~ Numerical Differentiation and Integration ~

Newton-Cotes Integration Formulas

Chapter 21

- *Calculus* is the mathematics of change. Since engineers continuously deal with systems and processes that change, *calculus* is an essential tool of engineering.
- Standing at the heart of *calculus* are the concepts of:

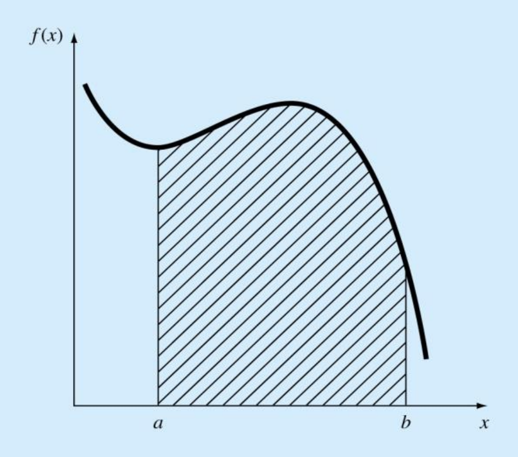
Differentiation

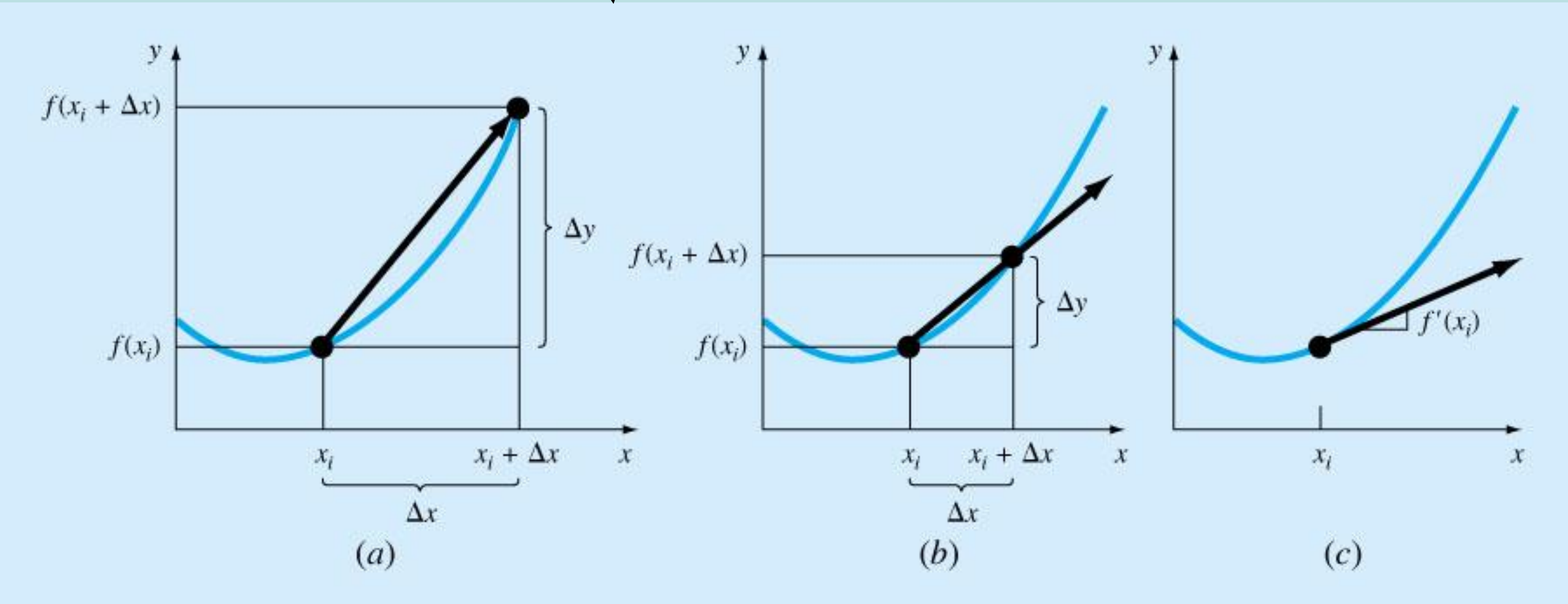
$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

