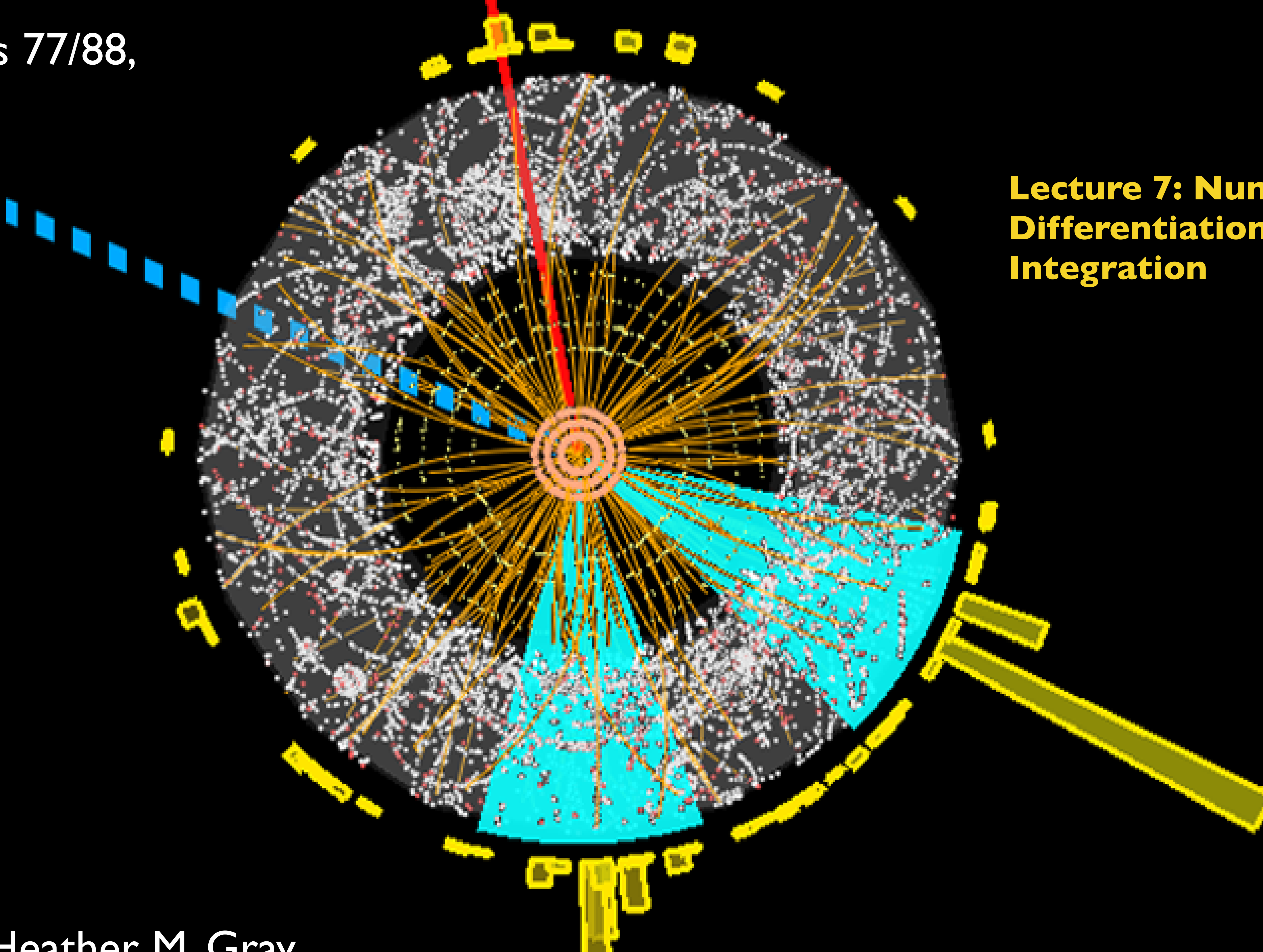
Introduction to Computational Techniques in Physics/Data Science Applications in Physics

Physics 77/88,



Lecture 7: Numerical Differentiation and Integration

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Numerical Differentiation

- Definition
  - $\dfrac{df(x)}{dx} = \lim$
- Approximation
  - $\dfrac{df(x)}{dx} =$
- Similarly
  - $\Delta^n f(x) =$

Numerical Differentiation

- The difference of a of degree is a constant, , and the difference is
- Let's take $f(x) = x^2$ as an example

x_i	$f(x_i)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$
2	$f(2) =$			
		$\Delta f(2) =$		
3	$f(3) =$		$\Delta^2 f(2) =$	
		$\Delta f(3) =$		$\Delta^3 f(2) =$
4	$f(4) =$		$\Delta^2 f(3) =$	
		$\Delta f(4) =$		$\Delta^3 f(3) =$
5	$f(5) =$		$\Delta^2 f(4) =$	
		$\Delta f(5) =$		
6	$f(6) =$			

Taylor Series

- Expand any function $f(x)$
  - $f(x_0 + kh) =$
- Rearrange to solve for $f'(x)$
-
- Backward difference ($k =$)
- Forward difference ($k =$)
-

Taylor Series: Central Difference

- $f(x_0 + kh) = f(x_0) + khf'(x_0) + \frac{(kh)^2 h''(x_0)}{2!} + \ldots + \frac{(kh^n) f^n(x_0)}{n!}$
- $f(x_0 - kh) =$
- Subtract the two and set k = 1:
-

Higher Order Approximations

- 1st order $f'(x) =$

- 2nd order $f'(x) =$

- 1st order $f''(x) =$

- 2n order $f''(x) =$

Numerical Integration

- Consider the integral
  - $I =$
- The integral can be by
  - $I \approx$
- The ω_ι are , and the x_i are
- Assuming that *f* is and on the interval [,] numerical integration leads to a solution
- The goal of any numerical integration method is to choose and such that are for the smallest n possible for a given function

