Numerical Integration - Lecture 01

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Today's Lecture

- Numerical integration plays a key role in many engineering applications. The integration methods that we will examine are:
  - Trapezoidal Rule
  - Simpson's 1/3 Rule
  - Mid-point Rule
  - Romberg Integration
  - Gauss Quadrature
  - Multiple Integrals

Numerical Integration covered in Chapters 21 & 22 of your textbook

Numerical Integration

In this section, we shall address the evaluation of

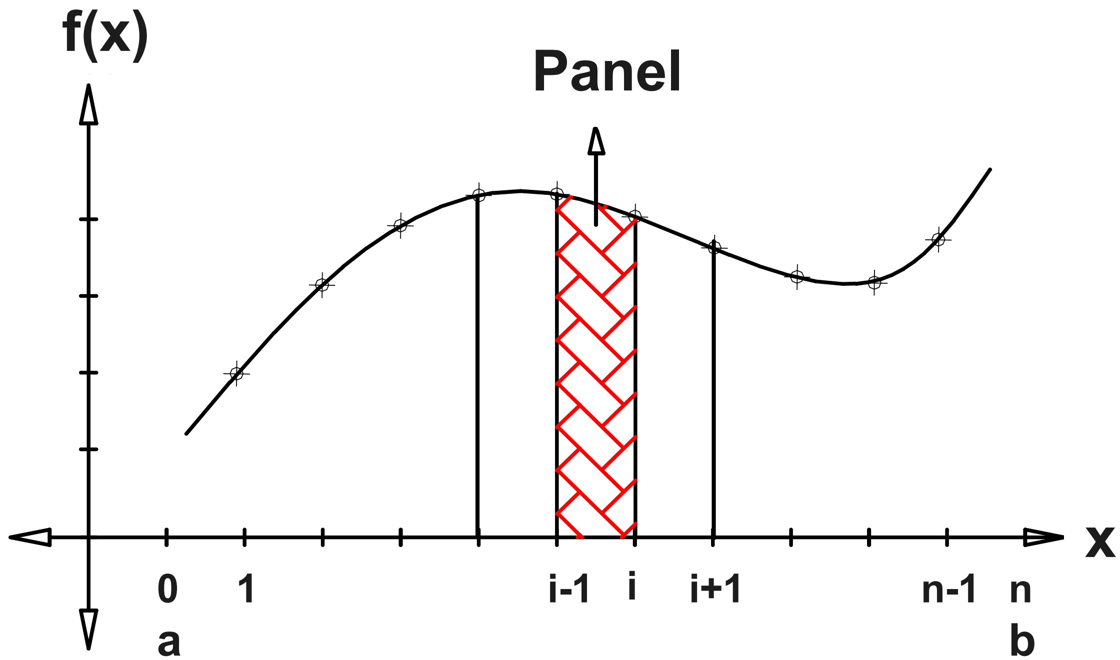
$$I = \int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

by **numerical quadrature**.

The scalar I denotes the area under the curve $f(x)$ on [a,b]. A ***panel*** is the area between two adjacent points. Between the points [a,b] we have n panels.

We shall consider an equally spaced grid in which the width h is given as

$$h = (b-a)/n = constant$$



It is a simple matter to extend the method to an unequally spaced grid.

Composite Trapezoidal Rule

By approximating the function with a straight line between adjacent points, it is clear that the each panel forms a trapezoid.

