

Physics 77

Introduction to Computational Techniques in Physics
Spring 2019

Numerical Integration
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See also Python workbook [Lecture08b.ipynb](#)

What is numerical integration really calculating?

- Consider the definite integral

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

- The integral can be approximated by weighted sum

$$I \approx \sum_{i=1}^n \omega_i f(x_i) \Delta x_i$$

- The ω_i are weights, and the x_i are abscissas
- Assuming that f is finite and continuous on the interval $[a,b]$ numerical integration leads to a unique solution
- The goal of any numerical integration method is to choose abscissas and weights such that errors are minimized for the smallest n possible for a given function

Numerical Integration

- What are the choices of evaluation points, x_i 's and weights w_i 's such that:

$$\int_a^b f(x)dx \approx \sum_{i=0}^n w_i f(x_i)\Delta x_i$$

- In general we have two sets of degree of freedom:
 - The spacing of evaluation points.
 - The weighted importance of each point.

Numerical Integration

- Numerical integration Methods:
 1. Upper and Lower Sums
 2. Newton-Cotes Methods:
 - a) Trapezoid Rule
 - b) Simpson Rules
 3. Romberg Method
 4. Gauss Quadrature

Upper and Lower Sums

The interval is divided into subintervals


$$\text{Partition } P = \{a = x_0 \leq x_1 \leq x_2 \leq \dots \leq x_n = b\}$$

Define

$$m_i = \min \{f(x) : x_i \leq x \leq x_{i+1}\}$$


$$M_i = \max \{f(x) : x_i \leq x \leq x_{i+1}\}$$

Lower sum

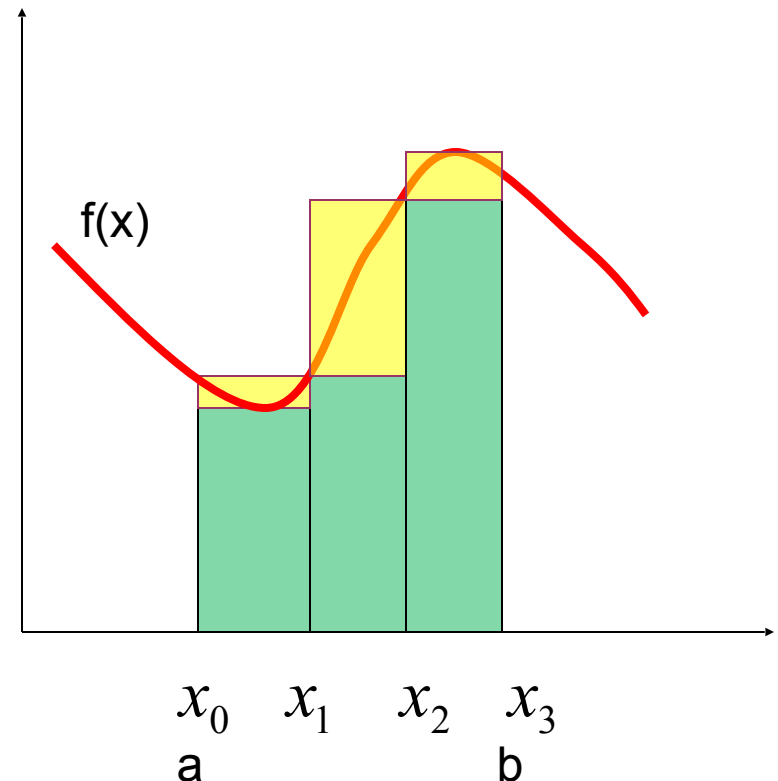


$$L(f, P) = \sum_{i=0}^{n-1} m_i (x_{i+1} - x_i)$$

Upper sum



$$U(f, P) = \sum_{i=0}^{n-1} M_i (x_{i+1} - x_i)$$



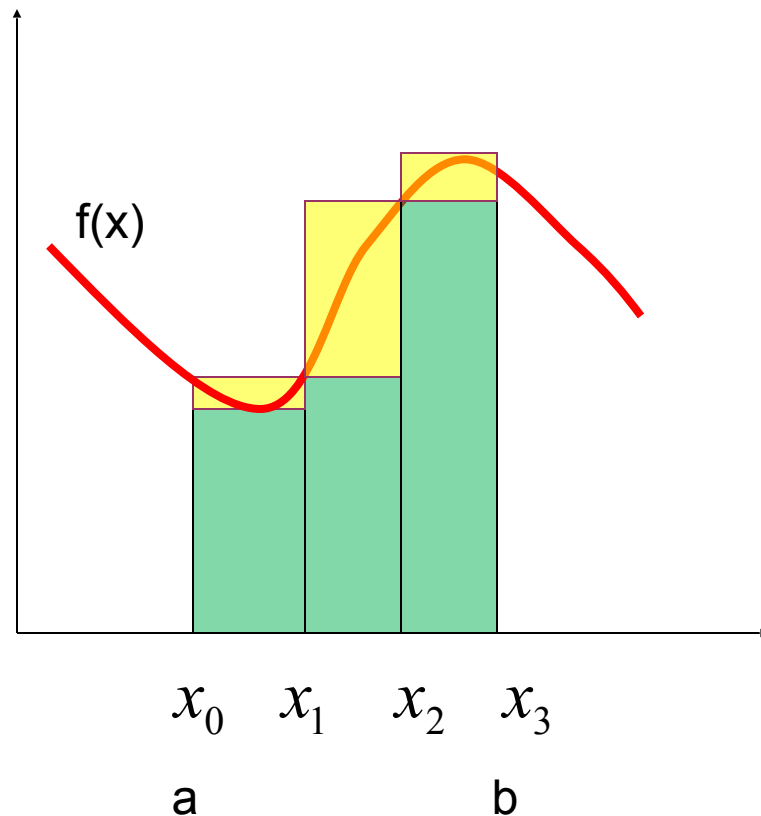
Upper and Lower Sums

Lower sum $L(f, P) = \sum_{i=0}^{n-1} m_i (x_{i+1} - x_i)$

Upper sum $U(f, P) = \sum_{i=0}^{n-1} M_i (x_{i+1} - x_i)$

Estimate of the integral $= \frac{L + U}{2}$

$Error \leq \frac{U - L}{2}$



Example

$$\int_0^1 x^2 dx = 1/3 \text{ (true value)}$$

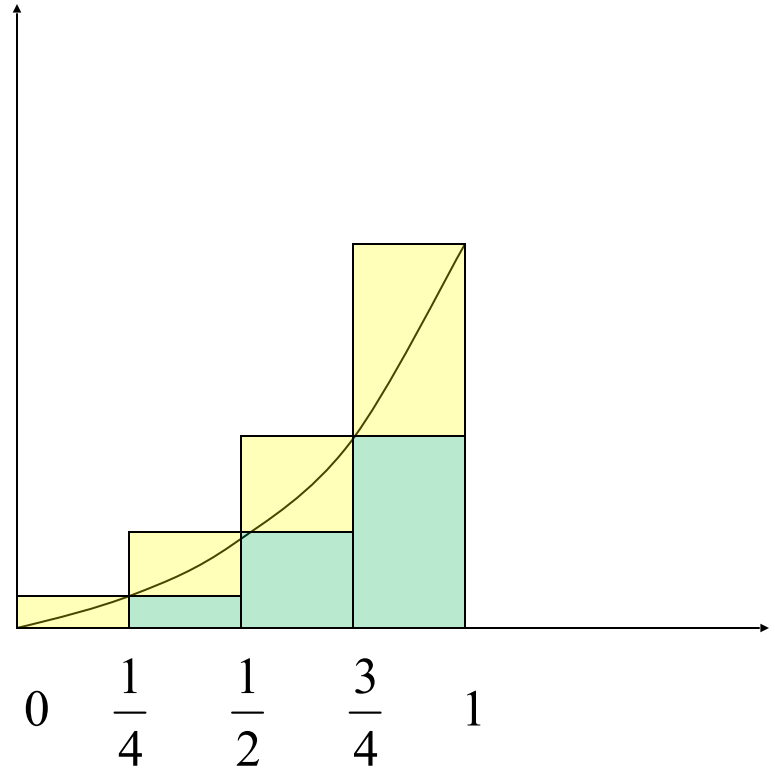
$$\text{Partition } P = \left\{0, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, 1\right\}$$

$n = 4$ (four equal intervals)

$$m_0 = 0, \quad m_1 = \frac{1}{16}, \quad m_2 = \frac{1}{4}, \quad m_3 = \frac{9}{16}$$

$$M_0 = \frac{1}{16}, \quad M_1 = \frac{1}{4}, \quad M_2 = \frac{9}{16}, \quad M_3 = 1$$

$$x_{i+1} - x_i = \frac{1}{4} \quad \text{for } i = 0, 1, 2, 3$$



Example

$$\text{Lower sum } L(f, P) = \sum_{i=0}^{n-1} m_i (x_{i+1} - x_i)$$

$$L(f, P) = \frac{1}{4} \left[0 + \frac{1}{16} + \frac{1}{4} + \frac{9}{16} \right] = \frac{14}{64}$$

