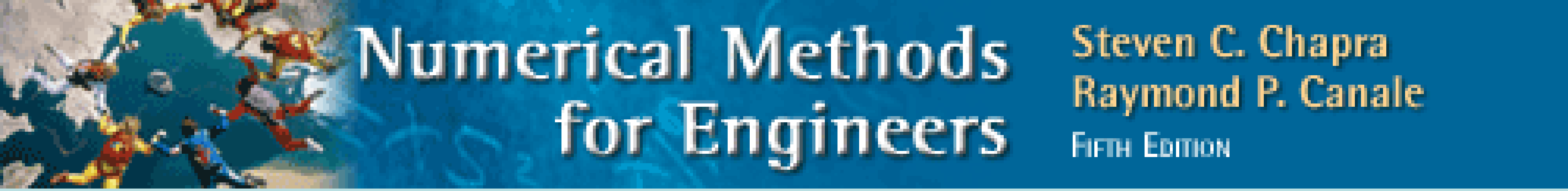


~ Numerical Differentiation and Integration ~

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:

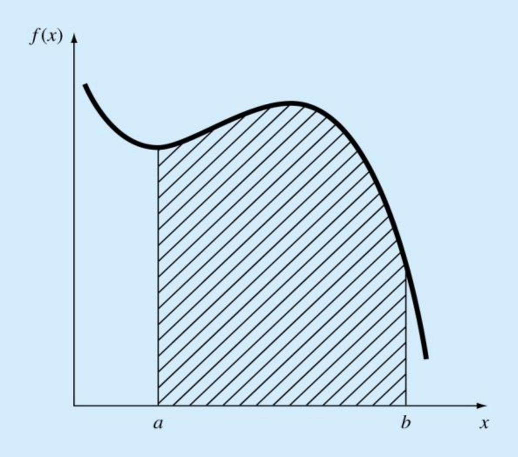
Differentiation

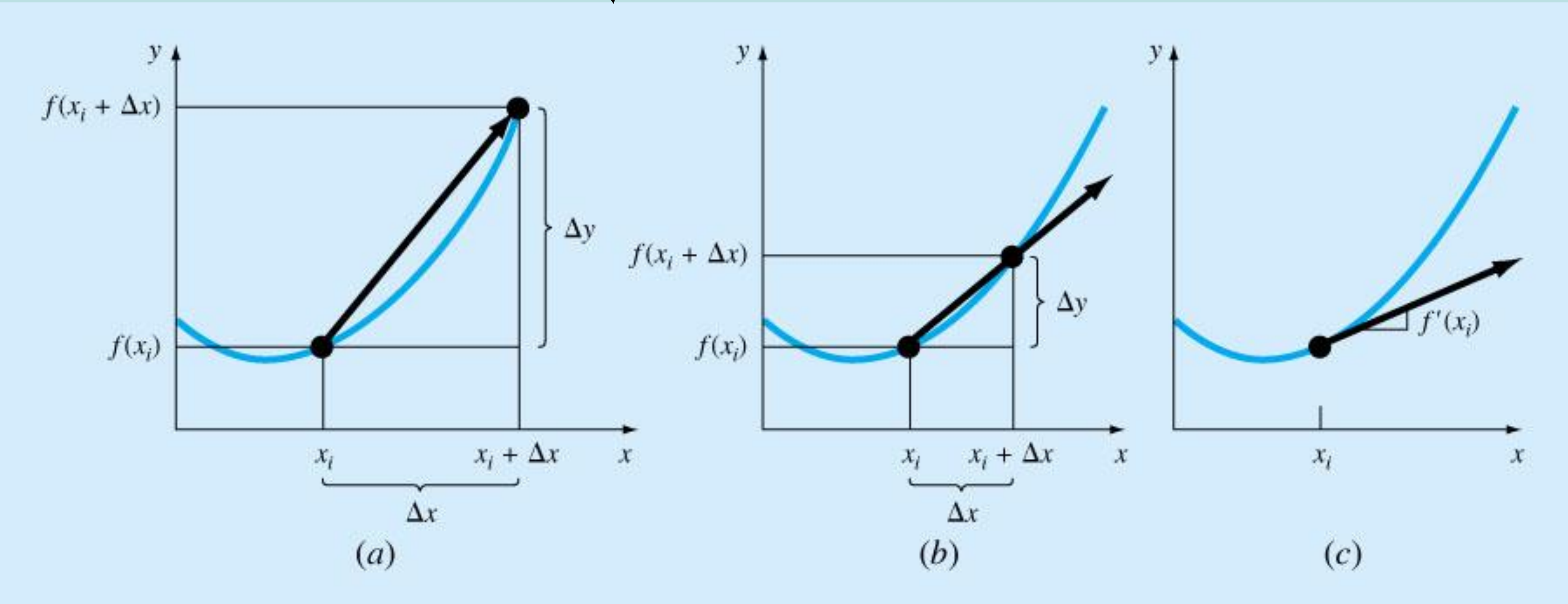
$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

