NUMERICAL METHODS

$$U^{n+1} = U^n + \Delta t\, f(U^n)$$

$$\frac{\partial v}{\partial t} + V \cdot \nabla v = \nabla \cdot (k \nabla v) + g(v)$$

$$(\lambda + \mu)\nabla(\nabla \cdot u) + \mu \nabla^2 u = \alpha(3\lambda + 2\mu)\nabla T - \rho b$$

Lecture 7

$$\rho\left(\frac{\partial u}{\partial t} + V \cdot \nabla u\right) = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho f_x$$

$$\nabla^2 u = f$$

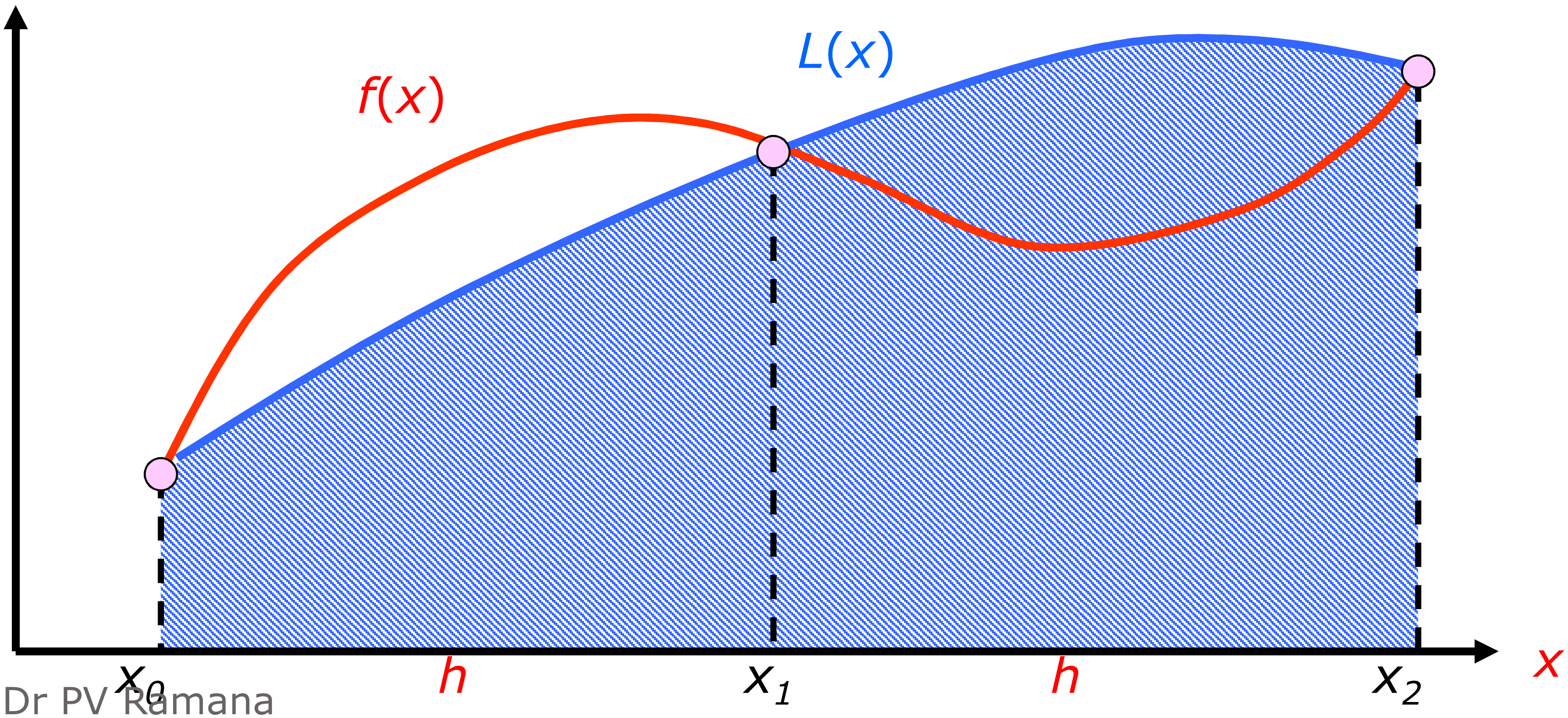
Dr. P V Ramana

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 1/3 - Rule

$$L(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1)$$

$$+ \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)$$

$$let \quad x_0 = a, x_2 = b, x_1 = \frac{a+b}{2}$$

$$h = \frac{b-a}{2}, \xi = \frac{x-x_1}{h}, \; d\xi = \frac{dx}{h}$$

$$\begin{cases} x = x_0 \Rightarrow \xi = -1 \\ x = x_1 \Rightarrow \xi = 0 \\ x = x_2 \Rightarrow \xi = 1 \end{cases}$$

$$\boxed{L(\xi) = \frac{\xi(\xi-1)}{2} f(x_0) + (1-\xi^2) f(x_1) + \frac{\xi(\xi+1)}{2} f(x_2)}$$

Simpson's 1/3 - Rule

$$L(\xi) = \frac{\xi(\xi-1)}{2} f(x_0) + (1-\xi^2) f(x_1) + \frac{\xi(\xi+1)}{2} f(x_2)$$

$$\int_a^b f(x)dx \approx h\int_{-1}^{1} L(\xi)d\xi = f(x_0)\frac{h}{2}\int_{-1}^{1}\xi(\xi-1)d\xi$$

$$+ f(x_1)h\int_0^1 (1-\xi^2)d\xi + f(x_2)\frac{h}{2}\int_{-1}^{1}\xi(\xi+1)d\xi$$

$$= f(x_0)\frac{h}{2}\left(\frac{\xi^3}{3}-\frac{\xi^2}{2}\right)\Bigg|_{-1}^{1} + f(x_1)h\left(\xi-\frac{\xi^3}{3}\right)\Bigg|_{-1}^{1}$$

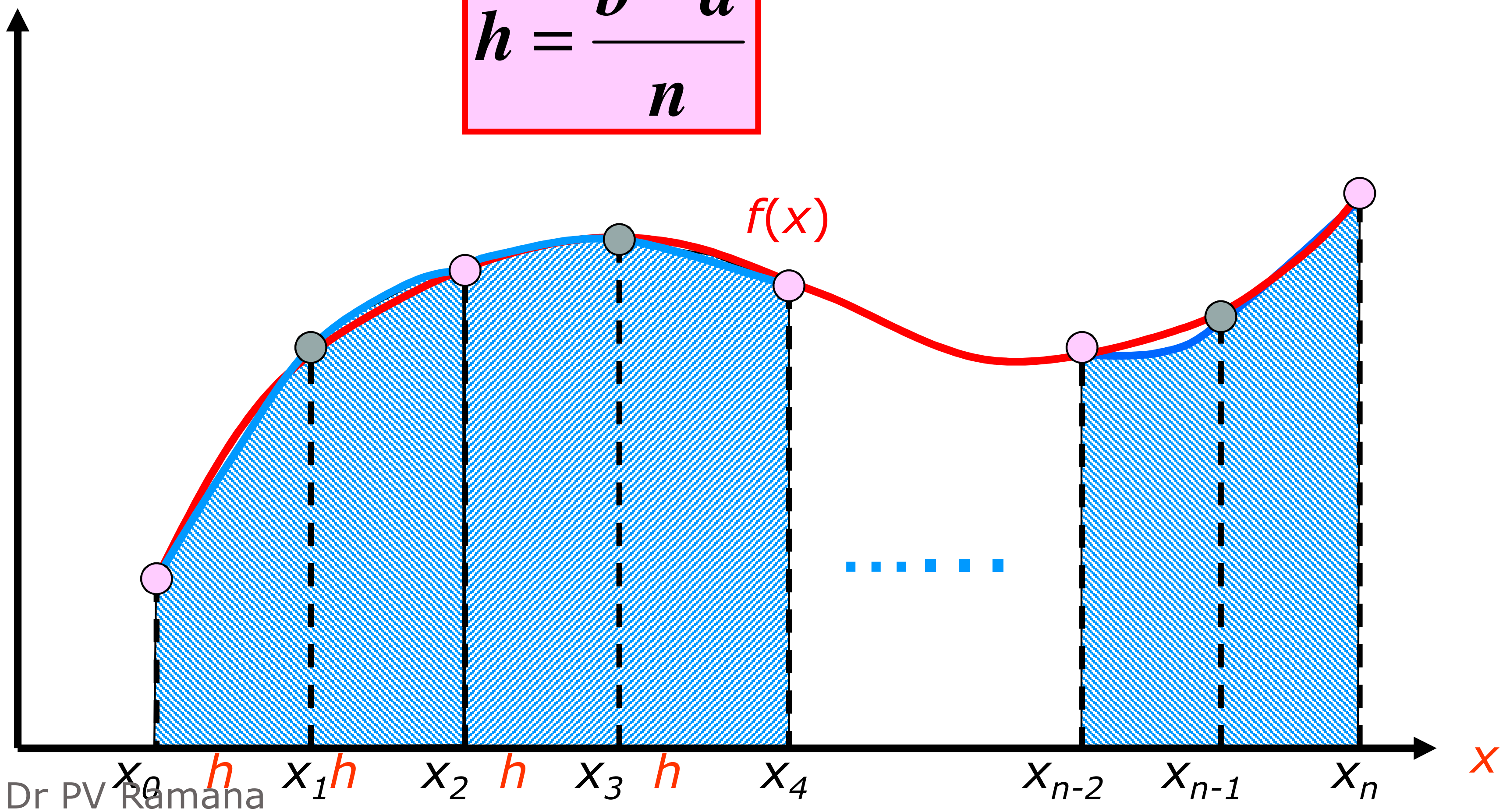
$$+ f(x_2)\frac{h}{2}\left(\frac{\xi^3}{3}+\frac{\xi^2}{2}\right)\Bigg|_{-1}^{1}$$