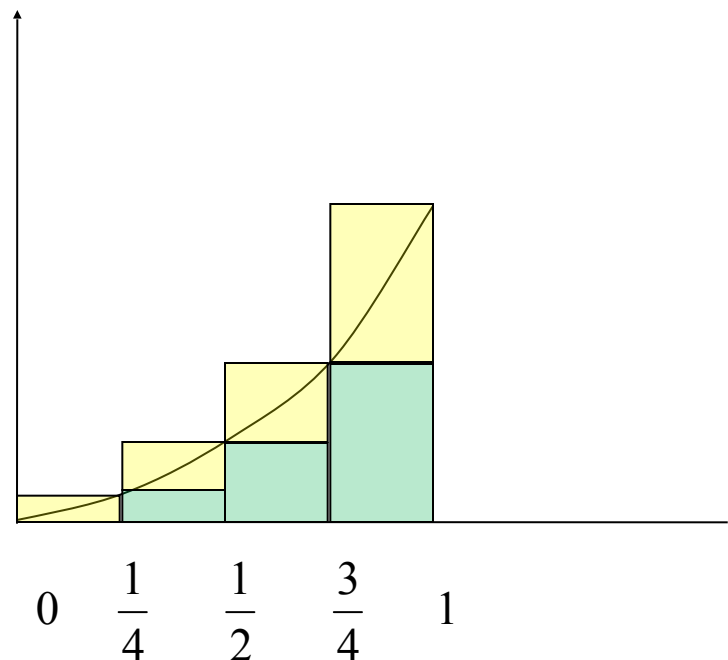
$$\text{Upper sum } U(f, P) = \sum_{i=0}^{n-1} M_i (x_{i+1} - x_i)$$

$$U(f, P) = \frac{1}{4} \left[\frac{1}{16} + \frac{1}{4} + \frac{9}{16} + 1 \right] = \frac{30}{64}$$

$$\text{Estimate of the integral} = \frac{1}{2} \left(\frac{30}{64} + \frac{14}{64} \right) = \frac{11}{32}$$

$$\text{Error} < \frac{1}{2} \left(\frac{30}{64} - \frac{14}{64} \right) = \frac{1}{8}$$

Estimate - True_Value = 0.01 << Error_Estimate



Upper and Lower Sums

- Estimates based on Upper and Lower Sums are easy to obtain for monotonic functions (**always increasing or always decreasing**).
- For non-monotonic functions, finding maximum and minimum of the function can be difficult and other methods can be more attractive.

Newton-Cotes Methods

- In **Newton-Cote Methods**, the function is approximated by a **polynomial of order n**
- Computing the integral of a polynomial is easy.

$$\int_a^b f(x)dx \approx \int_a^b (a_0 + a_1x + \dots + a_nx^n)dx$$

$$\int_a^b f(x)dx \approx a_0(b-a) + a_1 \frac{(b^2 - a^2)}{2} + \dots + a_n \frac{(b^{n+1} - a^{n+1})}{n+1}$$

Newton-Cotes Methods

- **Trapezoid Method** (First Order Polynomial are used)

$$\int_a^b f(x)dx \approx \int_a^b (a_0 + a_1x)dx$$

- **Simpson 1/3 Rule** (Second Order Polynomial are used),

$$\int_a^b f(x)dx \approx \int_a^b (a_0 + a_1x + a_2x^2)dx$$

Trapezoid Method

Derivation-One interval

$$I = \int_a^b f(x)dx \approx \int_a^b \left(f(a) + \frac{f(b) - f(a)}{b - a} (x - a) \right) dx$$

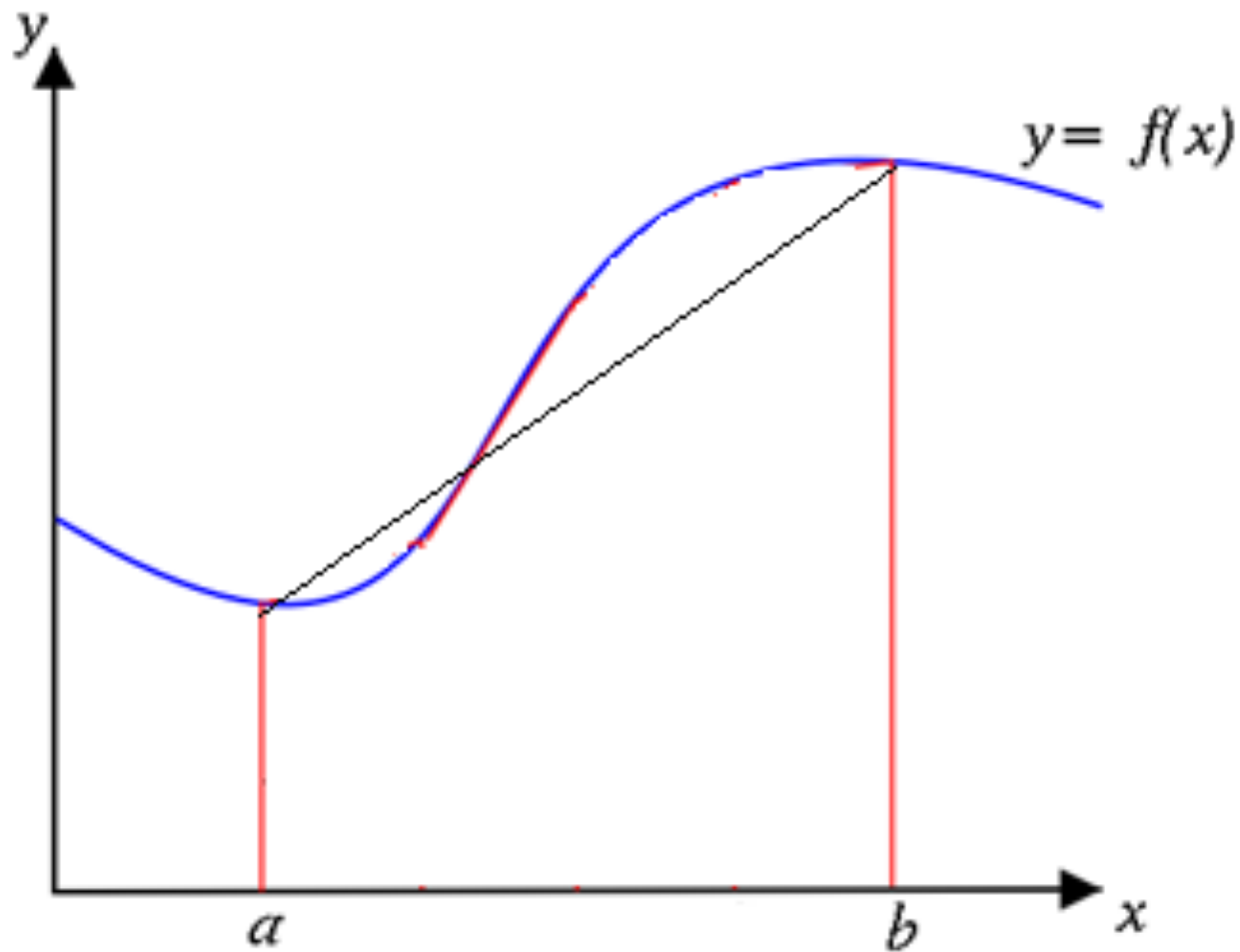
$$I \approx \int_a^b \left(f(a) - a \frac{f(b) - f(a)}{b - a} + \frac{f(b) - f(a)}{b - a} x \right) dx$$

$$= \left(f(a) - a \frac{f(b) - f(a)}{b - a} \right) x \Big|_a^b + \frac{f(b) - f(a)}{b - a} \frac{x^2}{2} \Big|_a^b$$

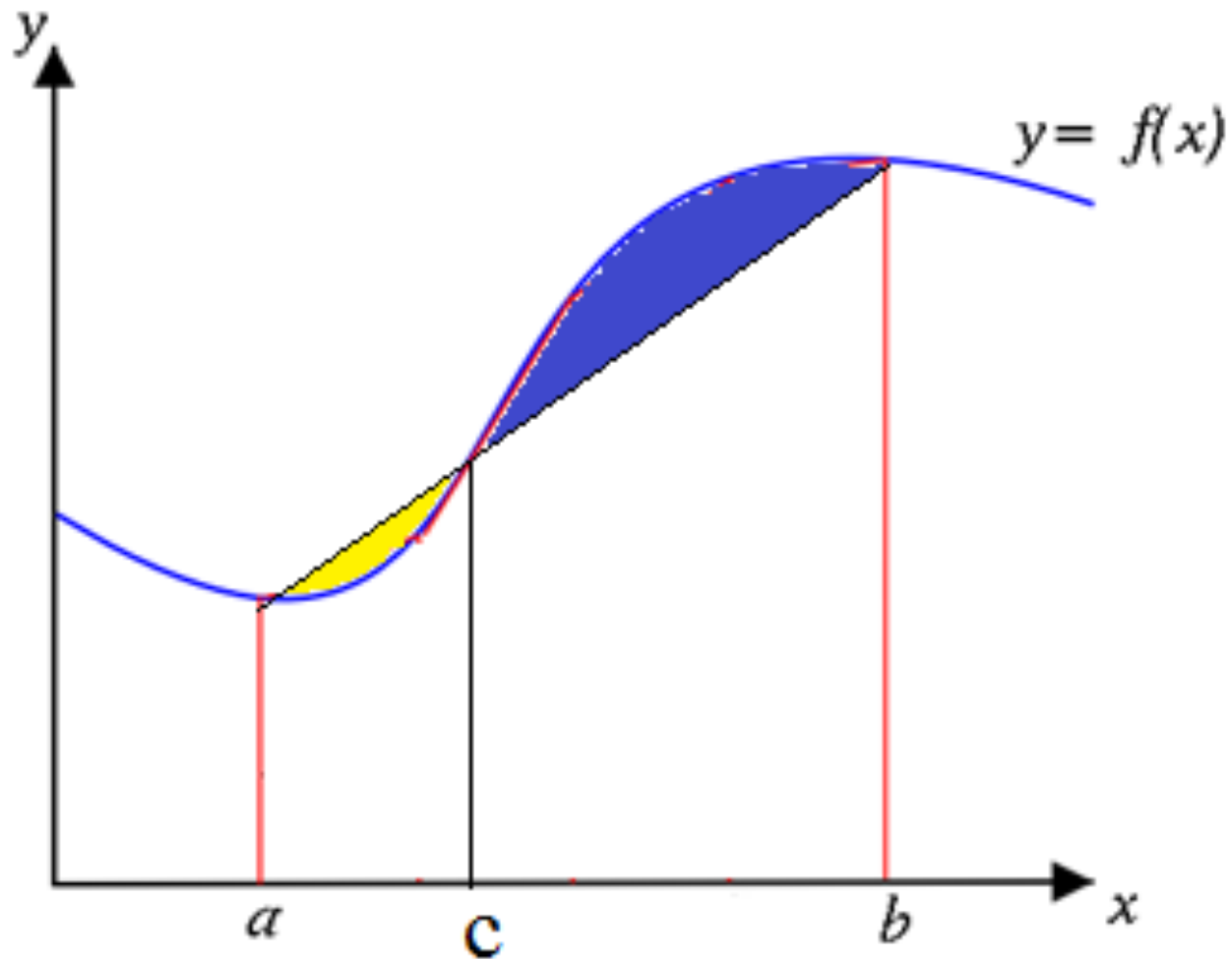
$$= \left(f(a) - a \frac{f(b) - f(a)}{b - a} \right) (b - a) + \frac{f(b) - f(a)}{2(b - a)} (b^2 - a^2)$$