Numerical Integration

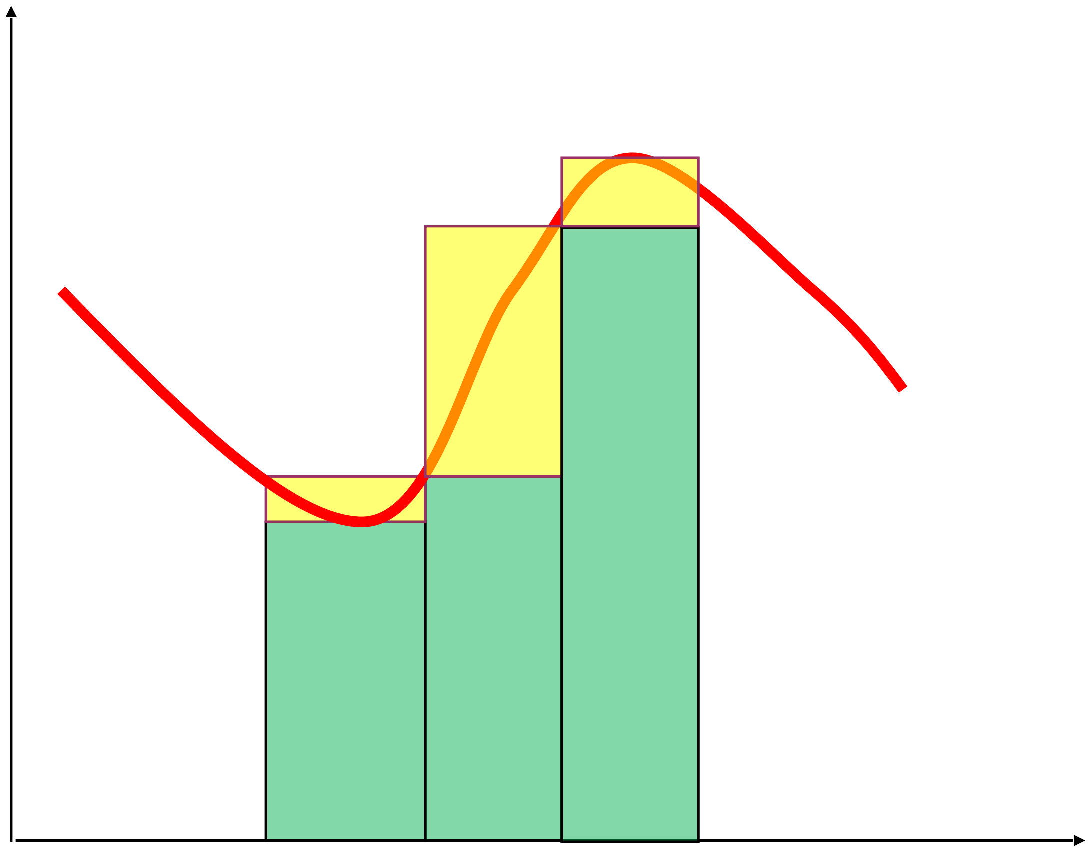
- How can we choose the points, , and the , , such that
  - $$\int_a^b f(x)dx \approx$$
- In general, there are sets of
  - The of the
  - The importance of

Numerical Integration Methods

- Upper and Lower Sums
- Newton-Cotes Methods:
  - a) Trapezoid Rule
  - b) Simpson Rules
- Romberg Method
- Gauss Quadrature

Upper and Lower Sums

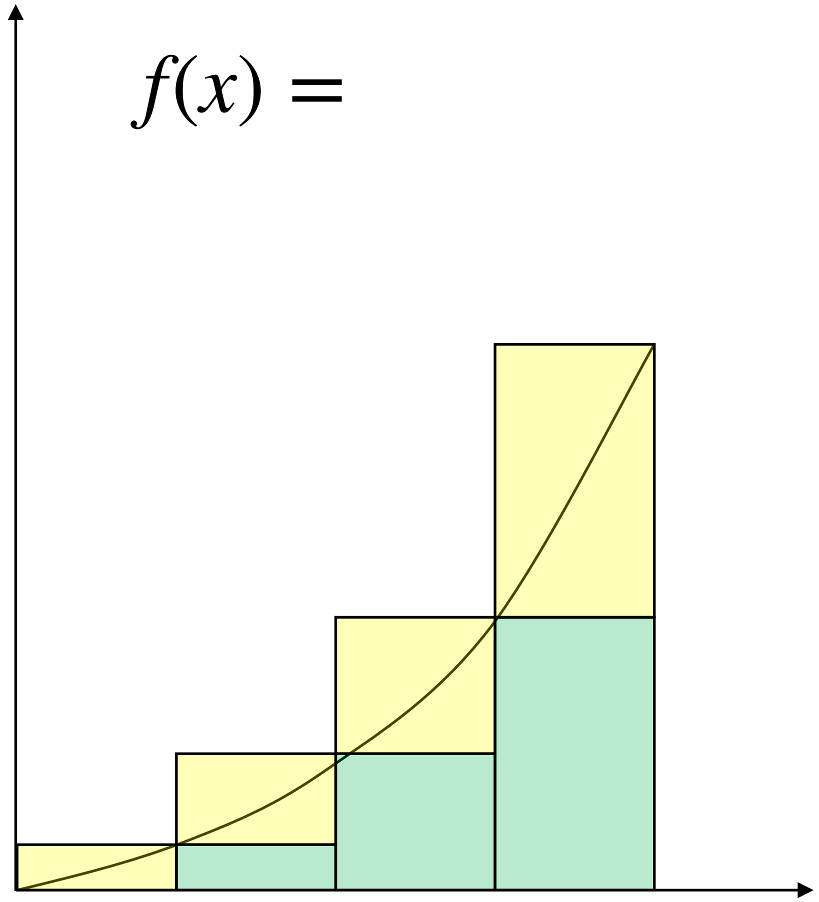
- Partition the into
  - $P =$
- Define
  - Minimum: $m_i =$
  - Maximum: $M_i =$
- Lower Sum
  - $L(f, P) =$
- Upper Sum
  - $U(f, P) =$
- Estimate of the integral =
- Error $\leq$



