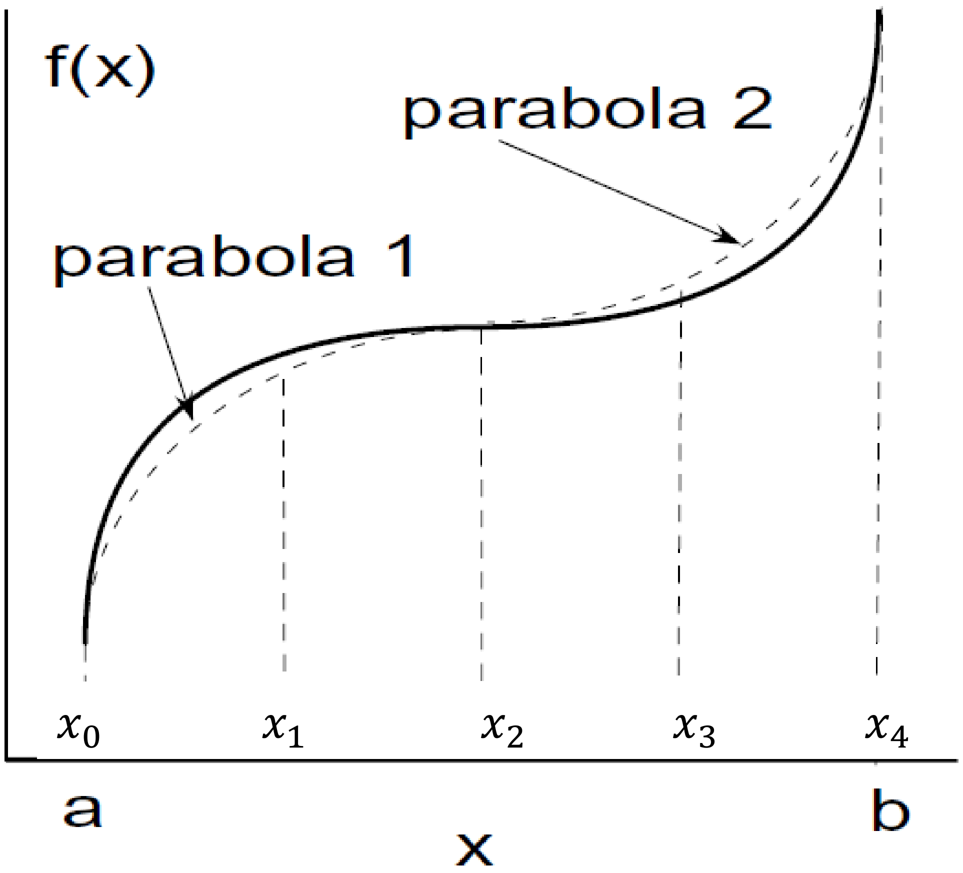
$$\int_{x_i-h}^{x_i+h} f(x)dx = \int_{x_i}^{x_i+h} f(x)dx + \int_{x_i-h}^{x_i} f(x)dx$$

$$\simeq \frac{h}{3}f_{i-1} + \frac{4h}{3}f_i + \frac{h}{3}f_{i+1}$$



Composite Simpson

- Pick up odd number of points



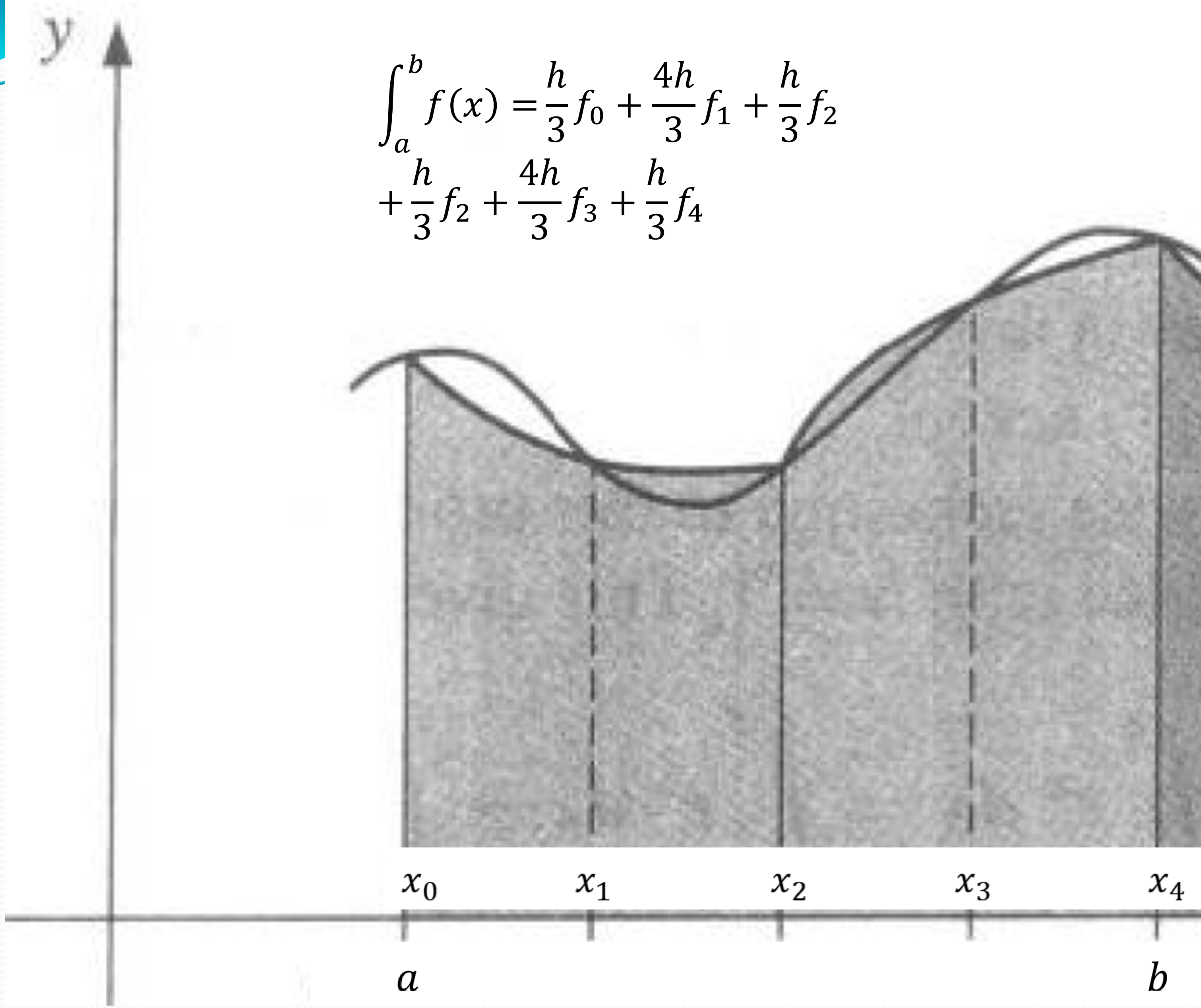
$$\int_{x_i-h}^{x_i+h} f(x)dx = \int_{x_i}^{x_i+h} f(x)dx + \int_{x_i-h}^{x_i} f(x)dx$$

