# NUMERICAL INTEGRATION

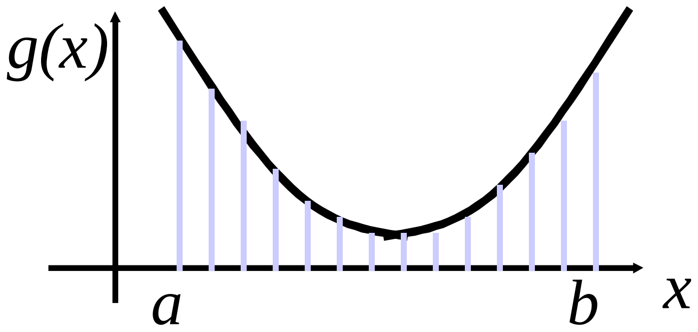
# Integration

Mathematically: the inverse operation to differentiation.

$$\frac{dI(x)}{dx} = g(x) \Rightarrow I(x) = \int g(x)dx$$

Practically: the integral of a function *g(x)* (integrand) between the limits $x_1$ and $x_2$ is equivalent to the net area between the integrand and the *x* axis.

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



# Numerical Integration

- Often *g(x)* cannot be integrated analytically to give a closed form expression for *I(x)*, e.g. solution to $y' = (1+xy)$. Motivates need to find approximate solutions for *I(x)*.

- In the differential limit, an integral is equivalent to a summation operation:

$$\int_{x_1}^{x_2} g(x)dx = \lim_{\Delta x \to 0} \sum_{x_1}^{x_2} g(x)\Delta x$$

- Approximate methods for determining integrals are mostly based on idea of area between integrand and axis.

# What Will We Learn?

## Basic Numerical Integration: *Set of Rules*

- Trapezoidal Rule
- Simpson's Rule
  - 1/3 Rule
  - 3/8 Rule

Closed form (end points are used)

- Midpoint → Open form (end points are not used)

- Gaussian Quadrature

# Basic Numerical Integration

We want to find integration of functions of various forms of the equation known as the Newton Cotes integration formulas.

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

*Quadrature*

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

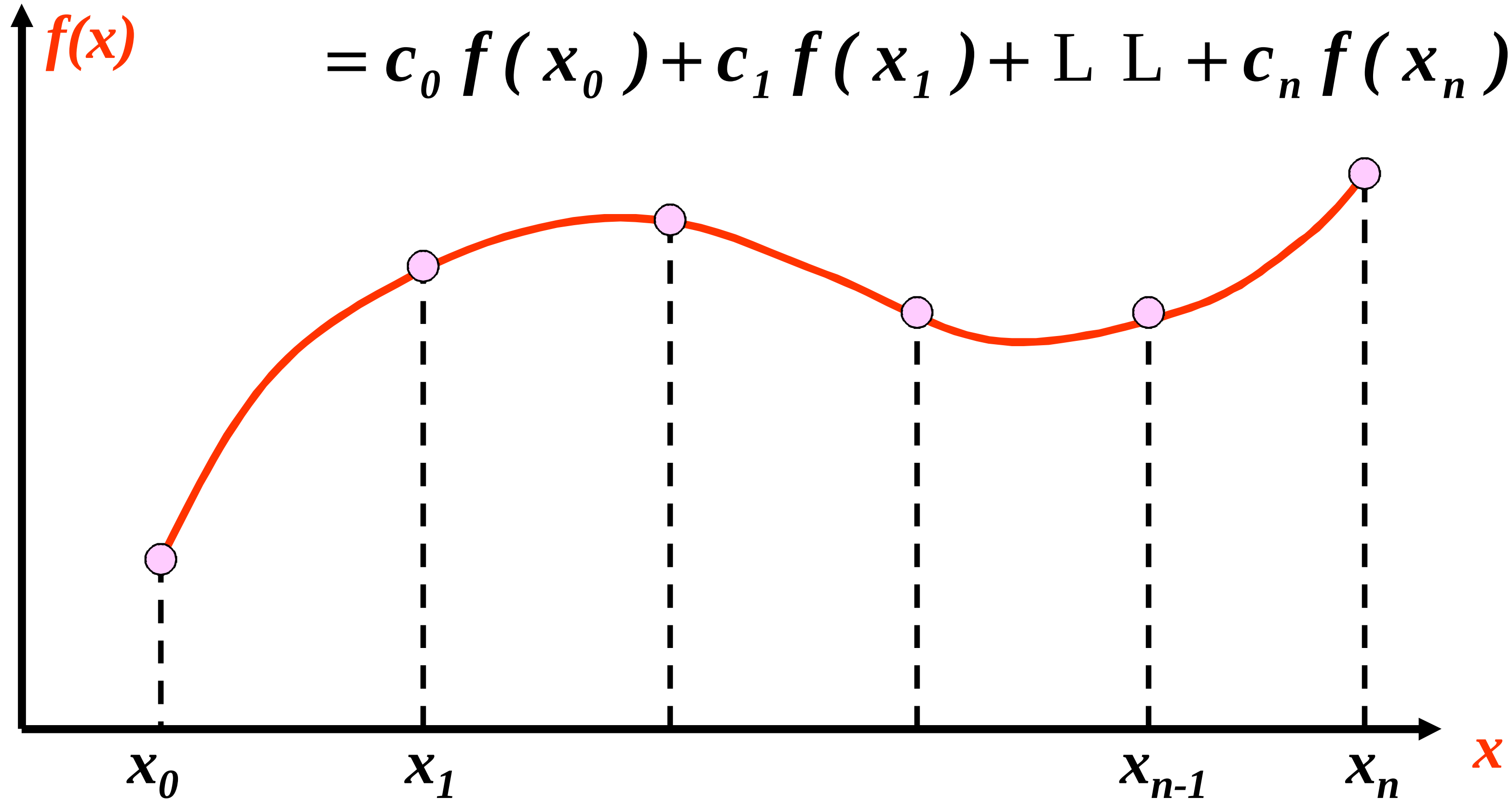
where $a \leq x_1 < x_2 < \ldots < x_n \leq b$

# Basic Numerical Integration

*Weighted sum of function values*

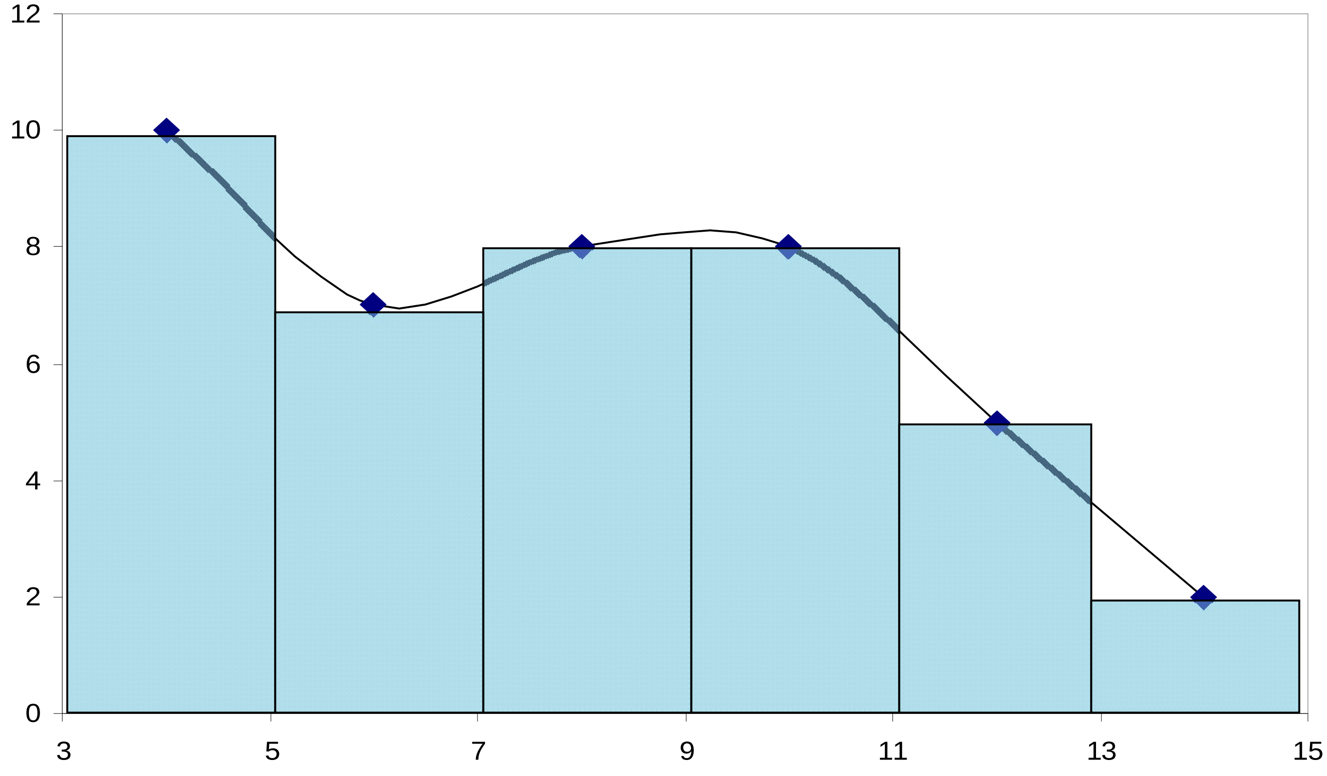
$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} c_i f(x_i)$$

$$= c_0 f(x_0) + c_1 f(x_1) + \cdots\cdots + c_n f(x_n)$$



# Numerical Integration

Idea is to do integral in small parts, like the way you first learned integration - a summation