Example

- $\int_0^1 x^2 dx =$
- Partition P =
- n =

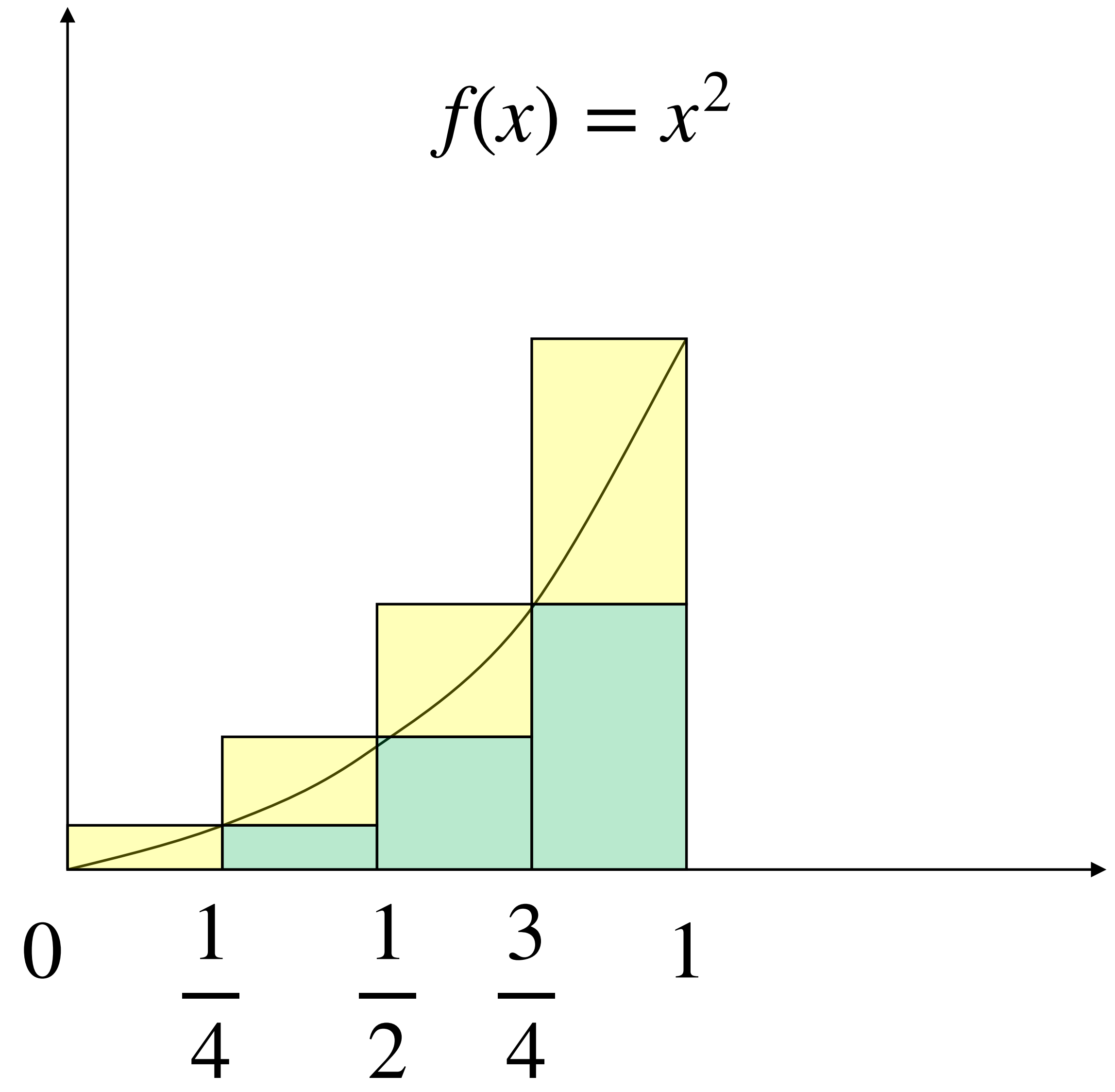
i				
m_i				
M_i				



- $x_{i+1} - x_i =$

Example (cont)

- Lower Sum
  - $L(f,P) = \sum_{i=0}^{n-1} m_i(x_{i+1} - x_i)$
  - =
  - =
- Upper Sum
  - $U(f,P) = \sum_{i=0}^{n-1} M_i(x_{i+1} - x_i)$
  - =
  - =
- I = $\dfrac{L+U}{2} =$
- Error $\leq \dfrac{U-L}{2} =$



Upper and Lower Sums

- Estimates based on and sums are easy to obtain for functions
  - functions that are always or
- For functions, finding the and of the function can be and are

Newton-Cotes Methods

- In , the function is by a

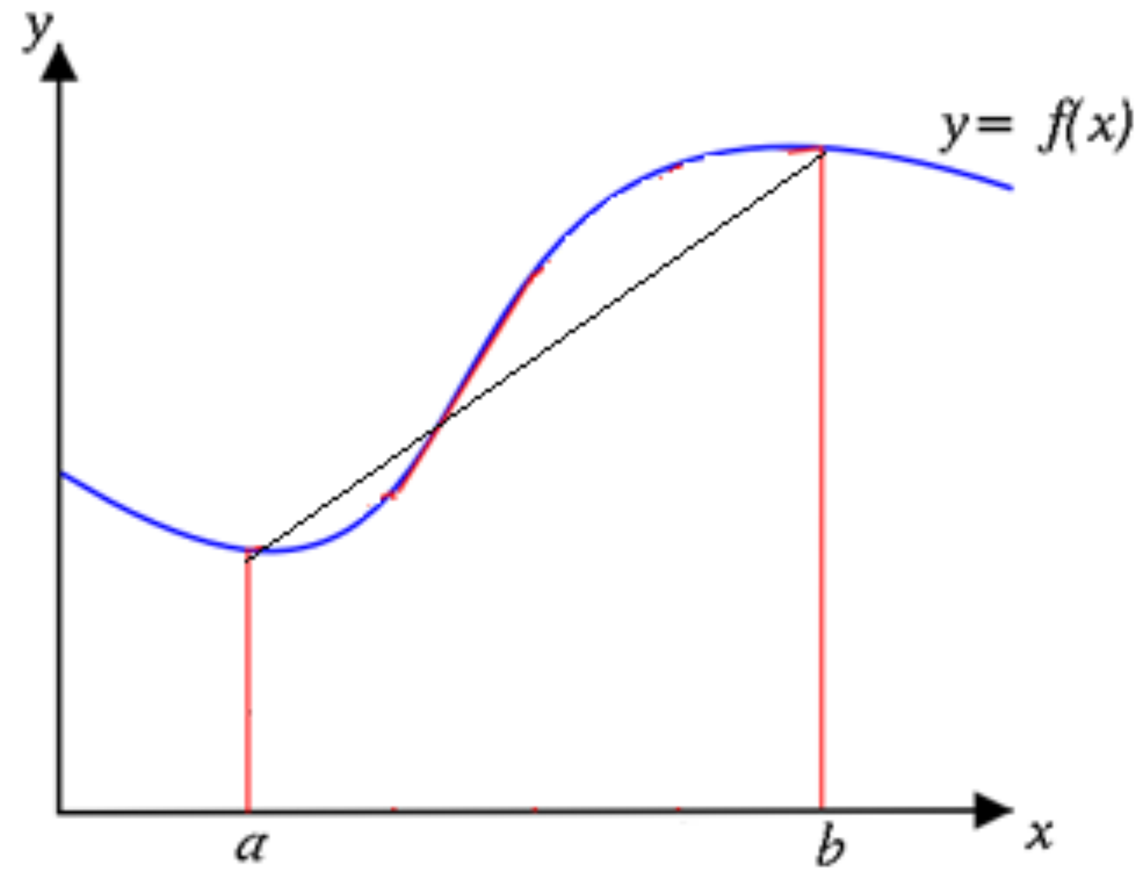
- Computing the of polynomial is
  - $\int_a^b f(x)d(x) \approx \int_a^b$
    - $\approx$

Newton-Cotes Methods

- Method
  - Uses polynomials
  - $\int_a^b f(x)dx \approx \int_a^b$
- Simpson's 1/3 Rule
  - Uses polynomials
  - $\int_a^b f(x)dx \approx \int_a^b$

