TMC: Numerical Differentiation and Integration

Presenter: Dr. Ha Viet Uyen Synh.

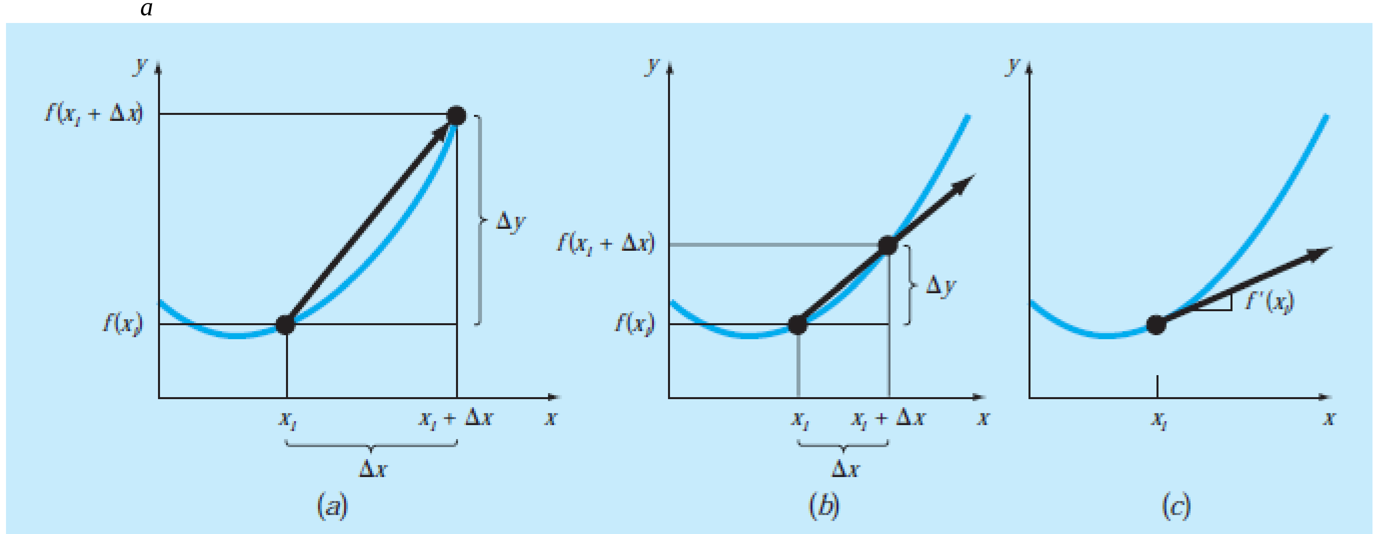
Differentiation and Integration

Standing in the heart of calculus are the mathematical concepts of *differentiation* and *integration*:

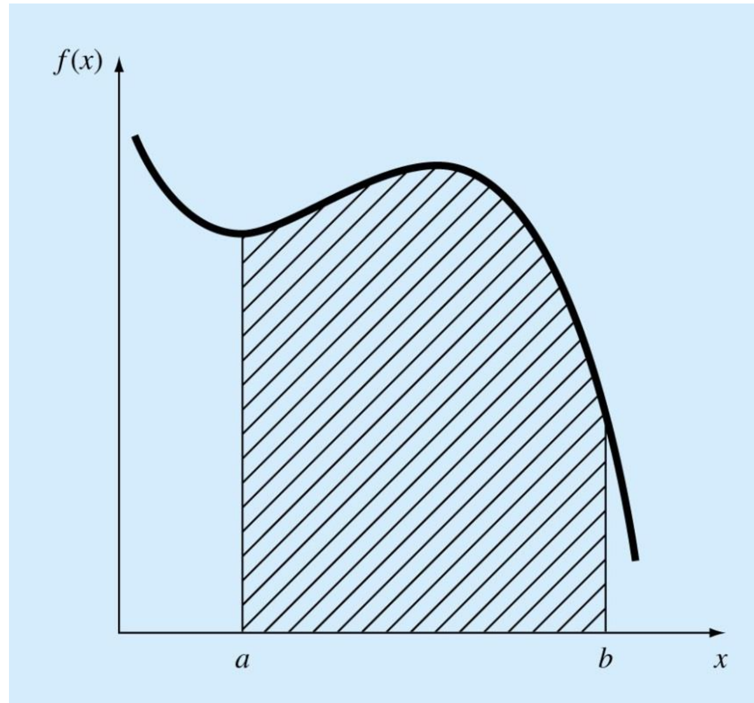
$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

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

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



Differentiation and Integration



Graphical representation of the integral of f(x) between the limits x = a to b. The integral is equivalent to the area under the curve.