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

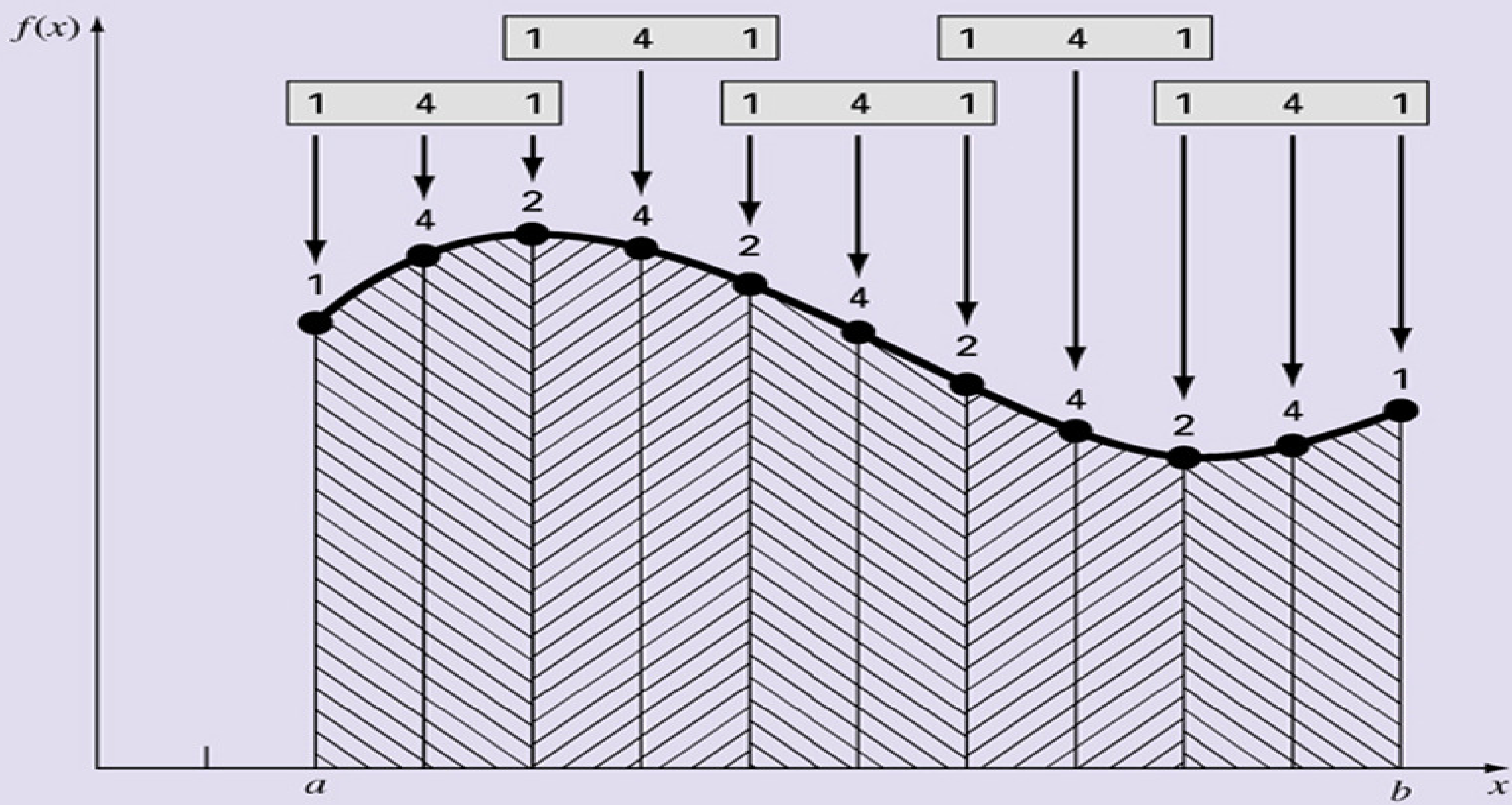
Simpson's 1/3 - Rule

Piecewise Quadratic approximations

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



Composite Simpson's 1/3 Rule



- Applicable only if the number of segments is even

Composite Simpson's 1/3 Rule

- **Applicable only if the number of segments is even**

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

- **Substitute Simpson's 1/3 rule for each integral**

$$I = 2h\frac{f(x_0)+4f(x_1)+f(x_2)}{6} + 2h\frac{f(x_2)+4f(x_3)+f(x_4)}{6} + \Lambda + 2h\frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6}$$

- **For uniform spacing (equal segments)**

$$\boxed{I = \frac{(b-a)}{3n}\left\{ f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n) \right\}}$$

Simpson's 1/3 Rule - Error

- **Truncation error (single application)**

$$E_t = -\frac{1}{90} h^5 f^{(4)}(\xi) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)\,; \quad h = \frac{b-a}{2}$$

- **Exact up to cubic polynomial ($f^{(4)} = 0$)**
- **Approximate error for ($n/2$) multiple applications**

$$E_a = -\frac{(b-a)^5}{180 n^4} \bar{f}^{(4)}$$

Composite Simpson's 1/3 Rule

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

- $n = 2, h = 2$

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

- $n = 4, h = 1$

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

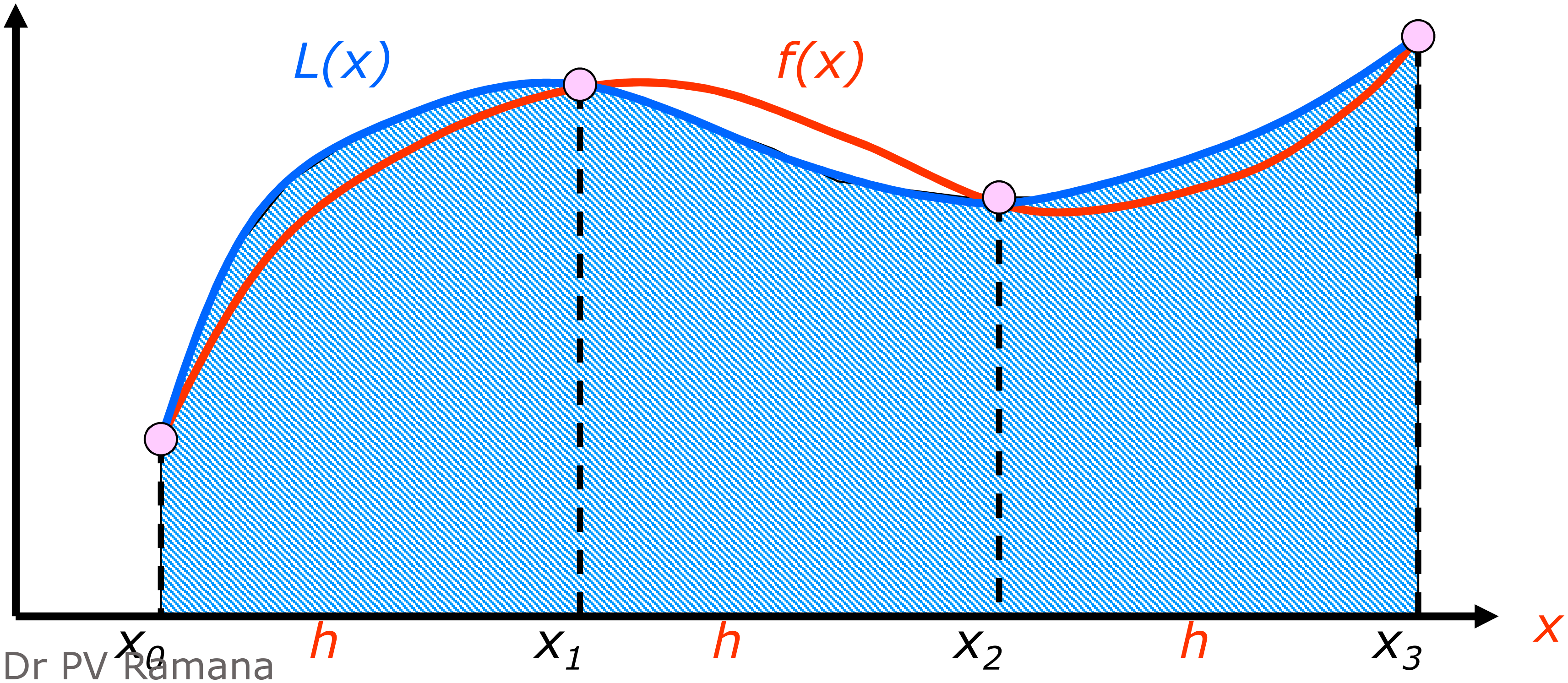
Simpson's 3/8 - Rule

$$\int_a^b f(x)\,dx \approx \int_a^b \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3\right)dx$$

- **Approximate by a cubic polynomial**

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

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



Simpson's 3/8- Rule

$$L(x) = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} f(x_0) + \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} f(x_1)$$

$$+ \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} f(x_2) + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} f(x_3)$$

$$\int_a^b f(x)dx \approx \int_a^b L(x)dx \quad ; \quad h = \frac{b-a}{3}$$

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

- Truncation error

$$E_t = -\frac{3}{80} h^5 f^{(4)}(\xi) = -\frac{(b-a)^5}{6480} f^{(4)}(\xi) \, ; \; h = \frac{b-a}{3}$$