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

and *Integration*

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





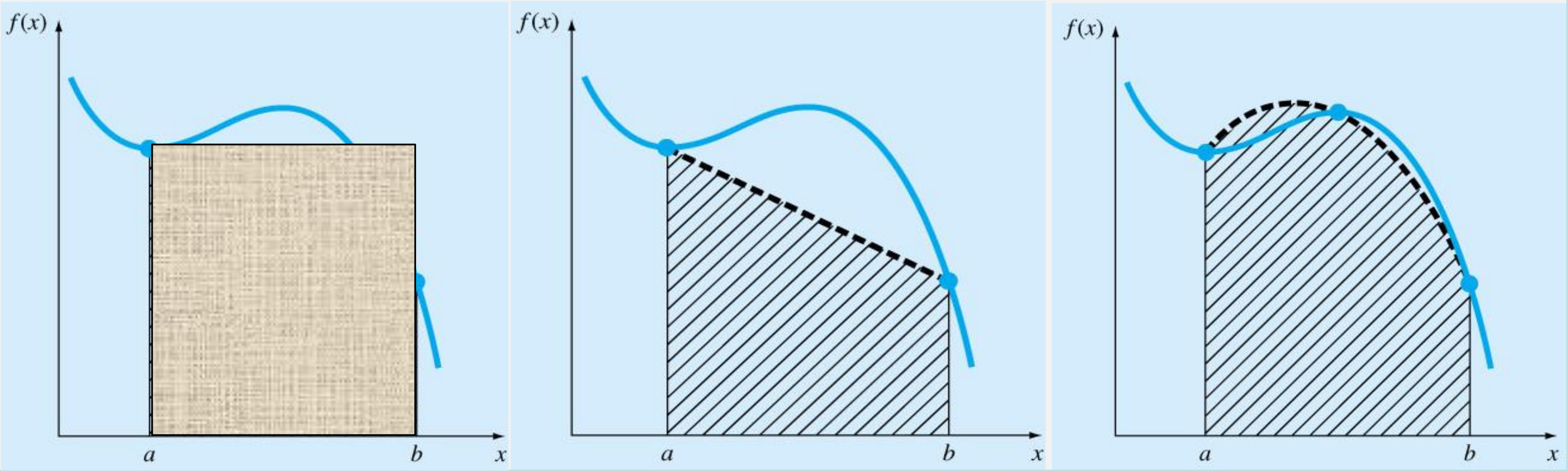
Newton-Cotes Integration Formulas

- 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

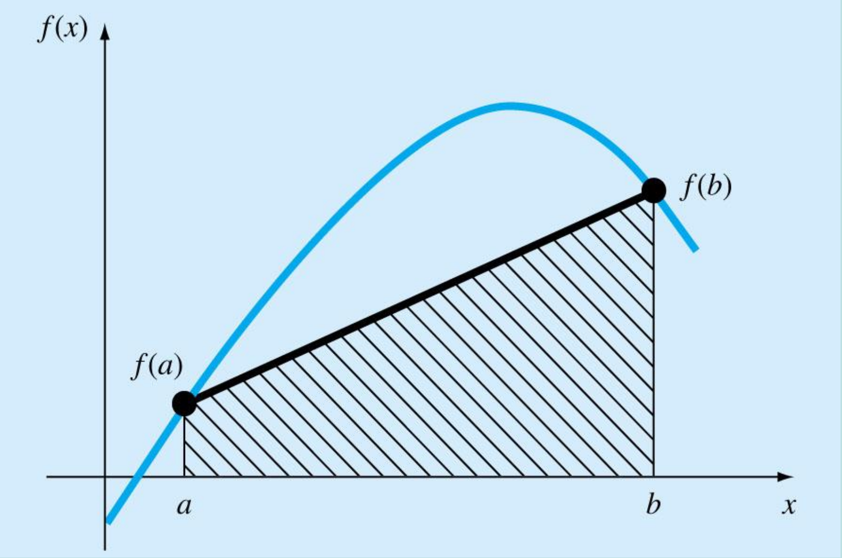
- Use a first order polynomial in approximating the function *f(x)*:

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

- 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

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

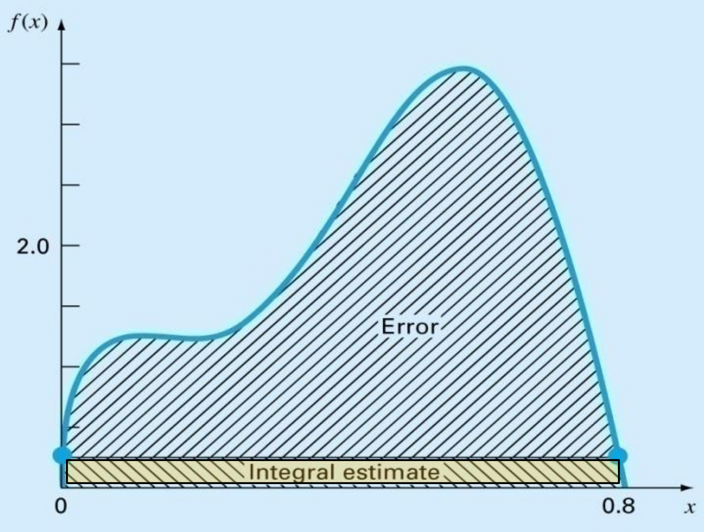
Solution: f(a)=f(0) = 0.2 and f(b)=f(0.8) = 0.232

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

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

which represents an error of :

$$E_t = 1.64053 - 0.1728 = 1.46773 \quad \varepsilon_t = 89.5\%$$



The Multiple-Application Trapezoidal Rule

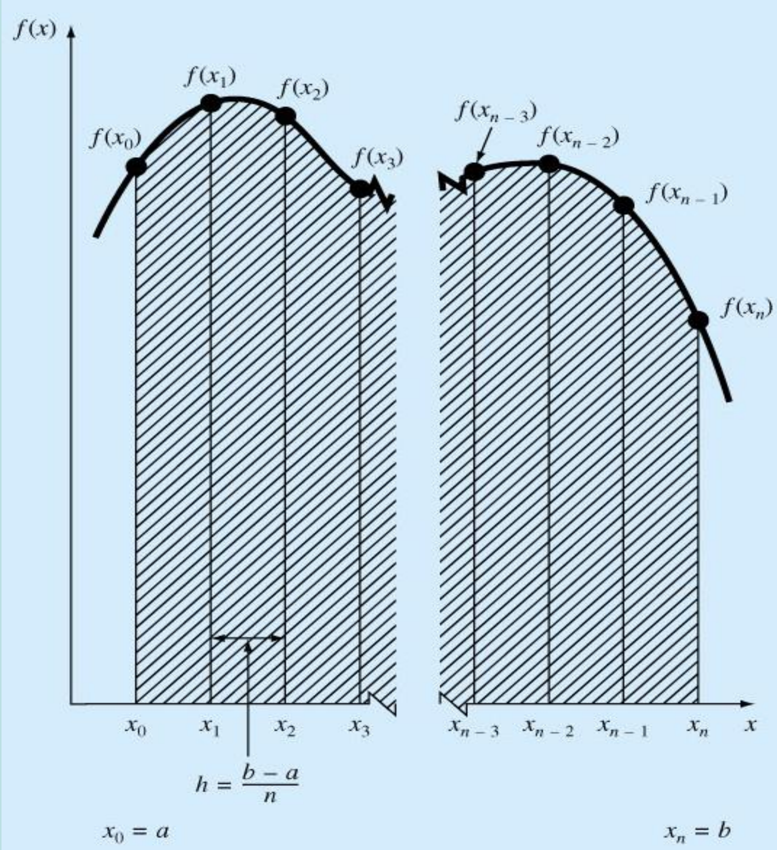
- The accuracy can be improved by dividing the interval from a to b into a number of segments and applying the method to each segment.

