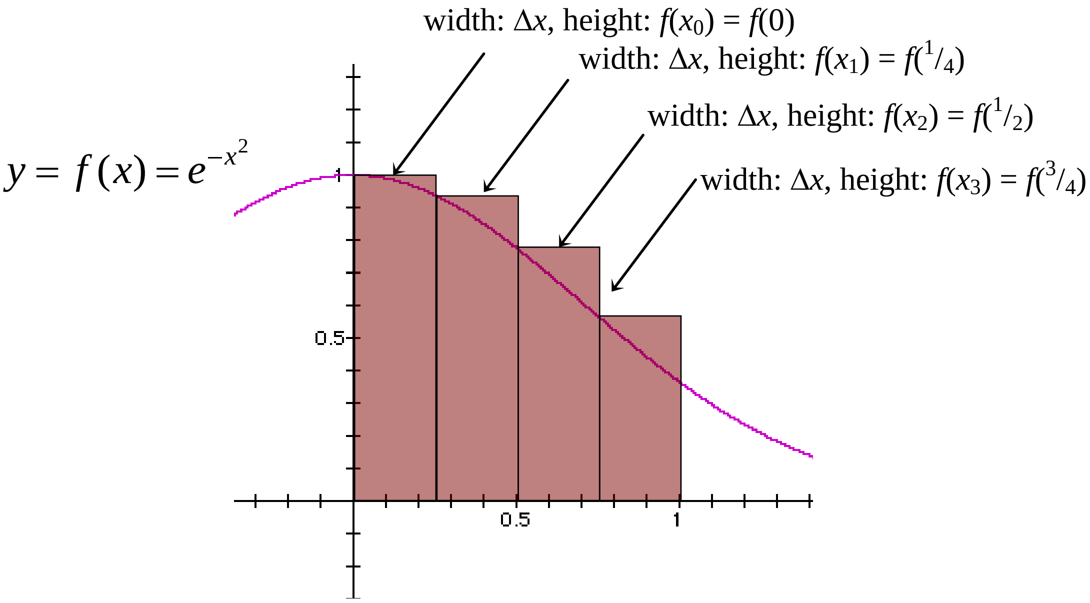
Numerical Integration Approximation.

Integration is the process of measuring the area under a function plotted on a graph. Sometimes, the evaluation of expressions involving these integrals can become daunting, if not indeterminate. For this reason, a wide variety of numerical methods have been developed to find the integral.

Here we discuss six different methods for approximating the value of a definite integral. Each method revolves around associating a definite integral with area under a curve. The first three use areas of rectangles, the fourth uses areas of trapezoids, and the final approximation technique uses areas of shapes that include a portion of a parabola.

4.1 Left-Endpoint Approximation

On each of the four subintervals shown below, we create a rectangle whose width is the length of the subdivision and whose height is determined by the function value at the ***left*** endpoint of each subdivision.



The sum of the areas of the four rectangles represents our approximation for the area under the curve and therefore represents an approximation for the value of the definite integral:

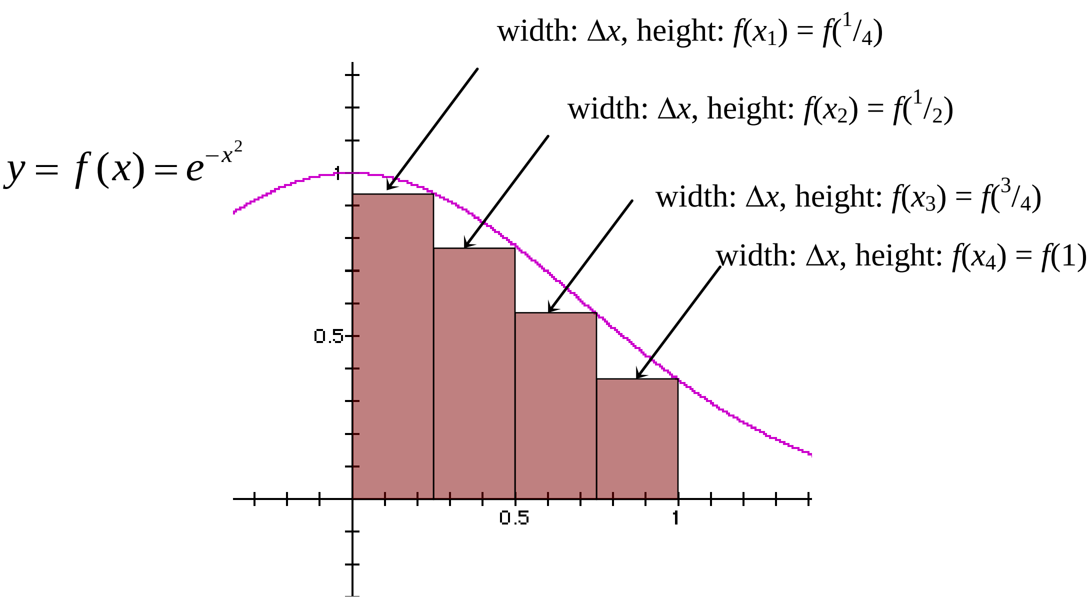
$$\int_0^1 e^{-x^2}dx \approx \Delta x\cdot f(x_0)+\Delta x\cdot f(x_1)+\Delta x\cdot f(x_2)+\Delta x\cdot f(x_3)$$
$$\approx \Delta x\big(f(x_0)+f(x_1)+f(x_2)+f(x_3)\big)$$
$$\approx \Delta x\sum_{i=0}^{3} f(x_i)$$

This same sequence of steps can be generalized for left-endpoint approximation of the definite integral $\int_a^b f(x)dx$ using n subdivisions:

$$\boxed{\begin{aligned}\int_a^b f(x)dx &\approx \Delta x\cdot f(x_0)+\Delta x\cdot f(x_1)+\Lambda\ +\Delta x\cdot f(x_{n-2})+\Delta x\cdot f(x_{n-1})\\ &\approx \Delta x\big(f(x_0)+f(x_1)+\Lambda\ +f(x_{n-2})+f(x_{n-1})\big)\\ &\approx \Delta x\sum_{i=0}^{n-1} f(x_i)\end{aligned}}$$

4.2 Right-Endpoint Approximation

Again we create rectangles whose widths are each the length of a subdivision, but here each height is determined by the function value at the ***right*** endpoint of each subinterval.



The sum of the areas of these four rectangles represents a right-endpoint approximation for the area under the curve and therefore is an approximation for the value of the definite integral:

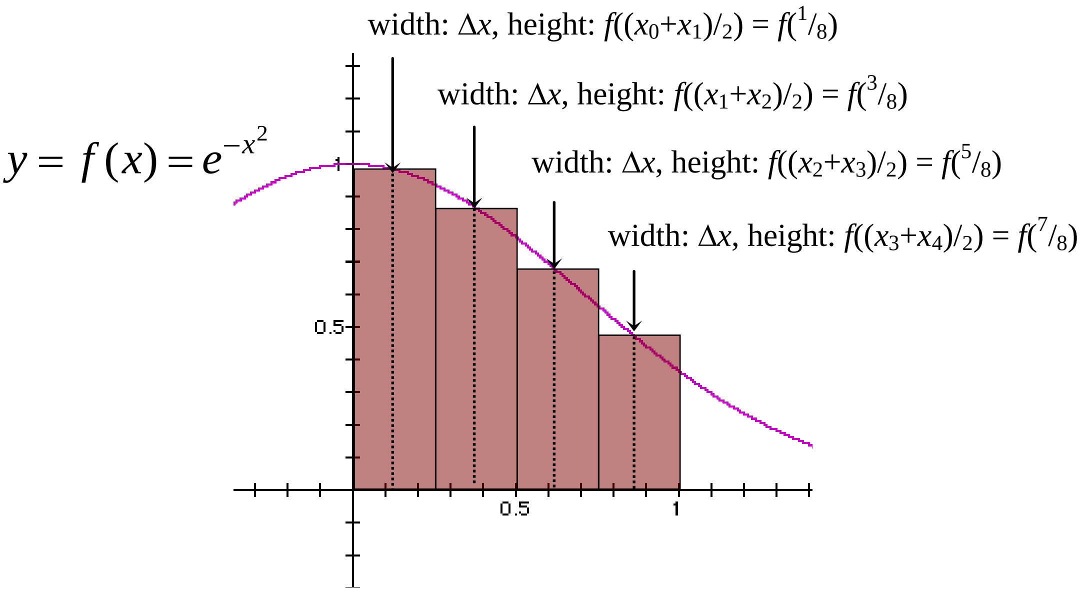
$$\int_0^1 e^{-x^2}dx \approx \Delta x \cdot f(x_1) + \Delta x \cdot f(x_2) + \Delta x \cdot f(x_3) + \Delta x \cdot f(x_4)$$
$$\approx \Delta x\big(f(x_1) + f(x_2) + f(x_3) + f(x_4)\big)$$
$$\approx \Delta x \sum_{i=1}^{4} f(x_i)$$

