Computational Methods
CMSC/AMSC/MAPL 460

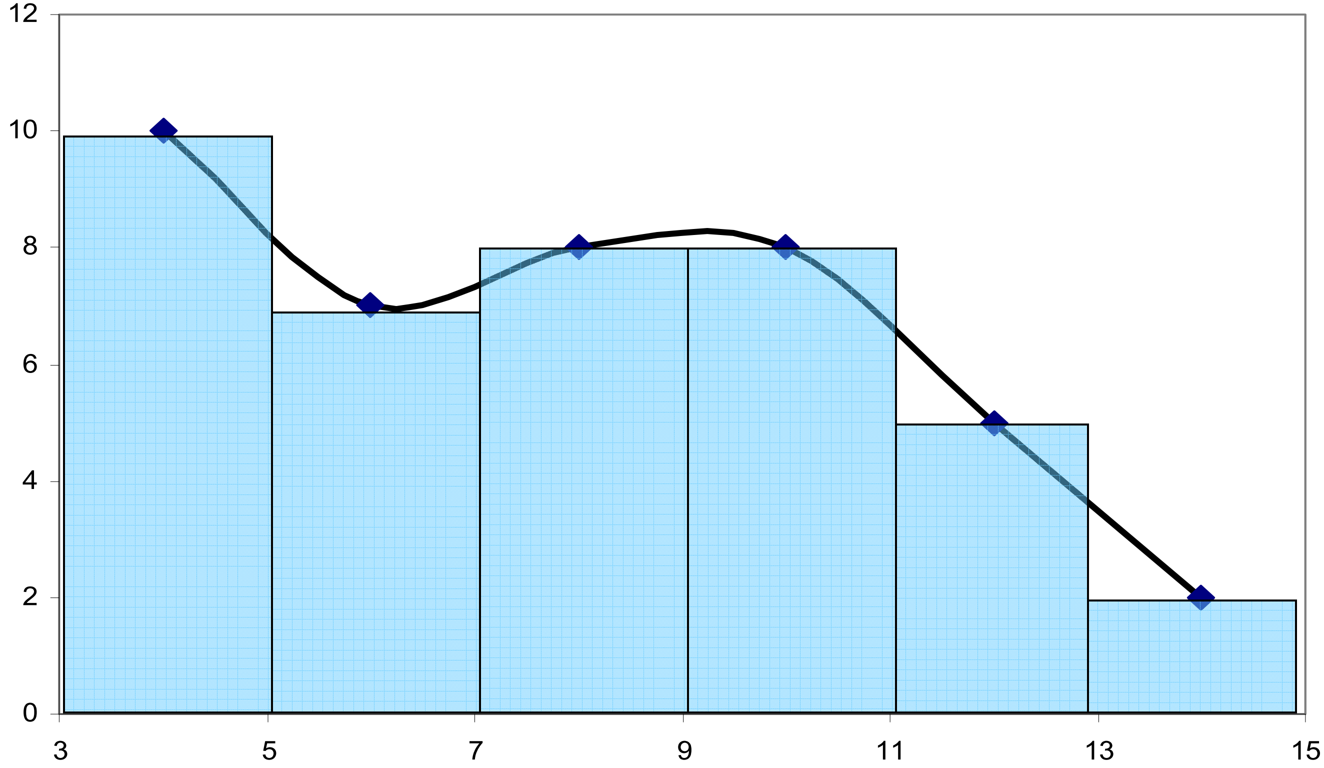
Numerical Integration

Ramani Duraiswami,
Dept. of Computer Science

Numerical Integration

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

Numerical methods just try to make it faster and more accurate

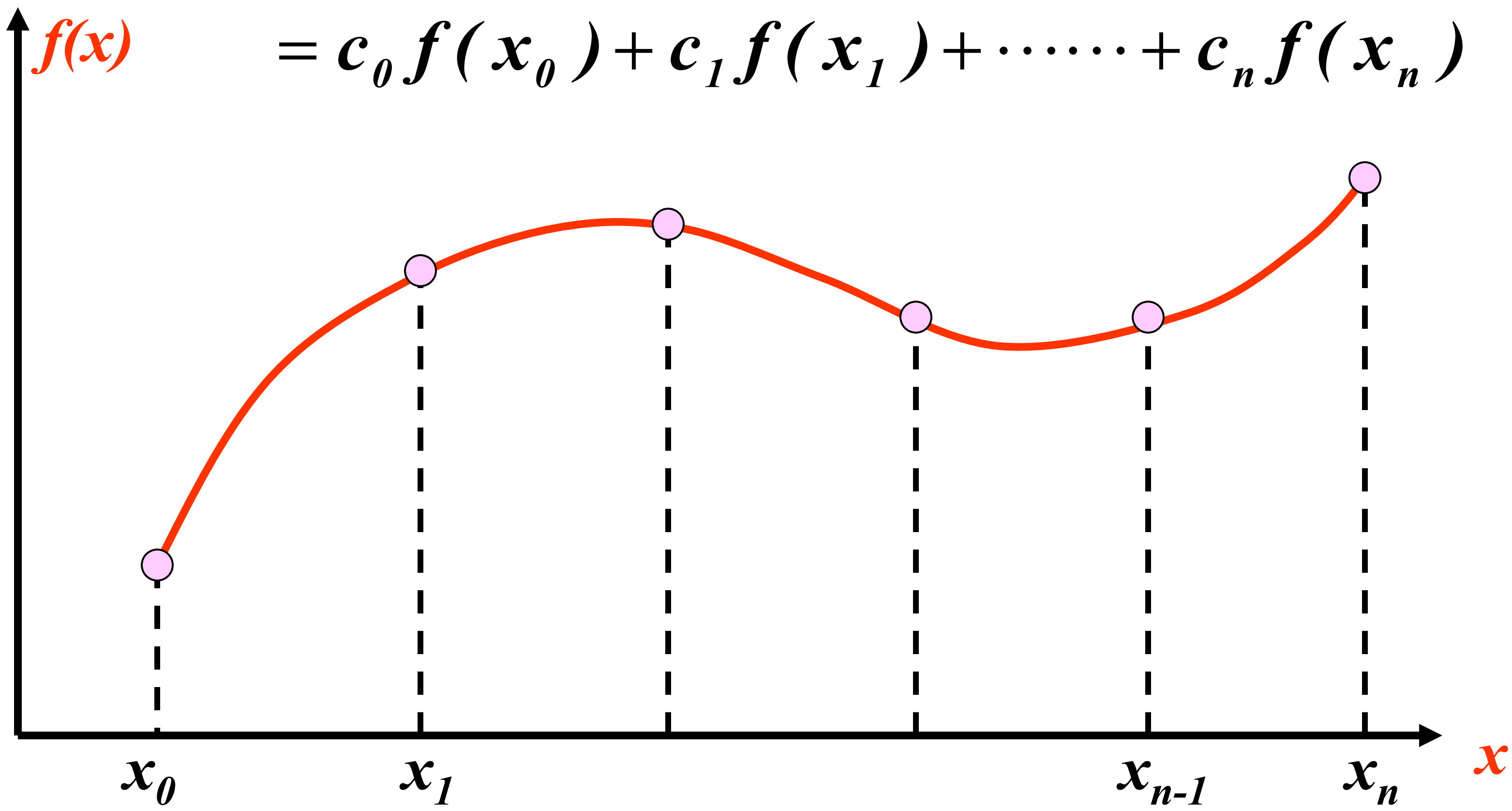


Basic Numerical Integration

- **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