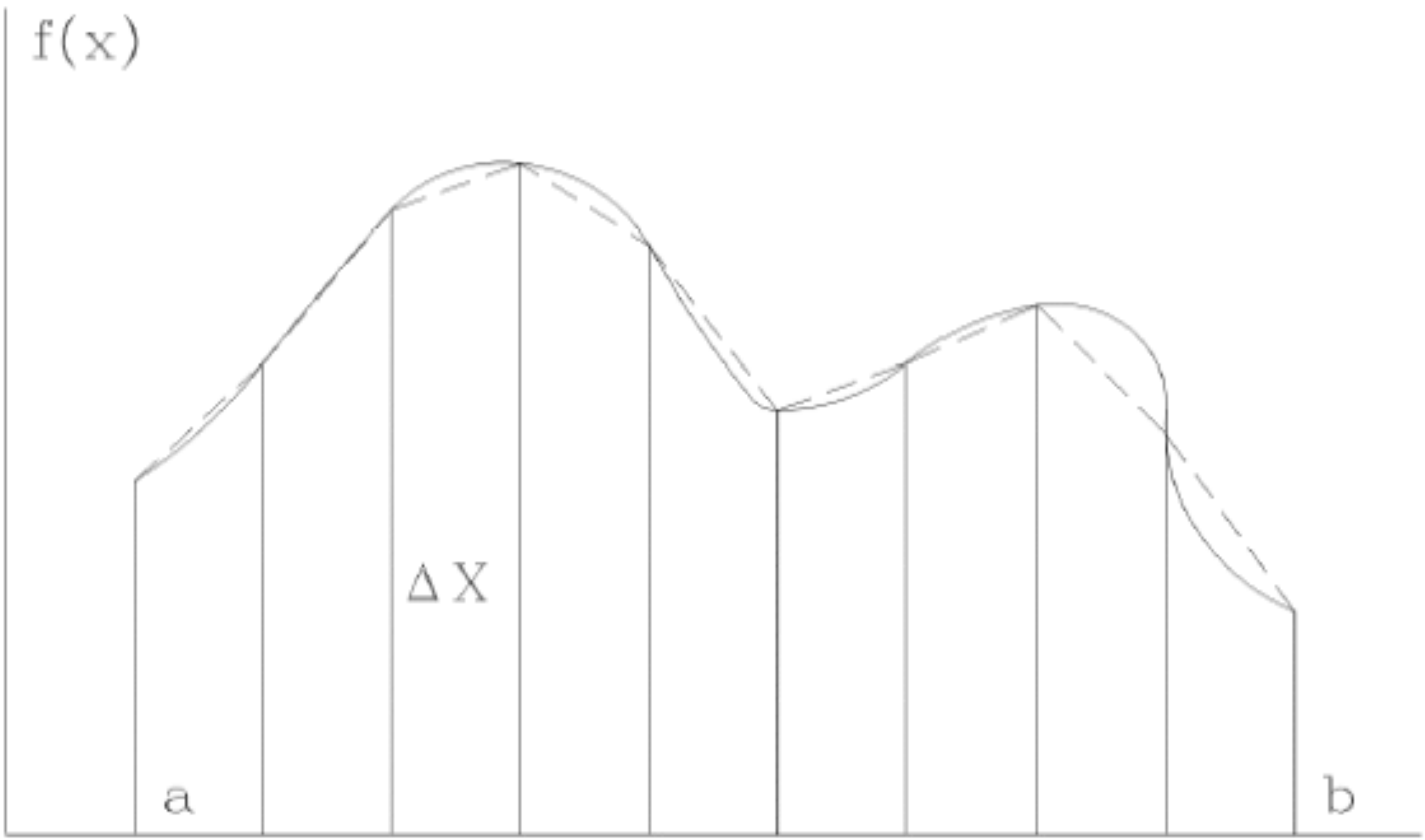
Trapezoid Method

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



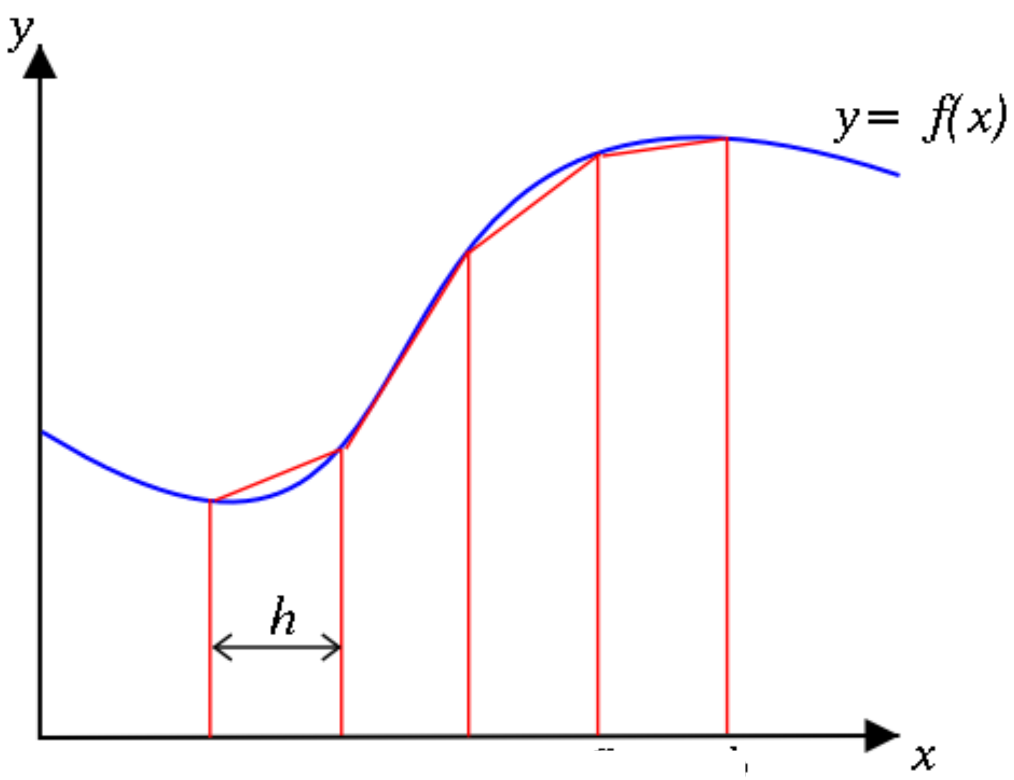
Numerical Integration

- Composite Trapezoid Rule



Trapezoid Rule

- Approximate using the areas of the



$$\int_a^b f(x)dx \approx \sum$$

$$=$$

$$=$$

For this to

$$\int_a^b f(x)dx \approx$$

Numerical Integration

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

Simpson’s Rule

- Trapezoidal rule was based on the by a polynomial, and then integrating
- Simpson’s is an of the trapezoidal rule where the is by a polynomial
  - $I = \int_a^b f(x)dx \approx$
  - Here, is a polynomial
    - $f_2(x) =$