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

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

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

Using the trapezoidal rule, we get:



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

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

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

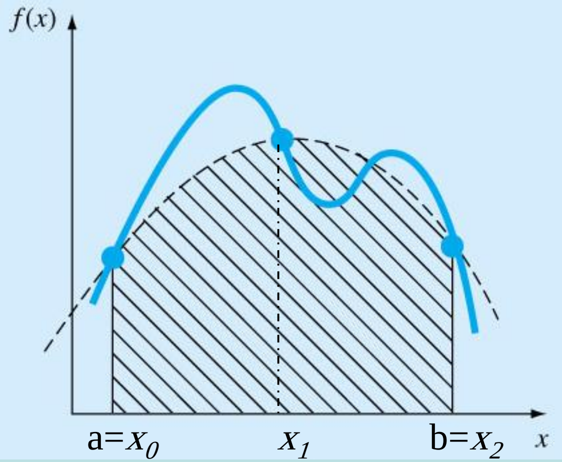
Since $h = \dfrac{(b-a)}{n}$

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

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 $a = x_0$ $b = x_2$

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

after integration and algebraic manipulation, the following formula results:

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

$\Leftarrow$ 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**.

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

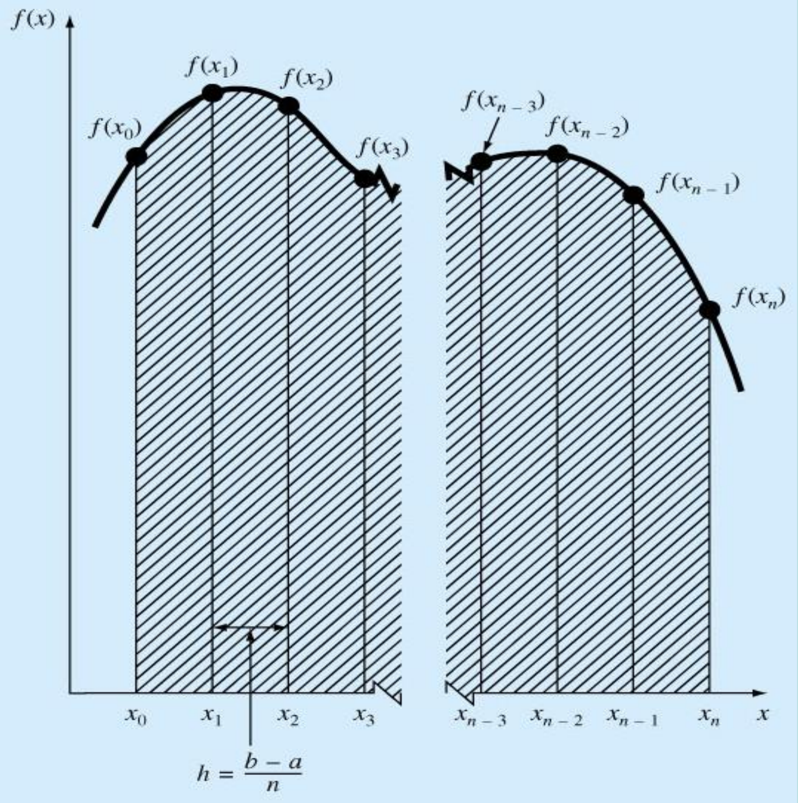
$$I = \int_{x_0}^{x_2} f^0(x)dx + \int_{x_2}^{x_4} f^2(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f^{n-2}(x)dx$$

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

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

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

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



Simpson's 3/8 Rule

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

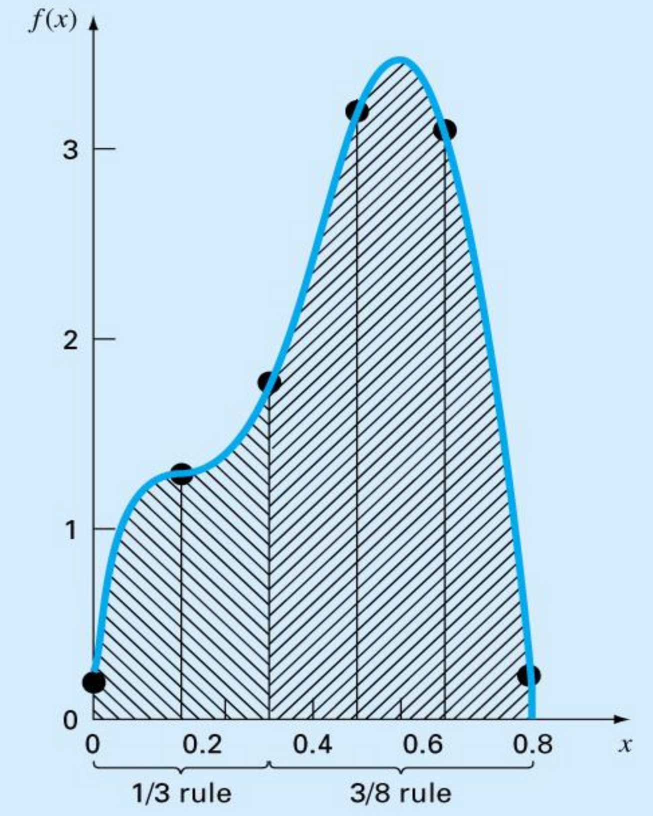
Simpson's 1/3 and 3/8 rules can be applied in tandem to handle multiple applications with odd number of intervals