and *Integration*

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





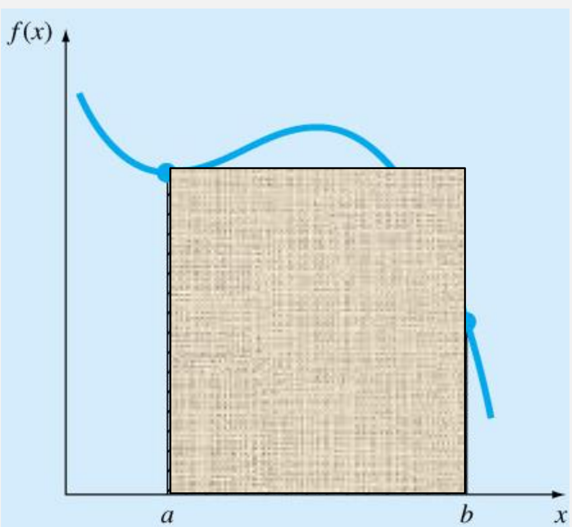
Newton-Cotes Integration Formulas

- Based on the strategy of replacing a complicated function or tabulated data with an approximating function that is easy to integrate:

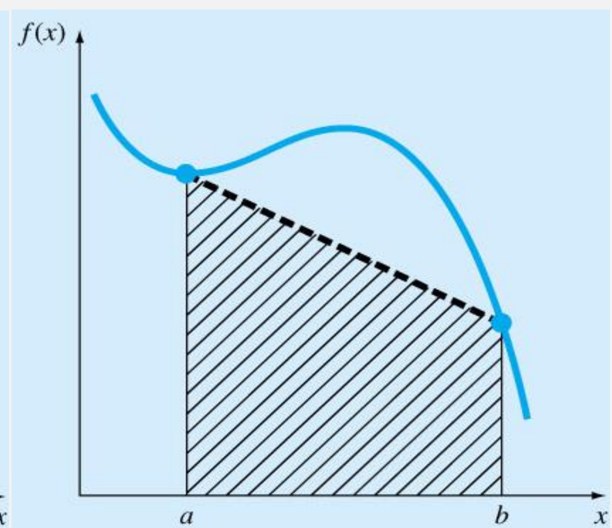
$$I = \int_a^b f(x)\,dx \cong \int_a^b f_n(x)\,dx$$