The area of the ***i***

The area of the i^{th} trapezoid formed by the panel is

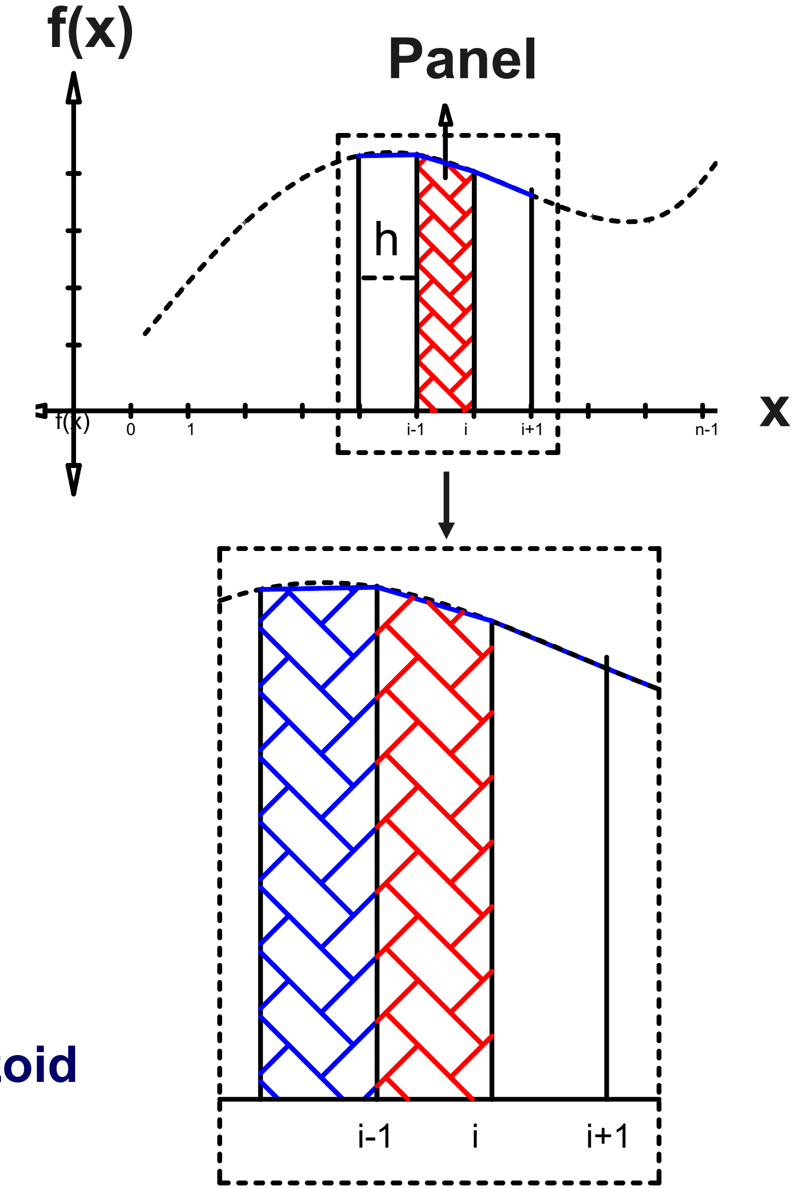
$$\int_{x_{i-1}}^{x_i} f(x)dx \approx h\frac{(f_i + f_{i-1})}{2}$$

Base x Average Height

Thus, the area under the curve on the interval [a,b] is:

$$\boxed{I \approx \sum_{i=1}^{n} \frac{h}{2}\left(f_i + f_{i-1}\right)}$$

Composite Trapezoid Rule



Trapezoidal Rule

If the interval does not remain constant, then the formula can be modified to accommodate varying interval widths and becomes

$$I = \sum_{i=1}^{n} \frac{h_i}{2}\left(f_i + f_{i-1}\right)$$

Accuracy of Trapezoidal Integration

Define
$$I(x) = \int_a^x f(\xi)d\xi$$

$I(x_i)$ is the area under the curve from a to x_i.

$I(x_{i+1})$ is the area under the curve from a to x_{i+1}.

Assume $I(x)$ is analytic in [a,b]. Then the function can be expanded in a Taylor's series, which can be used to obtain the accuracy of the method.