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

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

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

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



Newton-Cotes Closed Integration Formulas

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

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

Example 21.7

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

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

which represents a relative error of ε = 2.8%

Data for

f(x)= 0.2+25x-200x²+675x³-900x⁴+400x⁵

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

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

    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).

~ Numerical Differentiation and Integration ~

Integration of Equations

Chapter 22

Romberg Integration

Successive application of the *trapezoidal rule* to attain efficient numerical integrals of functions.

Richardson's Extrapolation: In numerical analysis, **Richardson extrapolation** is a sequence acceleration method, used to improve the rate of convergence of a sequence. Here we use two estimates of an integral to compute a third and more accurate approximation.

$$I = I(h) + E(h) \qquad h = (b-a)/n \qquad n = (b-a)/h$$

I = exact value of integral $E(h)$ = the truncation error

$I(h)$: trapezoidal rule (n segments, step size h)

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

$$E \cong \frac{b-a}{12} h^2 \bar{f}'' = O(h^2)$$

(assume $\bar{f}''$ is constant for different step sizes)

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

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

$$\boldsymbol{I = I(h_2) + E(h_2)}$$

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

Improved estimate of the integral. It is shown that the error of this estimate is $O(h^4)$. Trapezoidal rule had an error estimate of $O(h^2)$.

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

If $(h_2 = h_1/2) \Rightarrow$

$$I \cong I(h_2) + \frac{1}{2^2 - 1}\left[I(h_2) - I(h_1)\right] = \frac{4}{3}I(h_2) - \frac{1}{3}I(h_1)$$

Example

Evaluate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from a=0 to b=0.8.

I (*True Integral value*) = 1.6405

Segments	h	Integral	ε_{tr}%
1	0.8	0.1728	89.5
2	0.4	1.0688	34.9
4	0.2	1.4848	9.5

Segments 1 & 2 combined to give :

$$I \cong \frac{4}{3}(1.0688) - \frac{1}{3}(0.1728) = 1.3675$$

$$E_t = 1.6405 - 1.3675 = 0.273 \quad (\varepsilon_t = 16.6\%)$$

Segments 2 & 4 combined to give :

$$I \cong \frac{4}{3}(1.4848) - \frac{1}{3}(1.0688) = 1.6234$$

$$E_t = 1.6405 - 1.6234 = 0.0171 \quad (\varepsilon_t = 1\%)$$

In each case, two estimates with error $O(h^2)$ are combined to give a third estimate with error $O(h^4)$

In Example 22.1, we computed two improved estimates of **O(h⁴)**. These two estimates can, in turn, be combined to yield an even better value with error **O(h⁶)**.