$$f_n(x) = a_0 + a_1 x + \cdots + a_n x^n$$

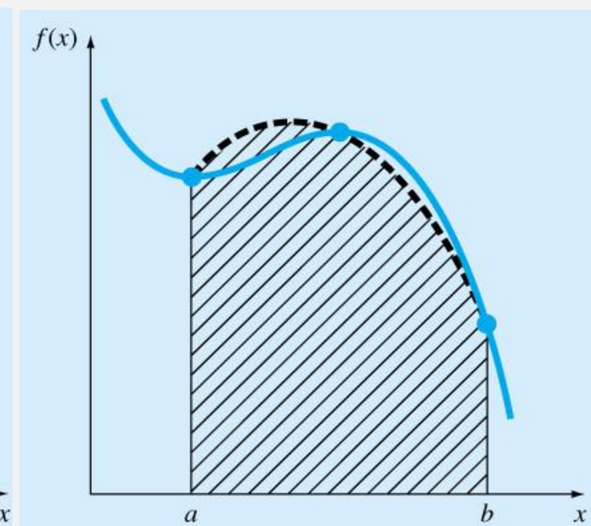
Zero order approximation



First-order



Second-order



The Trapezoidal Rule

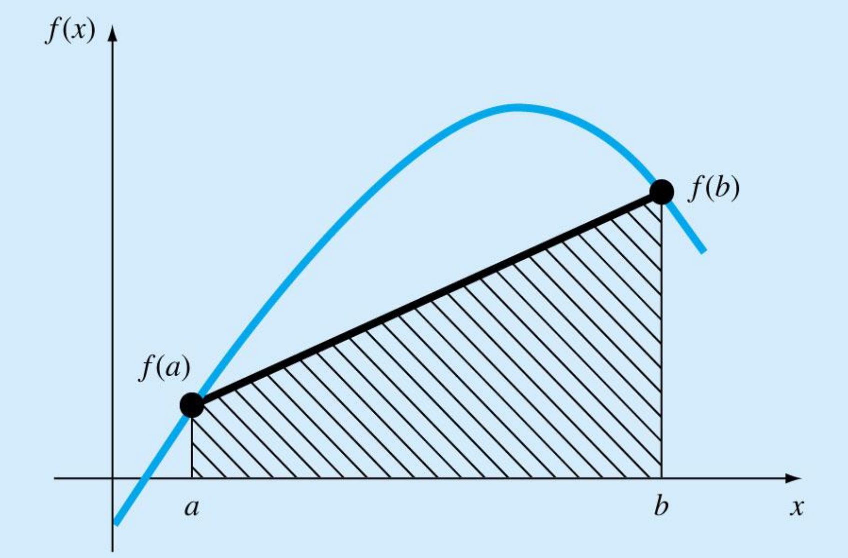
- Use a first order polynomial in approximating the function *f(x)* :

$$I = \int_a^b f(x)dx \cong \int_a^b f_1(x)dx$$

- The area under this first order polynomial is an estimate of the integral of *f(x)* between *a* and *b*:

$$I = (b-a)\frac{f(a)+f(b)}{2}$$

Trapezoidal rule



Error:

$$E_t = -\frac{1}{12} f''(\xi)(b-a)^3$$

where ξ lies somewhere in the interval from *a* to *b*

Example 21.1 Single Application of the Trapezoidal Rule

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

Integrate $f(x)$ from a=0 to b=0.8

True integral value : $\boldsymbol{I} = \int_{a=0}^{b=0.8} \boldsymbol{f(x)dx} = 1.64053$

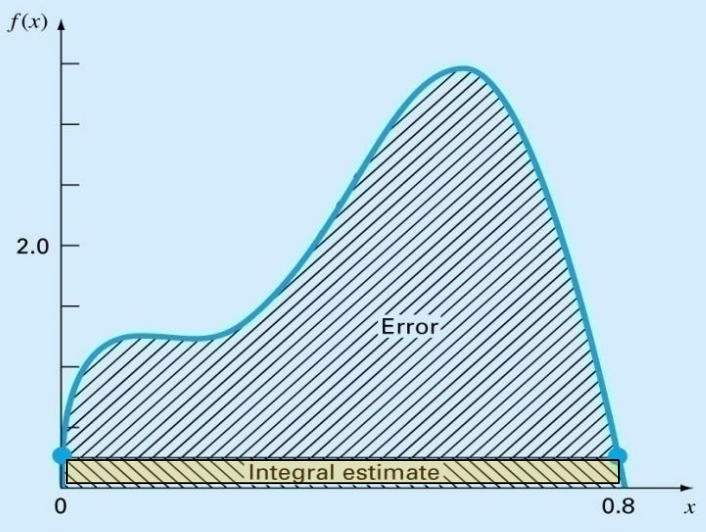
Solution: f(a)=f(0) = 0.2 and f(b)=f(0.8) = 0.232

Trapezoidal Rule: $I = (b-a)\dfrac{f(a)+f(b)}{2}$

$$= 0.8\frac{0.2+0.232}{2} = 0.1728$$

which represents an error of:

$$\varepsilon_t = \left|\frac{1.64053-0.1728}{1.64053}\right| = 89.5\%$$



The Multiple-Application Trapezoidal Rule

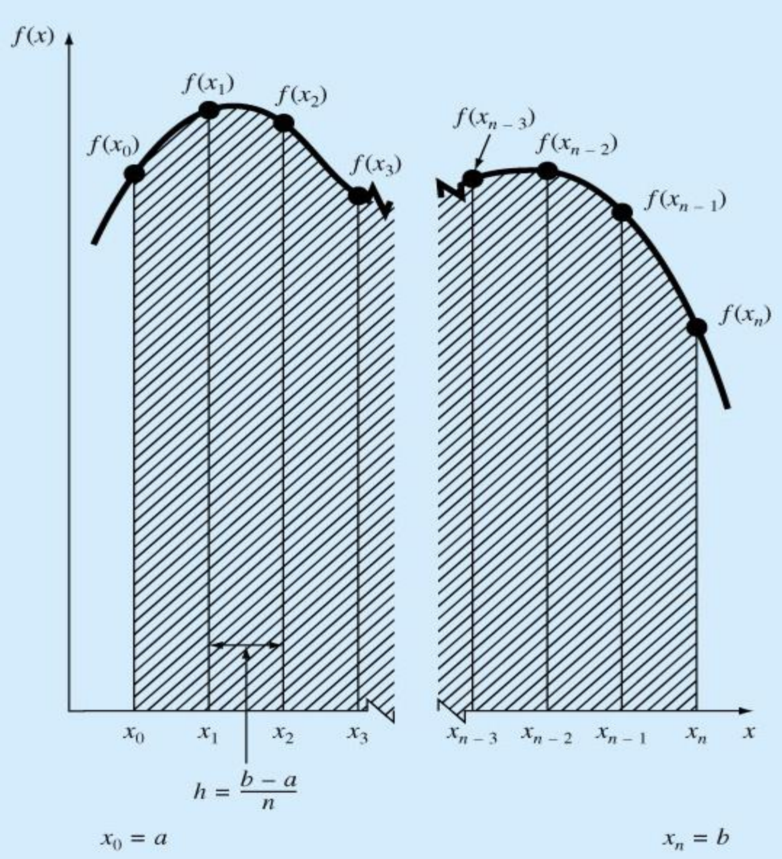
- The accuracy can be improved by dividing the interval from a to b into a number of segments and applying the method to each segment.

- The areas of individual segments are added to yield the integral for the entire interval.

$$h = \frac{b-a}{n} \quad \text{n = \# of seg.} \quad a = x_0 \quad b = x_n$$

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

Using the trapezoidal rule, we get:



$$\boldsymbol{I = h\frac{f(x_0)+f(x_1)}{2} + h\frac{f(x_1)+f(x_2)}{2} + \cdots + h\frac{f(x_{n-1})+f(x_n)}{2}}$$

$$\boldsymbol{I = \frac{b-a}{2n}\left[f(x_0)+f(x_n)+2\sum_{i=1}^{n-1} f(x_i)\right]}$$

The Error Estimate for The Multiple-Application Trapezoidal Rule

- Error estimate for **one segment** is given as:

$$E_t = \left| \frac{(b-a)^3}{12} f''(\xi) \right|$$

- An error for multiple-application trapezoidal rule can be obtained by summing the individual errors for each segment:

$$E_a = \frac{h^3}{12} \sum_{i=1}^{n} f''(\xi_i) \qquad \text{since} \qquad \sum f''(\xi_i) \cong n\bar{f}''$$

$$E_a = \frac{h^3}{12} n\bar{f}''$$ where $\bar{f}''$ is the mean of the second derivative over the interval

Since $h = \dfrac{(b-a)}{n}$

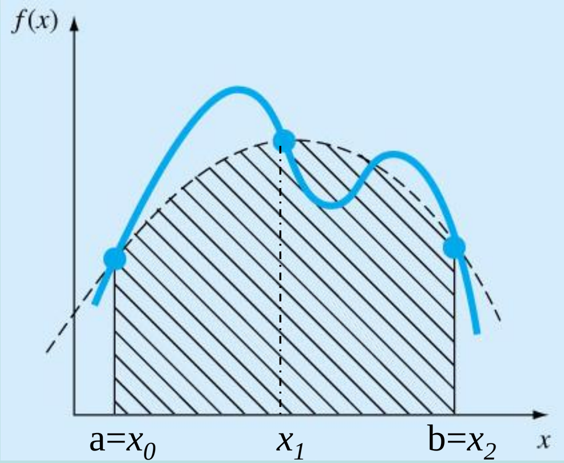
$$E_a = \frac{(b-a)^3}{12n^2} \bar{f}'' = \frac{(b-a)}{12} h^2 \bar{f}'' = \mathrm{O}(h^2)$$

Thus, if the number of segments is doubled, the truncation error will be quartered.

Simpson's Rules

- More accurate estimate of an integral is obtained if a high-order polynomial is used to connect the points. These formulas are called ***Simpson's rules*.**

Simpson's 1/3 Rule: results when a ***2nd order Lagrange*** *interpolating polynomial* is used for *f(x)*



$$I = \int_a^b f(x)dx \cong \int_a^b f_2(x)dx$$ where $f_2(x)$ is a second-order polynomial.