# Numerical Integration

- **Newton-Cotes Closed Formulae -- Use both end points**
  - **Trapezoidal Rule : Linear**
  - **Simpson's 1/3-Rule : Quadratic**
  - **Simpson's 3/8-Rule : Cubic**
  - **Boole's Rule : Fourth-order**

# Numerical Integration

- **Newton-Cotes Open Formulae –**

**Use only interior points**

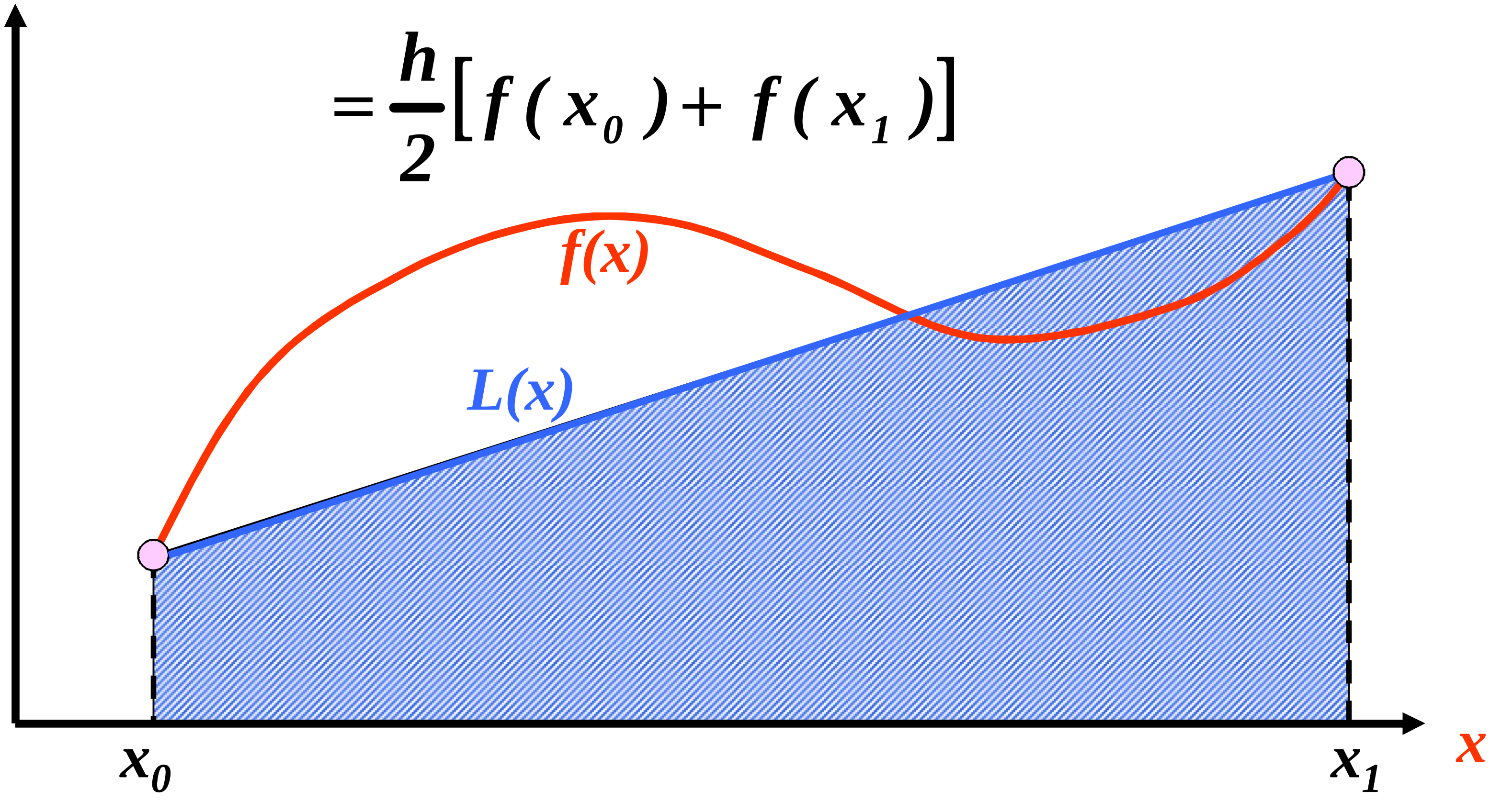
  - **midpoint rule**

# Trapezoid Rule

## Straight-line approximation (n=1)

$$\int_a^b f(x)dx \approx \sum_{i=0}^{1} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1)$$

$$= \frac{h}{2}\left[f(x_0) + f(x_1)\right]$$



# Example:Trapezoid Rule

**Evaluate the integral** $\int_0^4 xe^{2x}dx$

- **Exact solution**

$$\int_0^4 xe^{2x}dx = \left[\frac{x}{2}e^{2x} - \frac{1}{4}e^{2x}\right]_0^4$$

$$= \frac{1}{4}e^{2x}(2x-1)\Big|_0^1 = 5216.926477$$

- **Trapezoidal Rule**

$$I = \int_0^4 xe^{2x}dx \approx \frac{4-0}{2}[f(0)+f(4)] = 2(0+4e^8) = 23847.66$$

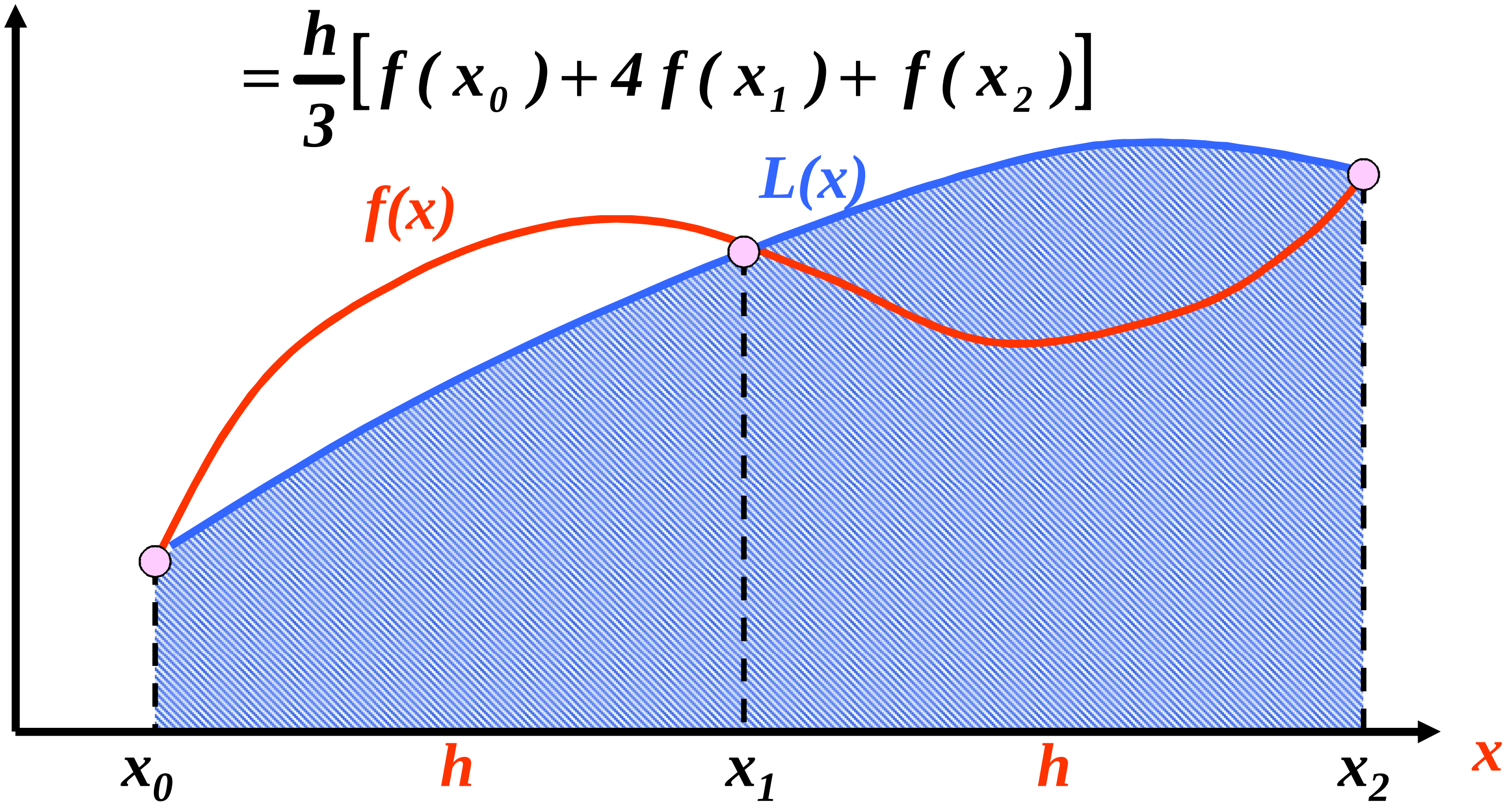
$$\varepsilon = \frac{5216.926 - 23847.66}{5216.926} = -357.12\%$$