This same sequence of steps can be generalized for right-endpoint approximation of the definite integral $\int_a^b f(x)dx$ using n subdivisions:

$$\boxed{\begin{aligned}\int_a^b f(x)dx &\approx \Delta x \cdot f(x_1) + \Delta x \cdot f(x_2) + \Lambda\ + \Delta x \cdot f(x_{n-1}) + \Delta x \cdot f(x_n)\\ &\approx \Delta x\big(f(x_1) + f(x_2) + \Lambda\ + f(x_{n-1}) + f(x_n)\big)\\ &\approx \Delta x \sum_{i=1}^{n} f(x_i)\end{aligned}}$$

4.3 Midpoint Approximation

For a third time we create rectangles each of whose width is the length of the subdivision, but now each height is determined by the function value at the ***midpoint*** of each subdivision.



The sum of the areas of these four rectangles represents a midpoint approximation for the area under the curve and therefore is another approximation for the value of the definite integral:

$$\int_0^1 e^{-x^2}dx \approx \Delta x \cdot f\left(\frac{x_0+x_1}{2}\right) + \Delta x \cdot f\left(\frac{x_1+x_2}{2}\right) + \Delta x \cdot f\left(\frac{x_2+x_3}{2}\right) + \Delta x \cdot f\left(\frac{x_3+x_4}{2}\right)$$

$$\approx \Delta x\left(f\left(\frac{x_0+x_1}{2}\right) + f\left(\frac{x_1+x_2}{2}\right) + f\left(\frac{x_2+x_3}{2}\right) + f\left(\frac{x_3+x_4}{2}\right)\right)$$