Using $a = x_0 \quad b = x_2$

$$I = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$

after integration and algebraic manipulation, the following formula results :

$$\boxed{I \cong \frac{h}{3}\left[f(x_0)+4f(x_1)+f(x_2)\right] \qquad h=\frac{b-a}{2}}$$

$\Leftarrow$ SIMPSON'S 1/3 RULE

The Multiple-Application Simpson's 1/3 Rule

- Just as the trapezoidal rule, Simpson's rule can be improved by dividing the integration interval into a number of segments of equal width.
- However, it is limited to cases where values are **equispaced**, there are an **even number of segments and odd number of points**.

$$h = \frac{b-a}{n} \quad \text{n =\# of seg.} \quad a = x_0 \quad b = x_n$$

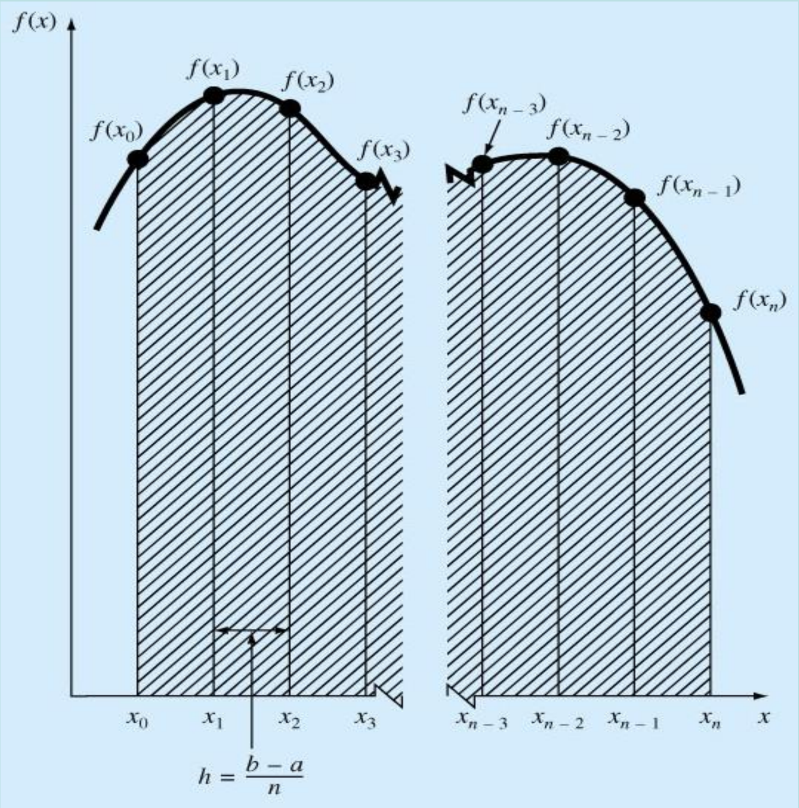
$$I = \int_{x_0}^{x_2} f^{0}(x)dx + \int_{x_2}^{x_4} f^{2}(x)dx + \ldots + \int_{x_{n-2}}^{x_n} f^{(n-2)}(x)dx$$

$$I = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2))$$

$$+ \frac{h}{3}(f(x_2) + 4f(x_3) + f(x_4)) +$$

$$\ldots\ldots + \frac{h}{3}(f(x_{n-2}) + 4f(x_{n-1}) + f(x_n))$$

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



*here Simpson's 3/8 Rule

Fit a ***3rd order Lagrange*** *interpolating polynomial* to four points and integrate