Trapezoidal Rule – Formal Derivation

Expanding $I(x_{i+1})$ about the point x_i, we have

$$I(x_{i+1}) = I(x_i) + hI'(x_i) + \frac{h^2}{2}I''(x_i) + \frac{h^3}{6}I'''(x_i) + \vartheta(h^4)$$

But $I'(x_i) = f(x_i) \quad \rightarrow (a)$

$I''(x_i) = f'(x_i) \rightarrow (b)$

$$\Rightarrow f'(x_i) = \frac{f_{i+1} - f_i}{h} - \frac{h}{2}f''(x_i) + \vartheta(h^2)$$

Similarly for higher order derivatives

See first order forward difference notes

Substitute (a) and (b) in $I(x_{i+1})$

$$I(x_{i+1}) = I(x_i) + hf_i + \frac{h^2}{2}\left[\frac{f_{i+1} - f_i}{h} - \frac{h}{2}f''(x_i) + \vartheta(h^2)\right] + \frac{h^3}{6}f''(x_i) + \vartheta(h^4)$$

$$\underbrace{I(x_{i+1}) - I(x_i)}_{\text{Exact area under Integral}} = \underbrace{h\left[\frac{f_{i+1} + f_i}{2}\right]}_{\text{Trap. rule for one panel}} \underbrace{- \frac{h^3}{12}f''(x_i) + \vartheta(h^4)}_{\text{Local Error for Trapezoidal Rule}}$$

Error of the Trapezoidal Rule

Local Error of the Trapezoidal rule is given by

$$-\frac{h^3}{12} f''(\xi_i), \quad x_i \le \xi_i \le x_{i+1}$$

The Global Error is obtained by adding the local errors.

$$\text{Global Error} = \sum_{\mathrm{i=1}}^{n} -\frac{h^3}{12} f''(\xi_i) = -\frac{h^3}{12} \sum_{\mathrm{i=1}}^{n} f''(\xi_i)$$

If f′′ is continuous on [a,b], then there is some $\xi \in [a,b]$ such that

$$\sum_{\mathrm{i=1}}^{n} f''(\xi_i) = n f''(\xi)$$

Thus, using the fact that ***n=(b-a)/h***, we obtain

$$\text{Global Error} = -\frac{\mathrm{h}^3}{12} n f''(\xi) = -\frac{\mathrm{h}^3}{12} . \frac{(b-a)}{h} f''(\xi) = -\frac{\mathrm{h}^2}{12} .(b-a) f''(\xi) = \vartheta(\mathrm{h}^2)$$

Simpson's 1/3 Rule

Simpson's Rule passes a parabola through a pair of panels.

$$I_{i+1} = I_i + hf_i + \frac{h^2}{2} f_i' + \frac{h^3}{6} f_i'' + \frac{h^4}{24} f_i''' + \frac{h^5}{120} f_i^{iv} + \frac{h^6}{720} f_i^{v} + ...$$

$$I_{i-1} = I_i - hf_i + \frac{h^2}{2} f_i' - \frac{h^3}{6} f_i'' + \frac{h^4}{24} f_i''' - \frac{h^5}{120} f_i^{iv} + \frac{h^6}{720} f_i^{v} - .....$$

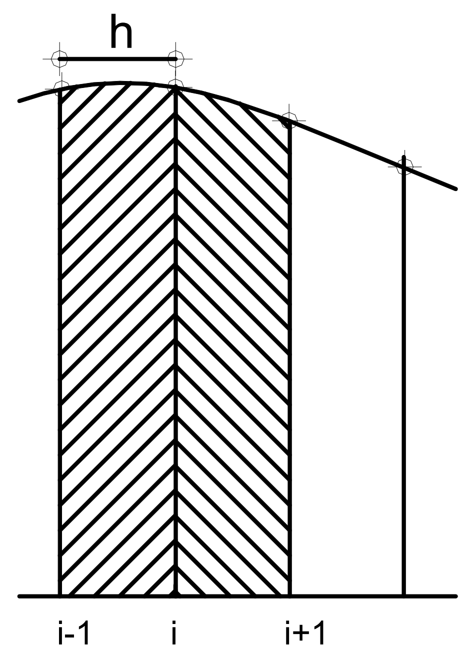
Subtracting

$$I_{i+1} - I_{i-1} = 2\left[hf_i + \frac{h^3}{3!} f_i'' + \frac{h^5}{5!} f_i^{v} + \frac{h^7}{7!} f_i^{vii} + \ldots \right]$$

$$I_{i+1} - I_{i-1} = 2hf_i + \frac{h^3}{3} f_i'' + \frac{h^5}{60} f_i^{v} + \vartheta(h^7)$$