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**

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

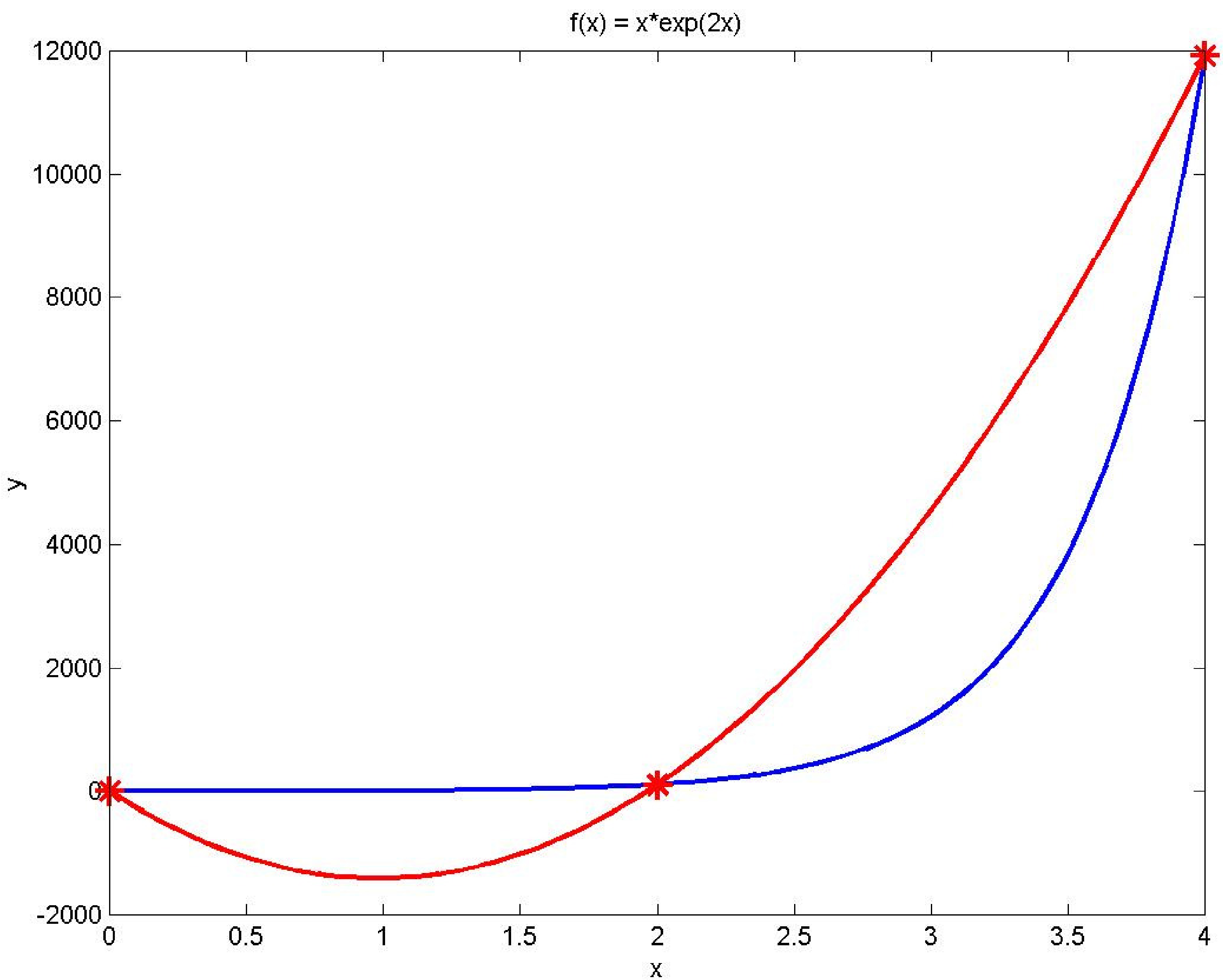
$$= \frac{3(4/3)}{8}\left[0 + 3(19.18922) + 3(552.33933) + 11923.832\right] = 6819.209$$

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

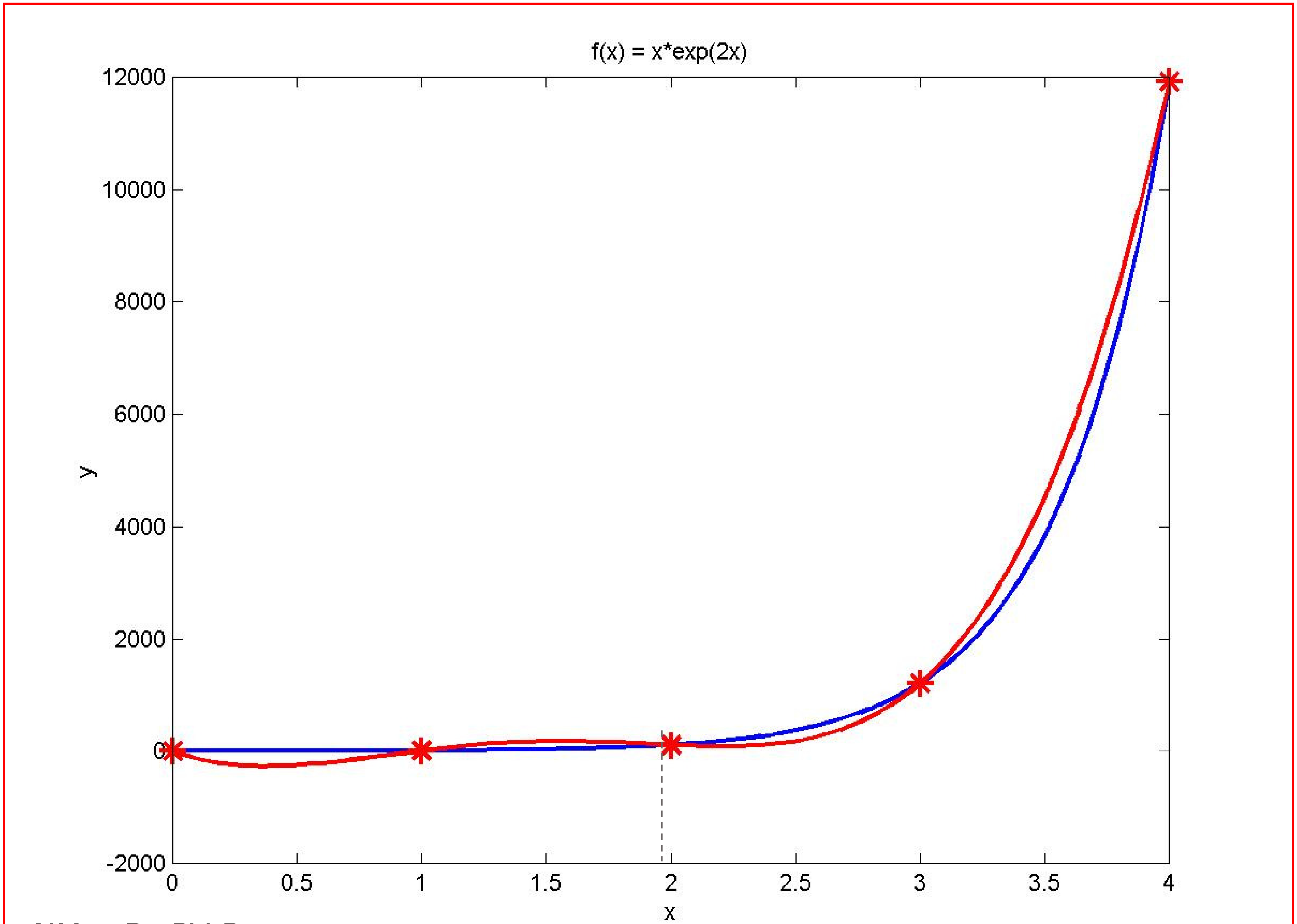
Matlab: Simpson's Rules

```
function I = Simp(f, a, b, n)
% integral of f using composite Simpson rule
% n must be even
h = (b - a)/n;
S = feval(f,a);
for i = 1 : 2 : n-1
    x(i) = a + h*i;
    S = S + 4*feval(f, x(i));
end
for i = 2 : 2 : n-2
    x(i) = a + h*i;
    S = S + 2*feval(f, x(i));
end
S = S + feval(f, b); I = h*S/3;
```