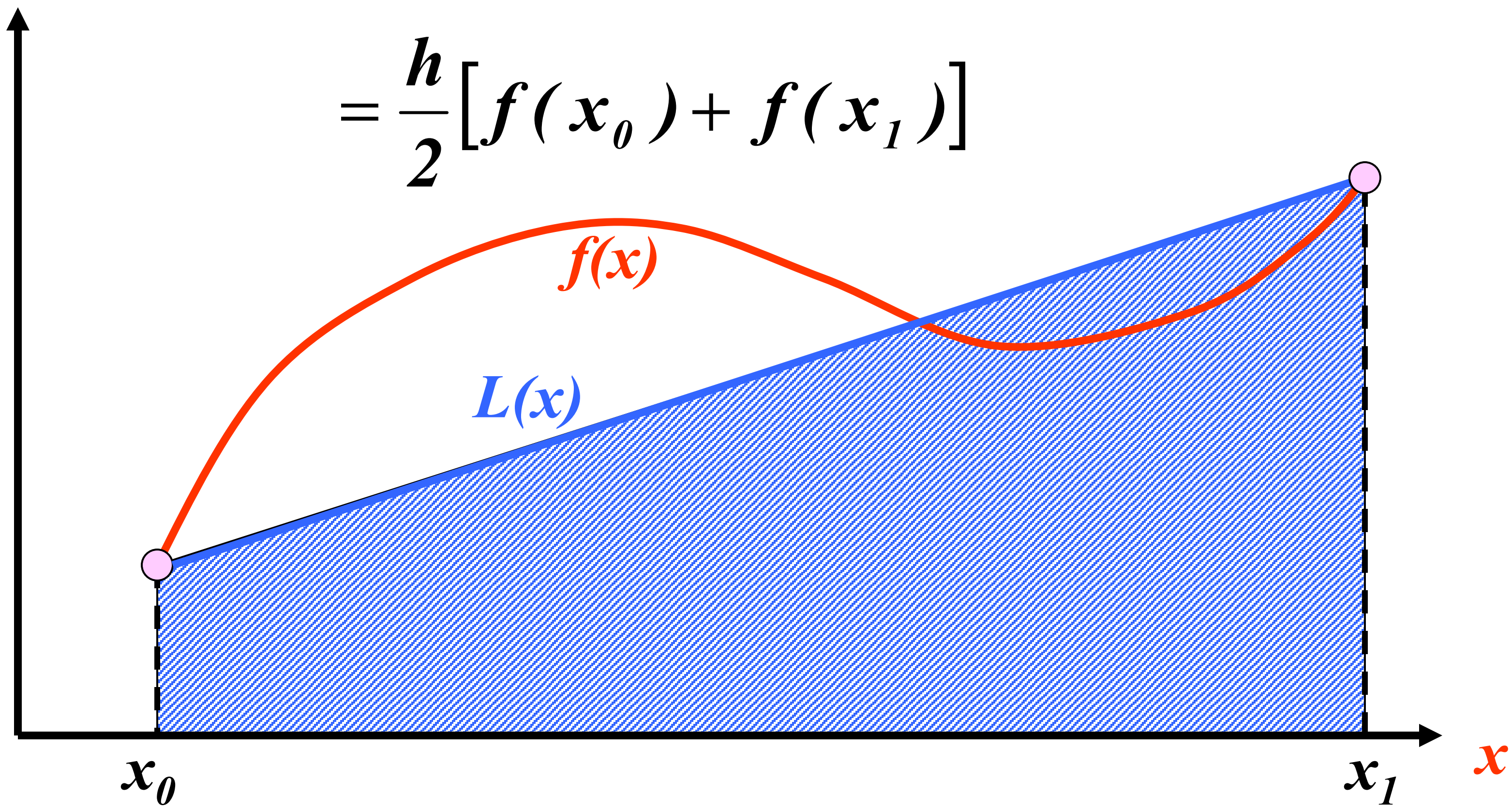
- **Characterized by where the function is evaluated**
- **Newton-Cotes Closed Formulae -- Use both end points**
  - **Trapezoidal Rule : Linear**
  - **Simpson’s 1/3-Rule : Quadratic**
  - **Simpson’s 3/8-Rule : Cubic**
  - **Boole’s Rule : Fourth-order**
- **Newton-Cotes Open Formulae -- Use only interior points**
  - **midpoint rule**