$$\simeq \frac{h}{3}f_{i-1} + \frac{4h}{3}f_i + \frac{h}{3}f_{i+1}$$

$$\int_a^b f(x) = \frac{h}{3}f_0 + \frac{4h}{3}f_1 + \frac{h}{3}f_2$$

$$+\frac{h}{3}f_2 + \frac{4h}{3}f_3 + \frac{h}{3}f_4$$

$$\int_a^b f(x) = \frac{h}{3} f_0 + \frac{4h}{3} f_1 + \frac{h}{3} f_2$$
$$+ \frac{h}{3} f_2 + \frac{4h}{3} f_3 + \frac{h}{3} f_4$$



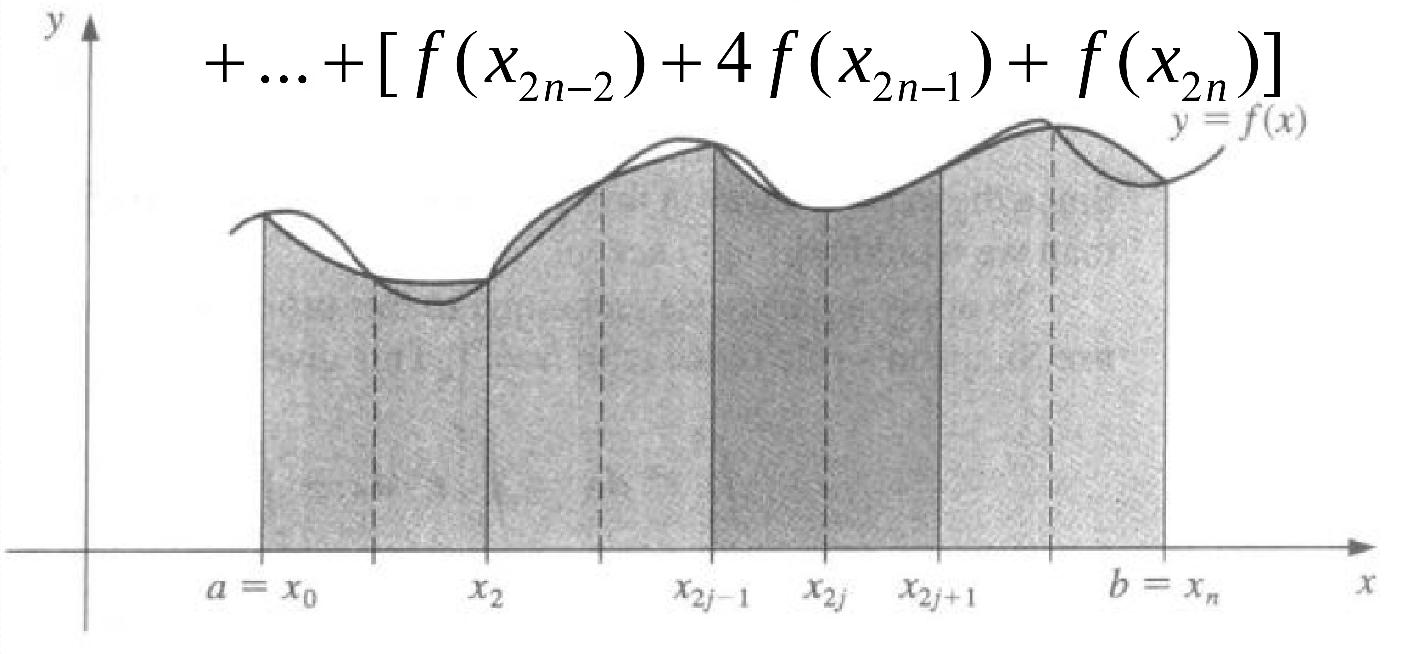
Composite Simpson