# Simpson's 1/3-Rule

**Approximate the function by a parabola (n=2)**

$$\int_a^b f(x)dx \approx \sum_{i=0}^{2} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1) + c_2 f(x_2)$$

$$= \frac{h}{3}\left[ f(x_0) + 4 f(x_1) + f(x_2) \right]$$

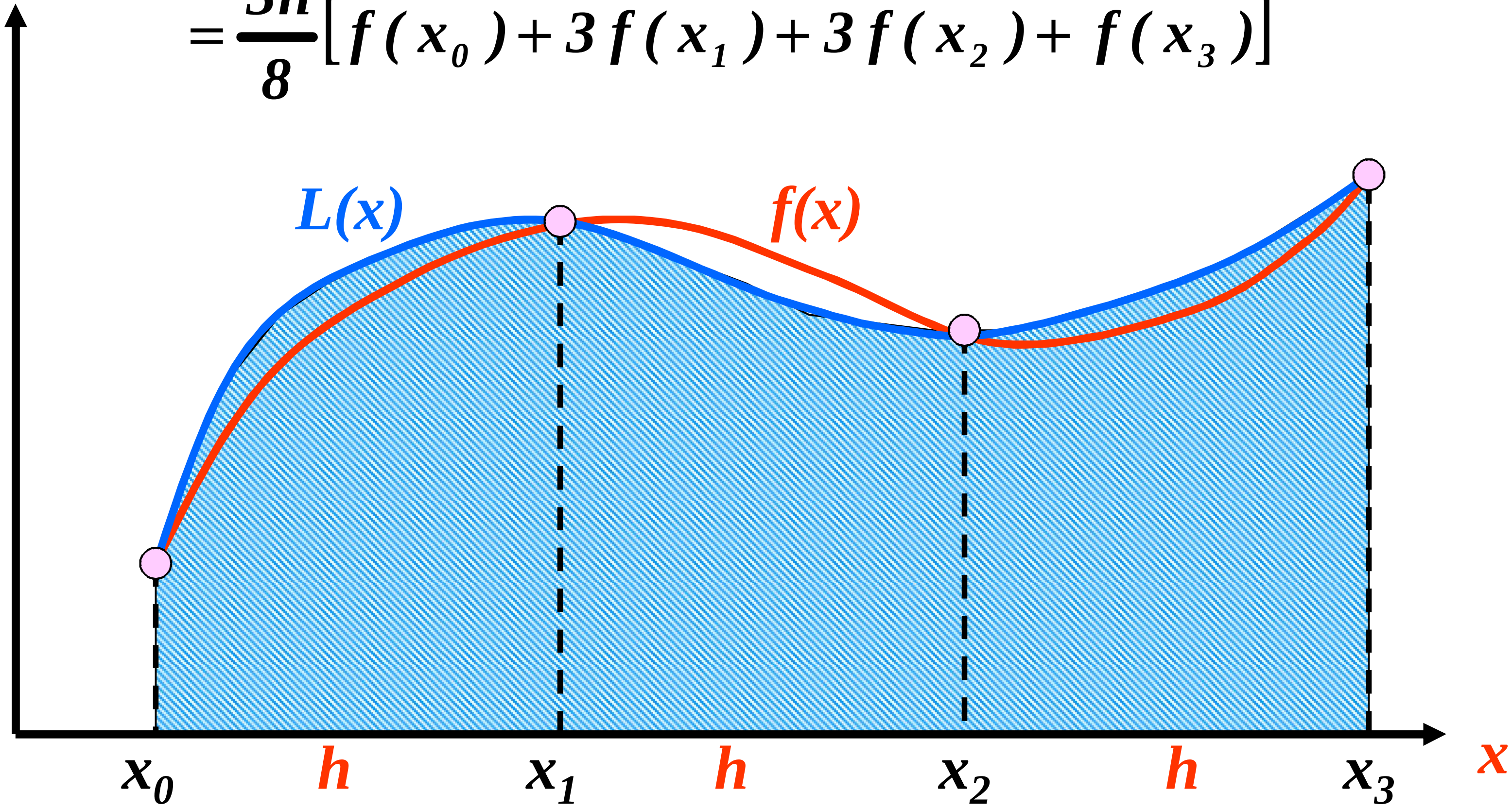


# Simpson's 3/8-Rule

**Approximate by a cubic polynomial (n=3)**

$$\int_a^b f(x)dx \approx \sum_{i=0}^{3} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$$

$$= \frac{3h}{8}\left[ f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3) \right]$$



# Example: Simpson's Rules

- **Evaluate the Integral** $\int_0^4 xe^{2x}dx$
- **Simpson's 1/3-Rule**

$$I = \int_0^4 xe^{2x}dx \approx \frac{h}{3}[f(0) + 4f(2) + f(4)]$$

$$= \frac{2}{3}\left[0 + 4(2e^4) + 4e^8\right] = 8240.411$$

$$\varepsilon = \frac{5216.926 - 8240.411}{5216.926} = -57.96\%$$

- **Simpson's 3/8-Rule**

$$I = \int_0^4 xe^{2x}dx \approx \frac{3h}{8}\left[f(0) + 3f(\frac{4}{3}) + 3f(\frac{8}{3}) + f(4)\right]$$