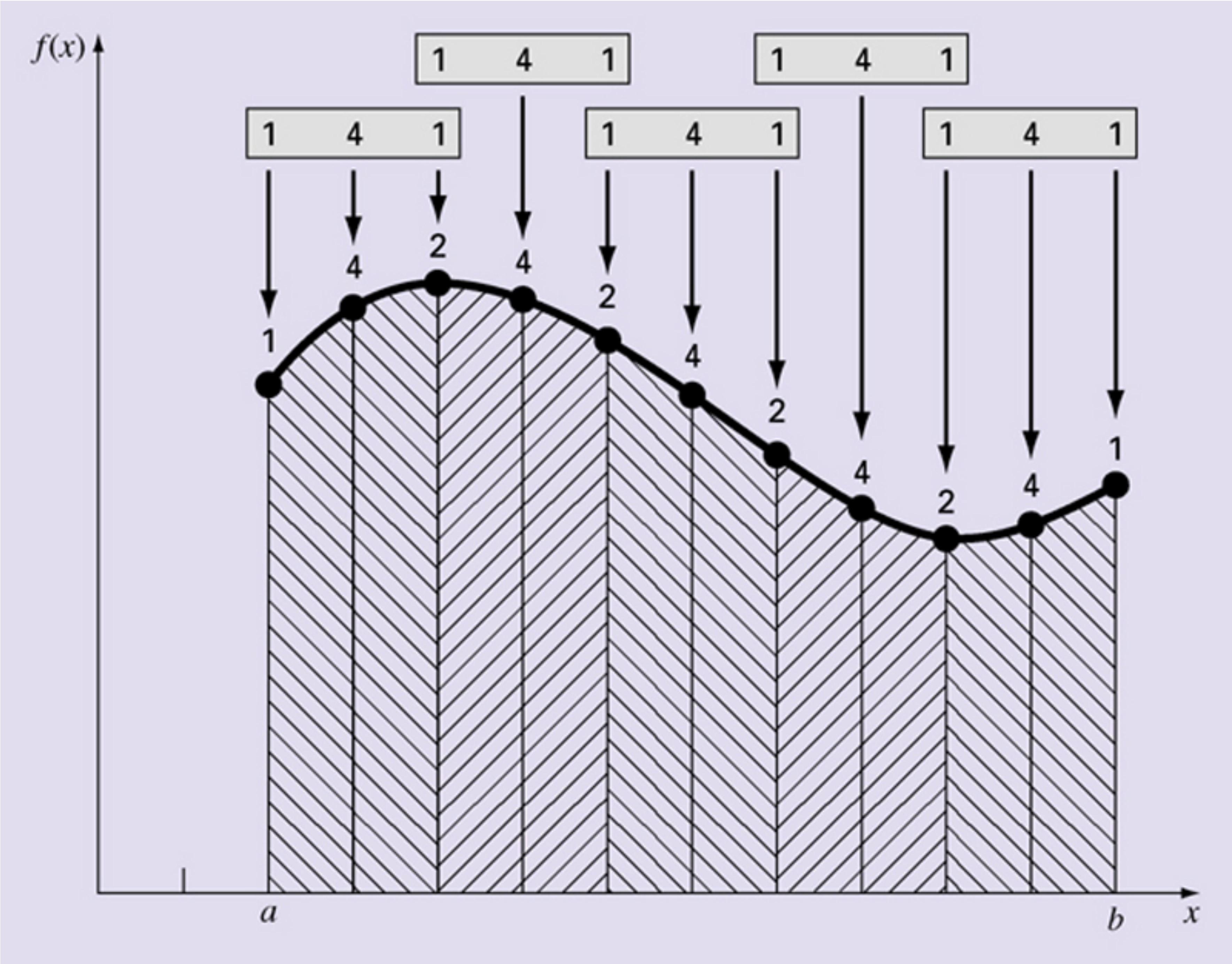
Simpson's Rule

- Simpson's rule:
  - $\int_a^b f(x)dx =$
    - where $\Delta x =$
- Simpson's rule can be when there are an number of
- $\int_{x_1}^{x_n} f(x)dx \approx \sum$

Composite Simpson's Rule

- Simpson's rule for is given as:
  - $\int_{x_0}^{x_2} p_1(x)dx =$
- We can do the same on to get
  - $\int_{x_2}^{x_4} p_1(x)dx =$
- Hence on the region
  - $\int_{x_0}^{x_4} f(x)dx =$
- In general for an number of intervals
  - $\int_{a}^{b} f(x)dx \approx$