- Pick up odd number of points

$$\int_a^b f(x)\,dx = \frac{h}{3}\{[f(x_0)+4f(x_1)+f(x_2)]+$$

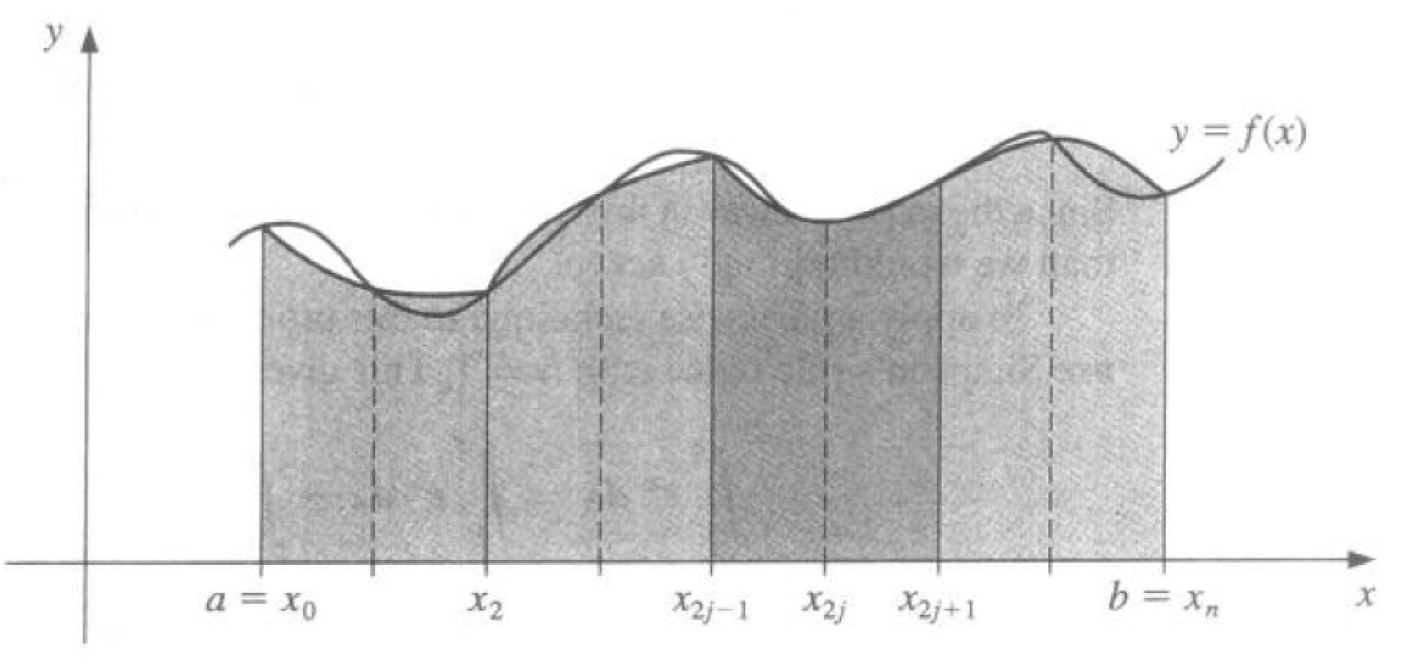
$$[f(x_2)+4f(x_3)+f(x_4)]$$

$$+\ldots+[f(x_{2n-2})+4f(x_{2n-1})+f(x_{2n})]$$

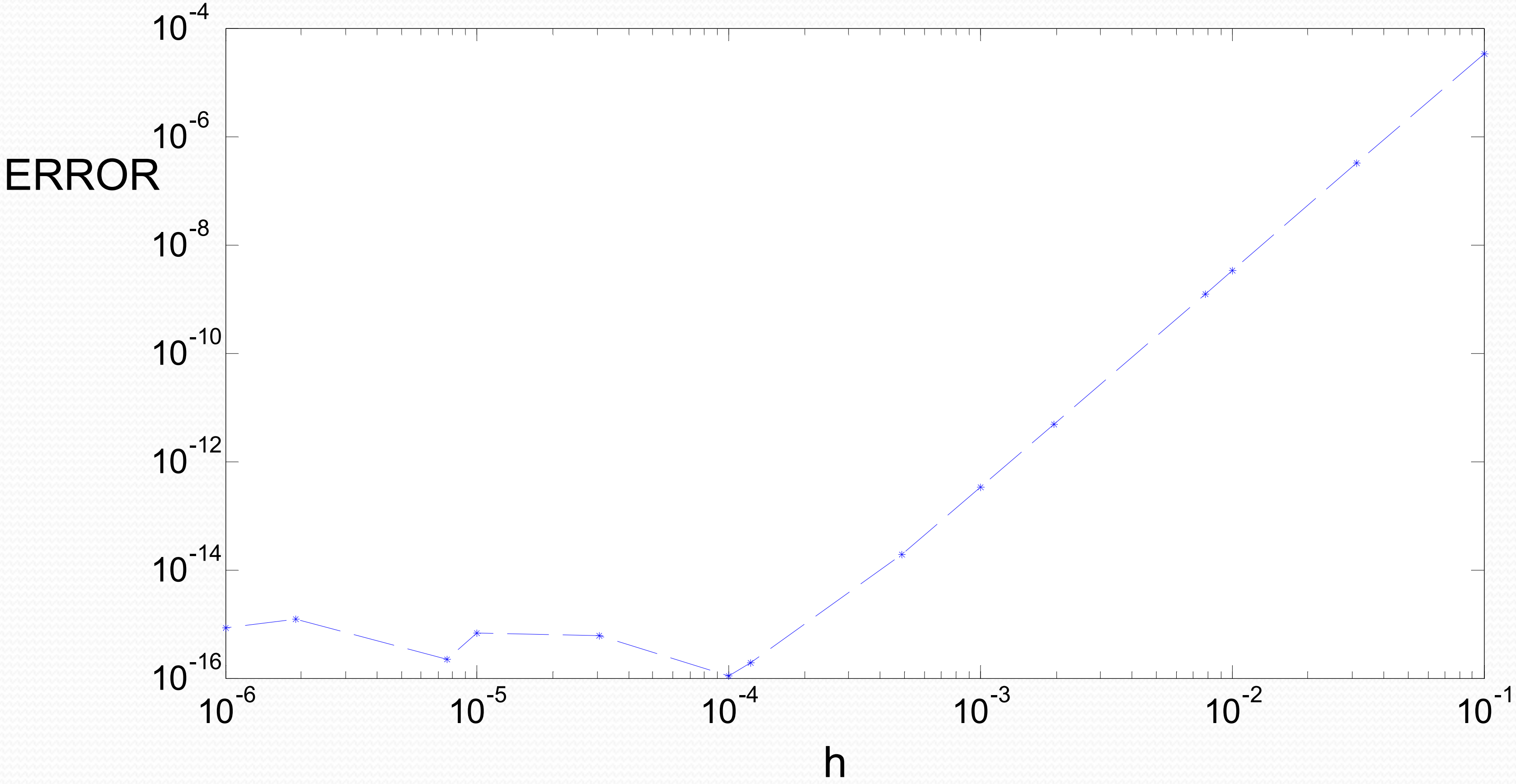


Composite Simpson

$$\int_{x_0}^{x_n} f(x)\,dx \approx \frac{h}{3}[f(x_0) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + f(x_n)]$$