$$= \frac{3(4/3)}{8}[0 + 3(19.18922) + 3(552.33933) + 11923.832] = 6819.209$$

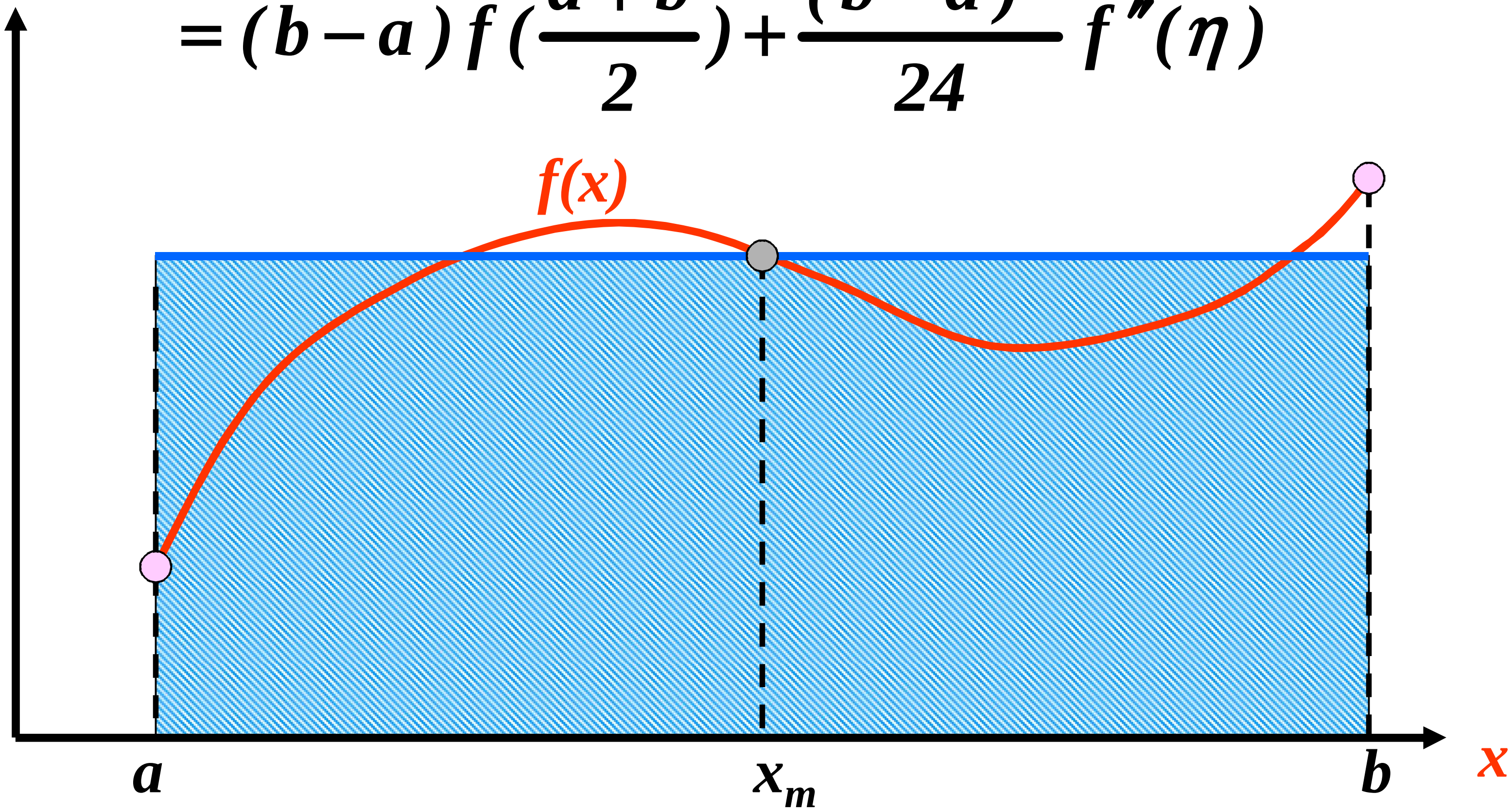
$$\varepsilon = \frac{5216.926 - 6819.209}{5216.926} = -30.71\%$$

# Midpoint Rule

## Newton-Cotes Open Formula

$$\int_a^b f(x)dx \approx (b-a)f(x_m)$$

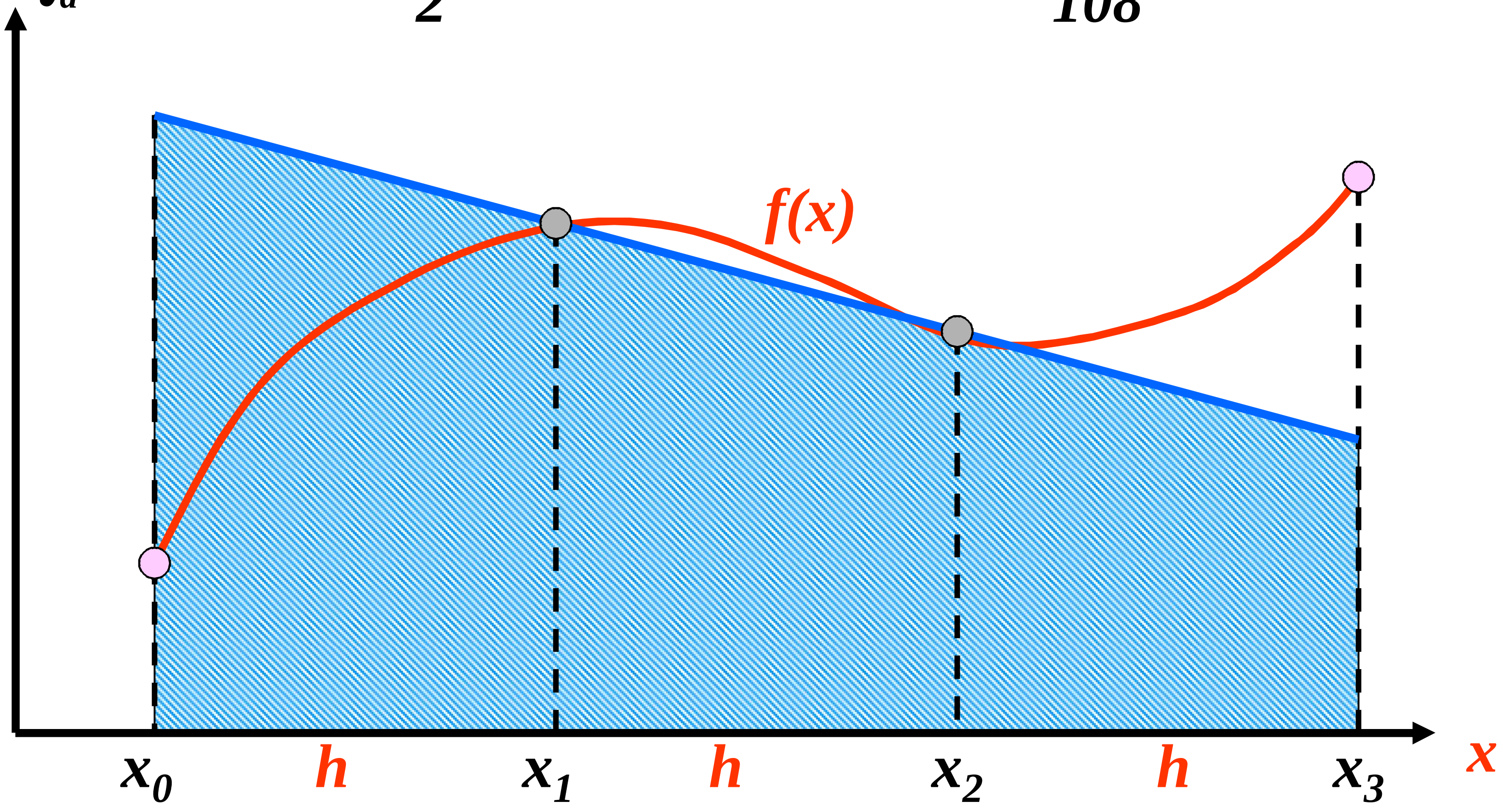
$$= (b-a)f\left(\frac{a+b}{2}\right) + \frac{(b-a)^3}{24} f''(\eta)$$



# Two-point Newton-Cotes Open Formula

## Approximate by a straight line

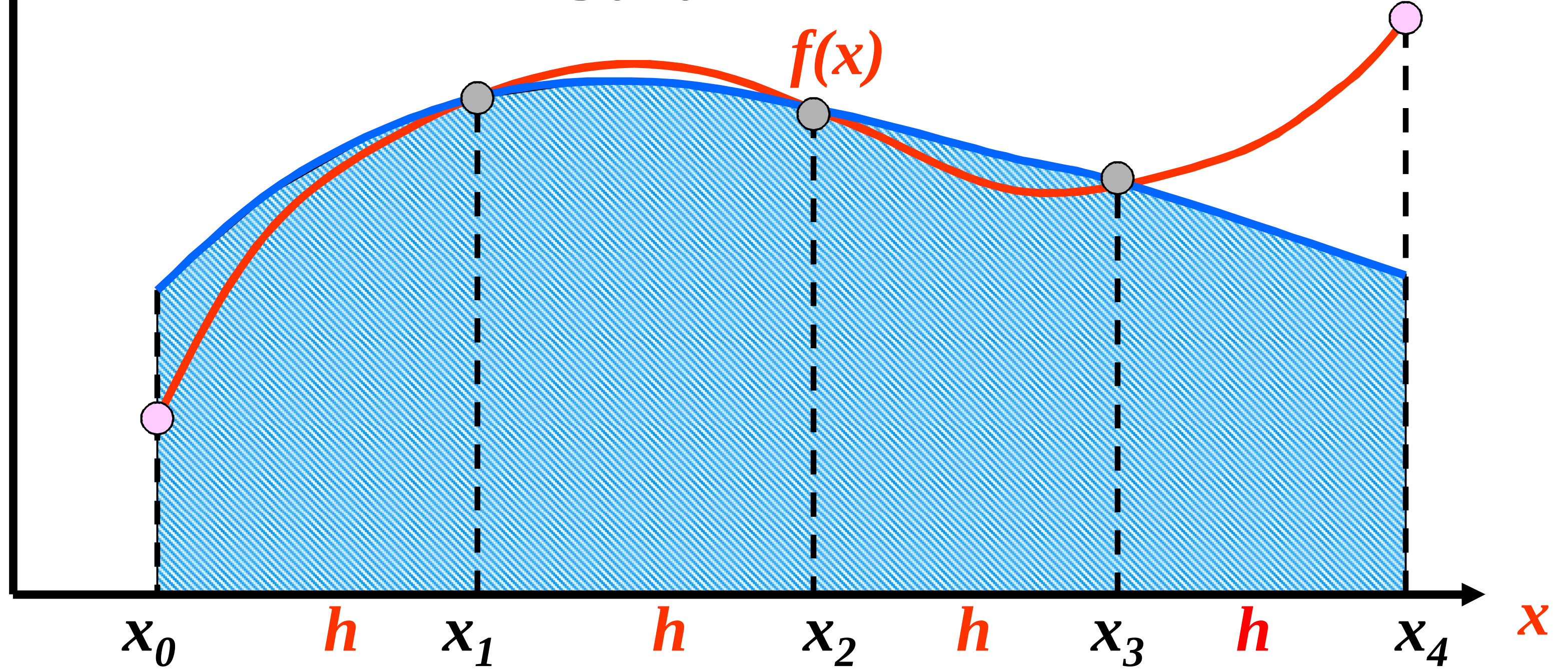
$$\int_a^b f(x)dx \approx \frac{b-a}{2}\left[f(x_1)+f(x_2)\right]+\frac{(b-a)^3}{108}f''(\eta)$$