$$= (b - a) \frac{f(b) + f(a)}{2}$$

Trapezoid Rule

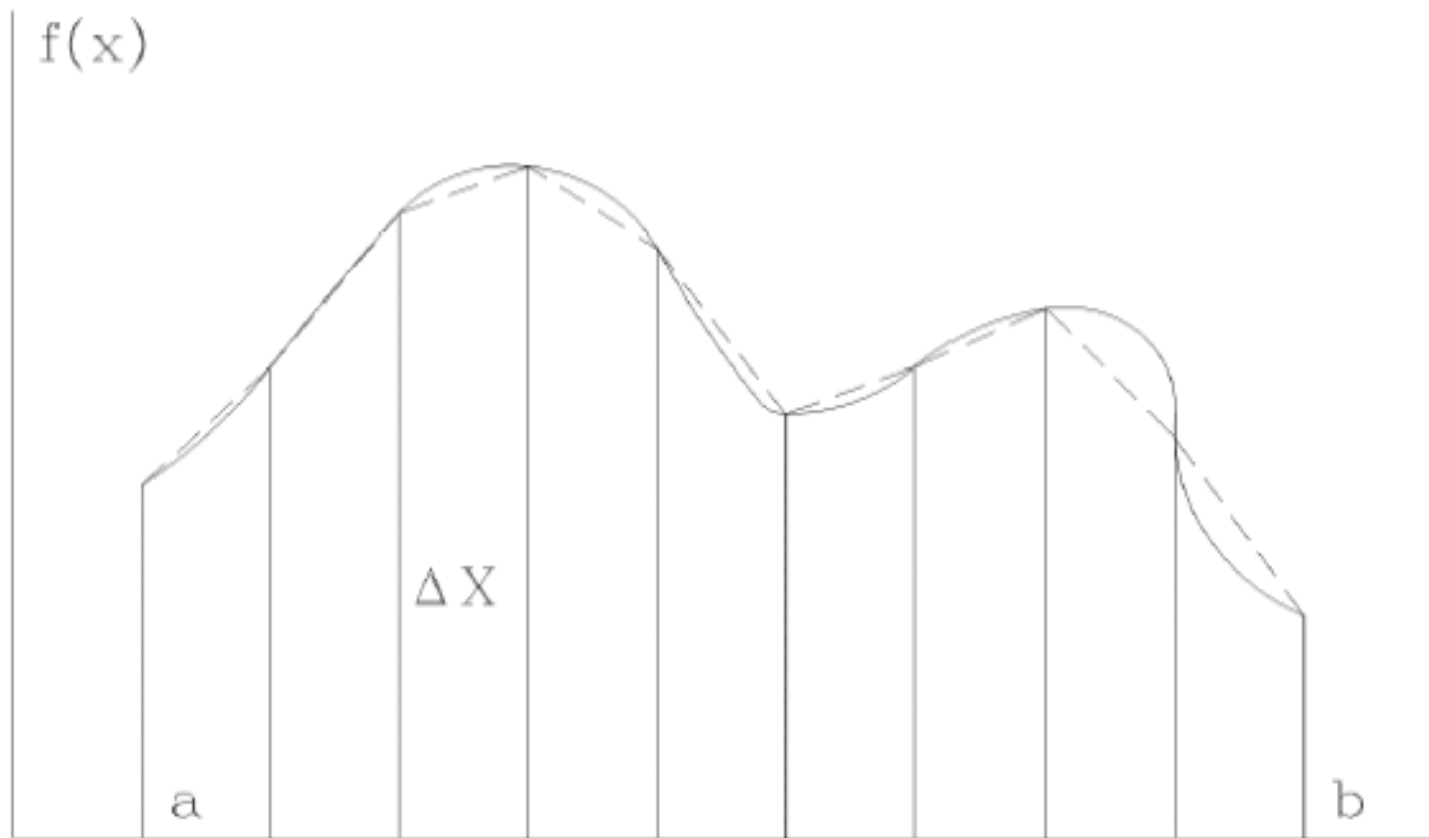


Trapezoid Rule

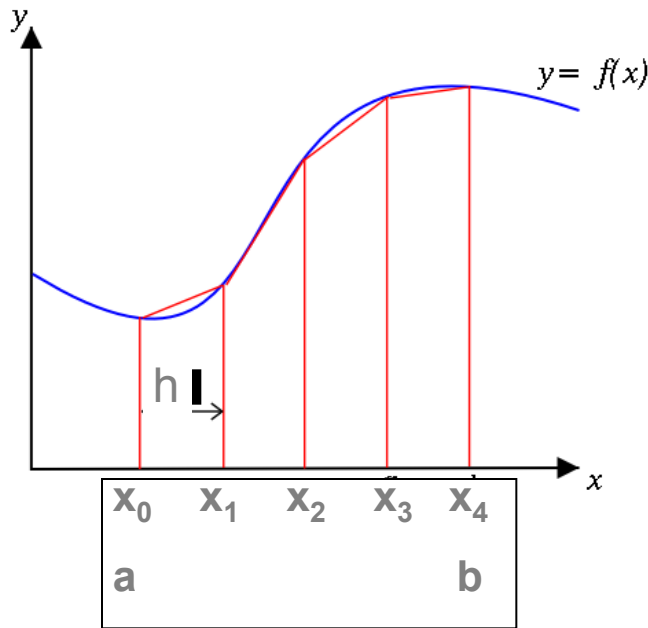


Numerical Integration

- Composite Trapezoid Rule



Trapezoid Rule



- Approximate integral using the areas of the trapezoids

$$\begin{aligned}
 \int_a^b f(x) dx &\cong \sum \text{area of trapezoids} \\
 &= h \frac{f(x_0) + f(x_1)}{2} + h \frac{f(x_1) + f(x_2)}{2} \\
 &\quad + h \frac{f(x_2) + f(x_3)}{2} + h \frac{f(x_3) + f(x_4)}{2} \\
 &= \frac{h}{2} [f(x_0) + 2f(x_1) + 2f(x_2) + 2f(x_3) + f(x_4)] \\
 &= \frac{h}{2} [f(x_0) + f(x_4)] + h[f(x_1) + f(x_2) + f(x_3)]
 \end{aligned}$$

For n intervals this generalizes to

$$\int_a^b f(x) dx \cong \frac{h}{2} [f(a) + f(b)] + h \sum_{i=1}^{n-1} f(x_i) \quad (1)$$

The trapezoidal rule.

Numerical Integration

- Trapezoid Rule

$$\int_a^b f(x)dx = \sum_{i=1}^{n-1} \frac{f(x_{i+1}) + f(x_i)}{2} \Delta x_i$$

$$\Delta x_i = (b - a) / (n - 1)$$

- So the weights are:

$$\{w_i\}_{i=0}^N : w_i \begin{cases} 0.5 & i = 0, N \\ 1 & \textit{otherwise} \end{cases}$$

Simpson's Rule

- Trapezoidal rule was based on approximating the integrand by a first order polynomial, and then integrating the line over the interval.
- Simpson's 1/3rd rule is an extension of Trapezoidal rule where the integrand is approximated by a second order polynomial.

$$I = \int_a^b f(x) dx \approx \int_a^b f_2(x) dx$$

Where $f_2(x)$ is a second order polynomial.

$$f_2(x) = a_0 + a_1x + a_2x^2$$

Simpson's Rule

- Simpson's rule:

$$\int_a^b f(x)dx = \frac{\Delta x}{3} [f(a) + 4f(a + \Delta x) + f(b)]$$

where $\Delta x = \frac{b-a}{2}$

- Simpson's rule can only be applied when there are an even number of subintervals:

$$\int_{x_1}^{x_n} f(x)dx \approx \sum_{i=1,3,5}^{n-2} \frac{x_{i+1} - x_i}{3} [f(x_i) + 4f(x_{i+1}) + f(x_{i+2})]$$