Non-computer Methods for Differentiation and Integration

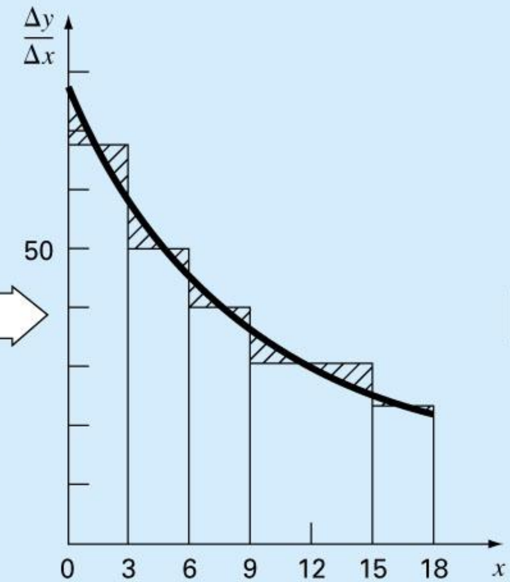
The function to be differentiated or integrated will typically be in one of the following three forms:

1. A simple continuous function such as polynomial, an exponential, or a trigonometric function.
2. A complicated continuous function that is difficult or impossible to differentiate or integrate directly.
3. A tabulated function where values of x and f(x) are given at a number of discrete points, as is often the case with experimental or field data.

Example #1

x	y	$\Delta y/\Delta x$
0	0	
		66.7
3	200	
		50
6	350	
		40
9	470	
		30
15	650	
		23.3
18	720	

(*a*)



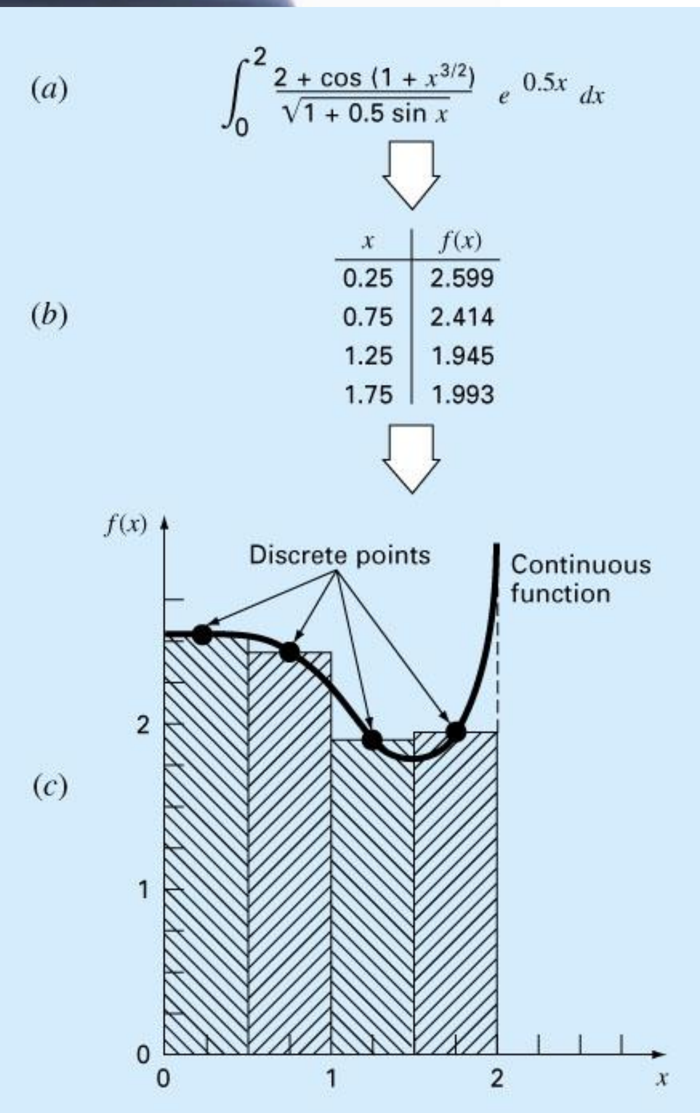
(*b*)