# Three-Point Newton-Cotes Open Formula

Approximate by a parabola

$$\int_a^b f(x)dx \approx \frac{b-a}{3}\left[2f(x_1) - f(x_2) + 2f(x_3)\right] + \frac{7(b-a)^5}{23040} f''''(\eta)$$

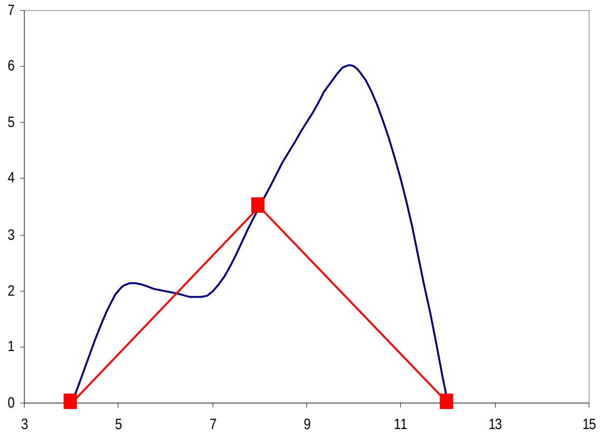


# Better Numerical Integration

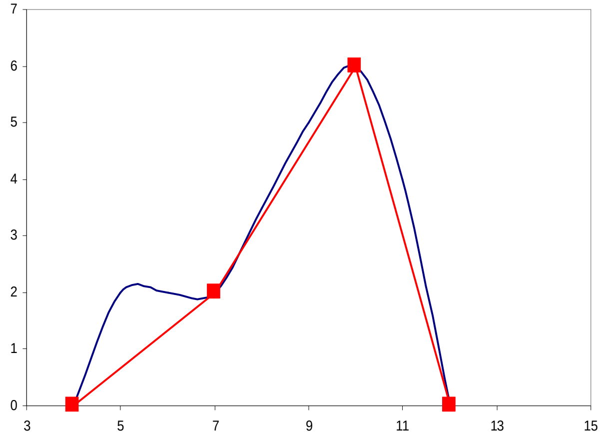
- Composite integration
  - Composite Trapezoidal Rule
  - Composite Simpson's Rule
- Romberg integration

# Apply Trapezoid Rule to Multiple Segments Over Integration Limits

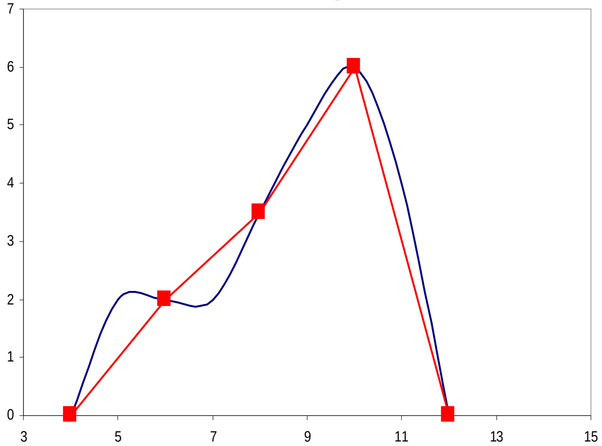
Two segments



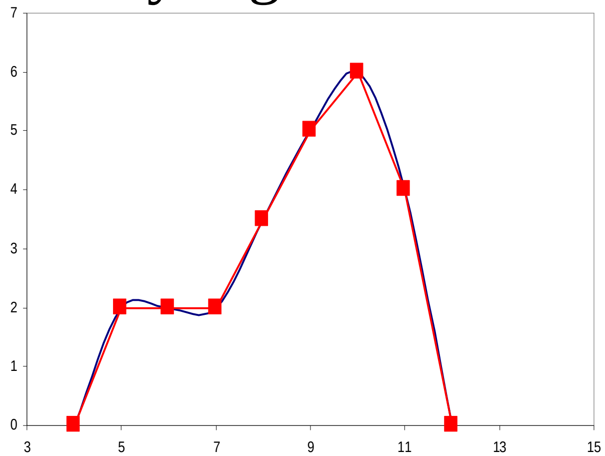

Three segments




Four segments




Many segments



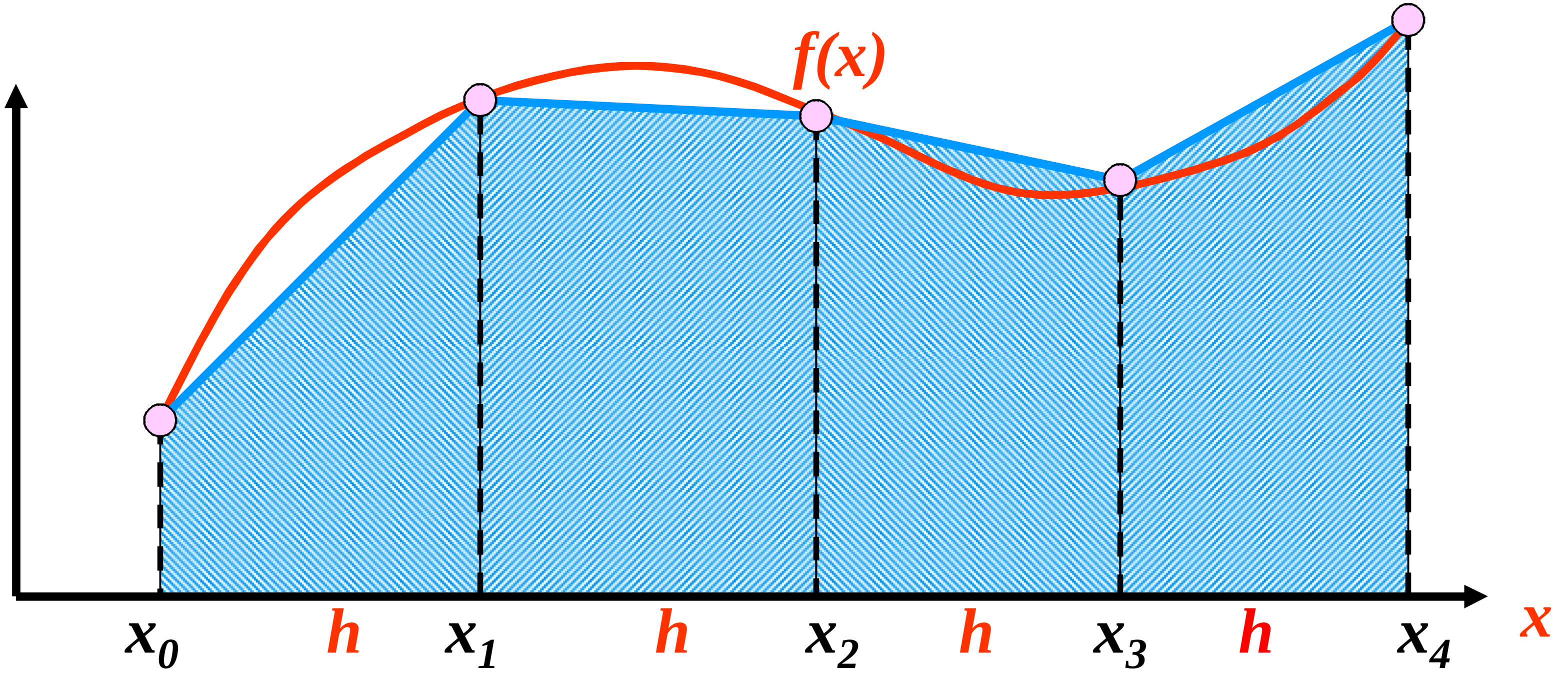
# Composite Trapezoid Rule

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots\cdots + \int_{x_{n-1}}^{x_n} f(x)dx$$