Composite Simpson's Rule

- The Simpson's rule for x_0, x_1, x_2 is given as:

$$\int_{x_0}^{x_2} p_1(x)dx = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)]$$

- We can do the same on x_2, x_3, x_4 to get

$$\int_{x_2}^{x_4} p_1(x)dx = \frac{h}{3} [f(x_2) + 4f(x_3) + f(x_4)]$$

- Hence on the entire region

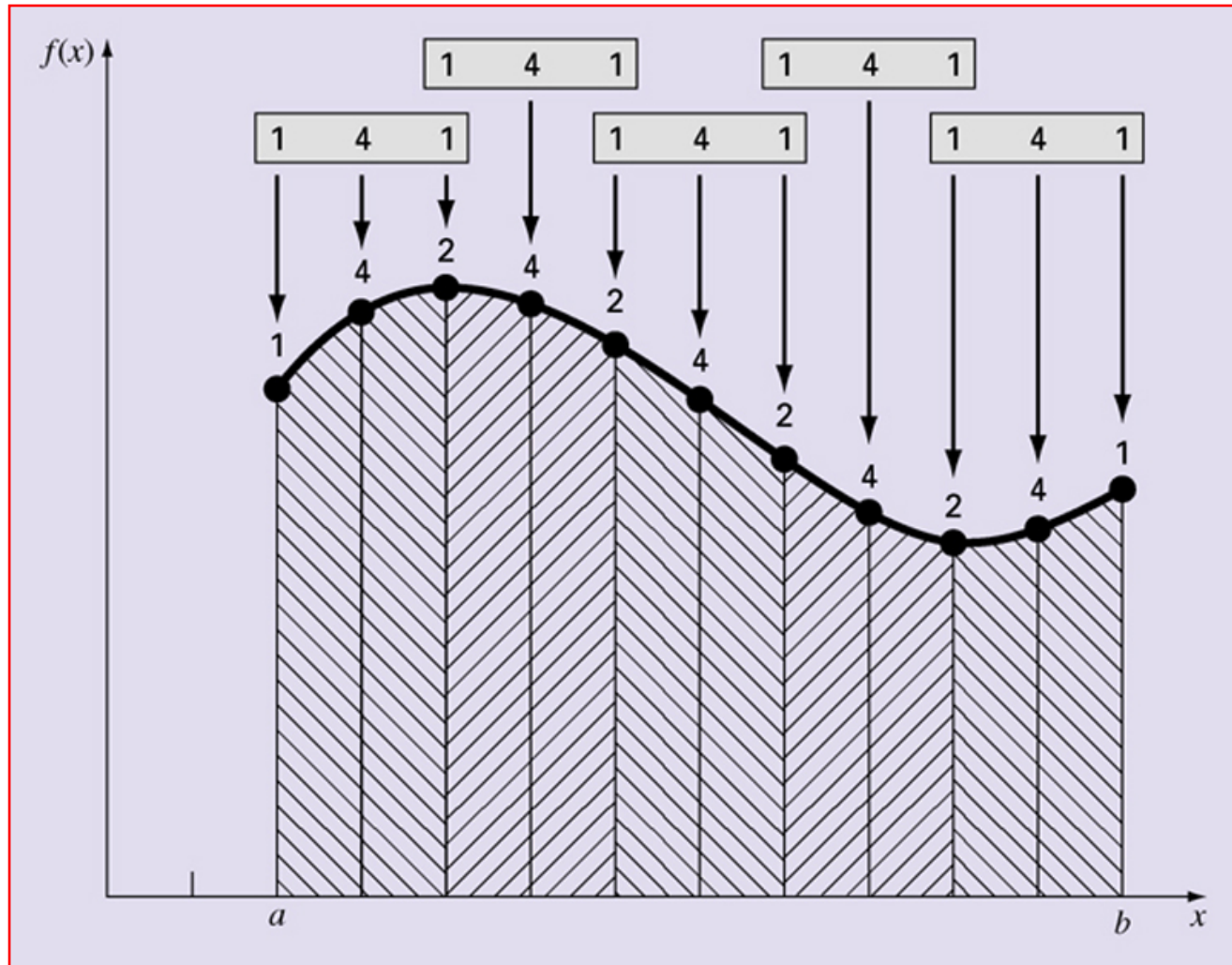
$$\int_{x_0}^{x_4} f(x)dx \cong \frac{h}{3} [f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)]$$

- In general for an even number of intervals n

$$\int_a^b f(x)dx \cong \frac{h}{3} [f(a) + f(b)] + \frac{4h}{3} \sum_{i=1}^{n/2} f(x_{2i-1}) + \frac{2h}{3} \sum_{i=1}^{n/2-1} f(x_{2i})$$

This is "Simpson's Composite Rule"

Composite Simpson's 1/3 Rule



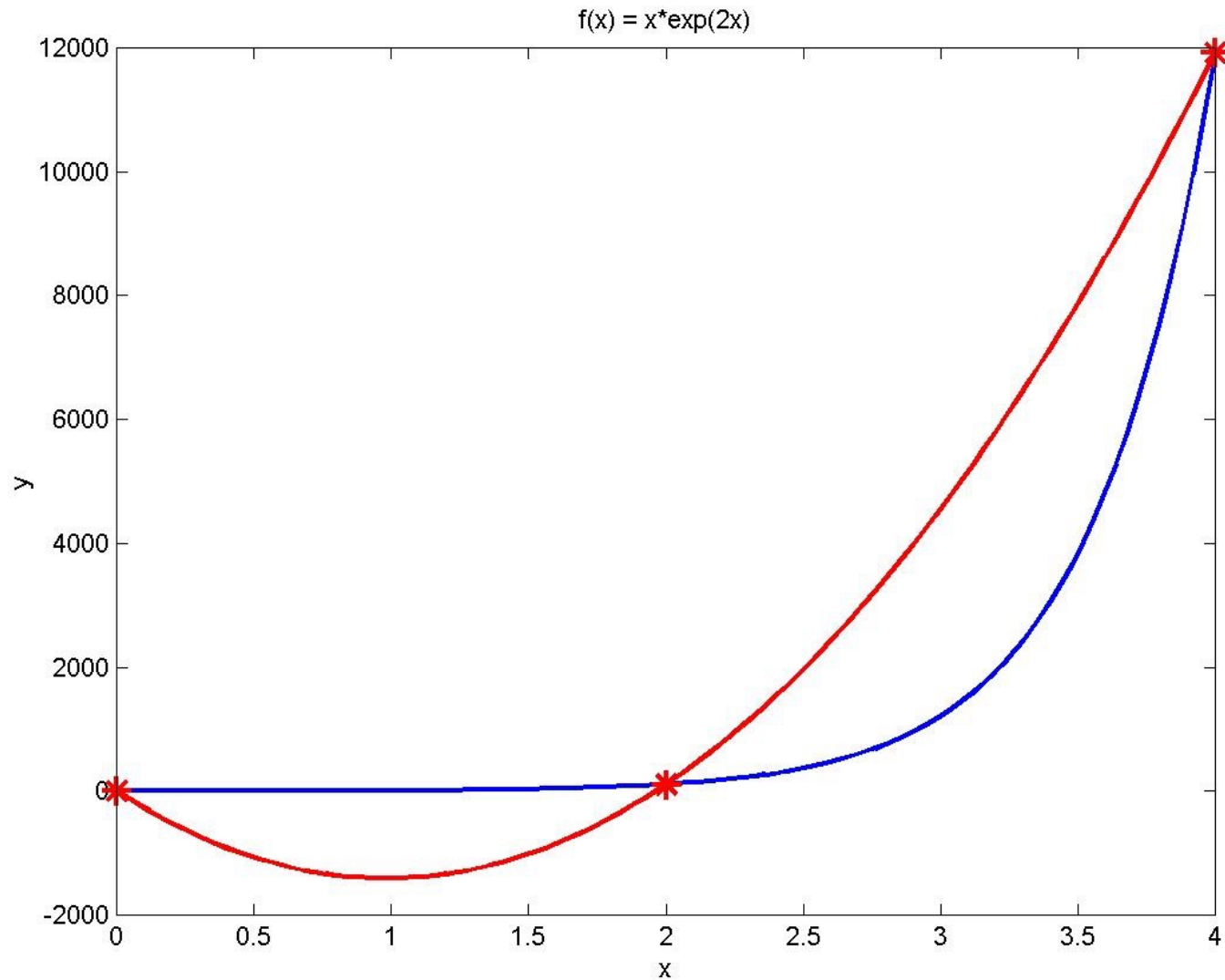
- Applicable only if the number of segments is even