Error of Simpson's Method



Simpson 3/8 RULE

$$\int_{x_0}^{x_n} f(x)\,dx \approx \frac{3h}{8}[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)+$$

$$f(x_3)+3f(x_4)+3f(x_5)+f(x_6)+$$

$$f(x_6)+3f(x_7)+3f(x_8)+f(x_9)+\ldots]$$

$$=\frac{3h}{8}[f(x_0)+3\sum_{j=0}^{n/3-1} f(x_{3j+1})+3\sum_{j=0}^{n/3-1} f(x_{3j+2})+2\sum_{j=1}^{n/3-1} f(x_{3j})+f(x_n)]$$

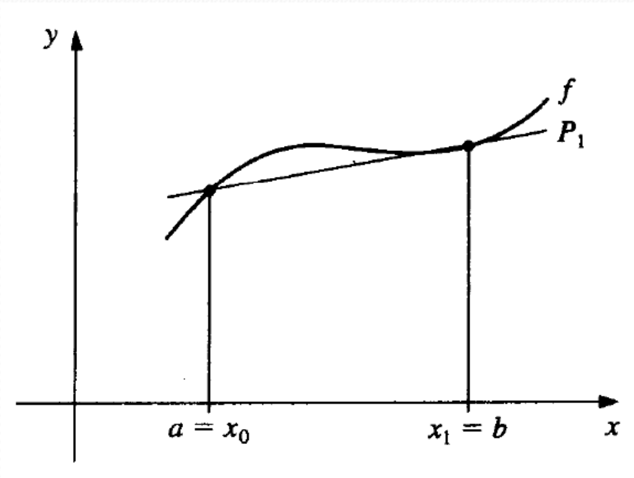
Integration Error

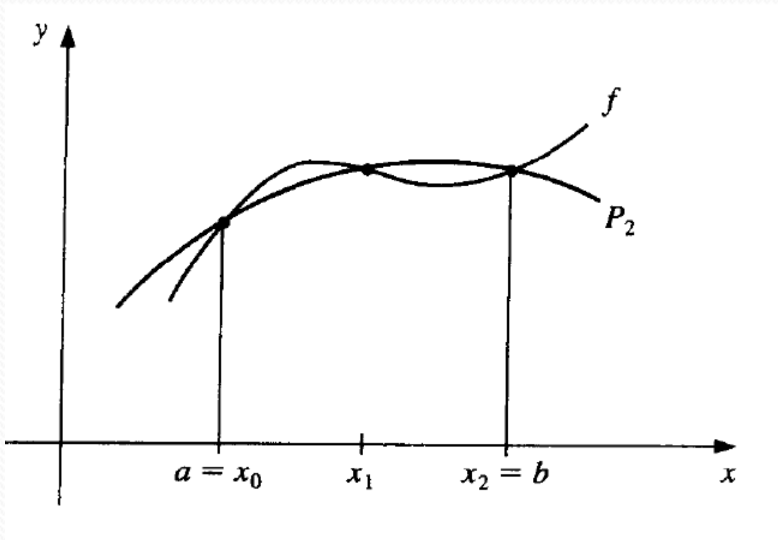
Integration Error

- Absolute Error=
  Round-off Error + Approximation Error

- Round-off Error : Very small

- Approximation Error:





Approximation Error

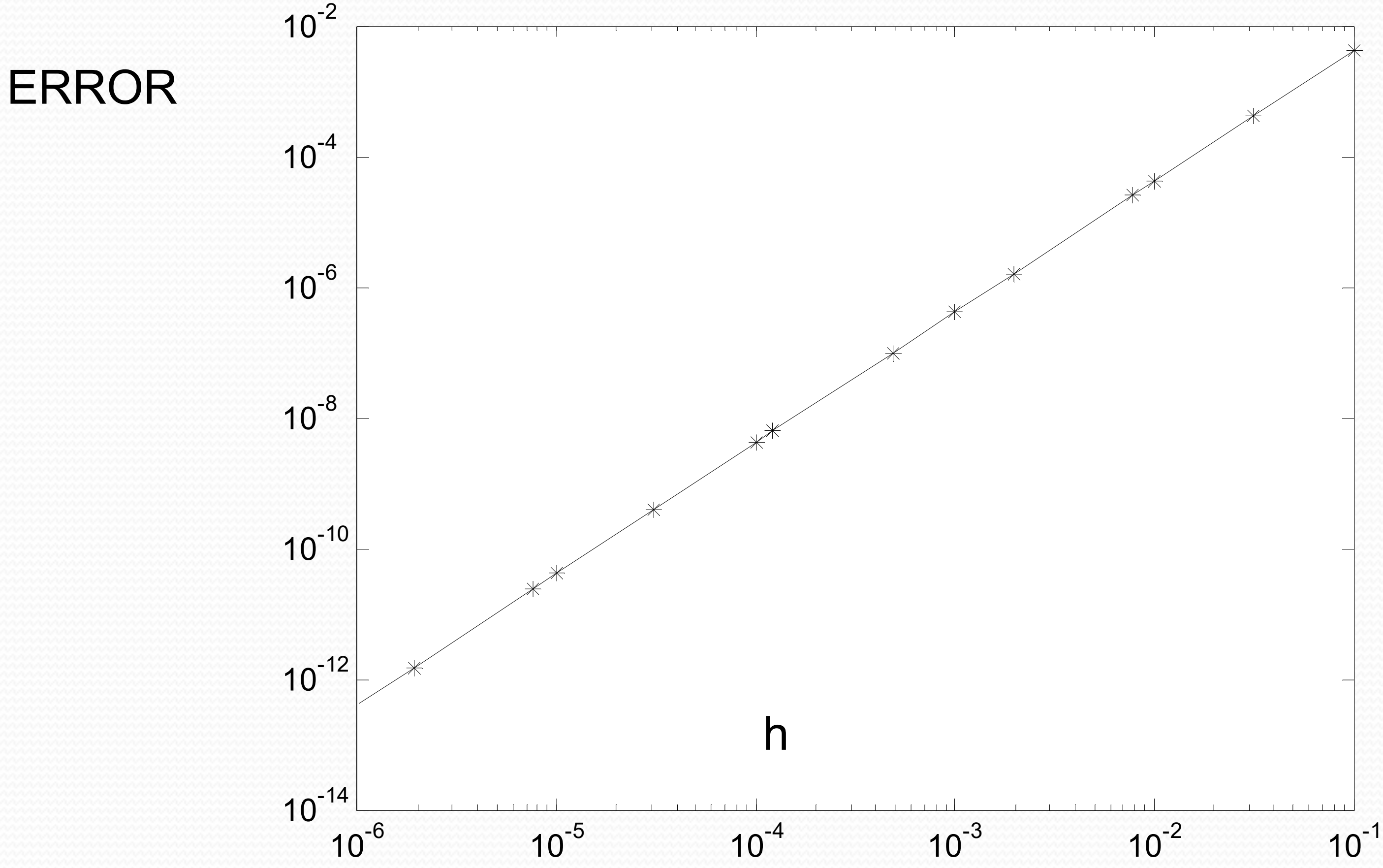
- Polynomial Approximation
  - Riemann Sum : Constant Approximation
  - Trapezoid Method: Linear Approximation