Trapezoid Rule

- **Straight-line approximation**

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

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



Example:Trapezoid Rule

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

- **Exact solution (integration by parts)`**

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

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

- **Trapezoidal Rule**

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

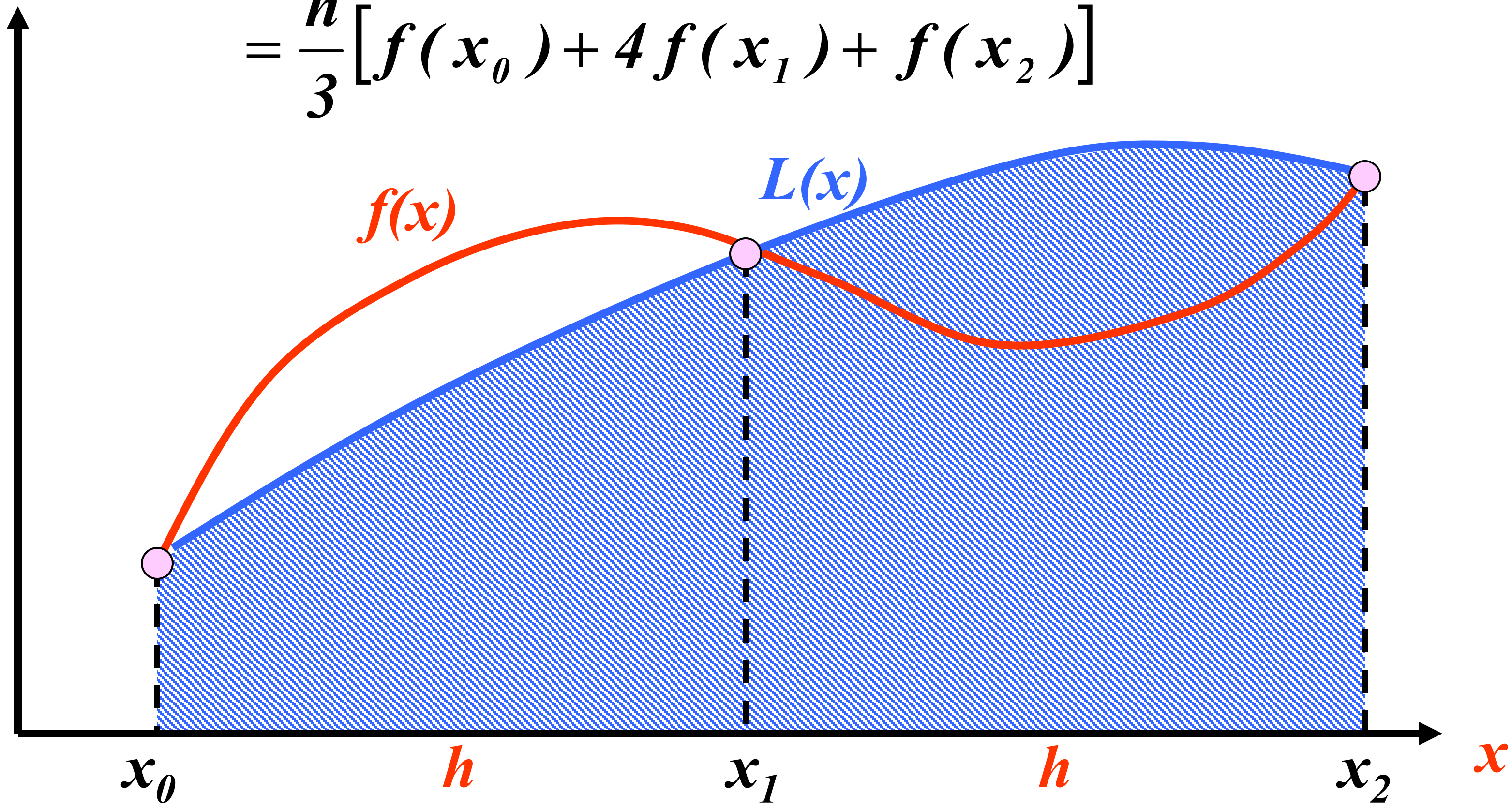
$$\varepsilon = \frac{5216.926 - 23847.66}{5216.926} = -357.12\%$$