Weights in Simpson's Rule

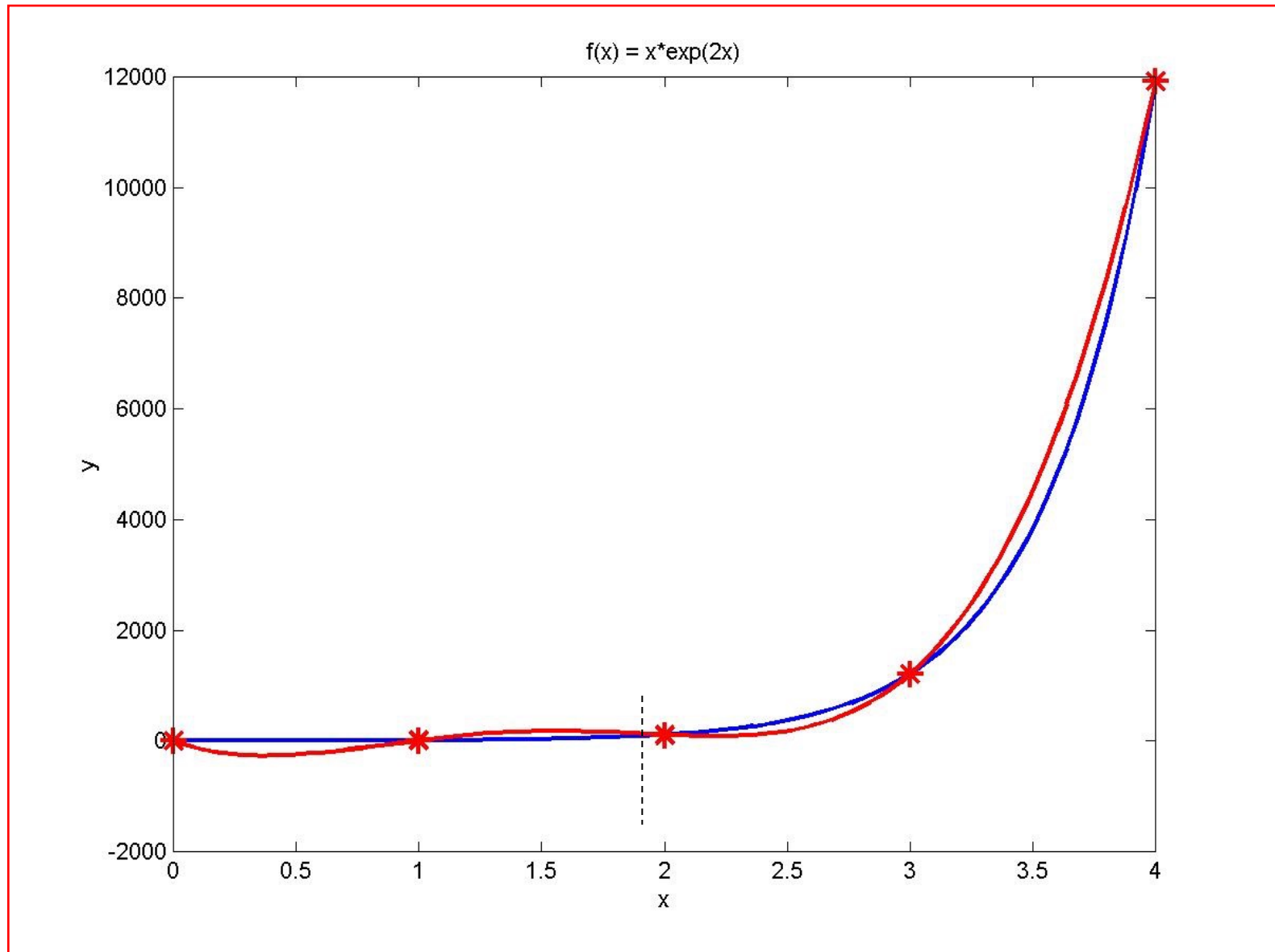
- For 1/3 Simpson' Rule the weights are:

$$\{w_i\}_{i=0}^N : w_i \left\{ \begin{array}{ll} 1/3 & \text{end points} \\ 4/3 & \text{odd points} \\ 2/3 & \text{even points} \end{array} \right\}$$

Simpson's 1/3 Rule



Composite Simpson's 1/3 Rule



Higher order fits

- Can increase the order of the fit to cubic, quartic etc.
- For a cubic fit over x_0, x_1, x_2, x_3 we find

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

Simpson's 3/8th Rule

- For a quartic fit over x_0, x_1, x_2, x_3, x_4

$$\int_{x_0}^{x_4} f(x) dx \cong \frac{2h}{45} [7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)]$$

Boole's Rule

- In practice these higher order formulas are not that useful, we can devise better methods if we first consider the errors involved

Error in the Trapezoid Rule

- Consider a Taylor expansions of $f(x)$ about a

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!} f''(a) + \frac{(x-a)^3}{3!} f'''(a) + \dots$$

- The integral of $f(x)$ written in this form is then

$$\begin{aligned} \int_a^b f(x) dx &= \left[xf(a) + \frac{(x-a)^2}{2!} f'(a) + \frac{(x-a)^3}{3!} f''(a) + \frac{(x-a)^4}{4!} f'''(a) \right. \\ &\quad \left. + \frac{(x-a)^5}{5!} f^{(4)}(a) + \dots \right]_a^b \\ &= hf(a) + \frac{h^2}{2} f'(a) + \frac{h^3}{6} f''(a) + \frac{h^4}{24} f'''(a) + \dots \quad (1) \quad \text{where } h=b-a \end{aligned}$$

Error in the Trapezoid Rule

- Perform the same expansion about b

$$\int_a^b f(x)dx = hf(b) - \frac{h^2}{2} f'(b) + \frac{h^3}{6} f''(b) - \frac{h^4}{24} f'''(b) + \dots \quad (2)$$

- If we take an average of (1) and (2) then

$$\begin{aligned} \int_a^b f(x)dx = & \frac{h}{2} [f(a) + f(b)] + \frac{h^2}{4} [f'(a) - f'(b)] + \frac{h^3}{12} [f''(a) + f''(b)] \\ & + \frac{h^4}{48} [f'''(a) - f'''(b)] + \frac{h^5}{240} [f^{iv}(a) + f^{iv}(b)] + \dots \quad (3) \end{aligned}$$

- Notice that odd derivatives are differenced while even derivatives are added

Error in the Trapezoid Rule

- We also make Taylor expansions of f' and f''' around both a & b , which allow us to substitute for terms in f'' and f^{iv} and to derive

$$\int_a^b f(x)dx = \frac{h}{2}[f(a) + f(b)] + \frac{h^2}{12}[f'(a) - f'(b)] + \frac{h^4}{720}[f'''(a) - f'''(b)] + \dots \quad (10)$$

- It takes *quite a bit of work* to get to this point, but the key issue is that we have now created correction terms which are all *differences*
- If we now use this formula in the composite trapezoid rule there will be a large number of cancellations

Error in the Composite Trapezoid

- We now sum over a series of trapezoids to get

$$\begin{aligned}
 \int_a^b f(x)dx &= \frac{h}{2}[(f(a) + f(x_1)) + (f(x_1) + f(x_2)) + \dots + (f(x_{n-2}) + f(x_{n-1})) + (f(x_{n-1}) + f(b))] \\
 &+ \frac{h^2}{12}[(f'(a) - f'(x_1)) + (f'(x_1) - f'(x_2)) + \dots + (f'(x_{n-2}) - f'(x_{n-1})) + (f'(x_{n-1}) - f'(b))] \\
 &+ \frac{h^4}{720}[(f'''(a) - f'''(x_1)) + (f'''(x_1) - f'''(x_2)) + \dots + (f'''(x_{n-2}) - f'''(x_{n-1})) + (f'''(x_{n-1}) - f'''(b))] \\
 &+ \dots \\
 &= \frac{h}{2}[f(a) + f(b)] + h \sum_{i=1}^{n-1} f(a + ih) + \frac{h^2}{12}[f'(a) - f'(b)] + \frac{h^4}{720}[f'''(a) - f'''(b)] + \dots \quad (11)
 \end{aligned}$$

- Note now $h=(b-a)/n$
- The expansion is in powers of h^{2i}

Error in estimating the integral

Error in estimating the integral

Assumption : $f'(x)$ is continuous on $[a,b]$

Equal intervals (width = h)

Theorem : If Trapezoid Method is used to

approximate $\int_a^b f(x)dx$ then

$$Error = \frac{b-a}{12} h^2 (f'(b) - f'(a))$$

$$|Error| \leq \frac{b-a}{12} h^2 \max_{x \in [a,b]} |f'(x)|$$

Estimating the Error

For Trapezoid method

- How many equally spaced intervals are needed to compute:
- To 5 decimal points accuracy?

Estimating the Error

For Trapezoid method

- How many equally spaced intervals are needed to compute:

$$\int_0^{\pi} \sin(x) dx$$

- To 5 decimal points accuracy?

Example



~750 equally-spaced points

Example

$$\int_0^{\pi} \sin(x) dx, \quad \text{find } h \text{ so that } |\text{error}| \leq \frac{1}{2} \times 10^{-5}$$

$$|\text{Error}| \leq \frac{b-a}{12} h^2 \max_{x \in [a,b]} |f'(x)|$$

$$b = \pi; \quad a = 0; \quad f'(x) = \cos(x);$$

$$|f'(x)| \leq 1 \quad \Rightarrow \quad |\text{Error}| \leq \frac{\pi}{12} h^2 \leq \frac{1}{2} \times 10^{-5}$$

$$\Rightarrow \quad h^2 \leq \frac{6}{\pi} \times 10^{-5} = 1.91 \times 10^{-5} \Rightarrow h \leq 0.004$$

~750 equally-spaced points

Gaussian Quadrature

- Thus far we have considered regular spaced abscissas, although we have considered the possibility of adapting spacing
- We've also looked solely at closed interval formulas
- Gaussian quadrature achieves high accuracy and efficiency by optimally selecting the abscissas
- It is usual to apply a change of variables to make the integral map to $[-1, 1]$
- There are also a number of different families of Gaussian quadrature, we'll look at Gauss-Legendre
- The following slides were adapted from:

http://numericalmethods.eng.usf.edu/topics/gauss_quadrature.html

See Numerical Recipes for a lengthy discussion

Theory of Gaussian Quadrature

Trapezoid Method

$$\int_a^b f(x)dx = h \left[\sum_{i=1}^{n-1} f(x_i) + \frac{1}{2} (f(x_0) + f(x_n)) \right]$$

It can be expressed as

$$\int_a^b f(x)dx = \sum_{i=0}^n c_i f(x_i)$$

$$\text{where } c_i = \begin{cases} h & i = 1, 2, \dots, n-1 \\ 0.5h & i = 0 \text{ and } n \end{cases}$$

Basis of the Gaussian Quadrature Rule

Previously, the Trapezoidal Rule was developed by the method of undetermined coefficients. The result of that development is summarized below.

$$\begin{aligned}\int_a^b f(x)dx &\approx c_1 f(a) + c_2 f(b) \\ &= \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b)\end{aligned}$$

Basis of the Gaussian Quadrature Rule

The two-point Gauss Quadrature Rule is an extension of the Trapezoidal Rule approximation where the arguments of the function are not predetermined as a and b but as unknowns x_1 and x_2 . In the two-point Gauss Quadrature Rule, the integral is approximated as

$$I = \int_a^b f(x) dx \approx c_1 f(x_1) + c_2 f(x_2)$$

Basis of the Gaussian Quadrature Rule

The four unknowns x_1, x_2, c_1 and c_2 are found by assuming that the formula gives exact results for integrating a general third order polynomial, $f(x) = a_0 + a_1x + a_2x^2 + a_3x^3$.