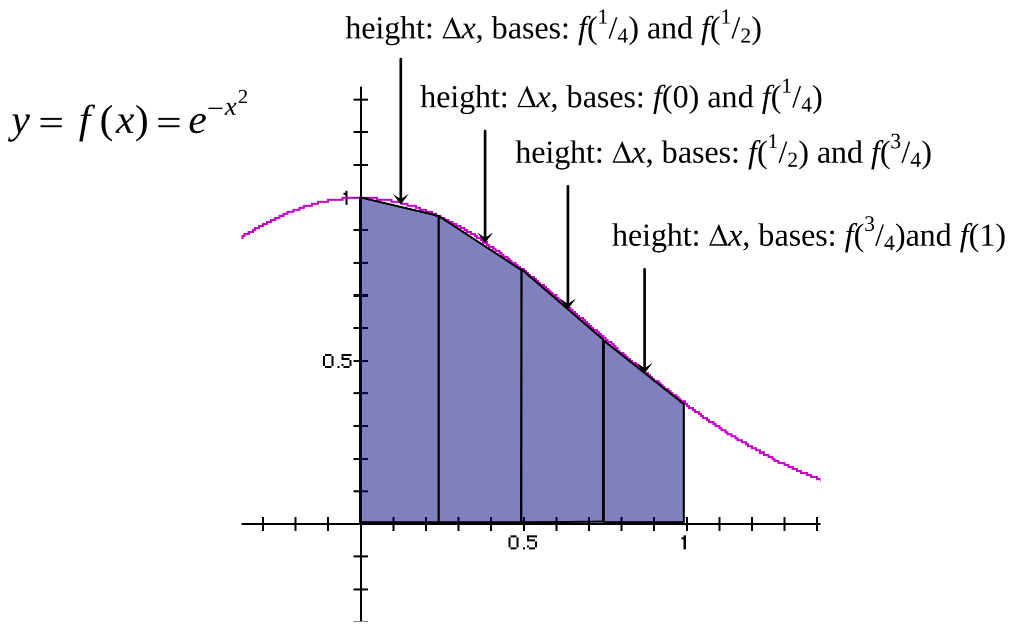
$$\approx \Delta x \sum_{i=0}^{3} f\left(\frac{x_i+x_{i+1}}{2}\right)$$

This same sequence of steps can be generalized for midpoint approximation of the definite integral $\int_a^b f(x)dx$ using n subdivisions:

$$\boxed{\begin{aligned}\int_a^b f(x)dx &\approx \left(\Delta x \cdot f\left(\frac{x_0+x_1}{2}\right)\right) + \left(\Delta x \cdot f\left(\frac{x_1+x_2}{2}\right)\right) + \Lambda + \left(\Delta x \cdot f\left(\frac{x_{n-1}+x_n}{2}\right)\right) + \left(\Delta x \cdot f\left(\frac{x_n+x_{n+1}}{2}\right)\right)\\ &\approx \Delta x\left(f\left(\frac{x_0+x_1}{2}\right) + f\left(\frac{x_1+x_2}{2}\right) + \Lambda + f\left(\frac{x_{n-1}+x_n}{2}\right) + f\left(\frac{x_n+x_{n+1}}{2}\right)\right)\\ &\approx \Delta x \sum_{i=0}^{n-1} f\left(\frac{x_i+x_{i+1}}{2}\right)\end{aligned}}$$

4.4 Trapezoidal Rule

Trapezoidal rule is based on the Newton-Cotes formula that if one approximates the integrand by an n^{th} order polynomial, then the integral of the function is approximated by the integral of that n^{th} order polynomial. Integrating polynomials is simple and is based on the calculus formula. The height of each trapezoid is the length of the subdivision. The two bases of each trapezoid correspond to the values of the function at the endpoints of the subinterval on which the trapezoid has been drawn.



It may be useful to remove the first of these trapezoids and rotate it into a more conventional orientation as we calculate its area.

base length: $f(0)$

height: Δx  Area = $\frac{1}{2}(\Delta x)\,(f(0) + f(\frac{1}{4}))$

base length: $f(\frac{1}{4})$

The sum of the areas of these four trapezoids represents an approximation for the area under the curve and therefore is one more approximation for the value of the definite integral:

$$\int_0^1 e^{-x^2}dx \approx \left(\frac{1}{2}\Delta x \cdot \left(f(x_0)+f(x_1)\right)\right)+\left(\frac{1}{2}\Delta x \cdot \left(f(x_1)+f(x_2)\right)\right)+$$
$$\left(\frac{1}{2}\Delta x \cdot \left(f(x_2)+f(x_3)\right)\right)+\left(\frac{1}{2}\Delta x \cdot \left(f(x_3)+f(x_4)\right)\right)$$
$$\approx \frac{1}{2}\Delta x\left(f(x_0)+2f(x_1)+2f(x_2)+2f(x_3)+f(x_4)\right)$$
$$\approx \frac{1}{2}\Delta x\sum_{i=0}^{3}\left(f(x_i)+f(x_{i+1})\right)$$