Simpson's 1/3-Rule

Approximate the function by a parabola

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

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

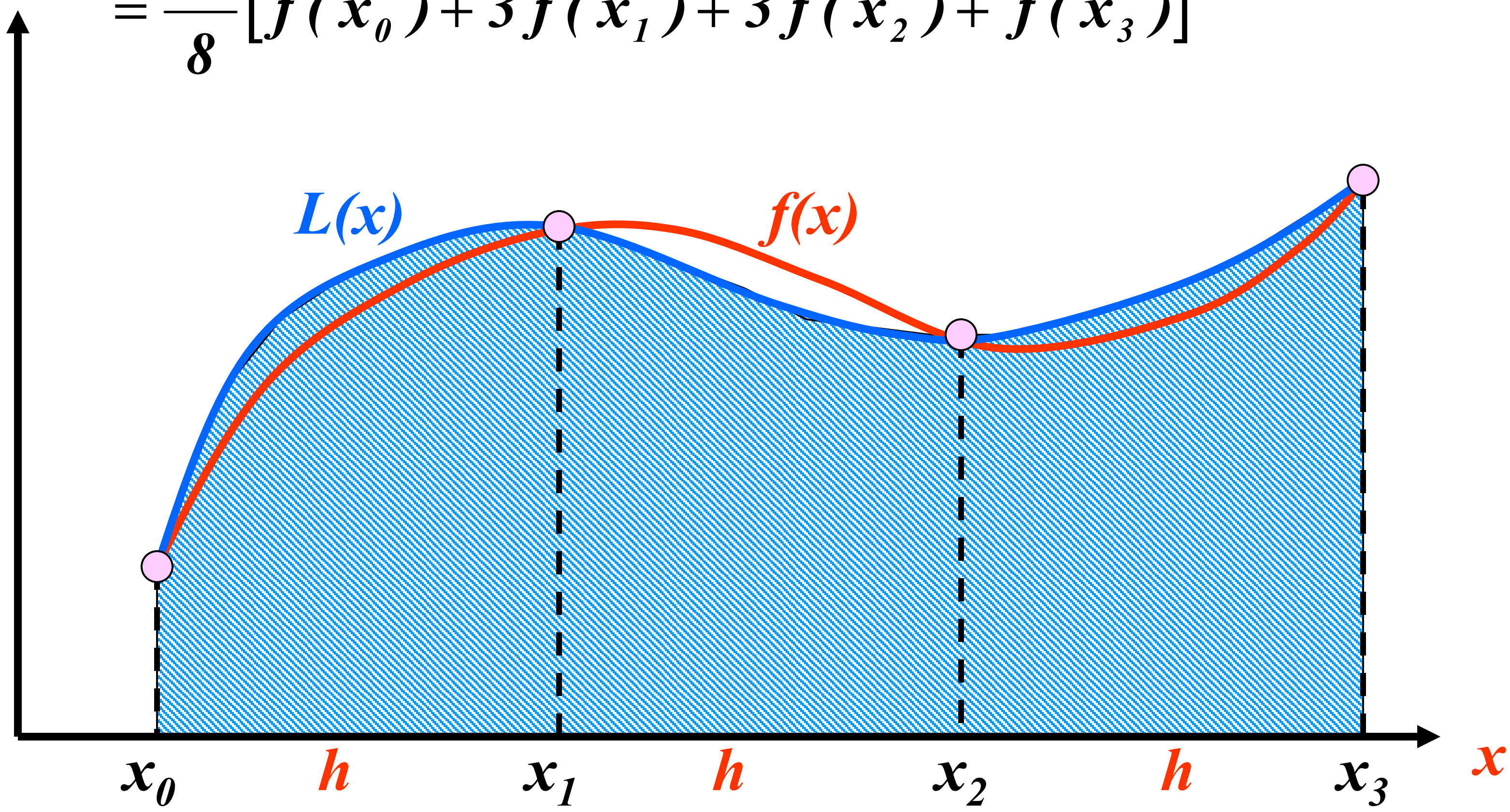


Simpson's 3/8-Rule

Approximate by a cubic polynomial

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

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



Example: Simpson's Rules

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

- **Simpson's 1/3-Rule**

$$I = \int_0^4 xe^{2x}dx \approx \frac{h}{3}\left[f(0) + 4f(2) + f(4)\right]$$
$$= \frac{2}{3}\left[0 + 4(2e^4) + 4e^8\right] = 8240.411$$
$$\varepsilon = \frac{5216.926 - 8240.411}{5216.926} = -57.96\%$$

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

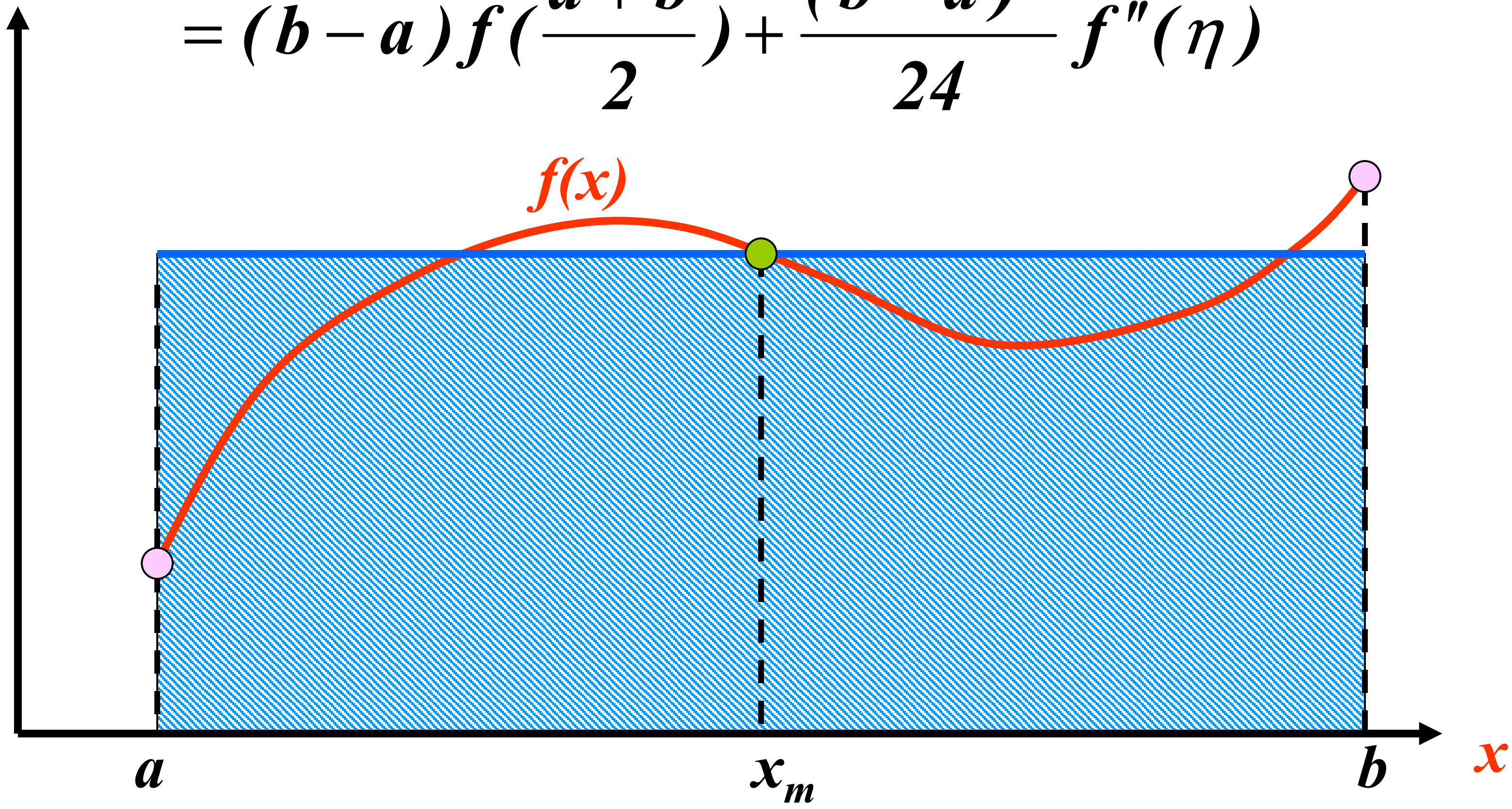
$$I = \int_0^4 xe^{2x}dx \approx \frac{3h}{8}\left[f(0) + 3f(\frac{4}{3}) + 3f(\frac{8}{3}) + f(4)\right]$$
$$= \frac{3(4/3)}{8}\left[0 + 3(19.18922) + 3(552.33933) + 11923.832\right] = 6819.209$$
$$\varepsilon = \frac{5216.926 - 6819.209}{5216.926} = -30.71\%$$