Hence

$$\begin{aligned}\int_a^b f(x) dx &= \int_a^b (a_0 + a_1x + a_2x^2 + a_3x^3) dx \\ &= \left[a_0x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3} + a_3 \frac{x^4}{4} \right]_a^b \\ &= a_0(b-a) + a_1 \left(\frac{b^2 - a^2}{2} \right) + a_2 \left(\frac{b^3 - a^3}{3} \right) + a_3 \left(\frac{b^4 - a^4}{4} \right)\end{aligned}$$

Basis of the Gaussian Quadrature Rule

It follows that

$$\int_a^b f(x) dx = c_1 (a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3) + c_2 (a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_2^3),$$

Equating Equations the two previous two expressions yield

$$\begin{aligned} & a_0(b-a) + a_1 \left(\frac{b^2 - a^2}{2} \right) + a_2 \left(\frac{b^3 - a^3}{3} \right) + a_3 \left(\frac{b^4 - a^4}{4} \right) \\ &= c_1 (a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3) + c_2 (a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_2^3), \\ &= a_0(c_1 + c_2) + a_1(c_1 x_1 + c_2 x_2) + a_2(c_1 x_1^2 + c_2 x_2^2) + a_3(c_1 x_1^3 + c_2 x_2^3), \end{aligned}$$

Basis of the Gaussian Quadrature Rule

Since the constants a_0, a_1, a_2, a_3 are arbitrary

$$b - a = c_1 + c_2$$

$$\frac{b^2 - a^2}{2} = c_1 x_1 + c_2 x_2$$

$$\frac{b^3 - a^3}{3} = c_1 x_1^2 + c_2 x_2^2$$

$$\frac{b^4 - a^4}{4} = c_1 x_1^3 + c_2 x_2^3$$

Basis of Gauss Quadrature

The previous four simultaneous nonlinear Equations have only one acceptable solution,

$$x_1 = \left(\frac{b-a}{2} \right) \left(-\frac{1}{\sqrt{3}} \right) + \frac{b+a}{2}$$

$$x_2 = \left(\frac{b-a}{2} \right) \left(\frac{1}{\sqrt{3}} \right) + \frac{b+a}{2}$$

$$c_1 = \frac{b-a}{2}$$

$$c_2 = \frac{b-a}{2}$$

Basis of Gauss Quadrature

Hence Two-Point Gaussian Quadrature Rule

$$\begin{aligned}\int_a^b f(x)dx &\approx c_1 f(x_1) + c_2 f(x_2) \\ &= \frac{b-a}{2} f\left(\frac{b-a}{2}\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}\right) + \frac{b-a}{2} f\left(\frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}\right)\end{aligned}$$

Higher Point Gaussian Quadrature Formulas

$$\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$$

is called the three-point Gauss Quadrature Rule.

The coefficients c_1 , c_2 , and c_3 , and the functional arguments x_1 , x_2 , and x_3 are calculated by assuming the formula gives exact expressions for integrating a fifth order polynomial

$$\int_a^b (a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5) dx$$

General n-point rules would approximate the integral

$$\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) + \dots + c_n f(x_n)$$

Arguments and Weighing Factors for n-point Gauss Quadrature Formulas

In handbooks, coefficients and arguments given for n-point Gauss Quadrature Rule are given for integrals

$$\int_{-1}^1 g(x) dx \cong \sum_{i=1}^n c_i g(x_i)$$

as shown in Table 1.

Table 1: Weighting factors c and function arguments x used in Gauss Quadrature Formulas.

Points	Weighting Factors	Function Arguments
2	$c_1 = 1.000000000$ $c_2 = 1.000000000$	$x_1 = -0.577350269$ $x_2 = 0.577350269$
3	$c_1 = 0.555555556$ $c_2 = 0.888888889$ $c_3 = 0.555555556$	$x_1 = -0.774596669$ $x_2 = 0.000000000$ $x_3 = 0.774596669$
4	$c_1 = 0.347854845$ $c_2 = 0.652145155$ $c_3 = 0.652145155$ $c_4 = 0.347854845$	$x_1 = -0.861136312$ $x_2 = -0.339981044$ $x_3 = 0.339981044$ $x_4 = 0.861136312$

Arguments and Weighing Factors for n-point Gauss Quadrature Formulas

So if the table is given for $\int_{-1}^1 g(x)dx$ integrals, how does one solve $\int_a^b f(x)dx$? The answer lies in that any integral with limits of $[a, b]$

can be converted into an integral with limits $[-1, 1]$ Let

$$x = mt + c$$

$$\text{If } x = a, \text{ then } t = -1$$

$$\text{If } x = b, \text{ then } t = 1$$

Such that:

$$m = \frac{b - a}{2}$$

Arguments and Weighing Factors for n-point Gauss Quadrature Formulas

Then $c = \frac{b+a}{2}$ Hence

$$x = \frac{b-a}{2}t + \frac{b+a}{2} \quad dx = \frac{b-a}{2}dt$$

Substituting our values of x , and dx into the integral gives us

$$\int_a^b f(x)dx = \int_{-1}^1 f\left(\frac{b-a}{2}t + \frac{b+a}{2}\right) \frac{b-a}{2} dt$$

See examples in Python workbook `Lecture07b.ipynb`

Basic Monte Carlo Algorithm

Basic Monte Carlo Algorithm

- Suppose we want to approximate

$$Z = \int_{\Omega} f(\mathbf{x}) d\mathbf{x}$$

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in a high-dimensional space

- For $i = 1$ to n
 - Pick a point x_i at random
 - Accept or reject the point based on criterion
 - If accepted, then add $f(x_i)$ to total sum
- Error estimates are “free” by calculating sums of squares

Basic Monte Carlo Algorithm

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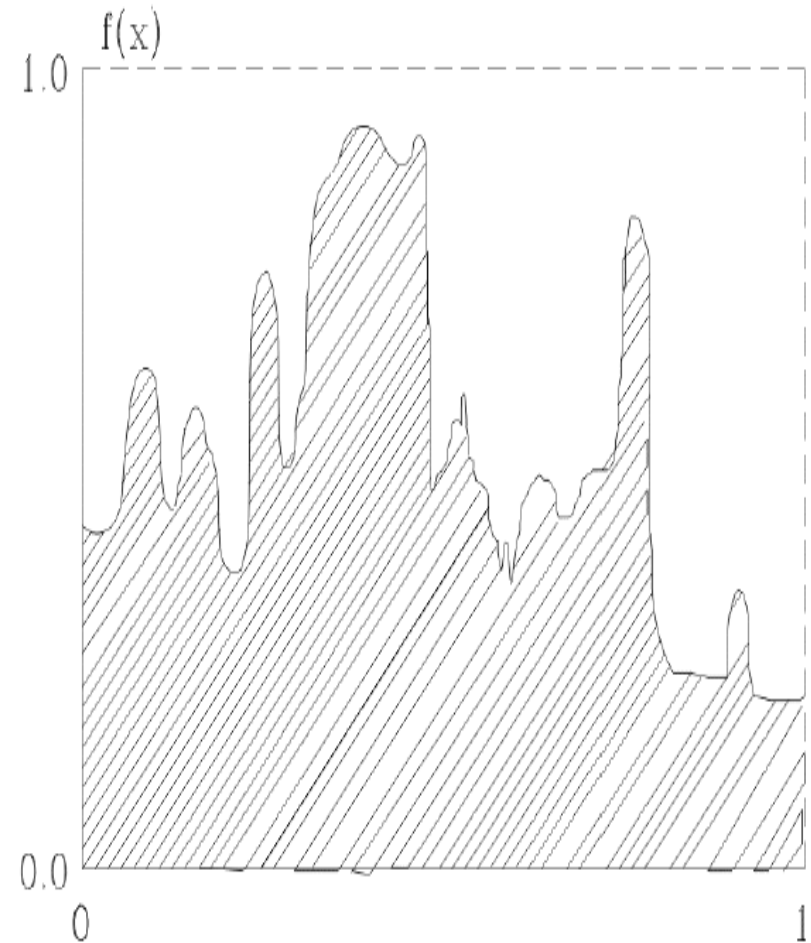
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 - Pick a point x_i at random
 - Accept or reject the point based on criterion
 - If accepted, then add $f(x_i)$ to total sum
- Error estimates are “free” by calculating sums of squares
- Error typically decays as