Replace f_i'' by the central difference approximation,

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} - \frac{h^2}{12} f_i^{iv} + \vartheta(h^4)$$



Simpson's 1/3 Rule

Substituting f_i'' into our expression for $I_{i+1} - I_{i-1}$, we obtain

$$I_{i+1} - I_{i-1} = 2hf_i + \frac{h^3}{3}\left[\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} - \frac{h^2}{12} f_i^{iv} + \vartheta(h^4)\right] + \frac{h^5}{60} f_i^{iv} + \vartheta(h^7)$$

$$I_{i+1} - I_{i-1} = \frac{h}{3}\left[f_{i+1} + 4f_i + f_{i-1}\right] - \frac{h^5}{90} f_i^{iv} + \vartheta(h^7)$$

Simpson's 1/3 Rule for a pair of panel is thus

$$I_{i+1} - I_{i-1} \approx \frac{h}{3}\left[f_{i+1} + 4f_i + f_{i-1}\right]$$

The local error term is

$$-\frac{h^5}{90} f_i^{iv} + \vartheta(h^7)$$

Composite Simpson's Rule

For a pair of panels, Simpson's 1/3 rule and error term are:

$$I_{i+1} - I_{i-1} = \frac{h}{3}\left[f_{i+1} + 4f_i + f_{i-1}\right] - \frac{h^5}{90} f_i^{iv} + \vartheta(h^7)$$

Total integral is given as:

$$\mathrm{I} = \int_a^b \mathrm{f(x)dx} = \sum_{\substack{i=1 \\ i\ odd}}^{n-1} \left(I_{i+1} - I_{i-1}\right) - \sum_{\substack{i=1 \\ i\ odd}}^{n-1} \frac{h^5}{90} f_i^{iv}(\xi_i)$$

$$= \frac{\mathrm{h}}{3}\left[f_0 + 4f_1 + 2f_2 + 4f_3 + \ldots + 2f_{n-2} + 4f_{n-1} + f_n\right]$$ **Composite Simpson's Rule**

$$-\frac{h^4}{180}(b-a) f^{iv}(\xi) \quad \text{where } \mathrm{a} \le \xi \le \mathrm{b}$$ **Error term**

This is a very common numerical integral evaluation technique.

Trapezoidal and Simpson's 1/3 Rule Example

Consider the numerical evaluation of

$$I = \int_1^2 \ln x dx = 0.3862943 \longleftarrow$$ **Exact value**

Trapezoidal: $$I \approx \frac{1}{2}\left[\ln(1) + \ln(2)\right] = 0.3465735$$

Simpson's 1/3: $$I \approx \frac{1/2}{3}\left[\ln(1) + 4\ln(1.5) + \ln(2)\right] = 0.3858346$$