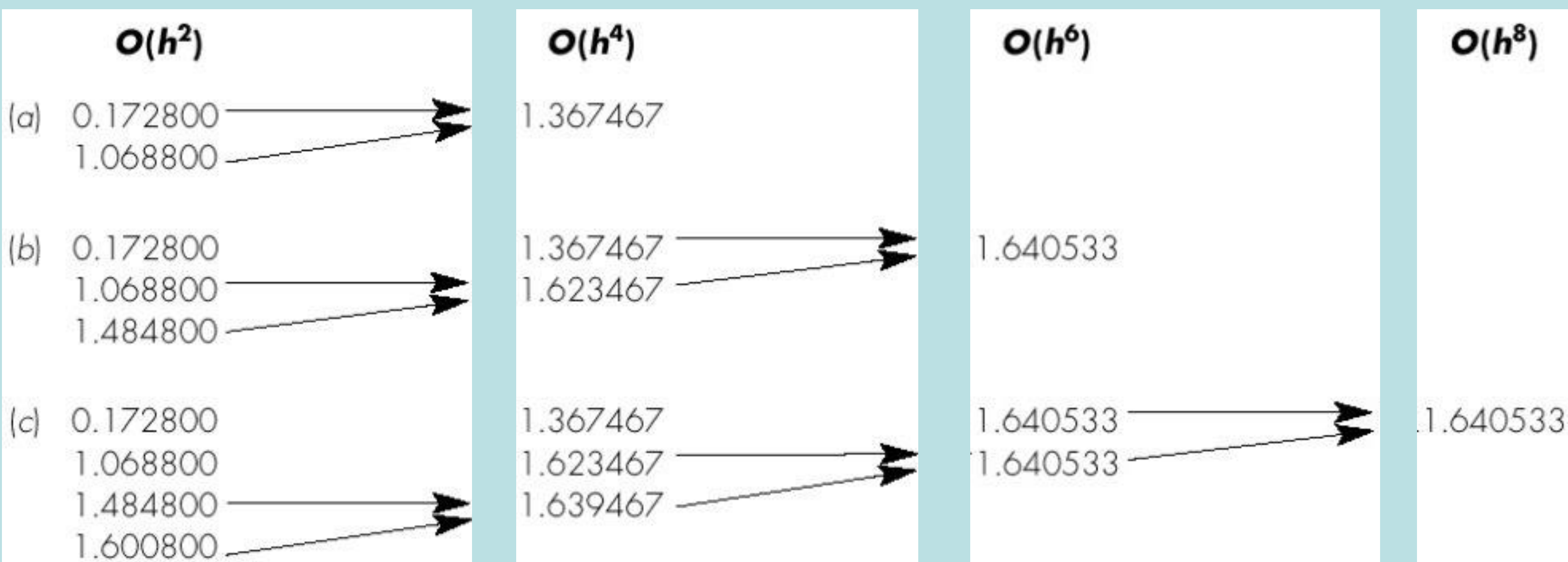
For the special case where the original trapezoidal estimates are based on ***successive halving*** of the step size, the equation used for **O(h⁶)** accuracy is:

$$I \cong \frac{16}{15} I_m - \frac{1}{15} I_l$$

where I_m and I_l are more and less accurate estimates

Similarly, two O(h^6) estimates can be combined to compute an I that is O(h^8).