This same sequence of steps can be generalized for trapezoid approximation of the definite integral $\int_a^b f(x)dx$ using n subdivisions:

$$\int_a^b f(x)dx \approx \left(\frac{1}{2}\Delta x \cdot \left(f(x_0)+f(x_1)\right)\right)+\left(\frac{1}{2}\Delta x \cdot \left(f(x_1)+f(x_2)\right)\right)+\Lambda$$
$$+\left(\frac{1}{2}\Delta x \cdot \left(f(x_{n-1})+f(x_{n-1})\right)\right)+\left(\frac{1}{2}\Delta x \cdot \left(f(x_{n-1})+f(x_n)\right)\right)$$
$$\approx \frac{1}{2}\Delta x\left(f(x_0)+2f(x_1)+2f(x_2)+\Lambda\right.$$
$$\left.+2f(x_{n-2})+2f(x_{n-1})+f(x_n)\right)$$

Single Segment Trapezoidal Rule

$$\boxed{\int_a^b f(x)dx \approx \frac{1}{2}\Delta x\left(f(x_i)+f(x_{i+1})\right)}$$

Multiple Segments Trapezoidal Rule

$$\boxed{\int_a^b f(x)dx \approx \frac{1}{2}\Delta x\sum_{i=0}^{n-1}\left(f(x_i)+f(x_{i+1})\right)}$$

Example 4.1

Evaluate the integral $I = \int_0^1 \frac{dx}{\sqrt{1+x^2}}$ by trapezoidal rule dividing the interval [0, 1] into five equal parts.

Solution

$n = 5$

$\Delta x = \frac{1-0}{5} = 0.2$

x	0	0.2	0.4	0.6	0.8	1.0
$\frac{1}{\sqrt{1+x^2}}$	1.0	0.98058	0.92848	0.85749	0.78087	0.70711

From Trapezoidal Rule;

$$I = \frac{\Delta x}{2}[f(x_1) + 2(f(x_2) + f(x_3) + f(x_4) + f(x_5)) + f(x_6)]$$

$$= \frac{0.2}{2}[1 + 2(0.98058 + 0.92848 + 0.85749 + 0.78087) + 0.70711]$$

$$= 0.88016$$

Example 4.2

Use Multiple-segment Trapezoidal Rule to find the area under the curve $f(x) = \frac{300x}{1+e^x}$ from $x = 0$ to $x = 10$.

Solution

Using two segments, we get

$$\Delta x = \frac{10-0}{2} = 5$$

$$f(0) = \frac{300(0)}{1+e^0} = 0$$

$$f(5) = \frac{300(5)}{1+e^5} = 10.039$$

$$f(10) = \frac{300(10)}{1+e^{10}} = 0.136$$

$$\text{Area} = \frac{5}{2}\left[f(0) + 2f(5) + f(10)\right] = \frac{5}{2}\left[0 + 2(10.039) + 0.136\right] = 50.535$$

So what is the true value of this integral? $\int_0^{10} \frac{300x}{1+e^x} dx = 246.59$

Making the relative true error $|\in_t| = \left| \frac{246.59 - 50.535}{246.59} \right| \times 100\% = 79.506\%$

Table: Values obtained using Multiple-segment Trapezoidal Rule for $\int_0^{10} \frac{300x}{1+e^x} dx$

n	Approximate Value	E_t	$\lvert\in_t\rvert$
1	0.681	245.91	99.724%
2	50.535	196.05	79.505%
4	170.61	75.978	30.812%
8	227.04	19.546	7.927%
16	241.70	4.887	1.982%
32	245.37	1.222	0.495%
64	246.28	0.305	0.124%

Example 4.3

The average values of a function can be determined by:-

$$Cp_{mh} = \frac{\int_{T_1}^{T_2} \mathrm{C}p dT}{T_2 - T_1}$$

C_p= 0.99403 +1.617×10^{-4}T+9.7215×$10^{-8}$$T^2$ – 9.5838 × 10^{-11} T^3 + 1.9520 × 10^{-14} T^4

C_p in KJ/(Kg K)