$$E_t = O\left(\frac{[b-a]^3}{N^2}\right) f^{(2)}$$

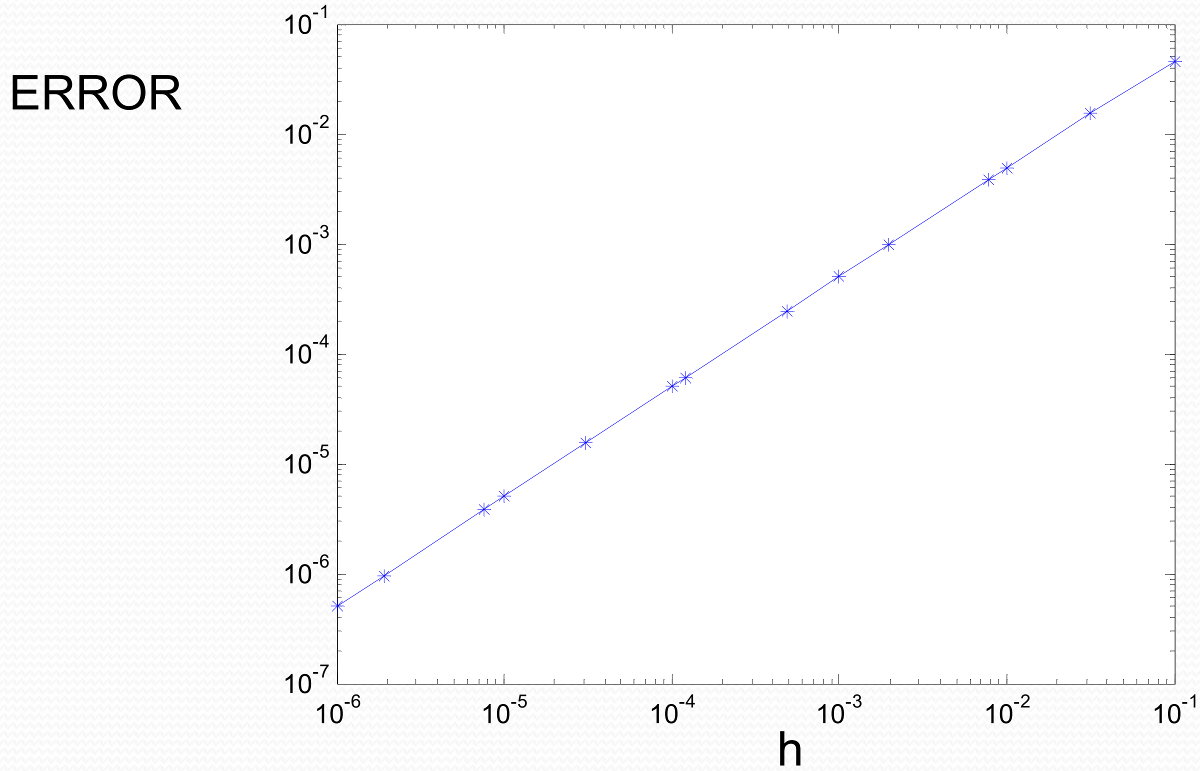
  - Simpson Method : 2nd order approximation