Composite Simpson's Rule



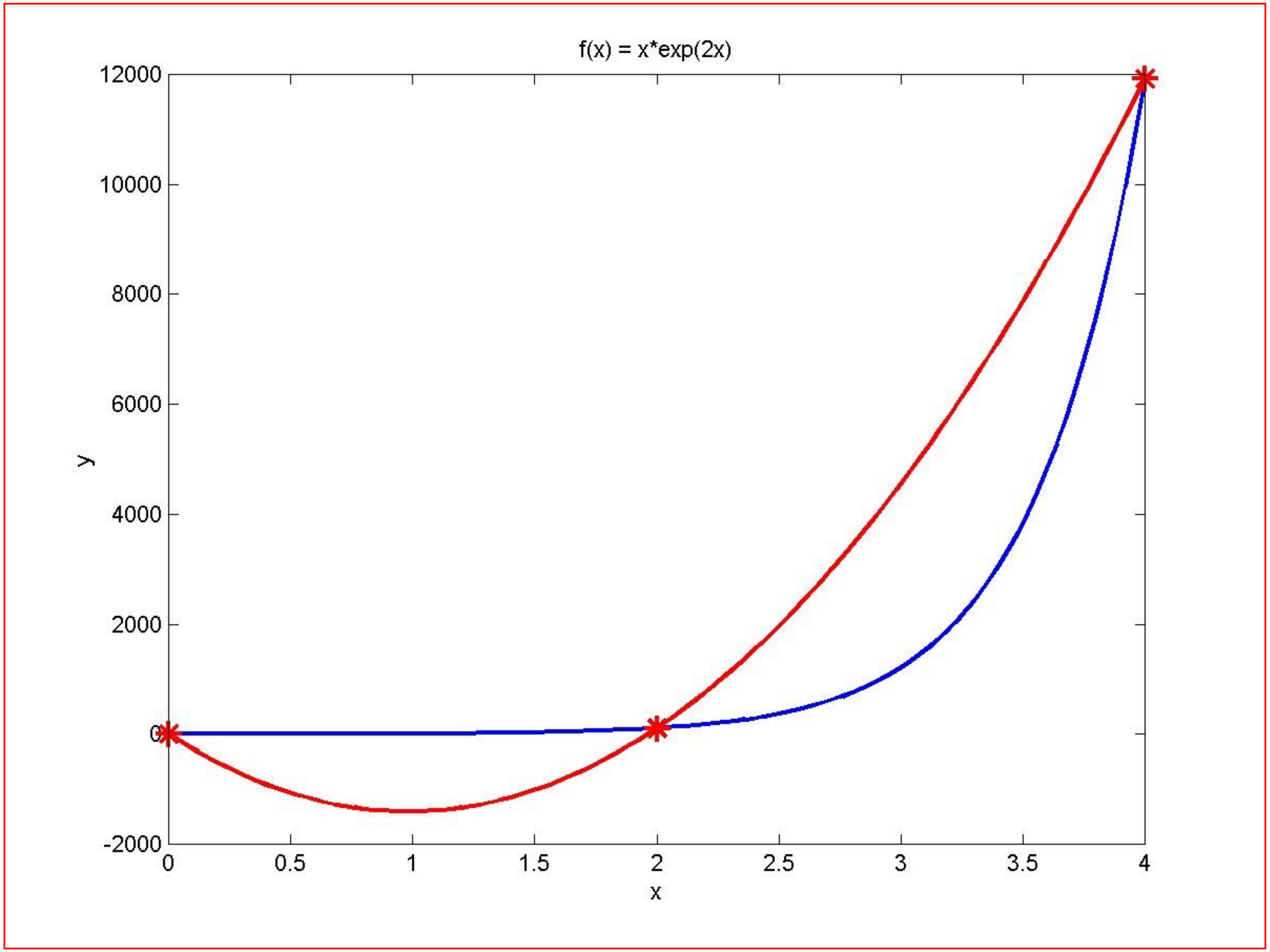
Applicable if the number of segments is

Weights in Simpson's Rule

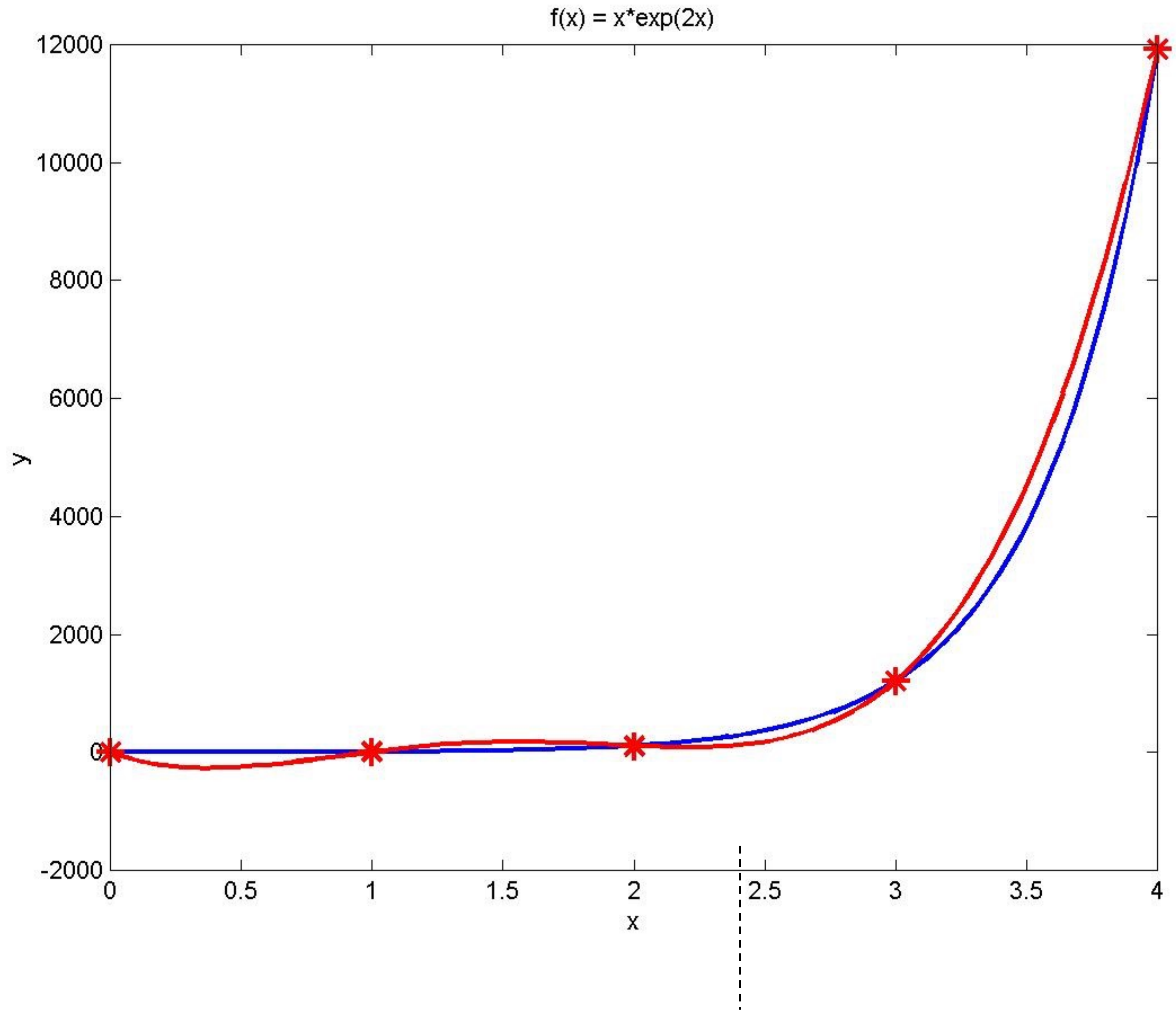
- For 1/3 Simpson' Rule the weights are:

- $w_i = \quad \{$

Simpson’s 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

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

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

Simpson's 3/8th Rule

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

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 of f(x)

$$f(x) =$$

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

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

$$=$$

Error in the Trapezoid Rule

- Perform the same expansion about

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

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

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

- Notice that derivatives are while derivatives are

Error in the Trapezoid Rule

- We also make Taylor expansions of and around both which allow us to for terms in and and to derive

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

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

Error in the Composite Trapzoid

- We now sum over a series of trapezoids to get

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

- Note now
- The expansion is in powers of

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

$Error =$

$|Error| \leq$

Estimating error for trapezoid rule

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

$$|Error| \ \leq$$

$$b = \qquad a = \qquad f'(x) =$$

$$|f'(x)| \leq \quad \Rightarrow |Error| \leq$$

$$\Rightarrow \qquad h^2 \leq$$

Gaussian Quadrature

- So far, we've considered spaced
- We've also only looked at formulae
- Gaussian quadrature achieves and by the
- We generally apply a to make the map
- There are a number of of Gaussian quadrature, we'll look at
- Slides were adapted from http://numericalmethods.eng.usf.edu/topics/gauss_quadrature.html

See <u>here</u> for further details

Theory of Gaussian Quadrature

- Recall the trapezoid method
  - $\int_a^b f(x)dx =$
- Let's express it as
  - $\int_a^b f(x)dx = \sum$
  - where

Basis of Gaussian Quadrature Rule

- Previously we discussed how the rule was developed using the method coefficients
  - $\int_a^b f(x)dx \approx c_1 f(a) + c_2 f(b)$
- The Gaussian Quadrature Rule is an of the Trapezoidal Rule approximation
  - where the of the function are not predetermined as and , but as and
  - $I = \int_a^b f(x)dx \approx$