Use this relationship to verity the average value of specific heat of dry air in the range from 300 K to 450 K:

1) Analytically

2) Numerically using five points Trapezoidal Rule

Solution

1) $$Cp_{mh} = \frac{\int_{300}^{450} 0.99403 + 1.617\times10^{-4}\mathrm{T} + 9.7215\times10^{-8}\mathrm{T}^2 - 9.5838\times10^{-11}\mathrm{T}^3 + 1.9520\times10^{-14}\mathrm{T}^4 dT}{450-300}$$

$$Cp_{mh} = \frac{\left. 0.99403\,\mathrm{T} + \frac{1.617\times10^{-4}}{2}\mathrm{T}^2 + \frac{9.7215\times10^{-8}}{3}\mathrm{T}^3 - \frac{9.5838\times10^{-11}}{4}\mathrm{T}^4 + \frac{1.9520\times10^{-14}}{5}\mathrm{T}^5 \right|_{300}^{450}}{450-300}$$

$$Cp_{mh} = \frac{465.73 - 306.18}{450 - 300} = 1.0637$$

2) $\Delta T = \dfrac{450 - 150}{4} = 37.5$

T	300	337.5	375	412.5	450
Cp	1.0489	1.0562	1.0637	1.0711	1.0785

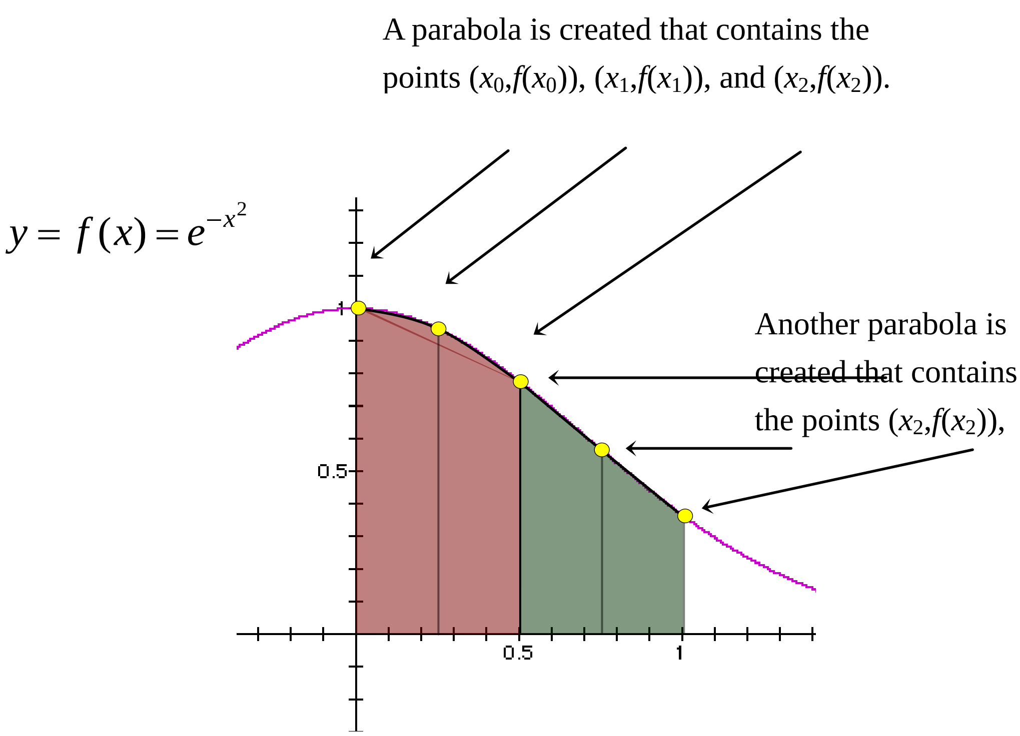
$$Cp_{mh} = \frac{(\mathrm{dT}/2) * (\mathrm{Cp}(1) + 2 * (\mathrm{Cp}(2) + \mathrm{Cp}(3) + \mathrm{Cp}(4)) + \mathrm{Cp}(5))}{T_2 - T_1}$$