$$\frac{1}{\sqrt{N}}$$

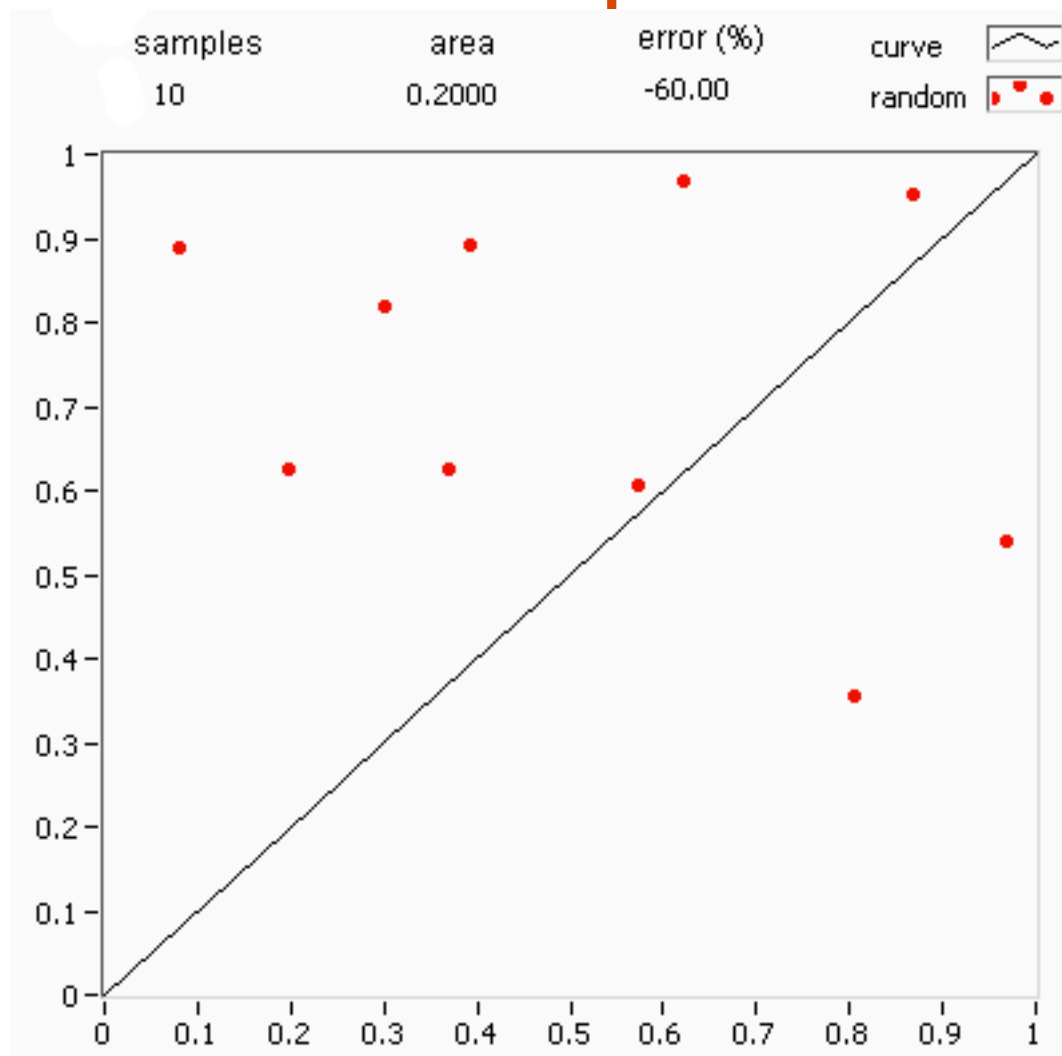
1-dimensional MC Integration

- Suppose we want to find the area under the curve for $Y=f(X)$ for a given interval.
- Now let's assume we are throwing darts at the picture of $f(x)$. Each dart will land on a point (x_i, y_i) , where $0 < x_i < 1$ and $0 < y_i < 1$.
- If the value of $y_i < f(x_i)$, then we count it as a hit. Repeat the process for a large number of i .
- The area under the curve = number of hits / total number of throws.



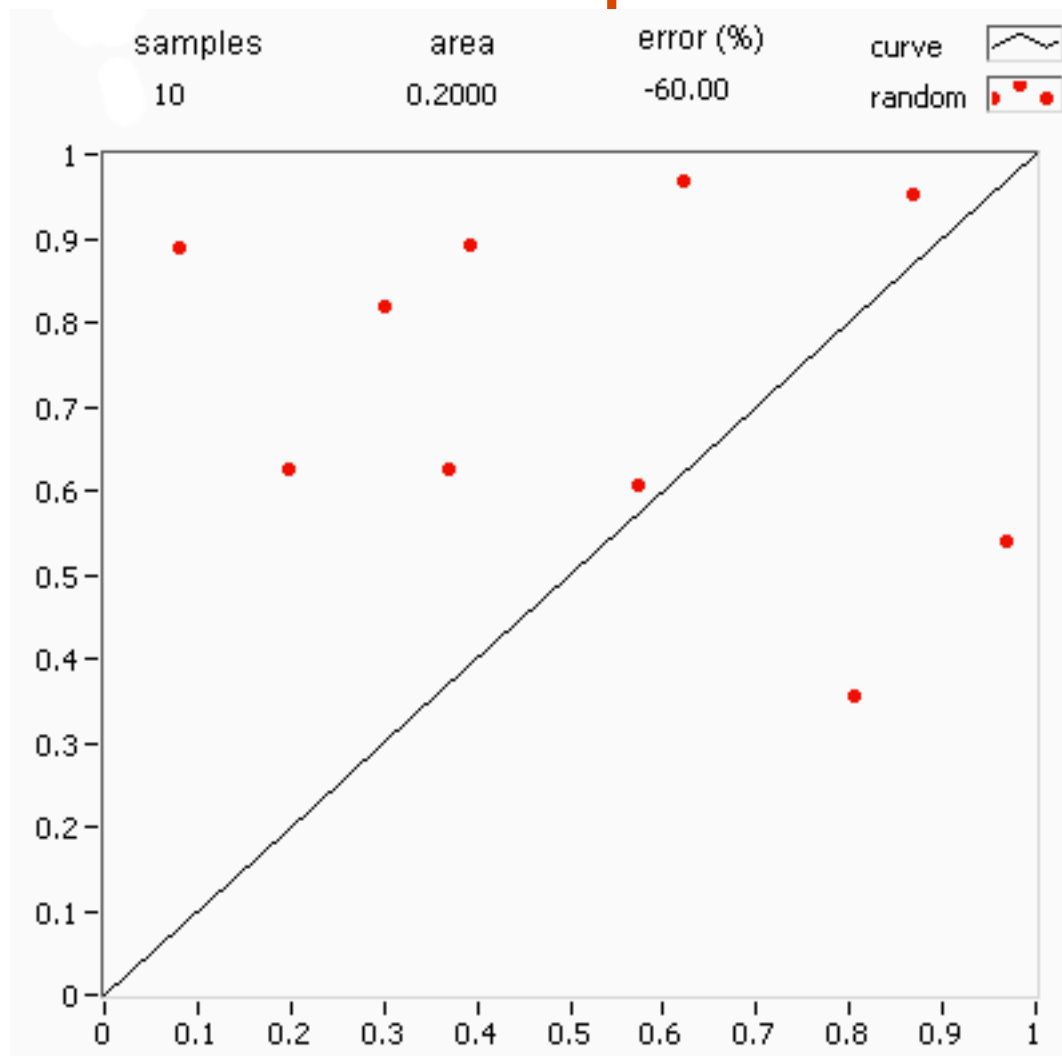
Amin Jazaeri

Example



https://en.wikipedia.org/wiki/Monte_Carlo_method

Example



https://en.wikipedia.org/wiki/Monte_Carlo_method

Error Estimate for MC Integrals

- Uncertainties for MC integrals follow the *binomial* distribution:
 - Let the area under the curve be S , and the area populated by random points (“darts”) is S_0 . Let N_0 be the number of points thrown, and N the number of points accepted. Then the estimator of S is:

$$\hat{S} = S_0 \frac{N}{N_0}$$

- Define the “efficiency” of accepting the events as

$$\epsilon \equiv \frac{S}{S_0} \approx \hat{\epsilon} = \frac{N}{N_0}$$

Error Estimate for MC Integrals

- N is a random variable, which follows a binomial distribution (“choose N out of N_0 ”). Estimator of $\epsilon = N/N_0$ is therefore also a random variable. Its uncertainty is given by