Midpoint Rule

Newton-Cotes Open Formula

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

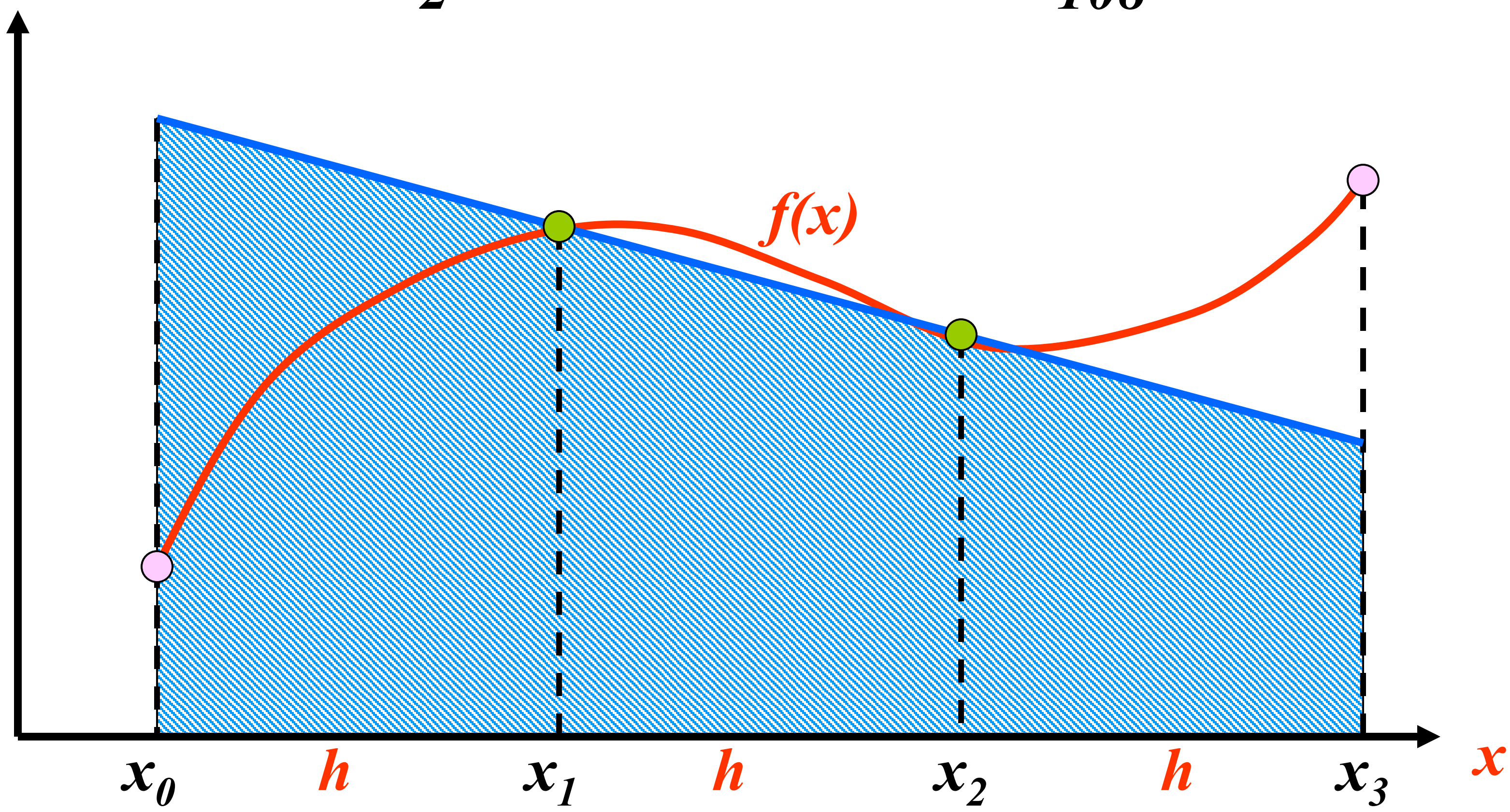
$$= (b-a)f\left(\frac{a+b}{2}\right) + \frac{(b-a)^3}{24} f''(\eta)$$