Simpson's 1/3 Rule

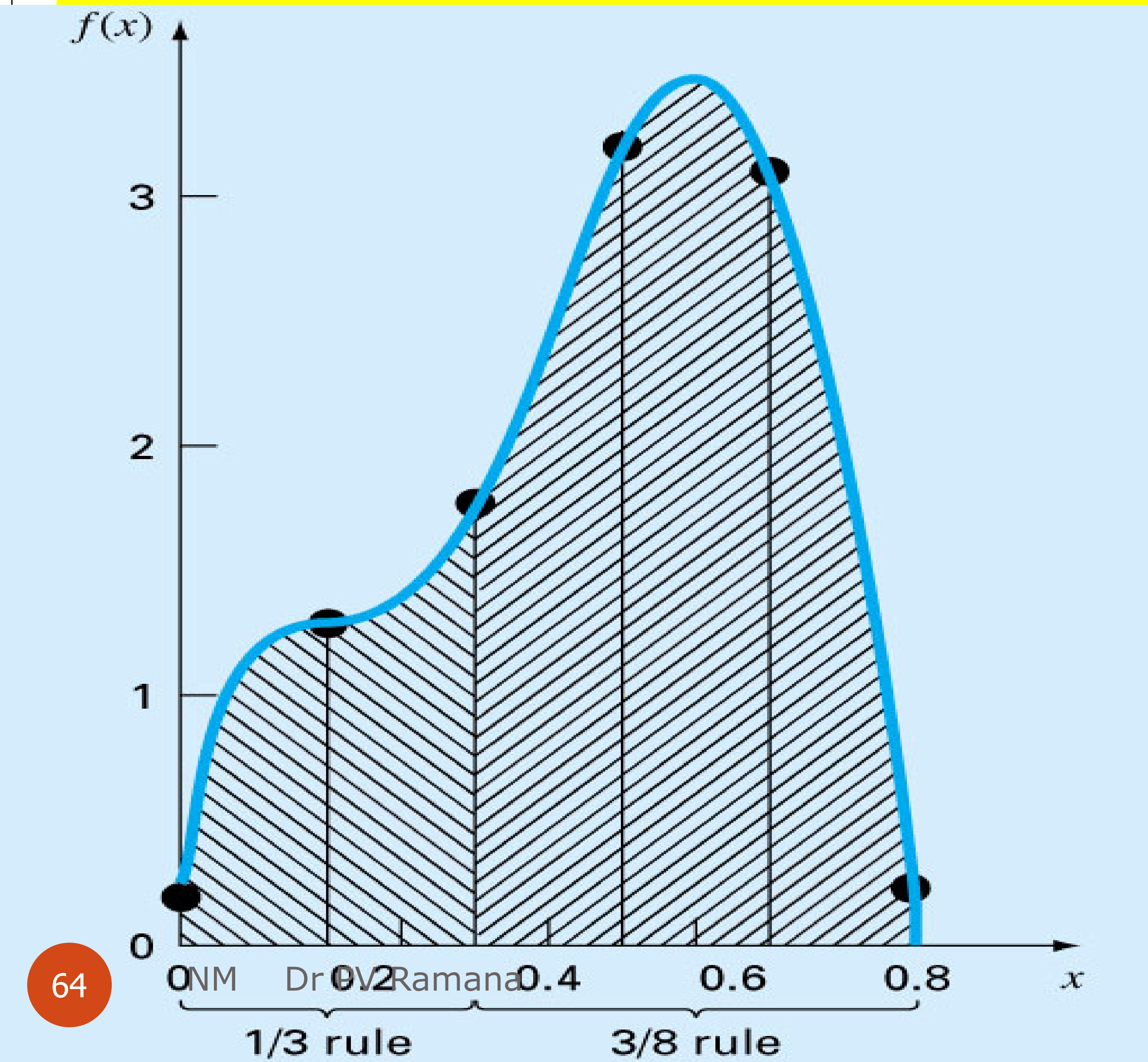


Composite Simpson's 1/3 Rule



```
» x=0:0.04:4; y=example(x);
» x1=0:2:4; y1=example(x1);
» c=Lagrange_coef(x1,y1); p1=Lagrange_eval(x,x1,c);
» H=plot(x,y,x1,y1,'r*',x,p1,'r');
» xlabel('x'); ylabel('y'); title('f(x) = x*exp(2x)');
» set(H,'LineWidth',3,'MarkerSize',12);
» x2=0:1:4; y2=example(x2);
» c=Lagrange_coef(x2,y2); p2=Lagrange_eval(x,x2,c);
» H=plot(x,y,x2,y2,'r*',x,p2,'r');
» xlabel('x'); ylabel('y'); title('f(x) = x*exp(2x)');
» set(H,'LineWidth',3,'MarkerSize',12);
»
» I=Simp('example',0,4,2)                  ←  n = 2
I =
  8.2404e+003
» I=Simp('example',0,4,4)                  ←  n = 4
I =
  5.6710e+003
» I=Simp('example',0,4,8)                  ←  n = 8
I =
  5.2568e+003
» I=Simp('example',0,4,16)                 ←  n = 16
I =
  5.2197e+003
» Q=Quad8('example',0,4)                   ← MATLAB fun
Q =
  2169e+003
```

Multiple applications of Simpson’s rule with odd number of intervals



Hybrid Simpson’s 1/3 & 3/8 rules

Newton-Cotes Closed Integration Formulae

n	Name	Formula	Truncation Error
1	Trapezoidal rule	$(b-a)\dfrac{f(x_0)+f(x_1)}{2}$	$-\dfrac{1}{12}h^3 f''(\xi)$
2	Simpson's 1/3 rule	$(b-a)\dfrac{f(x_0)+4f(x_1)+f(x_2)}{6}$	$-\dfrac{1}{90}h^5 f^{(4)}(\xi)$
3	Simpson's 3/8 rule	$(b-a)\dfrac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}$	$-\dfrac{3}{80}h^5 f^{(4)}(\xi)$
4	Boole's rule	$(b-a)\dfrac{7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)}{90}$	$-\dfrac{8}{945}h^7 f^{(6)}(\xi)$
5		$(b-a)\dfrac{19f(x_0)+75f(x_1)+50f(x_2)+50f(x_3)+75f(x_4)+19f(x_5)}{288}$	$-\dfrac{275}{12096}h^7 f^{(6)}(\xi)$

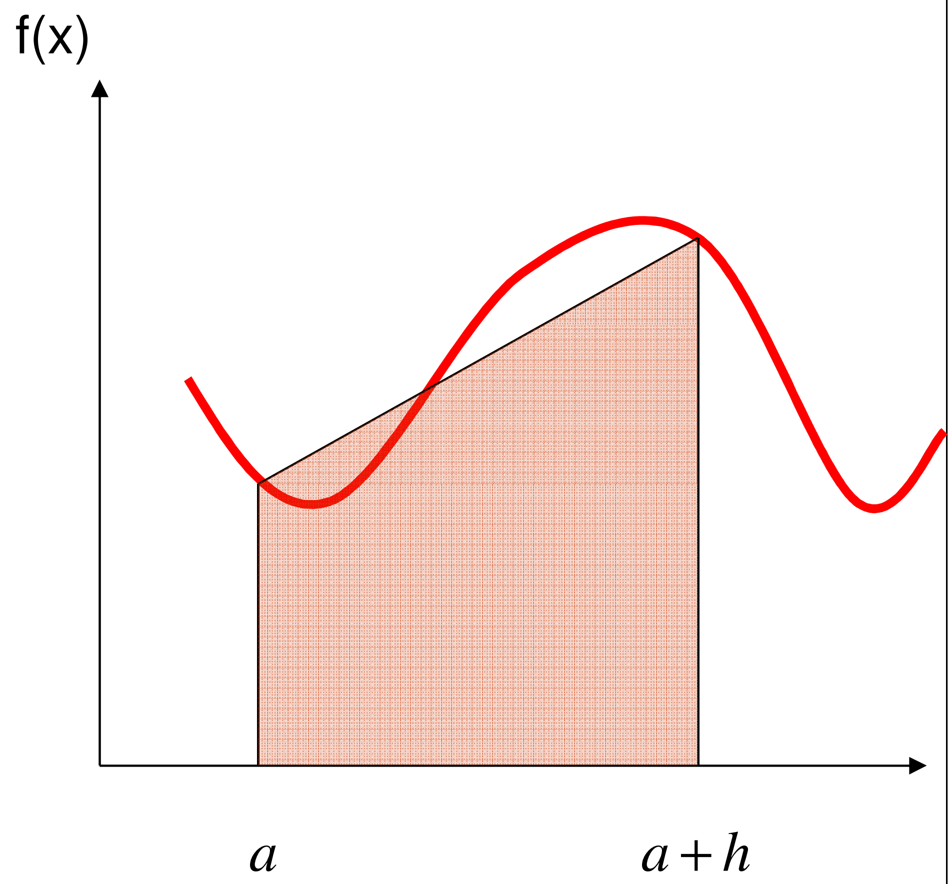
$$h = \frac{b-a}{n}$$

Recursive Trapezoid Method

Estimate based on one interval:

$$h = \frac{b-a}{2^0}$$

$$R(0,0) = \frac{b-a}{2}\left(f(a) + f(b)\right)$$



$$h = \frac{b-a}{2^0}; \mathrm{R}(0,0) = \frac{b-a}{2}\left(f(a) + f(b)\right)$$

Recursive Trapezoid Method

Estimate based on 2 intervals:

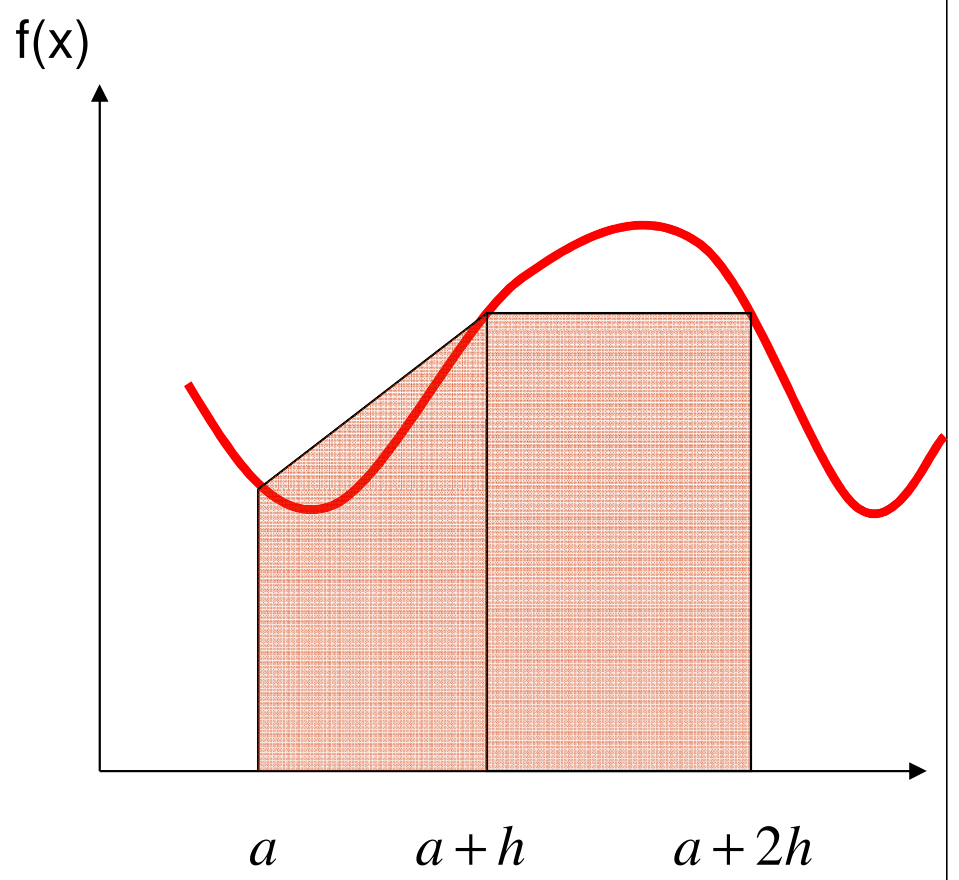
$$h = \frac{b-a}{2^1}$$

$$\mathrm{R}(1,0) = \frac{b-a}{2}\left[f(a+h) + \frac{1}{2}\left(f(a) + f(b)\right)\right]$$

$$R(1,0) = \frac{1}{2}R(0,0) + h\left[f(a+h)\right]$$

Based on previous estimate

Based on new point



Recursive Trapezoid Method

$$h=\frac{b-a}{2^1};\mathrm{R}(1,0)=\frac{b-a}{2}\left[f(a+h)+\frac{1}{2}\big(f(a)+f(b)\big)\right]$$