$$E_s = O\left(\frac{[b-a]^5}{N^4}\right) f^{(4)}$$

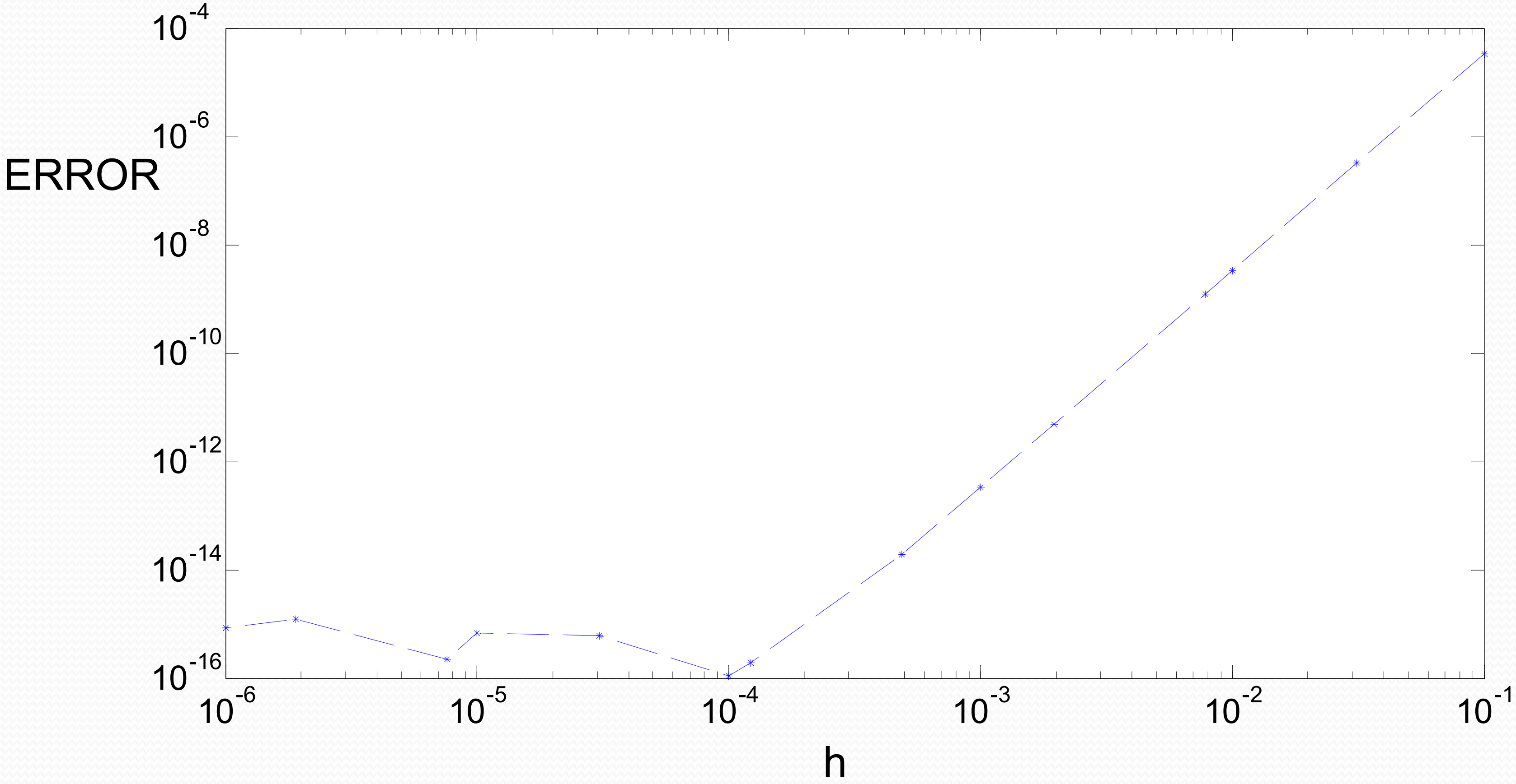
Error of Trapezoid method



Error of finite Riemann Sum



Error of Simpson's Method



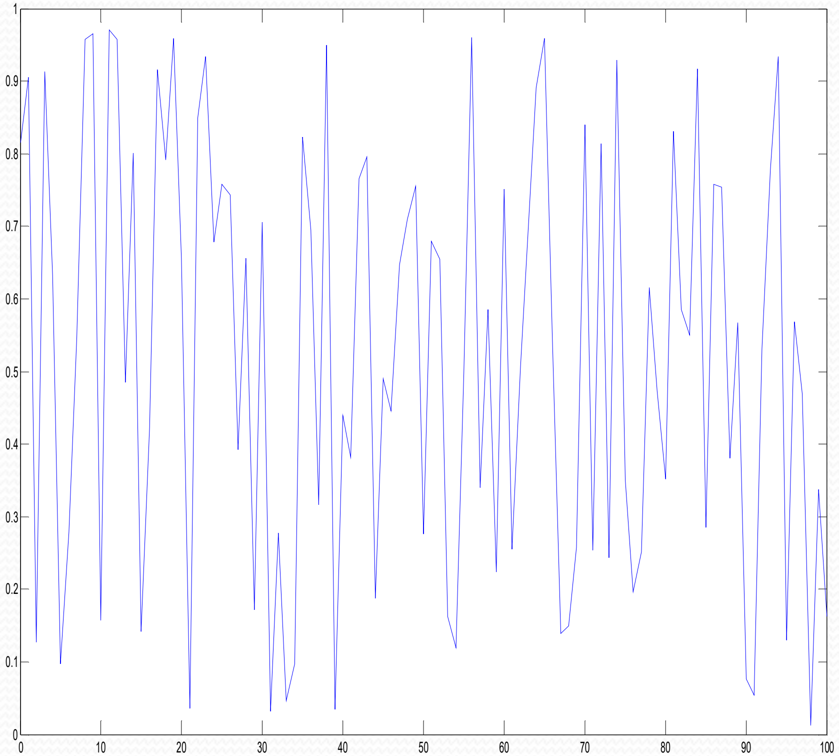
Monte Carlo Integration