Basis of the Gaussian Quadrature Rule

- We can find our by assuming that the formula gives for integrating a general polynomial
  - $f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$
- Then we find that
  - $\int_a^b f(x)dx = \int_a^b (a_0 + a_1 x + a_2 x^2 + a_3 x^3)dx$
  - =
  - =
- Recalling that $I \approx c_1 f(x_1) + c_2 f(x_2)$
- $\Rightarrow I =$

Basis of the Gaussian Quadrature Rule

- Equating the two expressions yields
  - $a_0(b-2) + a_1(\frac{b^2 - a^2}{2}) + a_2(\frac{b^3 - a^3}{3}) + a_3\frac{b^4 - a^4}{4})$

  =

- As the constants are
  -
  -
- Only one solution to the four equations
  - $x_1 =$; $x_2 =$
  - $c_1 =$; $c_2 =$

Gaussian Quadrature

- In conclusion, the Gaussian Quadrature Rule is
  - $\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2)$
  - =

Higher Point Gaussian Quadrature Formulae

- $\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$
- is called the Gaussian Quadrature Rule
- As for the two-point rule, one can calculate the and the by assuming that the formula gives for integrating a polynomial
  - $\int_a^b (a_0 + a_1 + a_2x^2 + a_3x^3 + a_4x^4 + a_5x^5)dx$
- General rules would approximate the integral
  - $\int_a^b f(x)dx \approx$

Arguments and Weighing Factors

- In handbooks, the and are given for Gaussian quadrature rules for integrals of the form
- $\int_{-1}^{+1} g(x)dx \approx$

Weighting factors c and function arguments x used in Gaussian Quadrature Formulae.

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

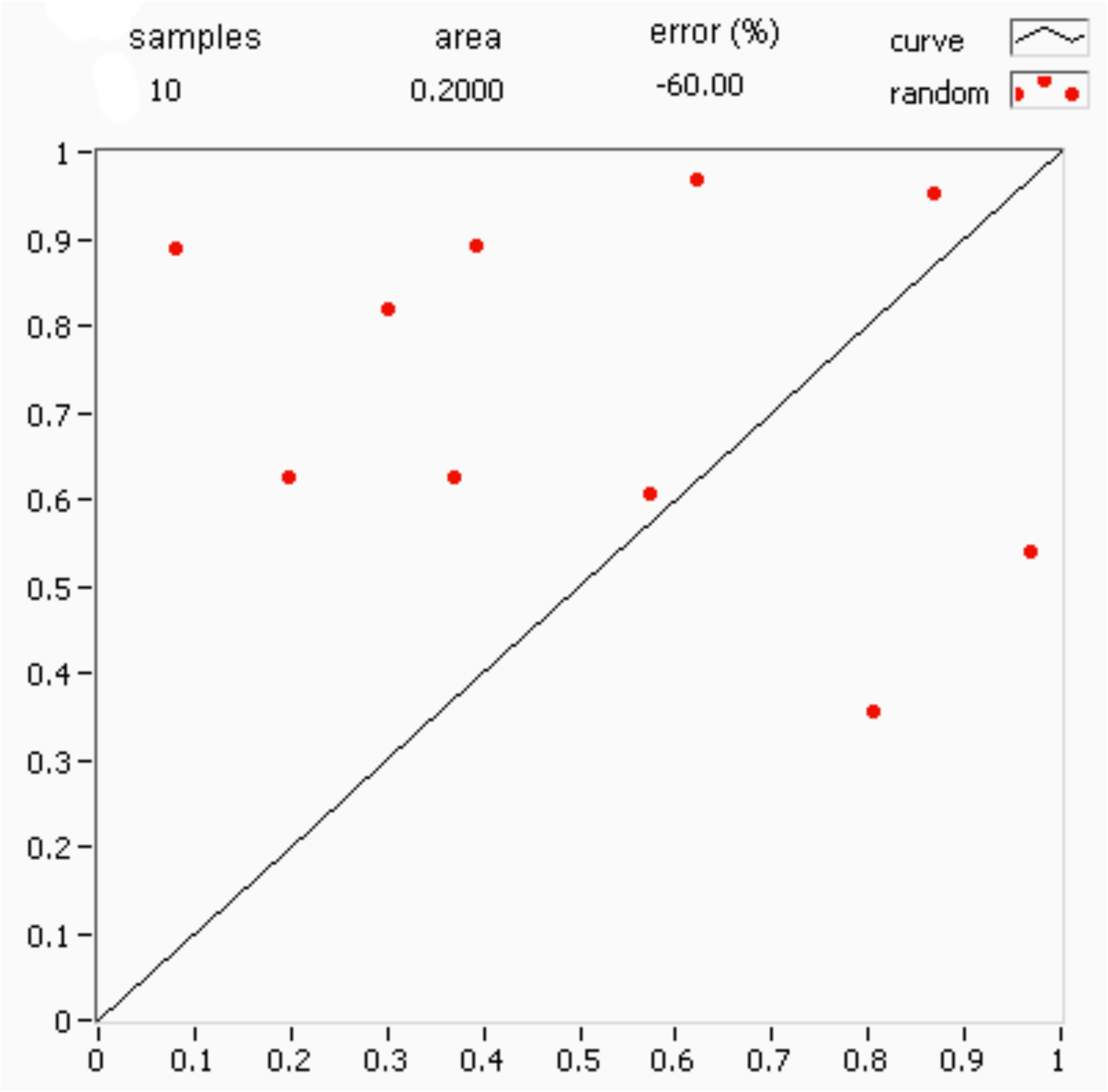
Arguments and Weighing Factors

- Now that we have a table for $\int_{-1}^{1} g(x)dx$ integrals,
  - how can we use it for integrals:
- Recall that with limits can be converted into with limits
- Let $x =$
  - If $x = a \Rightarrow$
  - If $x = b \Rightarrow$
- $\Rightarrow m =$ and $c =$
- i.e. $x =$; $dx =$
- Substituting x and dx yields

Recap: MC Integration

- Suppose we want to compute a
  - $Z = \int$
- Generate a (e.g. distributed in space)
- If is within , increment sum
- Repeat times
- Uncertainty on typically scales as