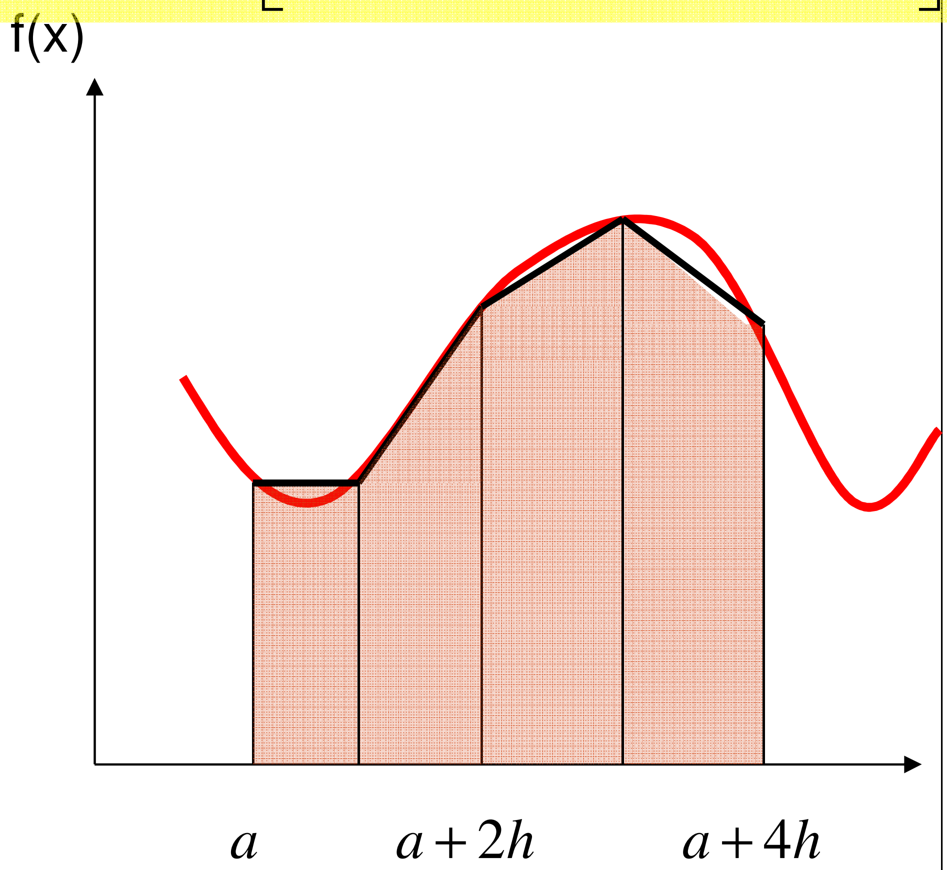
$$h=\frac{b-a}{2^2}$$

$$\mathrm{R}(2,0)=\frac{b-a}{4}\Big[f(a+h)+f(a+2h)+f(a+3h)$$
$$+\frac{1}{2}\big(f(a)+f(b)\big)\Big]$$

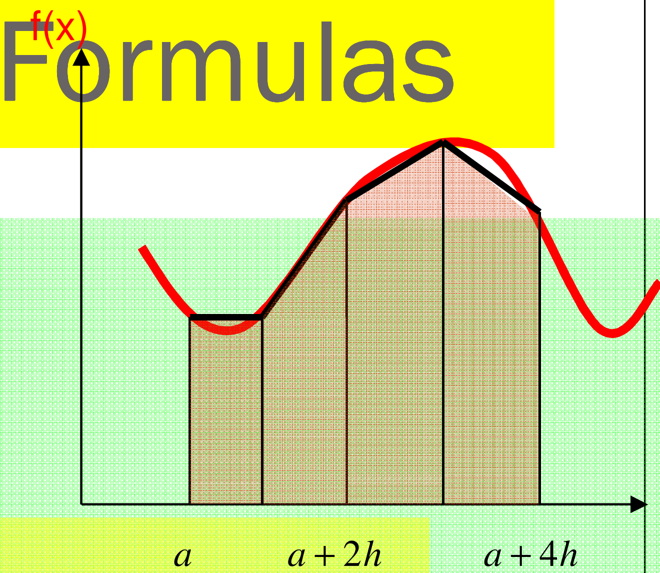
$$R(2,0)=\frac{1}{2}R(1,0)+h\big[f(a+h)+f(a+3h)\big]$$

Based on previous estimate

Based on new points



Recursive Trapezoid Method Formulas



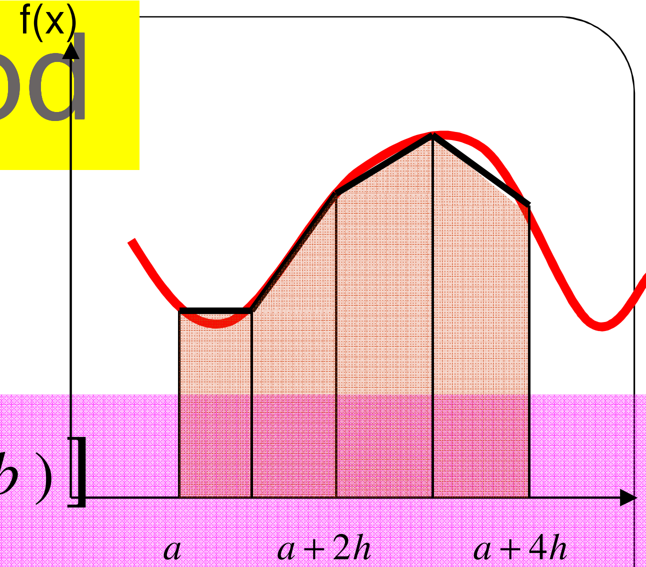
$$\mathrm{R}(0,0) = \frac{b-a}{2}\left[f(a) + f(b)\right]$$

$$h = \frac{b-a}{2^1}; \mathrm{R}(1,0) = \frac{b-a}{2}\left[f(a+h) + \frac{1}{2}\left(f(a) + f(b)\right)\right] = \frac{1}{2}R(0,0) + h[f(a+h)]$$

$$R(n,0) = \frac{1}{2}R(n-1,0) + h\left[\sum_{k=1}^{2^{(n-1)}} f\left(a + (2k-1)h\right)\right]$$

$$h = \frac{b-a}{2^n}$$

Recursive Trapezoid Method



$$h = b - a, \qquad R(0,0) = \frac{b-a}{2}\left[f(a) + f(b)\right]$$

$$h = \frac{b-a}{2}, \qquad R(1,0) = \frac{1}{2}R(0,0) + h\left[\sum_{k=1}^{1} f\left(a + (2k-1)h\right)\right]$$

$$h = \frac{b-a}{2^2}, \qquad R(2,0) = \frac{1}{2}R(1,0) + h\left[\sum_{k=1}^{2} f\left(a + (2k-1)h\right)\right]$$

$$h = \frac{b-a}{2^3}, \qquad R(3,0) = \frac{1}{2}R(2,0) + h\left[\sum_{k=1}^{2^2} f\left(a + (2k-1)h\right)\right]$$

....

$$h = \frac{b-a}{2^n}, \qquad R(n,0) = \frac{1}{2}R(n-1,0) + h\left[\sum_{k=1}^{2^{(n-1)}} f\left(a + (2k-1)h\right)\right]$$

Example on Recursive Trapezoid

Use Recursive Trapezoid method to estimate :

$$\int_0^{\pi/2} \sin(x)\,dx$$ by computing R(3,0) then estimate the error

$$h = \frac{b-a}{2^1}; \mathrm{R}(1,0) = \frac{b-a}{2}\left[f(a+h) + \frac{1}{2}\big(f(a) + f(b)\big)\right] = \frac{1}{2}R(1,0) + h[f(a+h)]$$

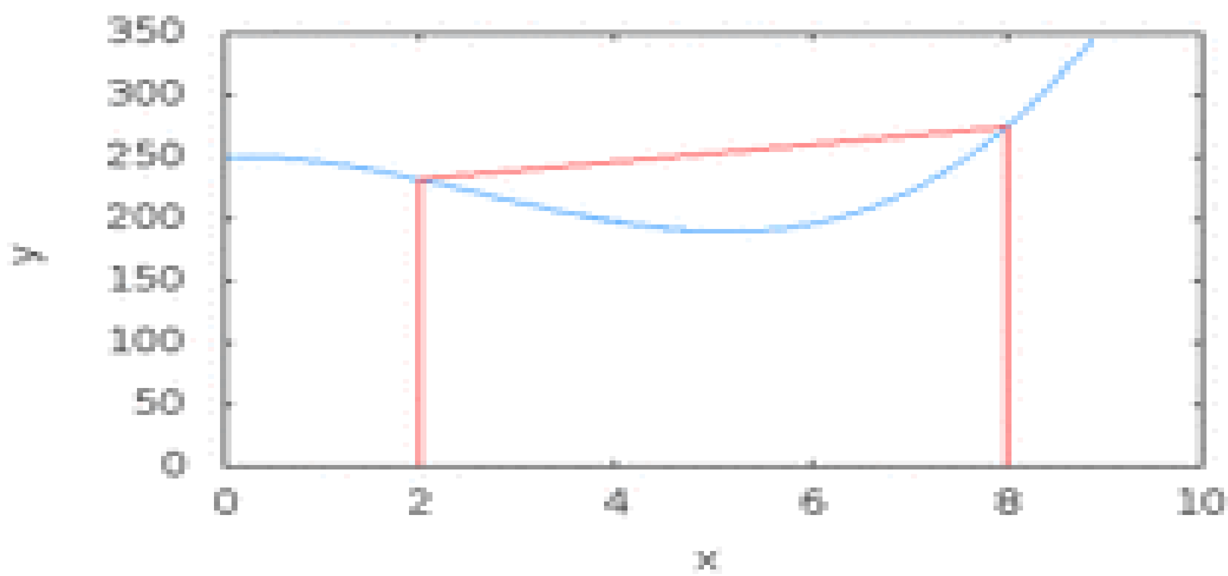
n	h	R(n,0)
0	(b-a)=π/2	(π/4)[sin(0) + sin(π/2)] = 0.785398
1	(b-a)/2=π/4	R(0,0)/2 + (π/4) sin(π/4) = 0.785398/2 + (π/4) x 1.42 = 0.948059
2	(b-a)/4=π/8	R(1,0)/2 + (π/8)[sin(π/8)+sin(3π/8)] = 0.948059/2 + (π/8) x 1.42 = 0.987116
3	(b-a)/8=π/16	R(2,0)/2 + (π/16)[sin(π/16)+sin(3π/16)+sin(5π/16)+ sin(7π/16)] = 0.996785

Estimated Error = |R(3,0) – R(2,0)| = 0.009669

Advantages of Recursive Trapezoid

Recursive Trapezoid:

- Gives the same answer as the standard Trapezoid method.
- Makes use of the available information to reduce the computation time.
- Useful if the number of iterations is not known in advance.