$$I \cong \frac{64}{63} I_m - \frac{1}{63} I_l$$



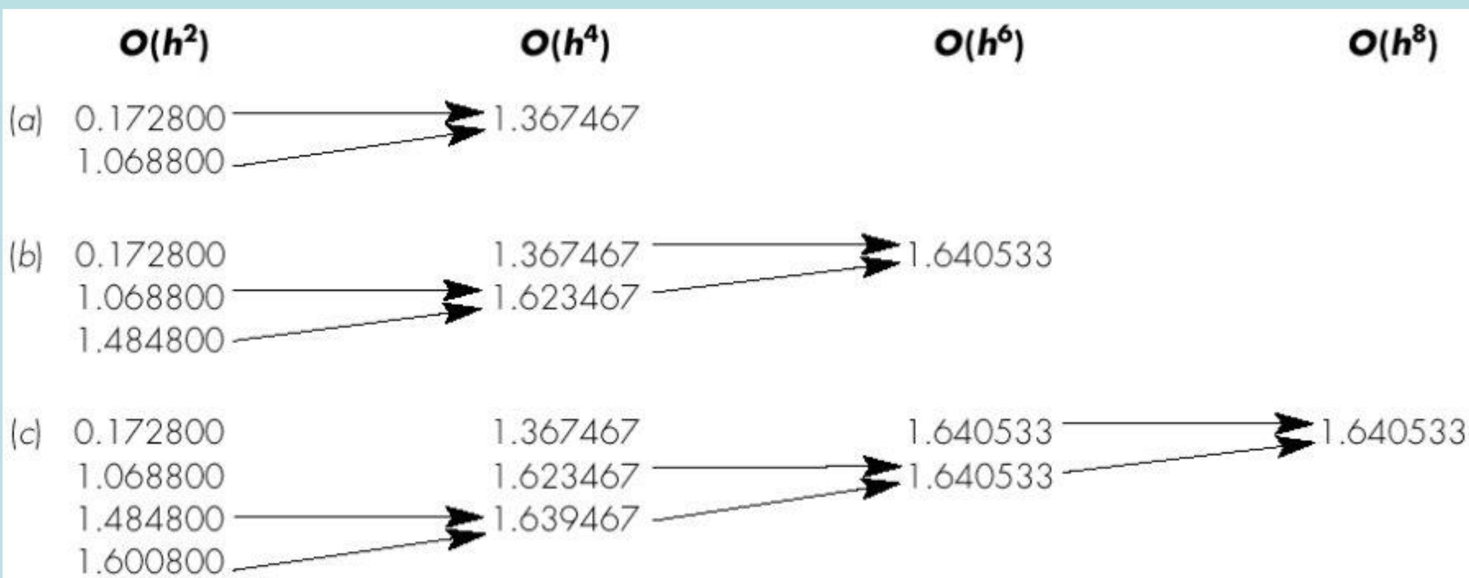
The Romberg Integration Algorithm

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

k=1 refers to *trapezoidal* rule, hence **O(h²)** accuracy.

k=2 refers to **$O(h^4)$** and k=3 ➔ **$O(h^6)$**

Index j is used to distinguish between the ***more*** (j+1) and the ***less*** (j) accurate estimates.



~ Numerical Differentiation and Integration ~

Numerical Differentiation

Chapter 23

High Accuracy Differentiation Formulas

- High-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion.

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2}h - \cdots$$

$$f''(x_i) = \frac{f'(x_{i+1}) - f'(x_i)}{h} = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

$$\boldsymbol{f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}h + O(h^2)}$$

$$\boldsymbol{f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)}$$

- Inclusion of the 2nd derivative term has improved the accuracy to *$O(h^2)$*.
- Similar improved versions can be developed for the *backward* and *centered* formulas

Forward finite-divided-difference formulas

First Derivative	Error
$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h}$	O(*h*)
$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	O(*h*[2])

Second Derivative	Error
$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	O(*h*)
$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	O(*h*[2])

Backward finite-divided-difference formulas

First Derivative	Error
$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	**O(*h*)**
$f'(x_i) = \dfrac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$	**O(*h*^{2})**

Second Derivative	Error
$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	**O(*h*)**
$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}$	**O(*h*^{2})**

Centered finite-divided-difference formulas

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	**O(h^2)**
$f'(x_i) = \dfrac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$	**O(h^4)**

Second Derivative	Error
$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	**O(h^2)**
$f''(x_i) = \dfrac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	**O(h^4)**

Derivation of the centered formula for *f''*(x_i)

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

$$f''(x_i) = \frac{2(f(x_{i+1}) - f(x_i) - f'(x_i)h)}{h^2}$$

$$= \frac{2\left(f(x_{i+1}) - f(x_i) - \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}h\right)}{h^2}$$

$$= \frac{2f(x_{i+1}) - 2f(x_i) - f(x_{i+1}) + f(x_{i-1})}{h^2}$$

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$$

Differentiation Using MATLAB

	x	*f(x)*
i-2	0	1.2
i-1	0.25	1.1035
i	0.50	0.925
i+1	0.75	0.6363
i+2	1	0.2

First, create a file called **fx1.m** which contains y=f(x):

```
function y = fx1(x)
    y = 1.2 - .25*x - .5*x.^2 - .15*x.^3 -.1*x.^4 ;
```

Command window:

```
>> x=0:.25:1
     0     0.25     0.5     0.75     1
>> y = fx1(x)

     1.2    1.1035    0.925    0.6363    0.2

>> d = diff(y) ./ diff(x)     % diff() takes differences between
                              % consecutive vector elements

     d =   -0.3859   -0.7141   -1.1547   -1.7453
```

Forward: x = 0 0.25 0.5 0.75 1

Backward: x = 0.25 0.5 0.75 1

Example :

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

At **x = 0.5** **True value** for First Derivative = **-0.9125**

Using finite divided differences and a step size of **h = 0.25** we obtain:

	x	*f(x)*
i-2	0	1.2
i-1	0.25	1.1035
i	0.50	0.925
i+1	0.75	0.6363
i+2	1	0.2

	Forward ***O(h)***	**Backward** ***O(h)***
Estimate	**-1.155**	**-0.714**
ε_t (%)	**26.5**	**21.7**

Forward difference of accuracy $O(h^2)$ is computed as:

$$f'(0.5) = \frac{-0.2 + 4(0.6363) - 3(0.925)}{2(0.25)} = -0.8593 \qquad \varepsilon_t = 5.82\%$$

Backward difference of accuracy $O(h^2)$ is computed as:

$$f'(0.5) = \frac{3(0.925) - 4(1.1035) + 1.2}{2(0.25)} = -0.8781 \qquad \varepsilon_t = 3.77\%$$