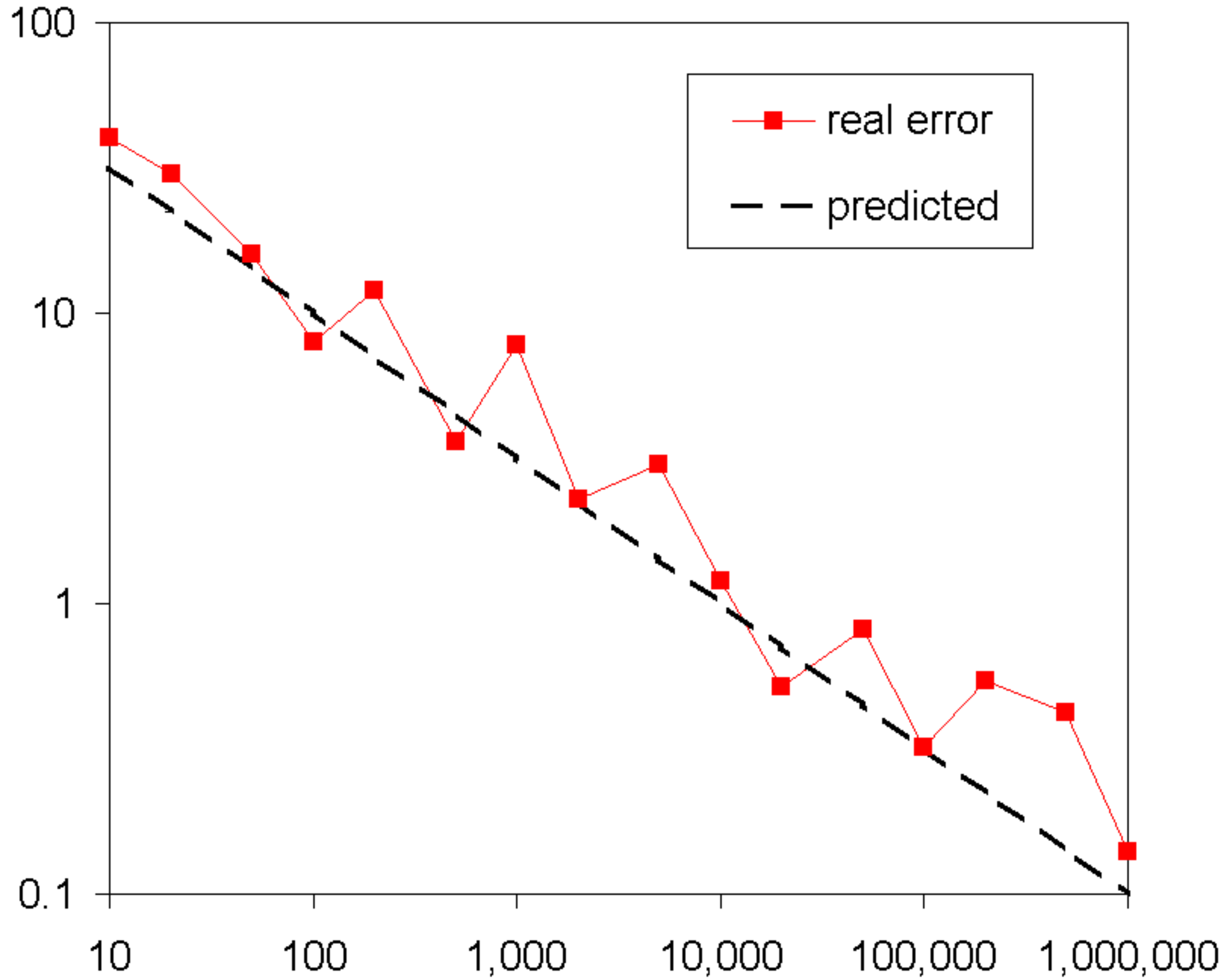
Example



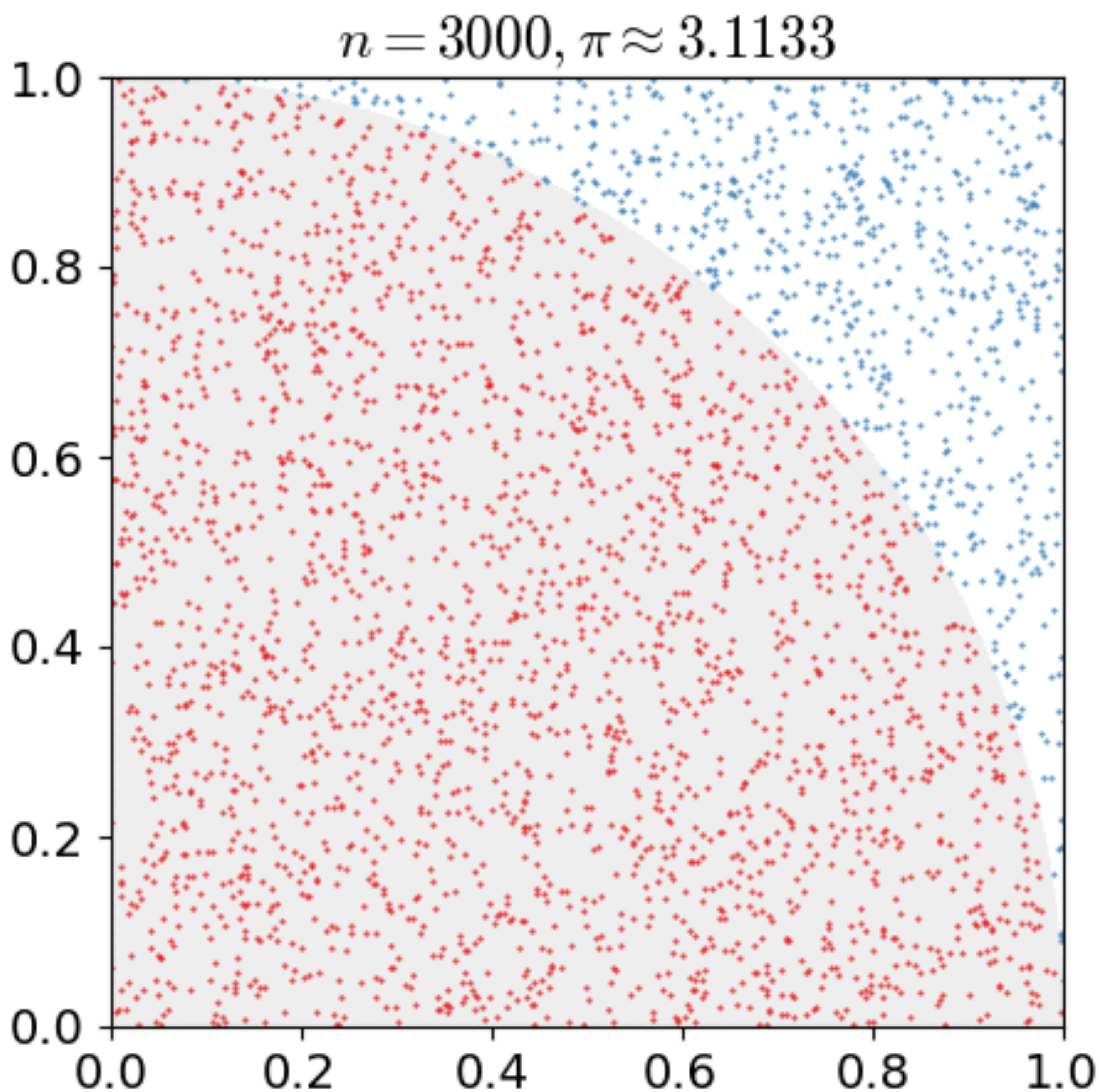
https://en.wikipedia.org/wiki/Monte_Carlo_method

Link to gif

Error Estimate



Example: Compute π by MC



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