Romberg Method

- Motivation
- Derivation of Romberg Method
- Romberg Method
- Example
- When to stop?

Romberg Integration

- More efficient methods to achieve better accuracy have been developed
- Romberg integration - uses Richardson extrapolation
- Idea behind Richardson extrapolation - improve the estimate by eliminating the leading term of truncation error at coarser grid levels

Romberg Integration

Motivation

- Trapezoid formula with a sub-interval h gives an error of the order $O(h^2)$.
- *One can combine two Trapezoid estimates with intervals h and $h/2$ to get a better estimate.*

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

Romberg Method

$$h = b - a, \qquad R(0,0) = \frac{b-a}{2}\left[f(a) + f(b)\right]$$

$$h = \frac{b-a}{2}, \qquad R(1,0) = \frac{1}{2}R(0,0) + h\left[\sum_{k=1}^{1} f\big(a + (2k-1)h\big)\right]$$

$$h = \frac{b-a}{2^2}, \qquad R(2,0) = \frac{1}{2}R(1,0) + h\left[\sum_{k=1}^{2} f\big(a + (2k-1)h\big)\right]$$

$$h = \frac{b-a}{2^3}, \qquad R(3,0) = \frac{1}{2}R(2,0) + h\left[\sum_{k=1}^{2^2} f\big(a + (2k-1)h\big)\right]$$

....

$$h = \frac{b-a}{2^n}, \qquad R(n,0) = \frac{1}{2}R(n-1,0) + h\left[\sum_{k=1}^{2^{(n-1)}} f\big(a + (2k-1)h\big)\right]$$

Estimates using Trapezoid method intervals of size h, h/2, h/4, h/8 ...

are combined to improve the approximat ion of $\int_a^b f(x)\,dx$

First column is obtained using Trapezoid Method

R(0,0)			
R(1,0)	R(1,1)		
R(2,0)	R(2,1)	R(2,2)	
R(3,0)	R(3,1)	R(3,2)	R(3,3)

The other elements are obtained using the Romberg Method

First Column
Recursive Trapezoid Method

$$\mathrm{R}(0,0) = \frac{b-a}{2}\left[f(a) + f(b)\right]$$

$$R(n,0) = \frac{1}{2}R(n-1,0) + h\left[\sum_{k=1}^{2^{(n-1)}} f\big(a + (2k-1)h\big)\right]$$

$$h = \frac{b-a}{2^n}$$

Derivation of Romberg Method

Method 1

$$\int_a^b f(x)\,dx = R(n-1,0) + O(h^2) \quad \text{Trapezoid method} \quad with \quad h = \frac{b-a}{2^{n-1}}$$

$$\int_a^b f(x)\,dx = R(n-1,0) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \ldots \qquad (eq\ 1)$$

More accurate estimate is obtained by R(n,0)

$$\int_a^b f(x)\,dx = R(n,0) + \frac{1}{4} a_2 h^2 + \frac{1}{16} a_4 h^4 + \frac{1}{64} a_6 h^6 + \ldots \qquad (eq\ 2)$$

$eq\ 1 - 4 * eq\ 2 \quad gives$

$$\int_a^b f(x)\,dx = \frac{1}{3}\left[4 \times R(n,0) - R(n-1,0)\right] + b_4 h^4 + b_6 h^6 + \ldots$$

Romberg Method

Method 1

$$\mathrm{R}(0,0) = \frac{b-a}{2}\left[f(a) + f(b)\right]$$

$$h = \frac{b-a}{2^{n}},$$

R(0,0)			
R(1,0)	R(1,1)		
R(2,0)	R(2,1)	R(2,2)	
R(3,0)	R(3,1)	R(3,2)	R(3,3)

$$R(n,0) = \frac{1}{2}R(n-1,0) + h\left[\sum_{k=1}^{2^{(n-1)}} f\left(a + (2k-1)h\right)\right]$$

$$R(n,m) = \frac{1}{4^{m}-1}\left[4^{m} \times R(n,m-1) - R(n-1,m-1)\right] \quad n \geq 1, \quad m \geq 1$$

Romberg Integration

Property

Theorem

$$\int_a^b f(x)dx = R(n,m) + O(h^{2m+2})$$

R(0,0)			
R(1,0)	R(1,1)		
R(2,0)	R(2,1)	R(2,2)	
R(3,0)	R(3,1)	R(3,2)	R(3,3)

Error Level $O(h^2)$ $O(h^4)$ $O(h^6)$ $O(h^8)$

$$R(n,m) = \frac{1}{4^m - 1}\left[4^m \times R(n,m-1) - R(n-1,m-1)\right] \quad n \geq 1, \quad m \geq 1$$

Example 1

0.5	
3/8	1/3

Method 1

Compute $\int_0^1 x^2\,dx$

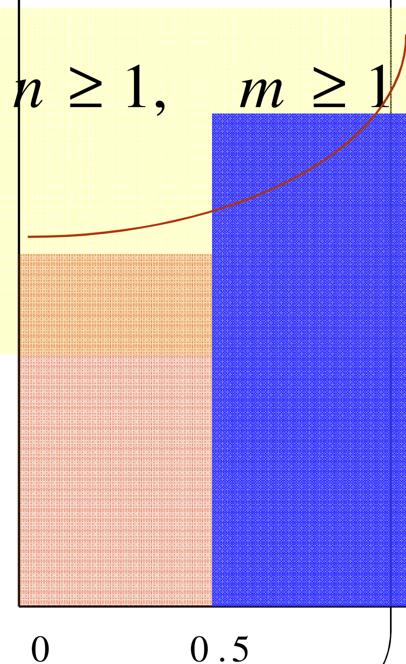
$$h = 1,\quad R(0,0) = \frac{b-a}{2}\left[f(a) + f(b)\right] = \frac{1}{2}\left[0+1\right] = 0.5$$

$$h = \frac{1}{2},\quad R(1,0) = \frac{1}{2}R(0,0) + h\left(f(a+h)\right) = \frac{1}{2}\left(\frac{1}{2}\right) + \frac{1}{2}\left(\frac{1}{4}\right) = \frac{3}{8}$$

$$R(n,m) = \frac{1}{4^m - 1}\left[4^m \times R(n,m-1) - R(n-1,m-1)\right] \quad for \quad n \geq 1, \quad m \geq 1$$

$$R(1,1) = \frac{1}{4^1 - 1}\left[4 \times R(1,0) - R(0,0)\right] = \frac{1}{3}\left[4 \times \frac{3}{8} - \frac{1}{2}\right] = \frac{1}{3}$$

x^2



Example 1

0.5	
3/8	1/3

Method 1

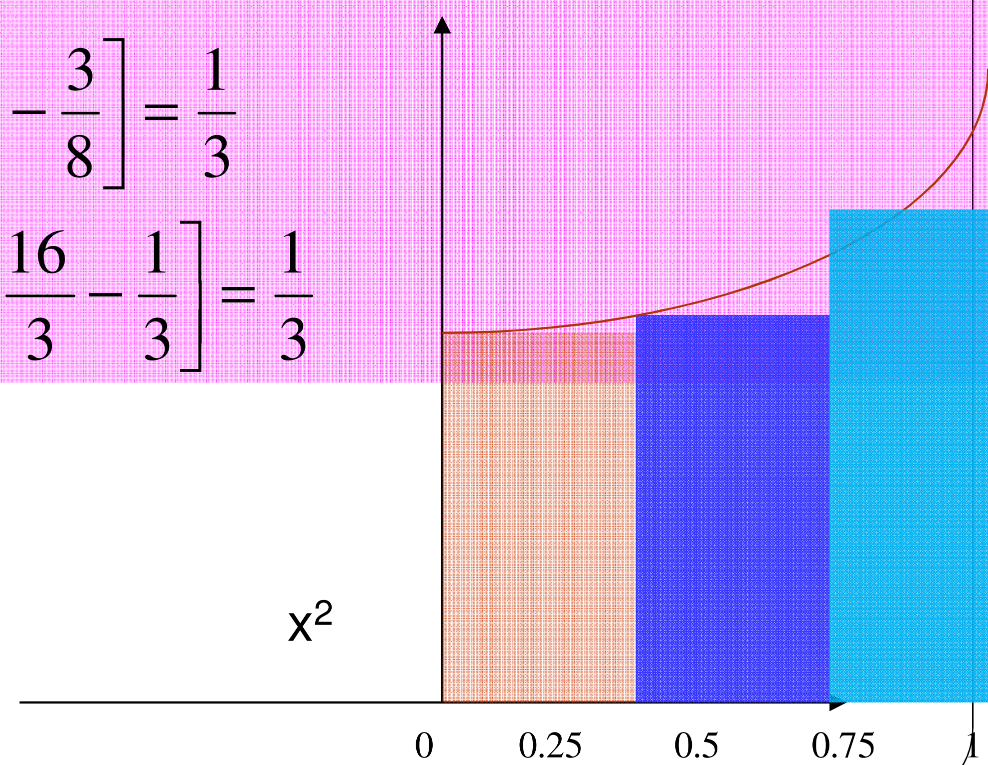
$$h=\frac{1}{4},\ R(2,0)=\frac{1}{2}R(1,0)+h(f(a+h)+f(a+3h))=\frac{1}{2}\left(\frac{3}{8}\right)+\frac{1}{4}\left(\frac{1}{16}+\frac{9}{16}\right)=\frac{11}{32}$$

$$R(n,m)=\frac{1}{4^m-1}\left[4^m\times R(n,m-1)-R(n-1,m-1)\right]$$

$$R(2,1)=\frac{1}{3}\left[4\times R(2,0)-R(1,0)\right]=\frac{1}{3}\left[4\times\frac{11}{32}-\frac{3}{8}\right]=\frac{1}{3}$$

$$R(2,2)=\frac{1}{4^2-1}\left[4^2\times R(2,1)-R(1,1)\right]=\frac{1}{15}\left[\frac{16}{3}-\frac{1}{3}\right]=\frac{1}{3}$$

0.5		
3/8	1/3	
11/32	1/3	1/3



Romberg Integration

When do stop?