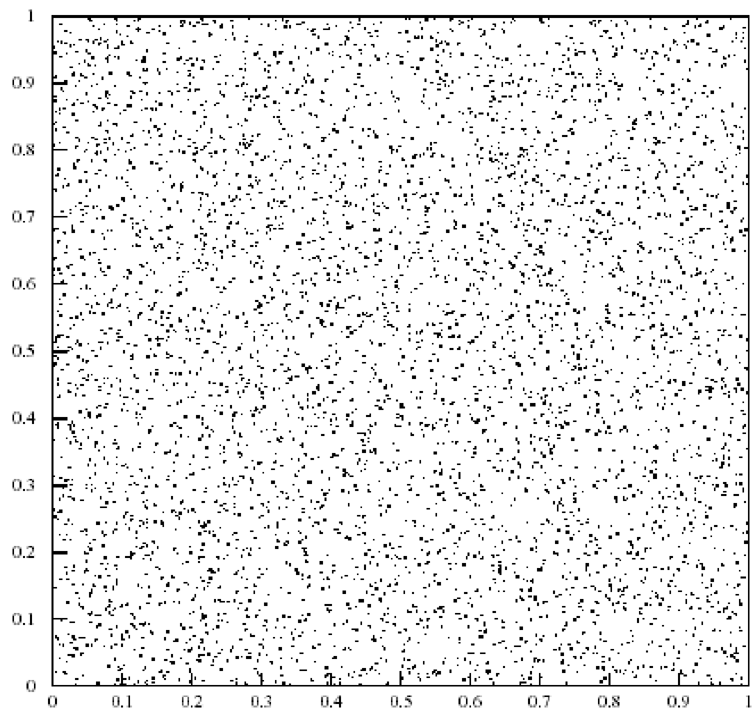
(Random Number Generator)

Random Number Generator

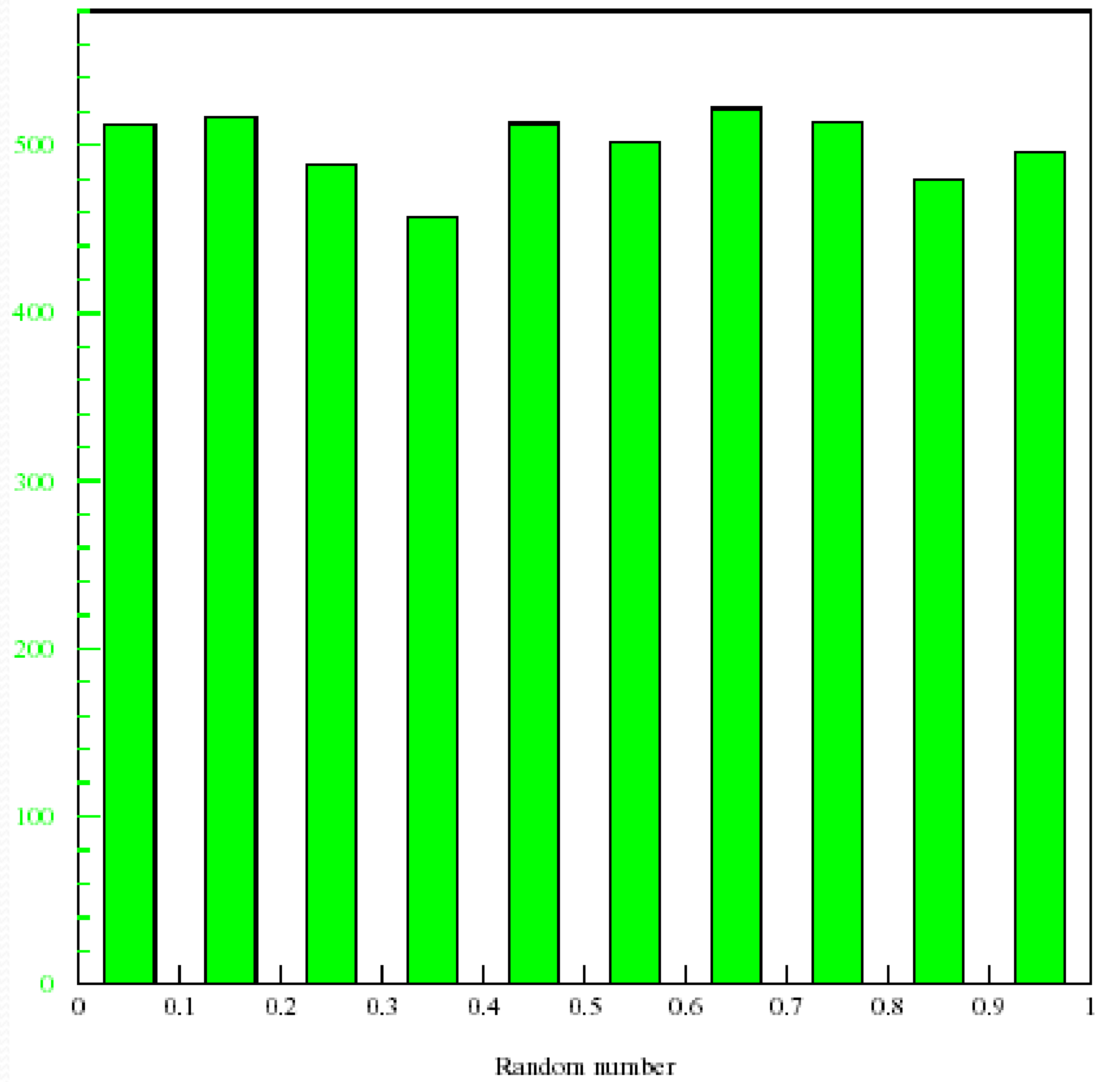
- Table of Random number
- Pseudo Random Number generator using program (in advanced Topic)
  - In Matlab: rand, randn