$$= \frac{h}{2}\left[f(x_0) + f(x_1)\right] + \frac{h}{2}\left[f(x_1) + f(x_2)\right] + \cdots + \frac{h}{2}\left[f(x_{n-1}) + f(x_n)\right]$$

$$= \frac{h}{2}\left[f(x_0) + 2f(x_1) + \cdots + 2f(x_i) + \cdots + 2f(x_{n-1}) + f(x_n)\right]$$

$$\boxed{h = \frac{b-a}{n}}$$



# Composite Trapezoid Rule

**Evaluate the integral**

$$\boxed{I = \int_0^4 x e^{2x} dx}$$

$$n = 1, h = 4 \Rightarrow I = \frac{h}{2}\left[f(0) + f(4)\right] = 23847.66 \qquad \varepsilon = -357.12\%$$

$$n = 2, h = 2 \Rightarrow I = \frac{h}{2}\left[f(0) + 2f(2) + f(4)\right] = 12142.23 \qquad \varepsilon = -132.75\%$$

$$\begin{aligned} n = 4, h = 1 \Rightarrow I = \frac{h}{2}\Big[ & f(0) + 2f(1) + 2f(2) \\ & + 2f(3) + f(4)\Big] = 7288.79 \qquad \varepsilon = -39.71\% \end{aligned}$$

$$\begin{aligned} n = 8, h = 0.5 \Rightarrow I = \frac{h}{2}\Big[ & f(0) + 2f(0.5) + 2f(1) \\ & + 2f(1.5) + 2f(2) + 2f(2.5) + 2f(3) \\ & + 2f(3.5) + f(4)\Big] = 5764.76 \qquad \varepsilon = -10.50\% \end{aligned}$$

$$\begin{aligned} n = 16, h = 0.25 \Rightarrow I = \frac{h}{2}\Big[ & f(0) + 2f(0.25) + 2f(0.5) + \cdots \\ & + 2f(3.5) + 2f(3.75) + f(4)\Big] \\ & = 5355.95 \qquad \varepsilon = -2.66\% \end{aligned}$$

# Composite Trapezoid Rule with Unequal Segments

**Evaluate the integral** $I = \int_0^4 xe^{2x}dx$

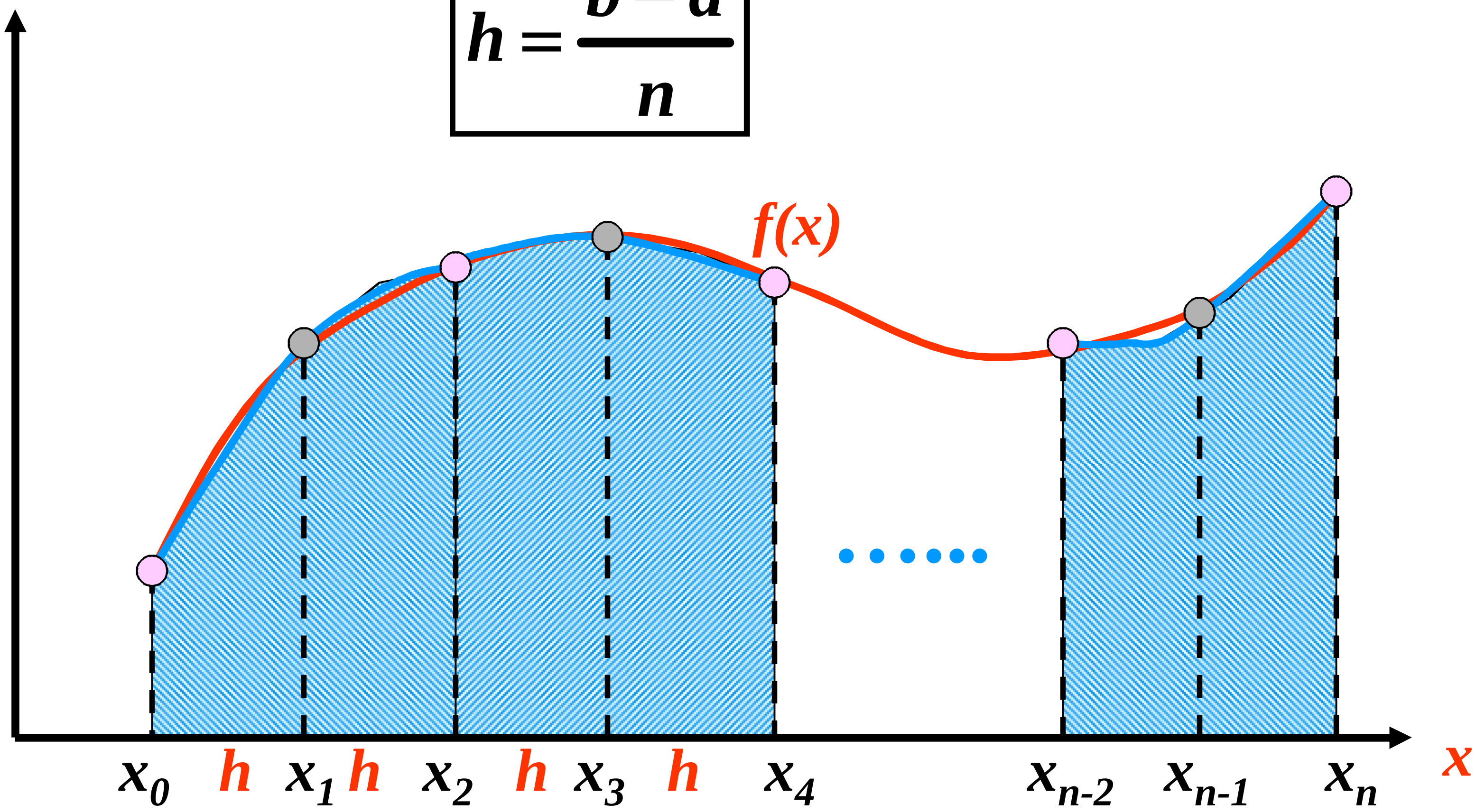
- $h_1 = 2,\ h_2 = 1,\ h_3 = 0.5,\ h_4 = 0.5$

$$\boxed{\begin{aligned} I &= \int_0^2 f(x)dx + \int_2^3 f(x)dx + \int_3^{3.5} f(x)dx + \int_{3.5}^4 f(x)dx \\ &= \frac{h_1}{2}\left[f(0) + f(2)\right] + \frac{h_2}{2}\left[f(2) + f(3)\right] \\ &+ \frac{h_3}{2}\left[f(3) + f(3.5)\right] + \frac{h_4}{2}\left[f(3.5) + f(4)\right] \\ &= \frac{2}{2}\left[0 + 2e^4\right] + \frac{1}{2}\left[2e^4 + 3e^6\right] + \frac{0.5}{2}\left[3e^6 + 3.5e^7\right] \\ &+ \frac{0.5}{2}\left[3.5e^7 + 4e^8\right] = 5971.58 \qquad \Rightarrow \varepsilon = -14.45\% \end{aligned}}$$

# Composite Simpson's Rule

**Piecewise Quadratic approximations**

$$h = \frac{b-a}{n}$$



# Composite Simpson's Rule

**Multiple applications of Simpson's rule**

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)dx$$

$$= \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] + \frac{h}{3}\left[f(x_2) + 4f(x_3) + f(x_4)\right]$$

$$+ \cdots + \frac{h}{3}\left[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right]$$

$$= \frac{h}{3}\Big[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots$$

$$+ 4f(x_{2i-1}) + 2f(x_{2i}) + 4f(x_{2i+1}) + \cdots$$

$$+ 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\Big]$$

# Composite Simpson's Rule

**Evaluate the integral** $I = \int_0^4 xe^{2x}dx$

- $n = 2, h = 2$

$$I = \frac{h}{3}[f(0)+4f(2)+f(4)]$$
$$= \frac{2}{3}\left[0+4(2e^4)+4e^8\right] = 8240.411 \quad \Rightarrow \varepsilon = -57.96\%$$

- $n = 4, h = 1$

$$I = \frac{h}{3}[f(0)+4f(1)+2f(2)+4f(3)+f(4)]$$
$$= \frac{1}{3}\left[0+4(e^2)+2(2e^4)+4(3e^6)+4e^8\right]$$
$$= 5670.975 \quad \Rightarrow \varepsilon = -8.70\%$$