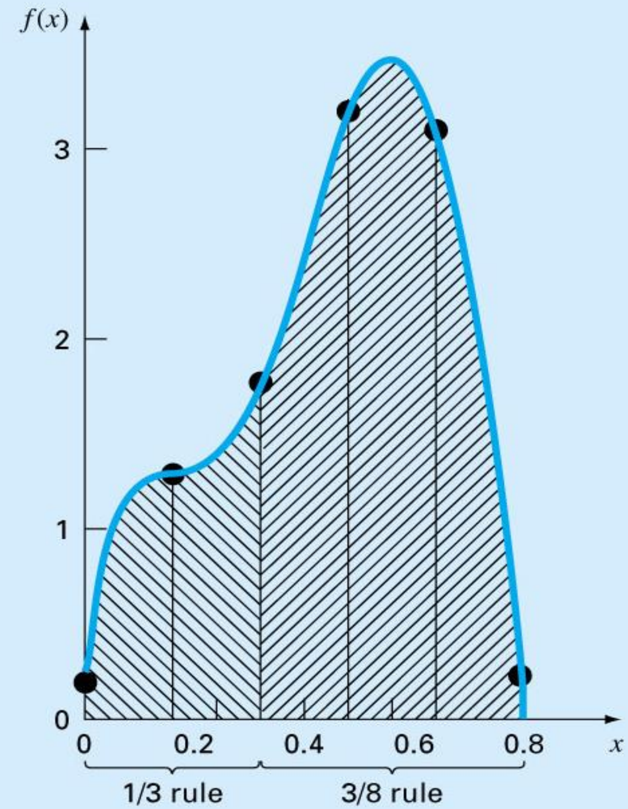
Simpson's 1/3 and 3/8 rules can be applied in tandem to handle multiple applications with odd number of intervals

$$I = \int_a^b f(x)dx \cong \int_a^b f_3(x)dx$$

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

$$h = \frac{(b-a)}{3}$$

$$I \cong (b-a)\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}$$



Newton-Cotes Closed Integration Formulas

Points	Name	Formula	Truncation Error
2	Trapezoidal	(b-a) * ($f(x_0)$+ $f(x_1)$)/2	(1/12)(b-a)$^3f''(\xi)$
3	Simpson's 1/3	(b-a) * ($f(x_0)$+ 4$f(x_1)$+$f(x_2)$)/6	(1/2880)(b-a)$^5f^{(4)}(\xi)$
4	Simpson's 3/8	(b-a) * ($f(x_0)$+ 3$f(x_1)$+ 3$f(x_2)$+ $f(x_3)$)/8	(1/6480)(b-a)$^5f^{(4)}(\xi)$
5	Boole's	(b-a) * (7$f(x_0)$ + 32$f(x_1)$ + 12$f(x_2)$ + 32$f(x_3)$ + 7$f(x_4)$)/90	proportional with (b-a)^7

Same order,

but Simpson's 3/8 is more accurate

In engineering practice, higher order (greater than 4-point) formulas are rarely used

Integration with Unequal Segments

Using Trapezoidal Rule

$$I = h_1 \frac{f(x_0)+f(x_1)}{2} + h_2 \frac{f(x_1)+f(x_2)}{2} + \cdots + h_n \frac{f(x_{n-1})+f(x_n)}{2}$$

<u>Example 21.7</u>

$$I = 0.12\frac{1.309+0.2}{2} + 0.10\frac{1.305+1.309}{2} + \cdots + 0.06\frac{0.363+3.181}{2} + 0.10\frac{0.232+2.363}{2}$$

$$= 0.0905 + 0.1307 + \ldots + 0.12975 = 1.594$$

which represents a relative error of ε = 2.8%

Data for

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

x	f(x)	x	f(x)
0.0	0.2	0.44	2.842
0.12	1.309	0.54	3.507
0.22	1.305	0.64	3.181
0.32	1.743	0.70	2.363
0.36	2.074	0.80	0.232
0.40	2.456		

Compute Integrals Using MATLAB

x	f(x)	x	f(x)
0.0	0.2	0.44	2.842
0.12	1.309	0.54	3.507
0.22	1.305	0.64	3.181
0.32	1.743	0.70	2.363
0.36	2.074	0.80	0.232
0.40	2.456		

First, create a file called **fx.m** which contains f(x):

```
function y = fx(x)
y = 0.2+25*x-200*x.^2+675*x.^3-900*x.^4+400*x.^5 ;
```

Then, execute in the *command window*:

```
>> Q=integral('fx', 0, 0.8)      % true integral
Or
>> Q=quad('fx', 0, 0.8)      % true integral

   Q =1.6405      ← true value

>> x=[0  .12  .22  .32  .36  .4  .44  .54  .64  .7  .8]

>> y = fx(x)
   y = 0.200   1.309   1.305   1.743   2.074   2.456
         2.843   3.507   3.181   2.363   0.232

>> I = trapz(x,y)          %  or   trapz(x, fx(x))
     Integral =1.5948
```

Demo: (how I changes wrt n) + (0^{th} order approx. With large n).