Richardson Extrapolation

- There are two ways to improve derivative estimates when employing finite divided differences:
  - Decrease the step size, or
  - Use a higher-order formula that employs more points.
- A third approach, based on **Richardson extrapolation**, uses two derivative estimates (with $O(h^2)$ error) to compute a third (with $O(h^4)$ error) , more accurate approximation. We can derive this formula following the same steps used in the case of the integrals:

$$h_2 = h_1 / 2 \quad \Rightarrow \quad D \cong \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1)$$

Example: using the previous example and Richardson's formula, estimate the first derivative at **x=0.5** Using **Centered Difference approx. (with error $O(h^2)$)** with **h=0.5** and **h=0.25** :

$D_{h=0.5}$**(x=0.5)** = (0.2-1.2)/1 = -1 [ε_t=|(-.9125+1)/-.9125| = **9.6%**]

$D_{h=0.25}$**(x=0.5)** = (0.6363-1.103)/0.5=-0.9343 [ε_t=|(-.9125+0.9343)/-.9125| = **2.4%**]

The improved estimate is:

D = 4/3(-0.9343) – 1/3(-1) = -0.9125 [ε_t=(-.9125+.9125)/-.9125 = **0%** ➔ **perfect!**]

Derivatives of Unequally Spaced Data

- Derivation formulas studied so far (especially the ones with $O(h^2)$ error) require multiple points to be spaced evenly.
- Data from experiments or field studies are often collected at unequal intervals.
- Fit a ***Lagrange interpolating polynomial***, and then calculate the 1st derivative.

  As an example, second order *Lagrange interpolating polynomial* is used below*:*

$$f(x) = f(x_{i-1})\frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})} + f(x_i)\frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})} + f(x_{i+1})\frac{(x-x_{i-1})(x-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}$$

$$f'(x) = f(x_{i-1})\frac{2x-x_i-x_{i+1}}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})} + f(x_i)\frac{2x-x_{i-1}-x_{i+1}}{(x_i-x_{i-1})(x_i-x_{i+1})} + f(x_{i+1})\frac{2x-x_{i-1}-x_i}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}$$

Note that any three points, x_{i-1} x_i and x_{i+1} can be used to calculate the derivative.* ***The points do not need to be spaced equally.*

Example:

The ***heat flux*** at the soil-air interface can be computed with *Fourier's Law*:

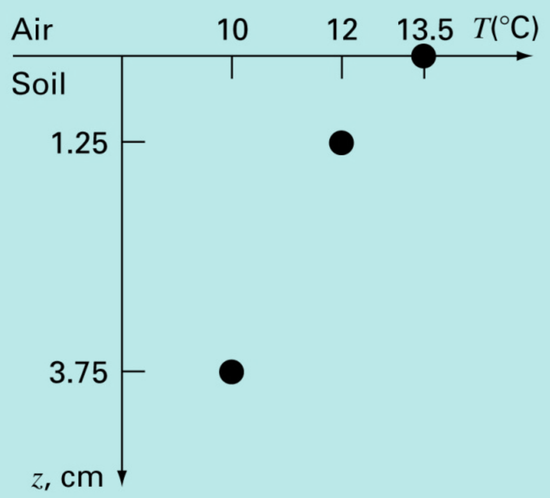
$$q(z=0) = -k\rho C \left.\frac{dT}{dz}\right|_{z=0}$$

q = heat flux
k = coefficient of thermal diffusivity in soil (≈$3.5\text{x}10^{-7}$ m^2/s)
ρ = soil density(≈ 1800 kg/m^3)
C = soil specific heat(≈ 840 J/kg . C°)
*Positive flux value means heat is transferred from the air to the soil

Calculate ***dT/dz*** (z=0) first and then and determine the heat flux.

A temperature gradient can be measured down into the soil as shown below.

MEASUREMENTS



$$f'(z=0) = 13.5\frac{2(0)-1.25-3.75}{(0-1.25)(0-3.75)} + 12\frac{2(0)-0-3.75}{(1.25-0)(1.25-3.75)} + 10\frac{2(0)-0-1.25}{(3.75-0)(3.75-1.25)}$$

$$= -14.4 + 14.4 - 1.333 = -1.333 \ \ {}^{0}C/cm$$

which can be used to compute the *heat flux* at z=0:

$q(z=0) = -3.5\text{x}10^{-7}(1800)(840)(-133.3\ {}^{0}C/m) = 70.56\ \ W/m^2$