$$\sigma(\hat{\epsilon}) = \sqrt{\frac{\epsilon(1 - \epsilon)}{N_0}}$$

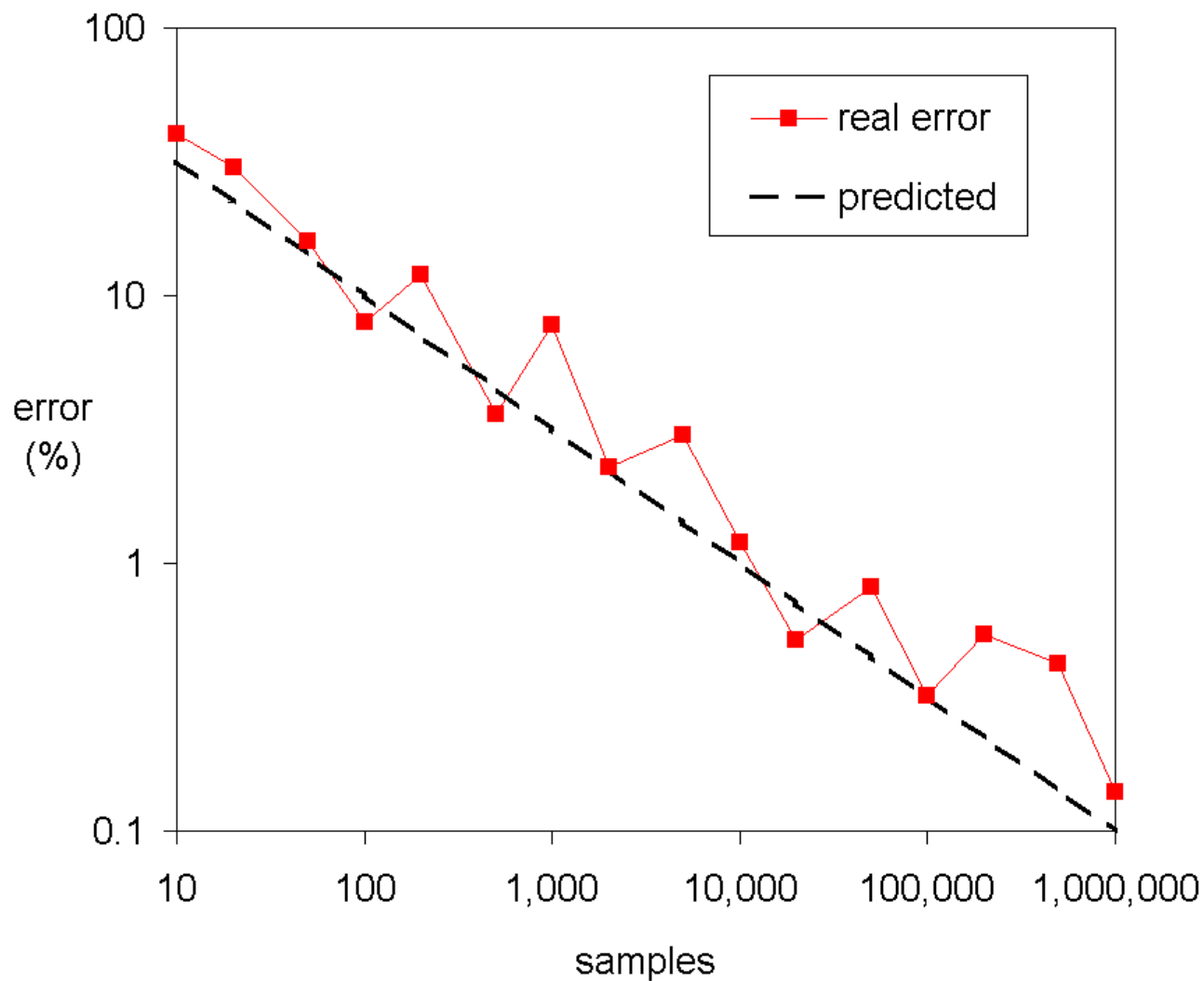
- You can show that in the limit $N \ll N_0$ ($\epsilon \rightarrow 0$),

$$\sigma(\hat{\epsilon}) \approx \sqrt{\frac{\epsilon}{N_0}} \approx \frac{\epsilon}{\sqrt{N}}$$

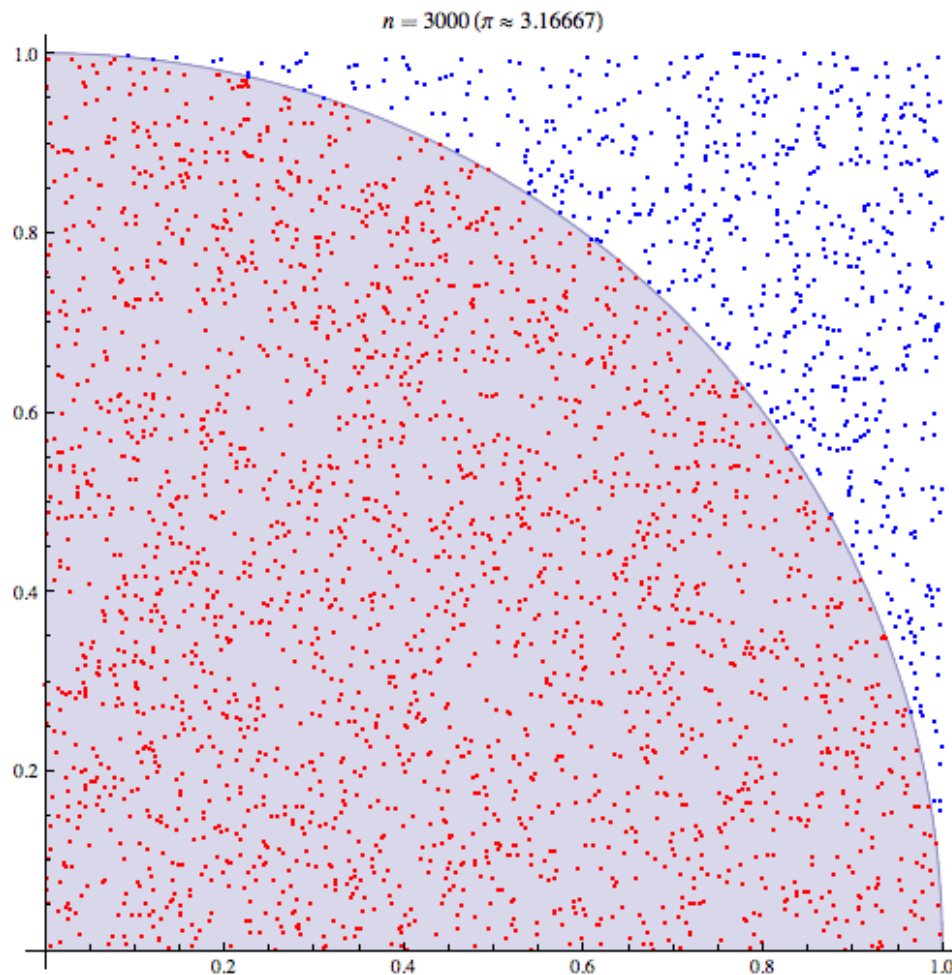
- and

$$\sigma(\hat{S}) = S_0 \sigma(\hat{\epsilon}) = \frac{S}{\sqrt{N}}$$

Error Estimate



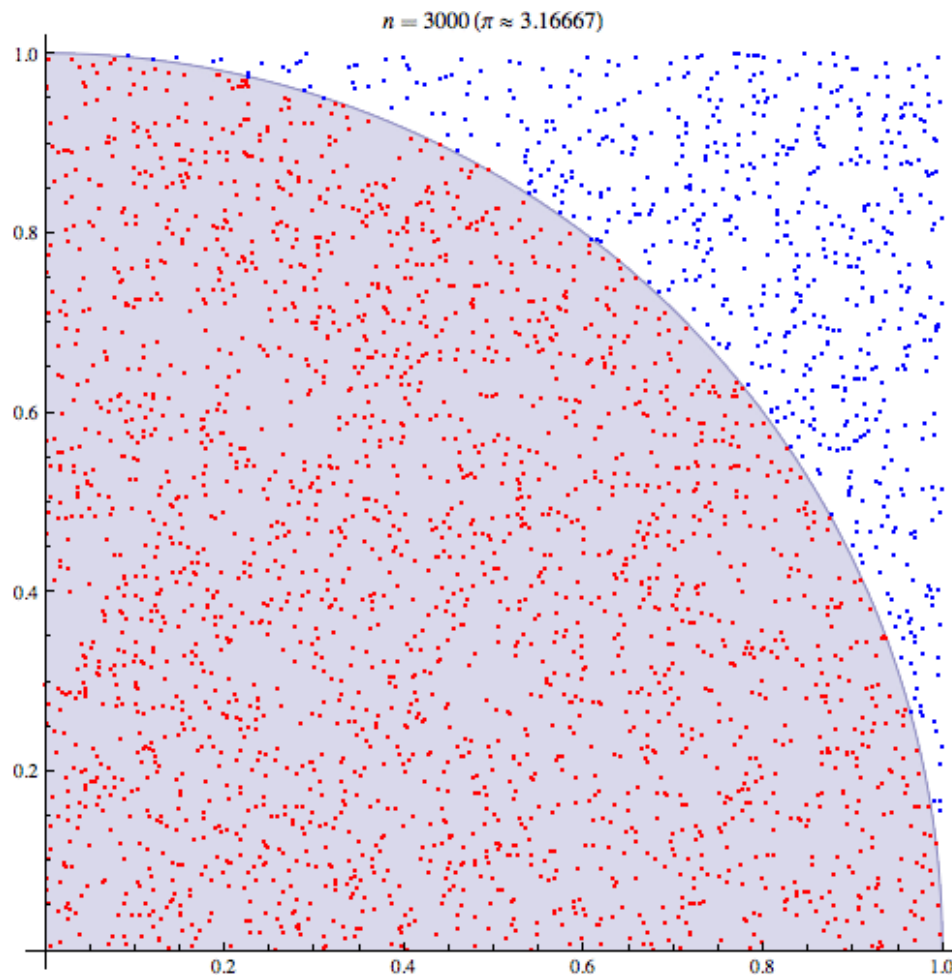
Example: Compute π by MC



Workshop 6 !

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Example: Compute π by MC



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