$STOP \quad if$

$$\left| R(n,n) - R(n,n-1) \right| \leq \varepsilon$$

or

After a given number of steps,

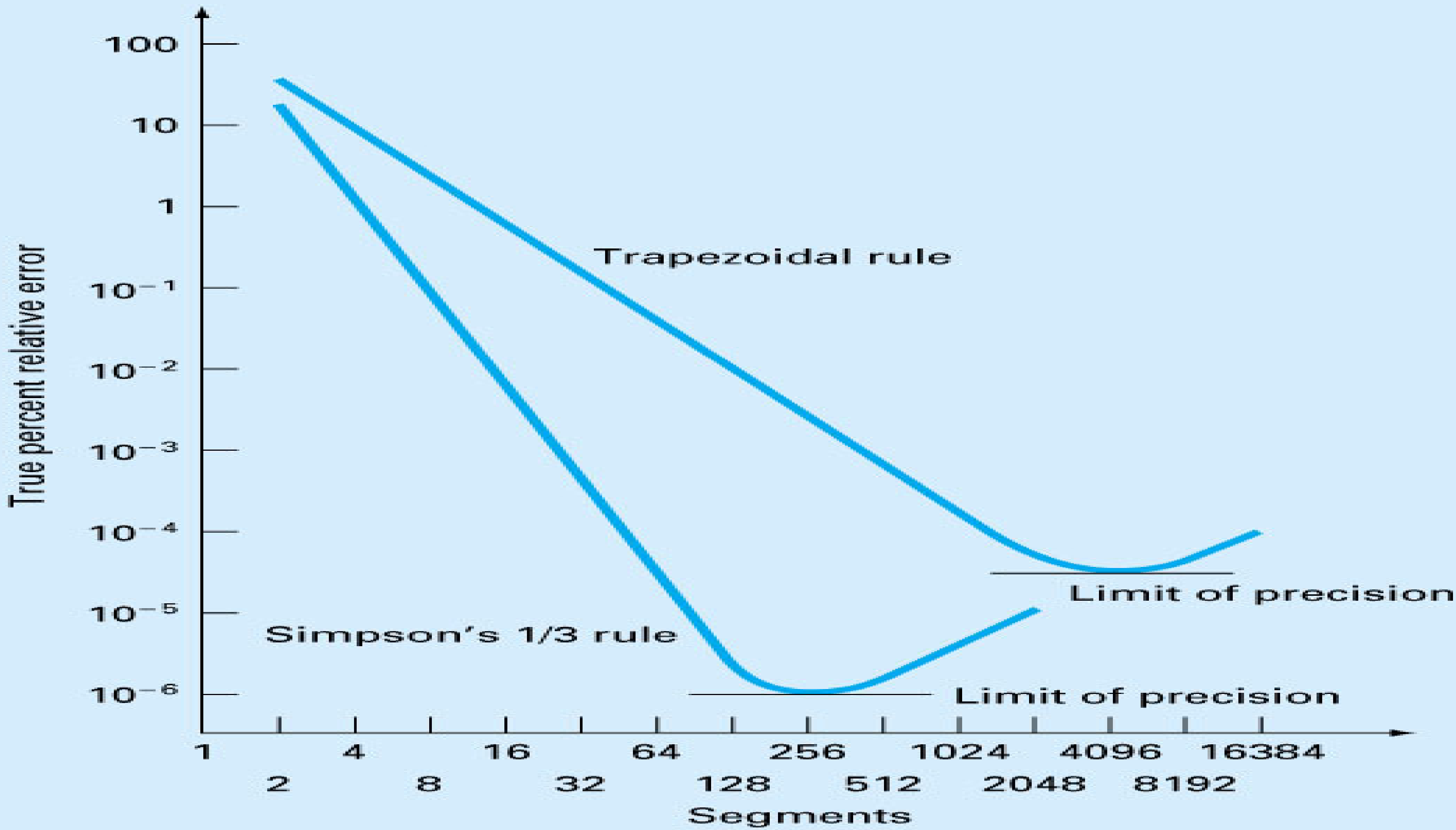
for example, STOP at R(4,4)

Numerical Integration

- Tabulated data – the accuracy of the integral is limited by the number of data points
- Continuous function – can generate as many f(x) as required to attain the required accuracy

- **Richardson extrapolation and Romberg integration**
- **Gauss Quadratures**

- Round-off errors may limit the precision of lower-order Newton-Cotes composite integration formula
- Use Romberg Integration for efficient integration



Richardson Extrapolation

Romberg Integration

Method 2

- The exact integral can be represented as

$$I = I(h) + E(h)$$

- **This is true for any *h* = (*b*–*a*)/*n***

$$I = I(h_1) + E(h_1) = I(h_2) + E(h_2)$$

- **Use trapezoidal rule as an example**

$$E = -\frac{(b-a)}{12} h^2 f''(\xi) \quad \Rightarrow \quad \frac{E(h_1)}{E(h_2)} \cong \frac{{h_1}^2}{{h_2}^2}$$

Richardson Extrapolation

- **Truncation error for trapezoidal rule**

$$\frac{E(h_1)}{E(h_2)} \cong \frac{h_1^{\,2}}{h_2^{\,2}}$$

$$E(h_1) \cong E(h_2)\left(\frac{h_1}{h_2}\right)^2$$

- **Substitute into the exact integral**

$$I = I(h_1) + E(h_1)$$

$$I = I(h_1) + E(h_2)\left(\frac{h_1}{h_2}\right)^2 \cong I(h_2) + E(h_2)$$

- **Which leads to**

$$\boxed{E(h_2) \cong \frac{I(h_1) - I(h_2)}{1 - (h_1/h_2)^2}}$$

Richardson Extrapolation

Method 2

- **Plugging back into $I = I(h) + E(h)$**

$$I \cong I(h_2) + \frac{1}{(h_1/h_2)^2 - 1}\left[I(h_2) - I(h_1)\right]$$

- **If $h_2 = h_1/2$, then**

$$I \cong I(h_2) + \frac{1}{2^2 - 1}\left[I(h_2) - I(h_1)\right]$$

$$I \cong \frac{4}{3} I(h_2) - \frac{1}{3} I(h_1)$$

Richardson Extrapolation

Method 2

- **Combine two O(h^2) estimates to get an O(h^4) estimate**
- **Can also combine two O(h^4) estimates to get an O(h^6) estimate**

$$I \cong \frac{16}{15} I(h_2) - \frac{1}{15} I(h_1) = \frac{16}{15} I_m - \frac{1}{15} I_l$$

- **Combine two O(h^6) estimates to get an O(h^8) estimate**

$$I \cong \frac{64}{63} I(h_2) - \frac{1}{63} I(h_1) = \frac{64}{63} I_m - \frac{1}{63} I_l$$

- **I_m and I_l are more and less accurate estimates, respectively**

Richardson Extrapolation

Romberg Integration **Method 2**

- General form is called Romberg Integration

$$\boxed{I_{j,k} \cong \frac{4^{k-1} I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1}}$$

- *j*: level of accuracy - j+1 is more accurate (more segments)

- *k*: level of integration - *k=1* is the original trapezoidal rule estimate ($O(h^2)$), *k=2* is improved ($O(h^4)$), *k=3* corresp's to $O(h^6)$, etc.

$$R(n,m) = \frac{1}{4^m - 1}\left[4^m \times R(n,m-1) - R(n-1,m-1)\right] \quad n \geq 1, \quad m \geq 1$$

Method 1

$$R(n,m)=\frac{1}{4^{m}-1}\left[4^{m}\times R(n,m-1)-R(n-1,m-1)\right]\quad n\ge 1,\quad m\ge 1$$

- **Accelerated Trapezoidal Rule**

Romberg Integration

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

	Trapezoid	Simpson's	Boole's		
	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$
	$O(h^{2})$	$O(h^{4})$	$O(h^{6})$	$O(h^{8})$	$O(h^{10})$
h	$I_{1,1}$	$I_{1,2}$	$I_{1,3}$	$I_{1,4}$	$I_{1,5}$
$h/2$	$I_{2,1}$	$I_{2,2}$	$I_{2,3}$	$I_{2,4}$	
$h/4$	$I_{3,1}$	$I_{3,2}$	$I_{3,3}$		
$h/8$	$I_{4,1}$	$I_{4,2}$			
$h/16$	$I_{5,1}$				
		$\frac{4I_{j+1,1}-I_{j,1}}{3}$	$\frac{16I_{j+1,2}-I_{j,2}}{15}$	$\frac{64I_{j+1,3}-I_{j,3}}{63}$	$\frac{256I_{j+1,4}-I_{j,4}}{255}$

Romberg Integration

- **Accelerated Trapezoid Rule**

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

	Trapezoid	Simpson's	Boole's		
	$k=1$	$k=2$	$k=3$	$k=4$	$k=5$
	$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$	$O(h^{10})$
$h=4$	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%

$$R(n,m) = \frac{1}{4^m - 1}\left[4^m \times R(n,m-1) - R(n-1,m-1)\right] \quad n \geq 1, \quad m \geq 1$$

Romberg Integration

```
function intg = romberg(func, a, b, es, maxit)
% romberg(func, a, b, es, maxit):
%   Romberg integration.
% input:
%   func = name of function to be integrated
%   a, b = integration limits
%   es = (optional) stop criterion (%); default = 0.00001
%   maxit = (optional) max allow iterations; default = 30
% output:
%   intg = integral estimate
% if necessary, assign default values
if nargin < 5, maxit = 30; end  % if maxit blank set to 30
if nargin < 4, es=0.00001; end  % if es blank set to 0.00001

n = 1;
I(1,1) = trap(func, a, b, n);
iter = 0;
while iter < maxit
iter = iter + 1;
n = 2^iter;
I(iter+1,1) = trap(func, a, b, n);
for k = 2:iter+1
   j = 2+iter-k
   I(j,k) = (4^(k-1)*I(j+1,k-1)-I(j,k-1))/(4^(k-1)-1)
end
ea = abs((I(1,iter+1)-I(2,iter))/I(1,iter+1))*100;
if ea <= es, break; end
end
intg = I(1,iter+1);
```