Two-point Newton-Cotes Open Formula

Approximate by a straight line

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

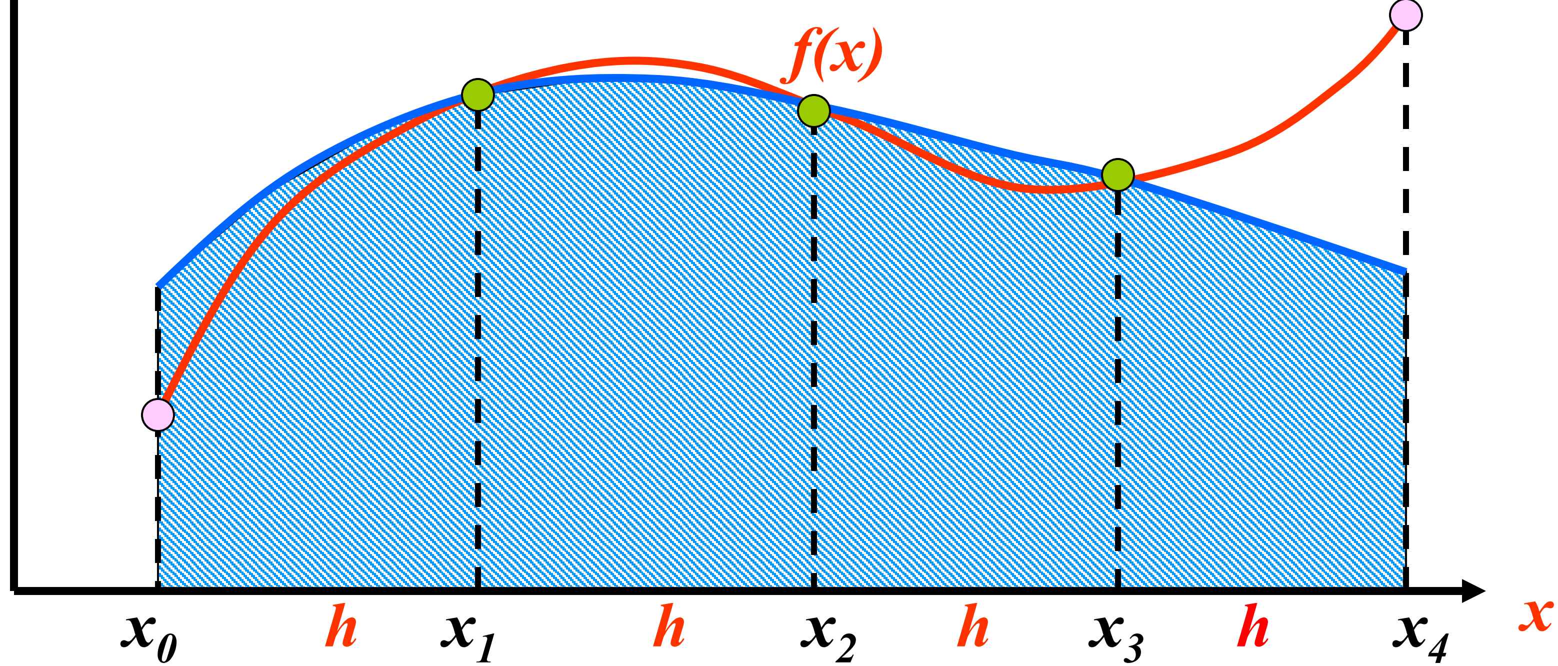


Three-point Newton-Cotes Open Formula

Approximate by a parabola

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

$$+\frac{7(b-a)^5}{23040} f''''(\eta)$$

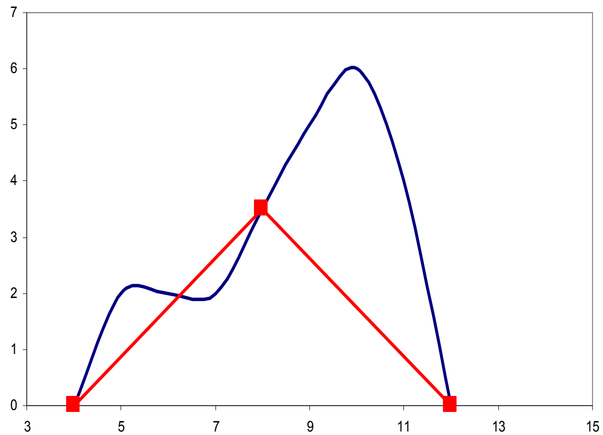


Better Numerical Integration

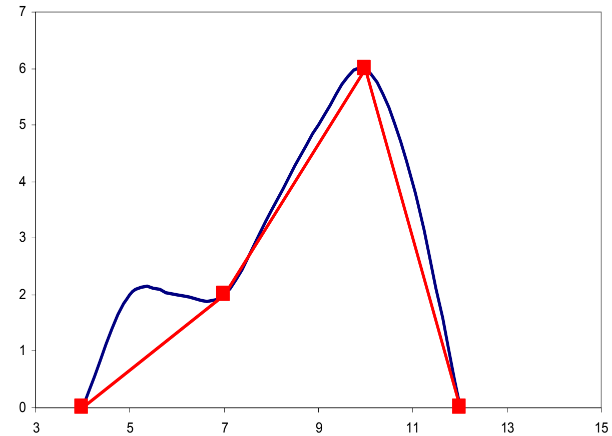
- **Composite integration**
  - **Composite Trapezoidal Rule**
  - **Composite Simpson's Rule**
- **Richardson Extrapolation**
- **Romberg integration**