$$= \frac{(37.5/2) * (1.0489 + 2 * (1.0562 + 1.0637 + 1.0711) + 1.0785)}{450 - 300} = 1.0637$$

$$\text{Realative Error \%} = \frac{\text{Analytical Solution - Numerical Solution}}{\text{Analytical Solution}} \% = \frac{1.0637 - 1.0637}{1.0637} \% = 0\%$$

4.5 Simpson's Rule (1/3 Simpson's Rule)

The final approximation technique we develop in this section is called Simpson's Rule. It is different from the first four methods because we are not creating polygons on each subinterval but rather we create a figure with a non-straight component to it. For this method, it is required that the number of subintervals be an **even** number.



Simpson's Rule uses pairs of subdivisions and creates over each pair a parabola that contains the points (x_{2i-2}, $f(x_{2i-2})$), (x_{2i-1}, $f(x_{2i-1})$), and (x_{2i}, $f(x_{2i})$) for i going from 1 to $^n/_2$. A shape is created using the resulting parabola, two vertical segments—one from (x_{2i-2},0) to (x_{2i-2}, $f(x_{2i-2})$) and one from (x_{2i+2},0) to (x_{2i+2}, $f(x_{2i+2})$)—and the segment on the x-axis with endpoints (x_{2i-2},0) and (x_{2i+2},0). The area of the resulting shape—such as of the red-shaded figure above or the green-shaded figure above-is calculated using the formula $\Delta x \cdot \frac{1}{3}\left(f(x_{2i-1}) + 4f(x_{2i}) + f(x_{2i+1})\right)$.

The sum of the areas of these shapes represents an approximation for the area under the curve and therefore is an approximation for the value of the definite integral:

$$\int_0^1 e^{-x^2}dx \approx \left(\Delta x \cdot \frac{1}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right)\right) + \left(\Delta x \cdot \frac{1}{3}\left(f(x_2) + 4f(x_3) + f(x_4)\right)\right)$$

This same sequence of steps can be generalized for the Simpson's Rule approximation of the definite integral $\int_a^b f(x)dx$ using n subdivisions:

$$\int_a^b f(x)dx \approx \left(\Delta x \cdot \frac{1}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right)\right) + \Lambda + \left(\Delta x \cdot \frac{1}{3}\left(f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right)\right)$$

$$\approx \Delta x \cdot \frac{1}{3}\left(f(x_0) + 4f(x_1) + f(x_2) + \Lambda + f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right)$$

Single Segment 1/3 Simpson's Rule

$$\boxed{\int_a^b f(x)dx \approx \frac{\Delta x}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right)}$$

Multiple Segment 1/3 Simpson's Rule

$$\boxed{\int_a^b f(x)dx \approx \frac{\Delta x}{3}\sum_{i=1}^{n/2}\left(f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})\right)}$$

Example 4.4

Evaluate the integral $I = \int_0^{0.8} \frac{dx}{\sqrt{1+x^2}}$ by 1/3 Simpson's rule dividing the interval [0, 0.8] to 4 equal sub-intervals.