Accelerated trapezoidal Rule

$$\int_0^{\pi} x^2 \sin(2x)dx$$

```
» intg = romberg('example1',0,pi,0.00001,2)
I =
    0.0000    0.0000   -5.5122
    0.0000   -5.1677         0
   -3.8758         0         0
» intg = Romberg('example1',0,pi,0.00001,3)
I =
    0.0000    0.0000   -5.5122   -4.9221
    0.0000   -5.1677   -4.9313         0
   -3.8758   -4.9461         0         0
   -4.6785         0         0         0
» intg = romberg('example1',0,pi,0.00001,4)
I =
    0.0000    0.0000   -5.5122   -4.9221   -4.9349
    0.0000   -5.1677   -4.9313   -4.9348         0
   -3.8758   -4.9461   -4.9348         0         0
   -4.6785   -4.9355         0         0         0
   -4.8712         0         0         0         0
» intg = romberg('example1',0,pi,0.00001,6)
I =
    0.0000    0.0000   -5.5122   -4.9221   -4.9349   -4.9348   -4.9348
    0.0000   -5.1677   -4.9313   -4.9348   -4.9348   -4.9348         0
   -3.8758   -4.9461   -4.9348   -4.9348   -4.9348         0         0
   -4.6785   -4.9355   -4.9348   -4.9348         0         0         0
   -4.8712   -4.9348   -4.9348         0         0         0         0
   -4.9189   -4.9348         0         0         0         0         0
   -4.9308         0         0         0         0         0
```

Gauss Quadrature

- Motivation
- General integration formula

Method 1 : Based on Natural Coordinates
Method 2 : Based on Polynomial functions
Method 3 : Based on Isoperimetric element

Motivation

Trapezoid Method :

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

It can be expressed as :

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

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

General Integration Formula

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

c_i : *Weights* x_i : *Nodes*

Problem :

How do select c_i *and* x_i so that th e formula gives a good approximat ion of the integral?

Lagrange Interpolation

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

where $P_n(x)$ is a polynomial that interpolat es f(x) at the nodes : $x_0, x_1, \ldots, x_n$

$$\int_a^b f(x)dx \approx \int_a^b P_n(x)dx = \int_a^b \left(\sum_{i=0}^{n} \lambda_i(x) f(x_i) \right) dx$$

$$\Rightarrow \int_a^b f(x)dx \approx \sum_{i=0}^{n} c_i \; f(x_i) \qquad where \quad c_i = \int_a^b \lambda_i(x)\, dx$$

Example

- Determine the Gauss Quadrature Formula of

  If the nodes are given as (-1, 0 , 1) $\int_{-2}^{2} f(x)dx$

- Solution: First need to find $l_0(x), l_1(x), l_2(x)$

- Then compute:

$$c_0 = \int_{-2}^{2} l_0(x)dx, \quad c_1 = \int_{-2}^{2} l_1(x)dx, \quad c_2 = \int_{-2}^{2} l_2(x)dx$$

(-1, 0 , 1)
(x0,x1,x2)

Solution

$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

$$l_0(x) = \frac{(x - x1)(x - x2)}{(x0 - x1)(x0 - x2)} = \frac{x(x-1)}{2}$$

$$l_1(x) = \frac{(x - x0)(x - x2)}{(x1 - x0)(x1 - x2)} = -(x+1)(x-1)$$

$$l_2(x) = \frac{(x - x0)(x - x1)}{(x2 - x0)(x2 - x1)} = \frac{x(x+1)}{2}$$

$$c_0 = \int_{-2}^{2} \frac{x(x-1)}{2} dx = \frac{8}{3}, \quad c_1 = \int_{-2}^{2} -(x+1)(x-1) dx = -\frac{4}{3}, \quad c_2 = \int_{-2}^{2} \frac{x(x+1)}{2} dx = \frac{8}{3}$$

$$\text{The Gauss Quadrature Formula for } \int_{-2}^{2} f(x)dx = \frac{8}{3} f(-1) - \frac{4}{3} f(0) + \frac{8}{3} f(1)$$

Using the Gauss Quadrature Formula

Case 1 : Let $f(x) = x^2$

The exact valu e for $\int_{-2}^{2} f(x)dx = \int_{-2}^{2} x^2 dx = \frac{16}{3}$

The Gauss Quadrature Formula $= \frac{8}{3} f(-1) - \frac{4}{3} f(0) + \frac{8}{3} f(1)$

$= \frac{8}{3}(-1)^2 - \frac{4}{3}(0)^2 + \frac{8}{3}(1)^2 = \frac{16}{3}$, which is the same exact answer

Using the Gauss Quadrature Formula

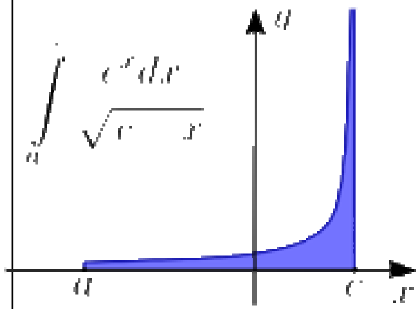
Case 2 : Let $f(x) = x^3$

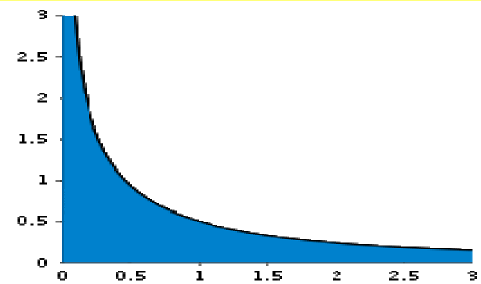
The exact valu e for $\displaystyle\int_{-2}^{2} f(x)\,dx = \int_{-2}^{2} x^3\,dx = 0$

The Gauss Quadrature Formula $= \dfrac{8}{3} f(-1) - \dfrac{4}{3} f(0) + \dfrac{8}{3} f(1)$

$= \dfrac{8}{3}(-1)^3 - \dfrac{4}{3}(0)^3 + \dfrac{8}{3}(1)^3 = 0$, which is the same exact answer

Improper Integrals





$$\int_0^\infty \frac{dx}{(x+1)\sqrt{x}} = \lim_{s\to 0}\int_s^1 \frac{dx}{(x+1)\sqrt{x}} + \lim_{t\to\infty}\int_1^t \frac{dx}{(x+1)\sqrt{x}}$$
$$= \lim_{s\to 0}\left(\frac{\pi}{2} - 2\arctan\sqrt{s}\right) + \lim_{t\to\infty}\left(2\arctan\sqrt{t} - \frac{\pi}{2}\right)$$
$$= \frac{\pi}{2} + \left(\pi - \frac{\pi}{2}\right)$$
$$= \pi.$$

Methods discussed earlier cannot be used directly to approximate improper integrals (one of the limits is ∞ or $-\infty$)

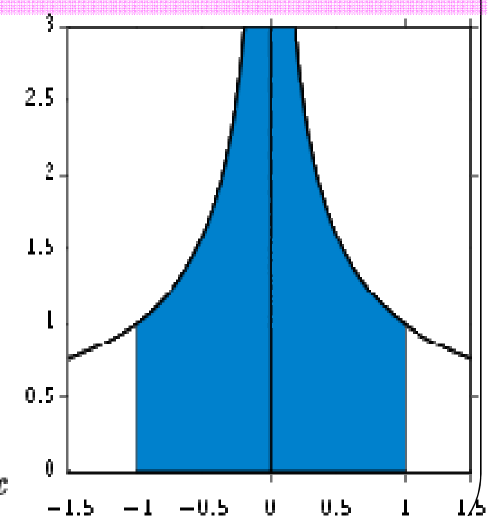
$\Rightarrow$ Use a transformation like the following

$$\int_a^b f(x)\,dx = \int_{\frac{1}{b}}^{\frac{1}{a}} \frac{1}{t^2} f\left(\frac{1}{t}\right) dt, \qquad (\text{assuming } ab > 0)$$

and apply the method on the new function.

$$Example \quad : \quad \int_1^\infty \frac{1}{x^2}\,dx = \int_0^1 \frac{1}{t^2}\left(\frac{1}{\left(\frac{1}{t}\right)^2}\right) dt$$

$$\int_{-\infty}^{\infty} f(x)\,dx = \lim_{a\to-\infty}\lim_{b\to\infty}\int_a^b f(x)\,dx$$



Gauss Quadrature - Example

Find the integral of:

$$f(x) = 0.2 + 25\,x - 200\,x^2 + 675\,x^3 - 900\,x^4 + 400\,x^5$$

Between the limits 0 to 0.8 using:

- 2 points integration points **(ans. 1.822578)**
- 3 points integration points **(ans. 1.640533)**

Improper Integral

- Improper integrals can be evaluated by making a change of variable that transforms the infinite range to one that is finite,

$$\int_a^b f(x)dx = \int_{1/b}^{1/a} \frac{1}{t^2} f\left(\frac{1}{t}\right)dt \qquad ab > 0$$

$$\int_{-\infty}^{b} f(x)dx = \boxed{\int_{-\infty}^{-A} f(x)dx} + \boxed{\int_{-A}^{b} f(x)dx}$$

$$\boxed{\int_{-\infty}^{-A} f(x)dx = \int_{-1/A}^{0} \frac{1}{t^2} f\left(\frac{1}{t}\right)dt}$$

Can be evaluated by Newton-Cotes closed formula

Improper Integral - Examples

$$\int_2^\infty \frac{dx}{x(x+2)} = \int_0^{0.5} \frac{1}{t^2}(t)\frac{1}{1/t+2}dt = \int_0^{0.5} \frac{1}{1+2t}dt$$

$$\int_0^\infty e^{-y}\sin^2 y\,dy = \int_0^2 e^{-y}\sin^2 y\,dy + \int_2^\infty e^{-y}\sin^2 y\,dy$$

$$\int_2^\infty e^{-y}\sin^2 y\,dy = \int_0^{1/2} \frac{1}{t^2} e^{-1/t}\sin^2(1/t)\,dt$$

$$\int_{-2}^\infty ye^{-y}\,dy = \int_{-2}^2 ye^{-y}\,dy + \int_2^\infty ye^{-y}\,dy$$

$$\int_2^\infty ye^{-y}\,dy = \int_0^{1/2} \frac{1}{t^3} e^{-1/t}\,dt$$

Gauss Quadrature

Method 1 : Based on Natural Coordinates

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

- Assume $$\boxed{I \cong c_0 f(a) + c_1 f(b)}$$
- a and b are limits of integration
- Trapezoidal rule should give exact results for constant and linear functions