Apply trapezoid rule to multiple segments over integration limits

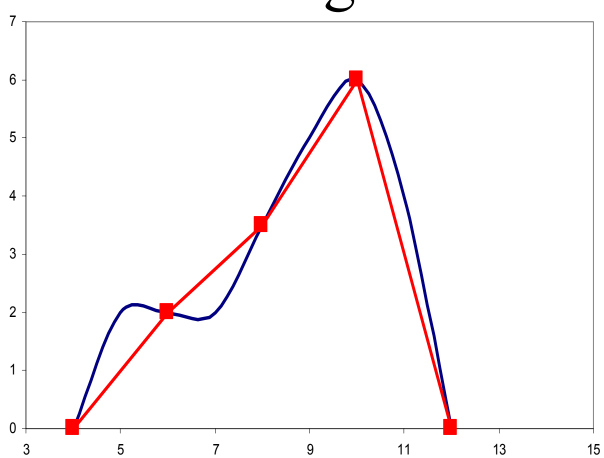
Two segments



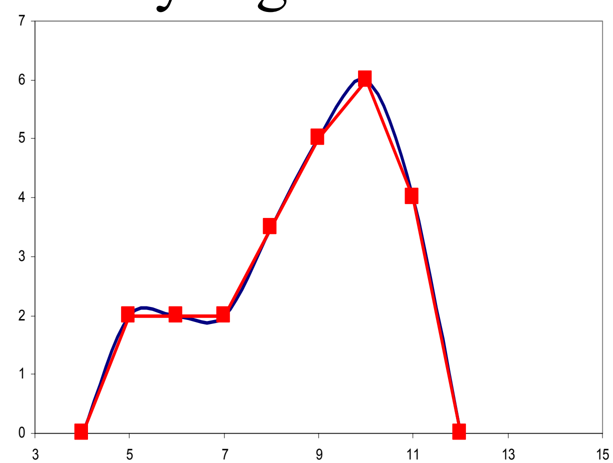
Three segments



Four segments



Many segments



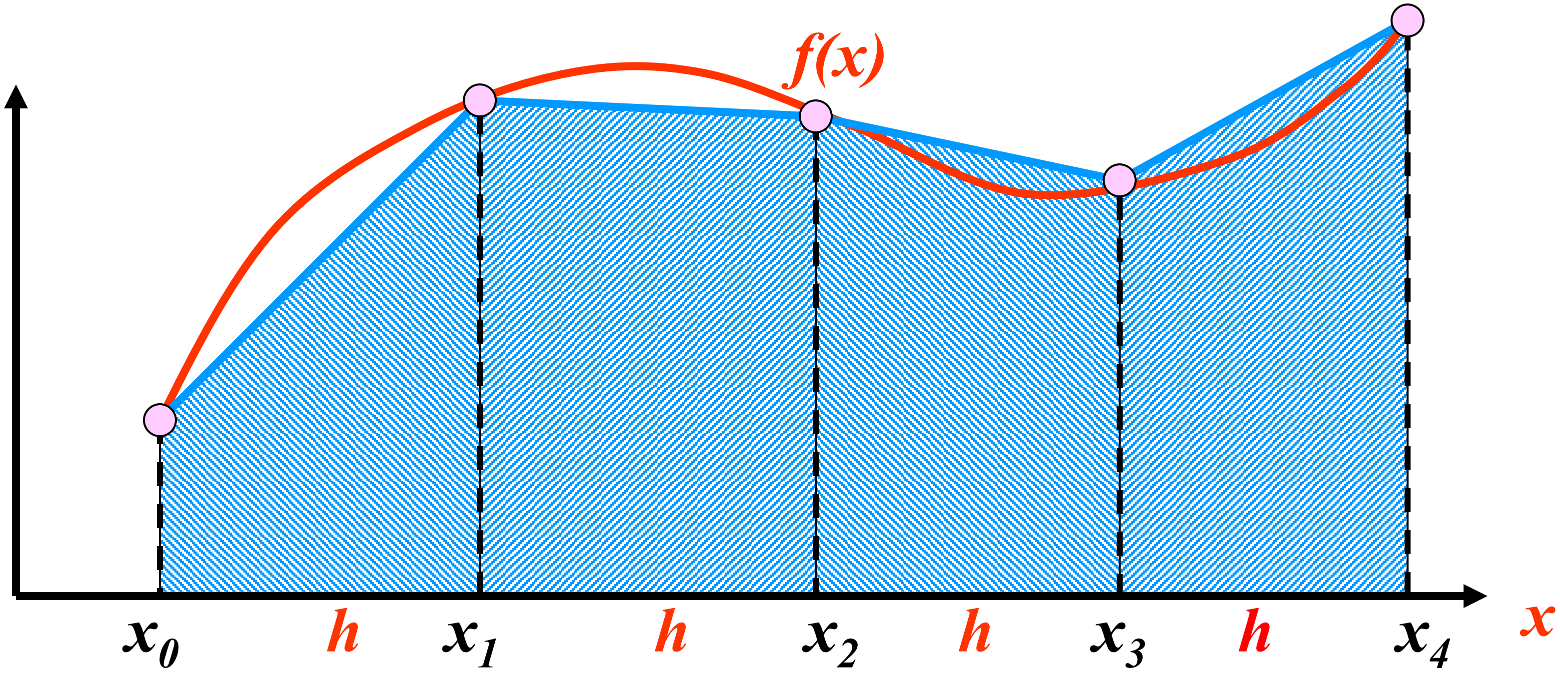
Composite Trapezoid Rule

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

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

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

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



Composite Trapezoid Rule

Evaluate the integral

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

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

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

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

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

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

Composite Trapezoid Rule with Unequal Segments

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

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

$$I = \int_0^2 f(x)dx + \int_2^3 f(x)dx + \int_3^{3.5} f(x)dx + \int_{3.5}^4 f(x)dx$$

$$= \frac{h_1}{2}\left[f(0) + f(2)\right] + \frac{h_2}{2}\left[f(2) + f(3)\right]$$

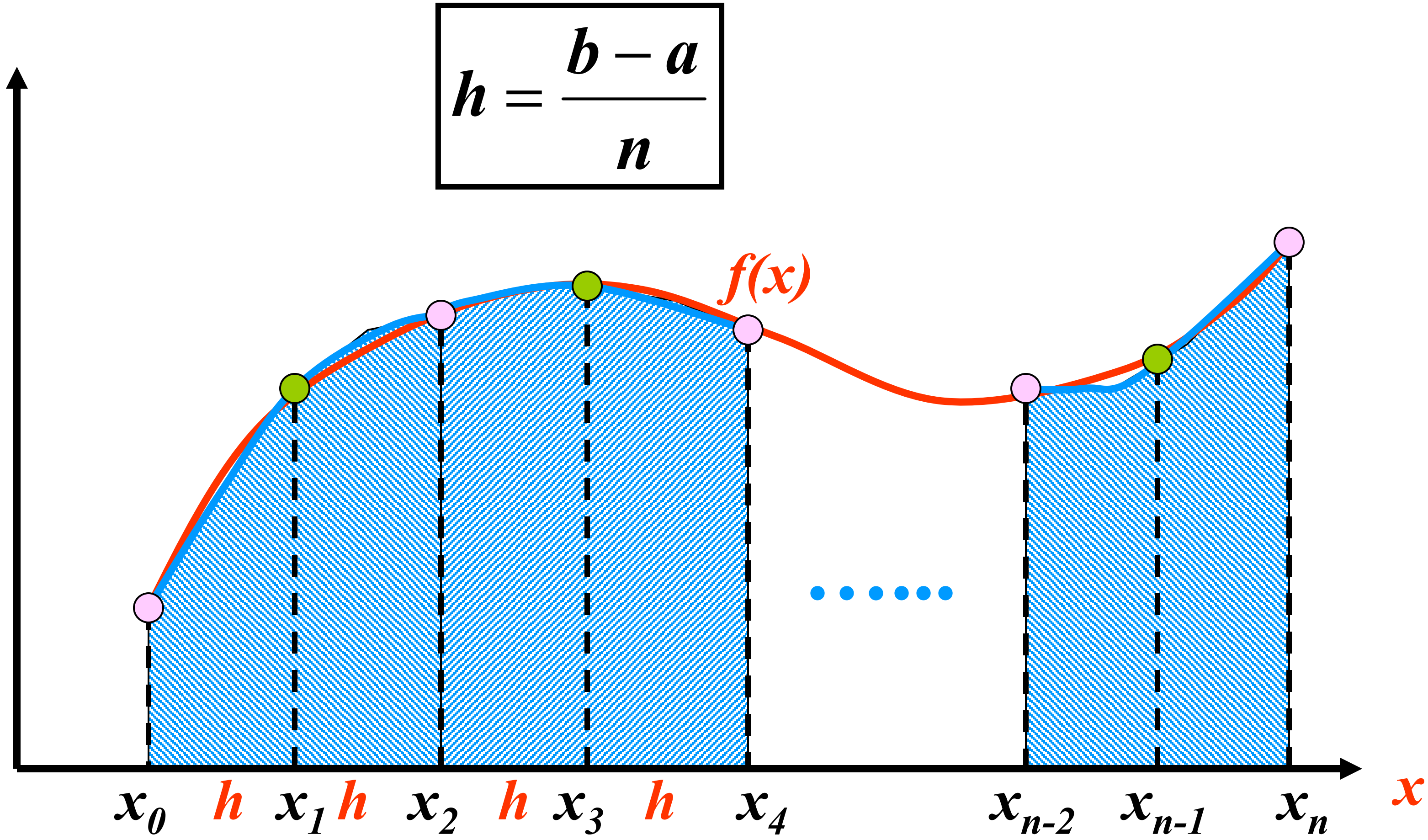
$$+ \frac{h_3}{2}\left[f(3) + f(3.5)\right] + \frac{h_4}{2}\left[f(3.5) + f(4)\right]$$