Effect of Mesh Refinement

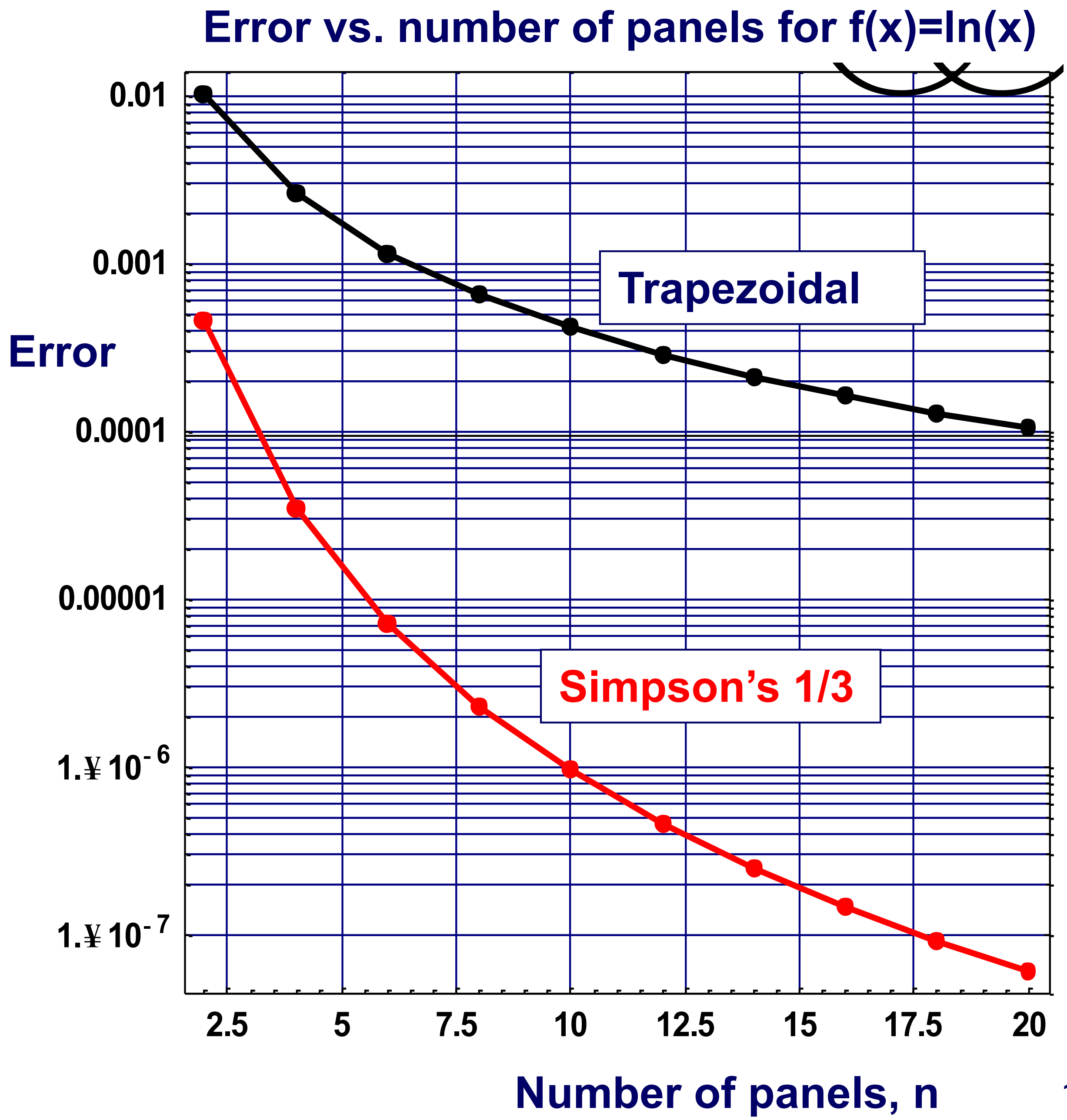
$$I = \int_1^2 \ln x\,dx = 0.3862943$$

# of panels	h	Trapezoidal	Error Trapezoidal	Simpson's 1/3	Error Simpson's 1/3
2	0.5	0.376019	0.010275	0.385835	0.000459759
4	0.25	0.3837	0.00259485	0.38626	0.0000347983
6	0.166667	0.385139	0.00115555	0.386287	7.19784×10^{-6}
8	0.125	0.385644	0.000650451	0.386292	2.31765×10^{-6}
10	0.1	0.385878	0.000416424	0.386293	9.57315×10^{-7}
12	0.0833333	0.386005	0.000289235	0.386294	4.63818×10^{-7}
14	0.0714286	0.386082	0.000212522	0.386294	2.51068×10^{-7}
16	0.0625	0.386132	0.000162723	0.386294	1.47444×10^{-7}
18	0.0555556	0.386166	0.000128578	0.386294	9.21661×10^{-8}
20	0.05	0.38619	0.000104151	0.386294	6.05255×10^{-8}