# Composite Simpson's Rule with Unequal Segments

**Evaluate the integral** $$I = \int_0^4 xe^{2x}dx$$

- $h_1 = 1.5,\ h_2 = 0.5$

$$
\begin{aligned}
I &= \int_0^3 f(x)dx + \int_3^4 f(x)dx \\
&= \frac{h_1}{3}\left[f(0) + 4f(1.5) + 2f(3)\right] \\
&\quad + \frac{h_2}{3}\left[f(3) + 4f(3.5) + 2f(4)\right] \\
&= \frac{1.5}{3}\left[0 + 4(1.5e^3) + 3e^6\right] + \frac{0.5}{3}\left[3e^6 + 4(3.5e^7) + 4e^8\right] \\
&= 5413.23 \quad \Rightarrow \varepsilon = -3.76\%
\end{aligned}
$$

# Romberg Integration

$$\boxed{I_{j,k} = \frac{4^k I_{j+1,k} - I_{j,k}}{4^k - 1}; \quad k = 1, 2, 3, \ldots}$$

| | *Trapezoid* | *Simpson's* | *Boole's* | | |
|---|---|---|---|---|---|
| | $k = 0$ | $k = 1$ | $k = 2$ | $k = 3$ | $k = 4$ |
| | $O(h^2)$ | $O(h^4)$ | $O(h^6)$ | $O(h^8)$ | $O(h^{10})$ |
| $h$ | $I_{0,0}$ | $I_{0,1}$ | $I_{0,2}$ | $I_{0,3}$ | $I_{0,4}$ |
| $h/2$ | $I_{1,0}$ | $I_{1,1}$ | $I_{1,2}$ | $I_{1,3}$ | |
| $h/4$ | $I_{2,0}$ | $I_{2,1}$ | $I_{2,2}$ | | |
| $h/8$ | $I_{3,0}$ | $I_{3,1}$ | | | |
| $h/16$ | $I_{4,0}$ | | | | |
| | | $\dfrac{4I_{j+1,0} - I_{j,0}}{3}$ | $\dfrac{16I_{j+1,1} - I_{j,1}}{15}$ | $\dfrac{64I_{j+1,2} - I_{j,2}}{63}$ | $\dfrac{256I_{j+1,3} - I_{j,3}}{255}$ |

# Romberg Integration

$$\boxed{I = \int_0^4 x e^{2x} dx = 5216.926477}$$

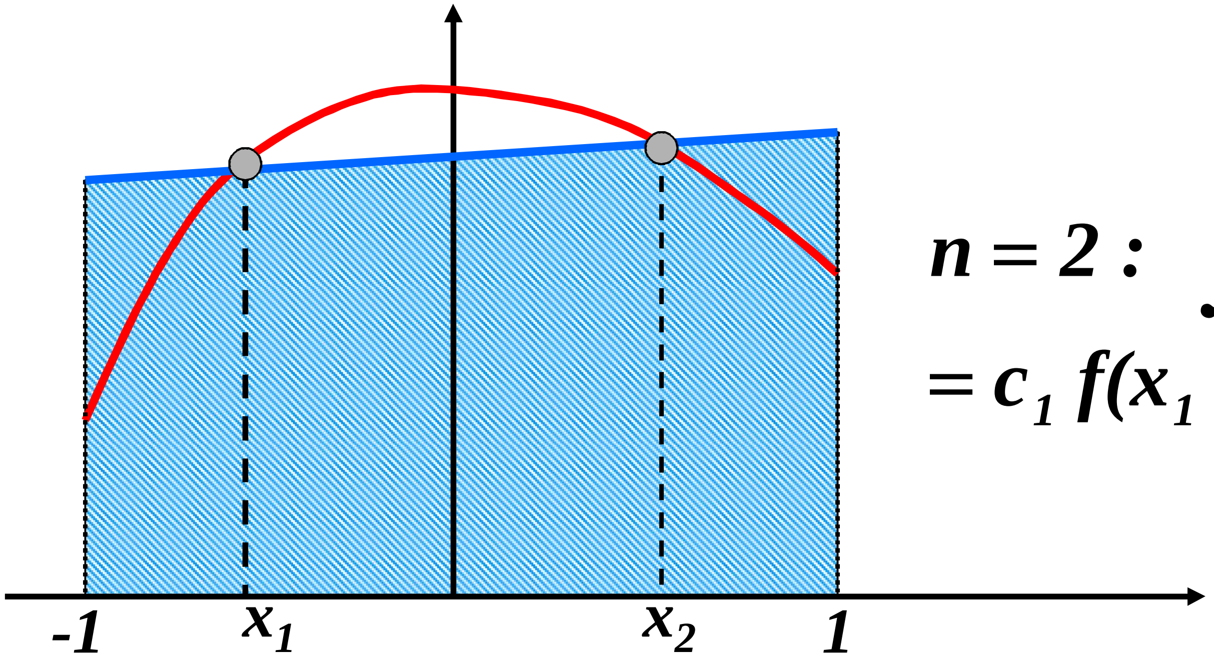
| | Trapezoid | Simpson's | Boole's | | |
|---|---|---|---|---|---|
| | $k = 0$ | $k = 1$ | $k = 2$ | $k = 3$ | $k = 4$ |
| | $O(h^2)$ | $O(h^4)$ | $O(h^6)$ | $O(h^8)$ | $O(h^{10})$ |
| $h = 4$ | 23847.7 | 8240.41 | 5499.68 | 5224.84 | 5216.95 |
| $h = 2$ | 12142.2 | 5670.98 | 5229.14 | 5217.01 | |
| $h = 1$ | 7288.79 | 5256.75 | 5217.20 | | |
| $h = 0.5$ | 5764.76 | 5219.68 | | | |
| $h = 0.25$ | 5355.95 | | | | |
| $\varepsilon =$ | $-2.66\%$ | $-0.0527\%$ | $-0.0053\%$ | $-0.00168\%$ | $-0.00050\%$ |

# Gaussian Quadratures

- **Newton-Cotes Formulae**
  - use evenly-spaced functional values
- **Gaussian Quadratures**
  - select functional values at non-uniformly distributed points to achieve higher accuracy
  - change of variables so that the interval of integration is [-1,1]

# Gaussian Quadrature on [-1, 1]

$$\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} c_i f(x_i) = c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n)$$




$$n = 2: \int_{-1}^{1} f(x)dx = c_1 f(x_1) + c_2 f(x_2)$$

- Choose $(c_1, c_2, x_1, x_2)$ such that the method yields "exact integral" for $f(x) = x^0, x^1, x^2, x^3$