$$= \frac{2}{2}\left[0 + 2e^4\right] + \frac{1}{2}\left[2e^4 + 3e^6\right] + \frac{0.5}{2}\left[3\mathrm{e}^6 + 3.5e^7\right]$$

$$+ \frac{0.5}{2}\left[3.5e^7 + 4e^8\right] = 5971.58 \qquad \Rightarrow \varepsilon = -14.45\%$$

Composite Simpson's Rule

Piecewise Quadratic approximations



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

- $n = 2, h = 2$

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

- $n = 4, h = 1$

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

Composite Simpson's Rule with Unequal Segments

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

- $h_1 = 1.5,\ h_2 = 0.5$

$$I = \int_0^3 f(x)dx + \int_3^4 f(x)dx$$

$$= \frac{h_1}{3}\left[f(0) + 4f(1.5) + 2f(3)\right]$$

$$+ \frac{h_2}{3}\left[f(3) + 4f(3.5) + 2f(4)\right]$$

$$= \frac{1.5}{3}\left[0 + 4(1.5e^3) + 3e^6\right] + \frac{0.5}{3}\left[3e^6 + 4(3.5e^7) + 4e^8\right]$$

$$= 5413.23 \quad \Rightarrow \varepsilon = -3.76\%$$

Richardson Extrapolation

Use trapezoidal rule as an example

- subintervals: $n = 2^j = 1, 2, 4, 8, 16, \ldots.$

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(x_0) + 2f(x_1) + \cdots + 2f(x_{n-1}) + f(x_n)\right] + \sum_{j=1}^{\infty} c_j h^{2j}$$

j	n	Formula
0	1	$I_0 = \frac{h}{2}\left[f(a) + f(b)\right]$
1	2	$I_1 = \frac{h}{4}\left[f(a) + 2f(x_1) + f(b)\right]$
2	4	$I_2 = \frac{h}{8}\left[f(a) + 2f(x_1) + 2f(x_2) + 2f(x_3) + f(b)\right]$
3	8	$I_3 = \frac{h}{16}\left[f(a) + 2f(x_1) + \cdots + 2f(x_7) + f(b)\right]$
$\vdots$	$\vdots$	$\vdots$
j	2^j	$I_j = \frac{h}{2^j}\left[f(a) + 2f(x_1) + \cdots + 2f(x_{n-1}) + f(b)\right]$

Richardson Extrapolation

For trapezoidal rule

$$A=\int_a^b f(x)dx = A(h)+c_1h^2+\cdots$$

$$\begin{cases} A = A(h)+c_1h^2+c_2h^4\cdots \\ A = A(\frac{h}{2})+c_1(\frac{h}{2})^2+c_2(\frac{h}{2})^4+\cdots \end{cases}$$

$$\Rightarrow A=\frac{1}{3}\left[4A(\frac{h}{2})-A(h)\right]-\frac{c_2}{4}h^4+\cdots = B(h)+b_2h^4+\cdots$$

– k^{th} level of extrapolation

$$\left.\begin{cases} A = B(h)+b_2h^4\cdots \\ A = B(\frac{h}{2})+b_2(\frac{h}{2})^4+\cdots \end{cases}\right\} \Rightarrow C(h)=\frac{1}{15}\left[16B(\frac{h}{2})-B(h)\right]$$

$$\boxed{D(h)=\frac{4^k C(h/2)-C(h)}{4^k-1}}$$

Romberg Integration

Accelerated Trapezoid Rule

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

	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	$I_{0,0}$	$I_{0,1}$	$I_{0,2}$	$I_{0,3}$	$I_{0,4}$
$h/2$	$I_{1,0}$	$I_{1,1}$	$I_{1,2}$	$I_{1,3}$	
$h/4$	$I_{2,0}$	$I_{2,1}$	$I_{2,2}$		
$h/8$	$I_{3,0}$	$I_{3,1}$			
$h/16$	$I_{4,0}$				
		$\frac{4I_{j+1,0} - I_{j,0}}{3}$	$\frac{16I_{j+1,1} - I_{j,1}}{15}$	$\frac{64I_{j+1,2} - I_{j,2}}{63}$	$\frac{256I_{j+1,3} - I_{j,3}}{255}$

Romberg Integration

Accelerated Trapezoid Rule

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

	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%