Mesh Refinement (1)

$$I = \int_1^2 \ln x \, dx$$

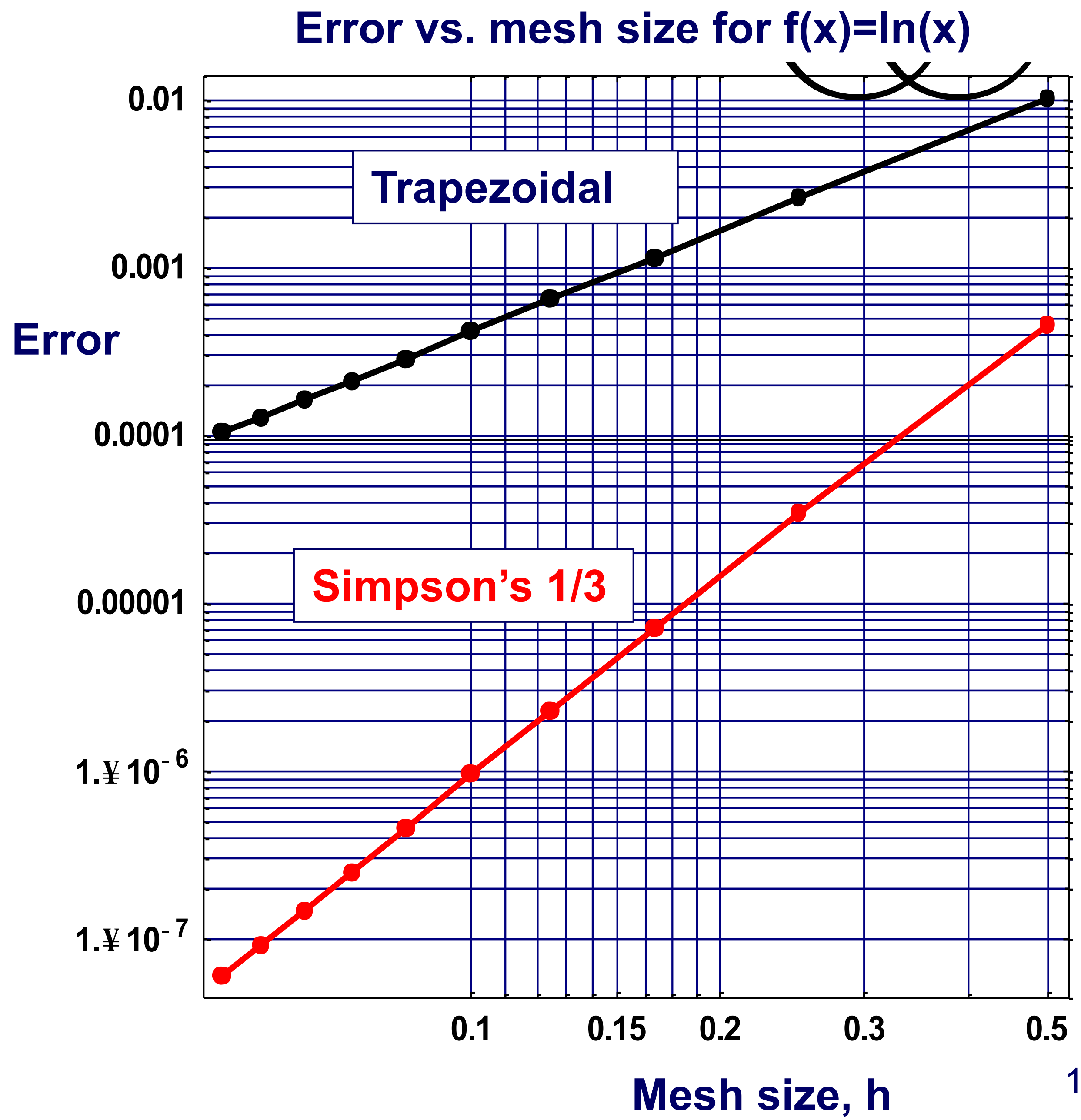
Simpson's rule is superior to the Trapezoidal rule in terms of the magnitude of the error and rate of convergence



Mesh Refinement (2)

$$I = \int_1^2 \ln x\,dx$$

On a log-log plot, the slope of the line indicates the order of the method as h is refined.



Summary

In this lecture we have

- started our discussion on numerical integration
- derived the Trapezoidal rule based on graphical considerations
- developed the truncation error of the trapezoidal rule using Taylor series expansions
- derived Simpson's 1/3 rule and it's error term
- worked on a numerical integration example and analyzed the accuracy of Trapezoidal and Simpson's rule with mesh refinement