Solution

$n = 4$

$\Delta x = \dfrac{0.8-0}{4} = 0.2$

x	0	0.2	0.4	0.6	0.8
$\dfrac{1}{\sqrt{1+x^2}}$	1.0	0.91287	0.84515	0.79057	0.74536

From Simpson's 1/3rd Rule

$$I = \int_0^{0.8} f(x)dx = \frac{\Delta x}{3}[(f(x_0)+4f(x_1)+f(x_2))+(f(x_2)+4f(x_3)+f(x_4))]$$

$$= \frac{\Delta x}{3}[f(x_0)+4[f(x_1)+f(x_3)]+2f(x_2)+f(x_4)]$$

$$= \frac{0.2}{3}[1.0+4[0.91287+0.79051]+2\times 0.84515+0.74536]$$
$$= 0.68329$$

4.6 Simpson's Rule (3/8 Simpson's Rule)

If we connect the points of the curve using a 3rd order Lagrange polynomial, the area under the curve can be approximated by the following formula:

$$\int_a^b f(x)\,dx \cong \frac{3\Delta x}{8}[f(x_0)+3f(x_1)+3f(x_2)+2f(x_3)+3f(x_4)+3f(x_5)$$
$$+2f(x_6)+.....+2f(x_{n-3})+3f(x_{n-2})+3f(x_{n-1})+f(x_n)]$$

Single Segment 3/8 Simpson's Rule

$$\boxed{\int_a^b f(x)dx \approx \frac{3\Delta x}{8}[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)]}$$

Multiple Segment 3/8 Simpson's Rule

$$\boxed{\int_a^b f(x)dx \approx \frac{3\Delta x}{8}\sum_{i=1}^{n/3}\left(f(x_{3i-3})+3f(x_{3i-2})+3f(x_{3i-1})+f(x_{3i})\right)}$$

Example 4.5

Evaluate the integral of the following tabular data with

(a) The trapezoidal rule.

(b) Simpson's rules.

x	0	0.1	0.2	0.3	0.4	0.5
F(x)	1	8	4	3.5	5	1

Solution

(a) Trapezoidal rule (n = 5):

$$I = \frac{0.1}{2}[1 + 2(8 + 4 + 3.5 + 5) + 1] = 2.15$$

(b) Simpson's rules (n = 5):

$$I = \frac{0.1}{3}[1 + 4(8) + 4] + 0.1\frac{3}{8}[4 + 3(3.5 + 5) + 1] = 1.233333 + 1.14375 = 2.377083$$

Example 4.6

The volume of is given by following expression:

$$V = \frac{F_{A0}}{CA_o}\int_0^{0.9}\frac{d\,x_A}{k(1-x_A)}$$

with $k = 2.7\times10^7 \exp(-6500/T) \quad \min^{-1}$ and $\qquad T = 325 + \dfrac{19000x_A}{120.35x_A + 143.75}$ using

$$F_{A0} = 1500 \text{mol/min}, \quad CA_0 = 2.5 \text{ mol L}^{-1}$$

Calculate the volume of the reactor using Simpsons rule with five points (4 steps).

Solution

Xa	T	k	$\dfrac{1}{k(1-x_A)}$
0	325.0000	0.0557	17.9691
0.2250	350.0251	0.2325	5.5491
0.4500	368.2020	0.5816	3.1263
0.6750	382.0035	1.1005	2.7958
0.9000	392.8396	1.7597	5.6827

$$V = (1500/2.5)*(0.225/3)*(23.1031 + 4*7.1346 + 2*4.0195 + 4*3.5947 + 7.3063)$$
$$= 3661.4 \text{ L}$$

A Matlab program for solving example 4.5 is listed in Table 4.1.

Table (4.1) Matlab code and results for solution example (4.5)	
Matlab Code	**Xa=0:0.225:0.9** **T=325+(19000*Xa)./(120.35*Xa+143.75)** **k=2.7e7*exp(-6500./T)** **f=1./(k.*(1-Xa))** **V=(1500/2.5)*(0.225/3)*(f(1)+4*f(2)+2*f(3)+4*f(4)+f(5))**
Results	**Xa =** **0 0.2250 0.4500 0.6750 0.9000** **T =** **325.0000 350.0251 368.2020 382.0035 392.8396** **k =** **0.0557 0.2325 0.5816 1.1005 1.7597** **f =** **17.9691 5.5491 3.1263 2.7958 5.6827** **V =** **2.8478e+03**