# Gaussian Quadrature on [-1, 1]

$$n = 2: \quad \int_{-1}^{1} f(x)dx = c_1 f(x_1) + c_2 f(x_2)$$

**Exact integral for $f = x^0, x^1, x^2, x^3$**

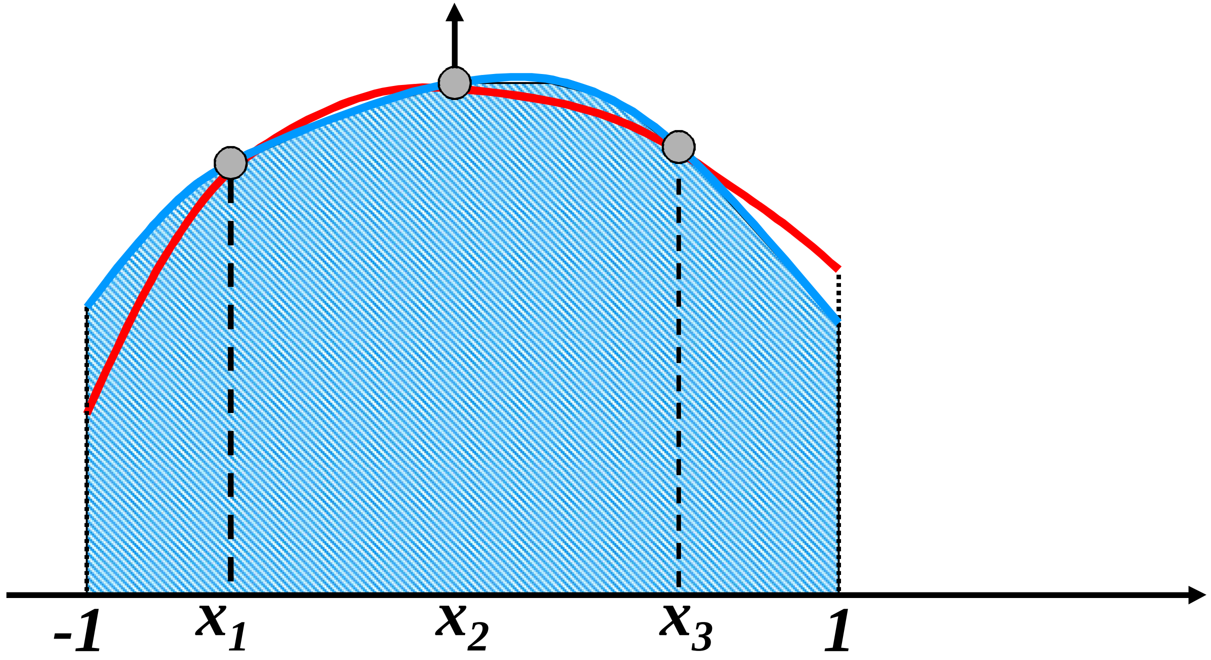
- **Four equations for four unknowns**

$$\begin{cases} f = 1 \Rightarrow \int_{-1}^{1} 1dx = 2 = c_1 + c_2 \\ f = x \Rightarrow \int_{-1}^{1} xdx = 0 = c_1 x_1 + c_2 x_2 \\ f = x^2 \Rightarrow \int_{-1}^{1} x^2 dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 \\ f = x^3 \Rightarrow \int_{-1}^{1} x^3 dx = 0 = c_1 x_1^3 + c_2 x_2^3 \end{cases} \Rightarrow \begin{cases} c_1 = 1 \\ c_2 = 1 \\ x_1 = \frac{-1}{\sqrt{3}} \\ x_2 = \frac{1}{\sqrt{3}} \end{cases}$$

$$\boxed{I = \int_{-1}^{1} f(x)dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)}$$

# Gaussian Quadrature on [-1, 1]

$$n = 3: \quad \int_{-1}^{1} f(x)dx = c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$$




- Choose $(c_1, c_2, c_3, x_1, x_2, x_3)$ such that the method yields "exact integral" for $f(x) = x^0, x^1, x^2, x^3, x^4, x^5$

# Gaussian Quadrature on [-1, 1]

$$f = 1 \Rightarrow \int_{-1}^{1} x dx = 2 = c_1 + c_2 + c_3$$

$$f = x \Rightarrow \int_{-1}^{1} x dx = 0 = c_1 x_1 + c_2 x_2 + c_3 x_3$$

$$f = x^2 \Rightarrow \int_{-1}^{1} x^2 dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 + c_3 x_3^2$$

$$f = x^3 \Rightarrow \int_{-1}^{1} x^3 dx = 0 = c_1 x_1^3 + c_2 x_2^3 + c_3 x_3^3$$

$$f = x^4 \Rightarrow \int_{-1}^{1} x^4 dx = \frac{2}{5} = c_1 x_1^4 + c_2 x_2^4 + c_3 x_3^4$$

$$f = x^5 \Rightarrow \int_{-1}^{1} x^5 dx = 0 = c_1 x_1^5 + c_2 x_2^5 + c_3 x_3^5$$

$$\Rightarrow \begin{cases} c_1 = 5/9 \\ c_2 = 8/9 \\ c_3 = 5/9 \\ x_1 = -\sqrt{3/5} \\ x_2 = 0 \\ x_3 = \sqrt{3/5} \end{cases}$$

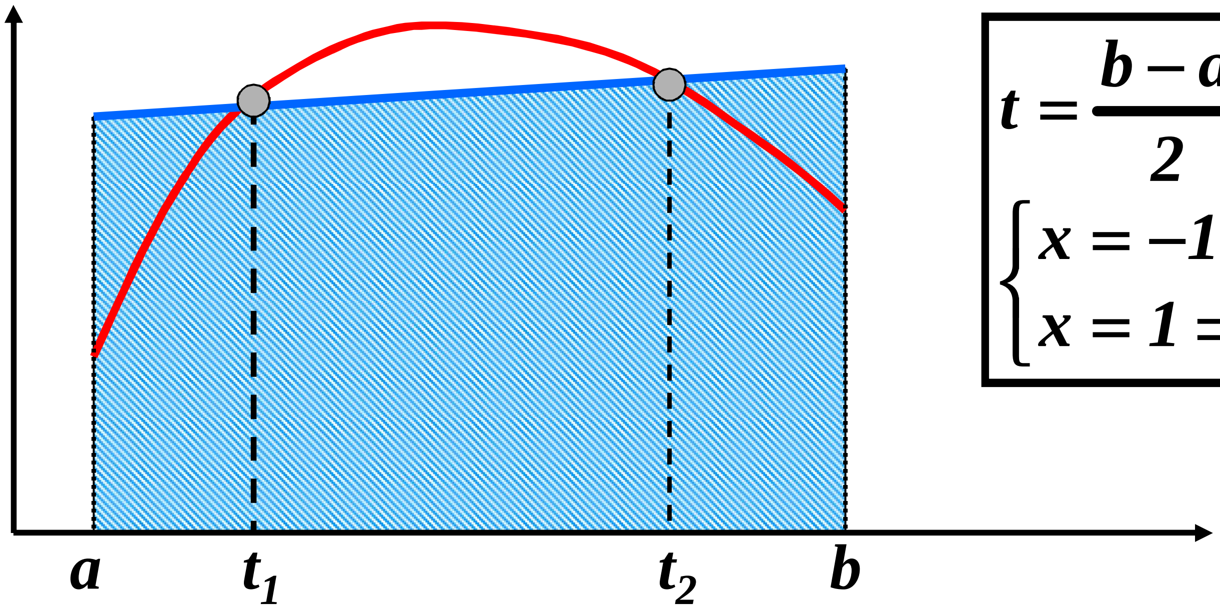
# Gaussian Quadrature on [-1, 1]

Exact integral for $f = x^0, x^1, x^2, x^3, x^4, x^5$

$$\boxed{I = \int_{-1}^{1} f(x)dx = \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)}$$

# Gaussian Quadrature on [a, b]

## Coordinate transformation from [a,b] to [-1,1]




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

$$\begin{cases} x = -1 \Rightarrow t = a \\ x = 1 \Rightarrow \quad t = b \end{cases}$$

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

# Example: Gaussian Quadrature

**Evaluate** $\quad I = \int_0^4 te^{2t}dt = 5216.926477$

**Coordinate transformation**

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

$$I = \int_0^4 te^{2t}dt = \int_{-1}^{1}(4x+4)e^{4x+4}dx = \int_{-1}^{1} f(x)dx$$

**Two-point formula**

$$I = \int_{-1}^{1} f(x)dx = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) = \left(4 - \frac{4}{\sqrt{3}}\right)e^{4-\frac{4}{\sqrt{3}}} + \left(4 + \frac{4}{\sqrt{3}}\right)e^{4+\frac{4}{\sqrt{3}}}$$

$$= 9.167657324 + 3468.376279 = 3477.543936 \qquad (\varepsilon = 33.34\%)$$

# Example: Gaussian Quadrature

## Three-point formula

$$I = \int_{-1}^{1} f(x)dx = \frac{5}{9} f(-\sqrt{0.6}) + \frac{8}{9} f(0) + \frac{5}{9} f(\sqrt{0.6})$$

$$= \frac{5}{9}(4 - 4\sqrt{0.6})e^{4-\sqrt{0.6}} + \frac{8}{9}(4)e^{4} + \frac{5}{9}(4 + 4\sqrt{0.6})e^{4+\sqrt{0.6}}$$

$$= \frac{5}{9}(2.221191545) + \frac{8}{9}(218.3926001) + \frac{5}{9}(8589.142689)$$

$$= 4967.106689 \qquad (\varepsilon = 4.79\%)$$

## Four-point formula

$$I = \int_{-1}^{1} f(x)dx = 0.34785\left[f(-0.861136) + f(0.861136)\right]$$

$$+ 0.652145\left[f(-0.339981) + f(0.339981)\right]$$

$$= 5197.54375 \qquad (\varepsilon = 0.37\%)$$

# Comparison of the Integration Formulae

Simpson's rule with 'n' points gives about as much accuracy as Trapezoidal rule with '2n' points.

If Gauss quadrature is used we may attain the same accuracy with 'n/2' points: An advantage over Simpson's rule.

But, there is no easy way of picking the intervals in Gauss method: So we end up using Trapezoidal/ Simpson's rules

We may be given tabulated functions already tabulated at equal intervals in which case only trapezoidal and Simpson's rules can be applied

If the given function is given at random unequal intervals only Trapezoidal rule can be applied

**Next Lecture: Introduction to numerical solutions of differential equations**