1D and 2D Distribution of a Random Number Generator





Property of Rand

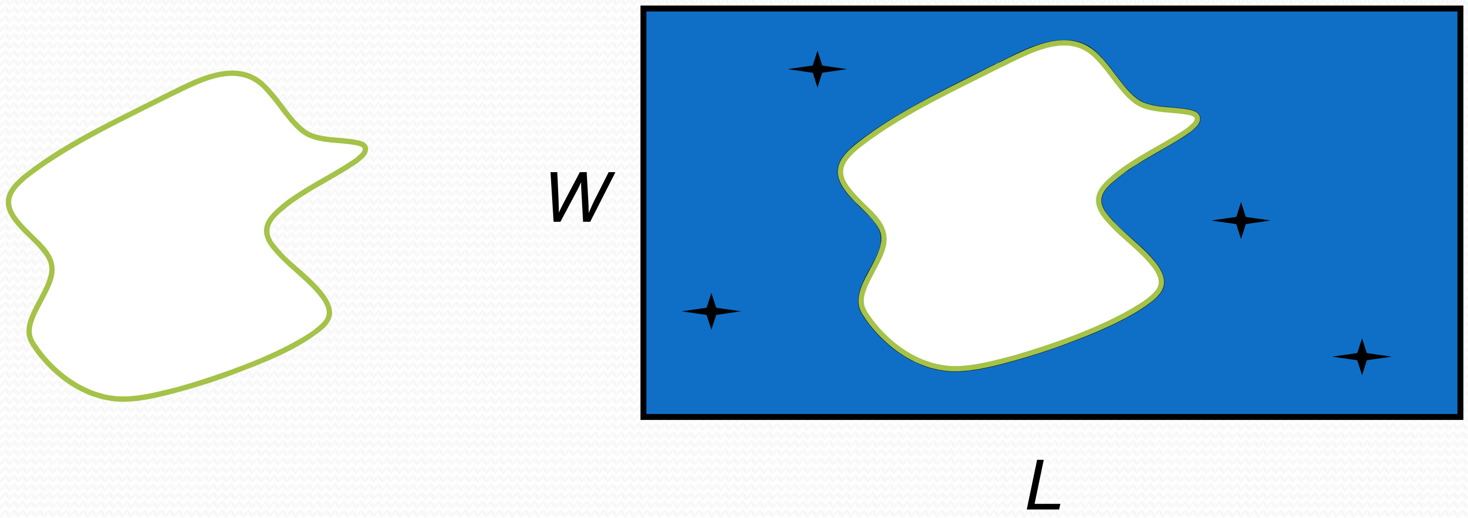


Monte Carlo Integration

The Hit or Miss Method, The Sample-Mean Method

- Hit or Miss Method

Suppose we would like to estimate the surface area of the irregularly shaped small pond



We would try

- Throwing a large number (n) of rocks to land randomly within a rectangular area of width W and Length L.
- Counting the number of 'hits' within the boundary of the pond.
- If the rock throwing was random, then

$$\frac{A_{pond}}{A_{rectangle}} = \frac{n_h}{n}$$

$$A_{pond} = \frac{n_h}{n}\left(W \times L\right)$$

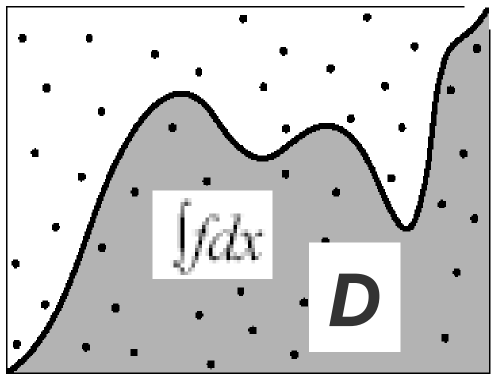
- The accuracy of such methods is poor for small n (number of trials), but the methods become exact as $n \to \infty$.

Monte-Carlo Integration

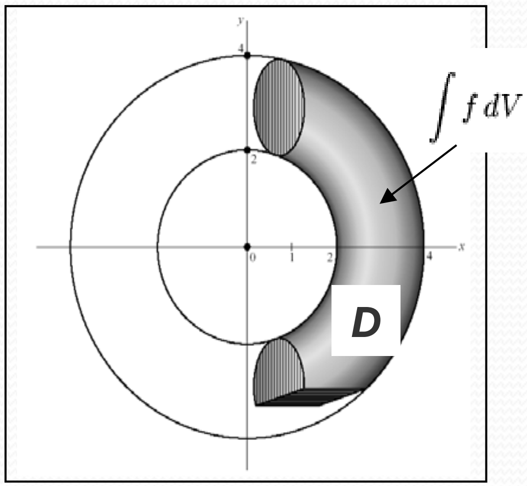
- **Integrate a function over a complicated domain**
  - **D: complicated domain.**
  - **D': Simple domain, superset of D.**
- **Pick random points over D':**
- **Counting: N: points over D**
- **N': points over D'**

$$\frac{Volume_D}{Volume_{D'}} \approx \frac{N}{N'}$$

***D':* rectangular**



***D':* circle**



Estimating π using Monte Carlo

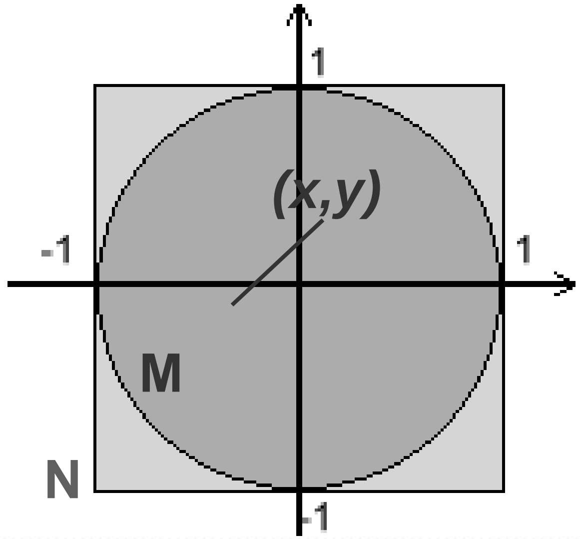
- **The probability of a random point lying inside the unit circle:**

$$\mathbf{P}\left(x^2+y^2<1\right)=\frac{A_{circle}}{A_{square}}=\frac{\pi}{4}$$

- **If pick a random point *N* times and *M* of those times the point lies inside the unit circle:**

$$\mathbf{P}^{\circ}\left(x^2+y^2<1\right)=\frac{M}{N}$$

- **If *N* becomes very large, P=P°**



$$\pi=\frac{4\cdot M}{N}$$

Estimating π using Monte Carlo

- Results:
  - N = 10,000 Pi= 3.104385
  - N = 100,000 Pi= 3.139545
  - N = 1,000,000 Pi= 3.139668
  - N = 10,000,000 Pi= 3.141774
  - …