x	dy/dx
0	76.50
3	57.50
6	45.00
9	36.25
15	25.00
18	21.50

(*c*)

Equal-area differentiation.
(a) Centered finite divided differences are used to estimate the derivative for each interval between the data points.
(b) The derivative estimates are plotted as a bar graph. A smooth curve is superimposed on this plot to approximate the area under the bar graph. This is accomplished by drawing the curve so that equal positive and negative areas are balanced.
(c) Values of dy/dx can then be read off the smooth curve.

Example #2



Application of a numerical integration method:
(a) A complicated, continuous function.
(b) Table of discrete values of f(x) generated from the function.
(c) Use of a numerical method to estimate the integral on the basis of the discrete points.

For a tabulated function, the data is already in tabular form (b); therefore, step (a) is unnecessary.

Mathematical Background

$$y = xn \quad \Rightarrow \quad \frac{dy}{dx} = nx^{n-1}$$

$$y = u^n \quad \Rightarrow \quad \frac{dy}{dx} = nu^{n-1}\frac{du}{dx}$$

$$y = uv \quad \Rightarrow \quad \frac{dy}{dx} = u\frac{dv}{dx} + v\frac{du}{dx}$$

$$y = \frac{u}{v} \quad \Rightarrow \quad \frac{dy}{dx} = \frac{v\frac{du}{dx} - u\frac{dv}{dx}}{v^2}$$

$$\frac{d}{dx}\sin x = \cos x \qquad \frac{d}{dx}\cot x = -\csc^2 x$$

$$\frac{d}{dx}\cos x = -\sin x \qquad \frac{d}{dx}\sec x = \sec x \tan x$$

$$\frac{d}{dx}\tan x = \sec^2 x \qquad \frac{d}{dx}\csc x = -\csc x \cot x$$

$$\frac{d}{dx}\ln x = \frac{1}{x} \qquad \frac{d}{dx}\log_a x = \frac{1}{x \ln a}$$

$$\frac{d}{dx}e^x = e^x \qquad \frac{d}{dx}a^x = a^x \ln a$$

Mathematical Background

$$\int u\,dv = uv - \int v\,du$$

$$\int u^n\,du = \frac{u^{n+1}}{n+1} + C \qquad n \neq -1$$

$$\int a^{bx}\,dx = \frac{a^{bx}}{b\ln a} + C \qquad a > 0,\ a \neq 1$$

$$\int \frac{dx}{x} = \ln|x| + C \qquad x \neq 0$$

$$\int \sin(ax+b)\,dx = -\frac{1}{a}\cos(ax+b) + C$$

$$\int \cos(ax+b)\,dx = \frac{1}{a}\sin(ax+b) + C$$

$$\int \ln|x|\,dx = x\ln|x| - x + C$$

$$\int e^{ax}\,dx = \frac{e^{ax}}{a} + C$$

$$\int xe^{ax}\,dx = \frac{e^{ax}}{a^2}(ax-1) + C$$

$$\int \frac{dx}{a+bx^2} = \frac{1}{\sqrt{ab}}\tan^{-1}\frac{\sqrt{ab}}{a}x + C$$

Part A

NEWTON-COTES INTEGRATION FORMULAS

Newton-Cotes formulas

The *Newton-Cotes formulas* are the most common numerical integration schemes.

They are based on the strategy of replacing a complicated function or tabulated data with an *approximating function* that is easy to integrate:

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

$$f_n(x) = a_0 + a_1 x + \cdots + a_{n-1} x^{n-1} + a_n x^n$$

The Trapezoidal Rule

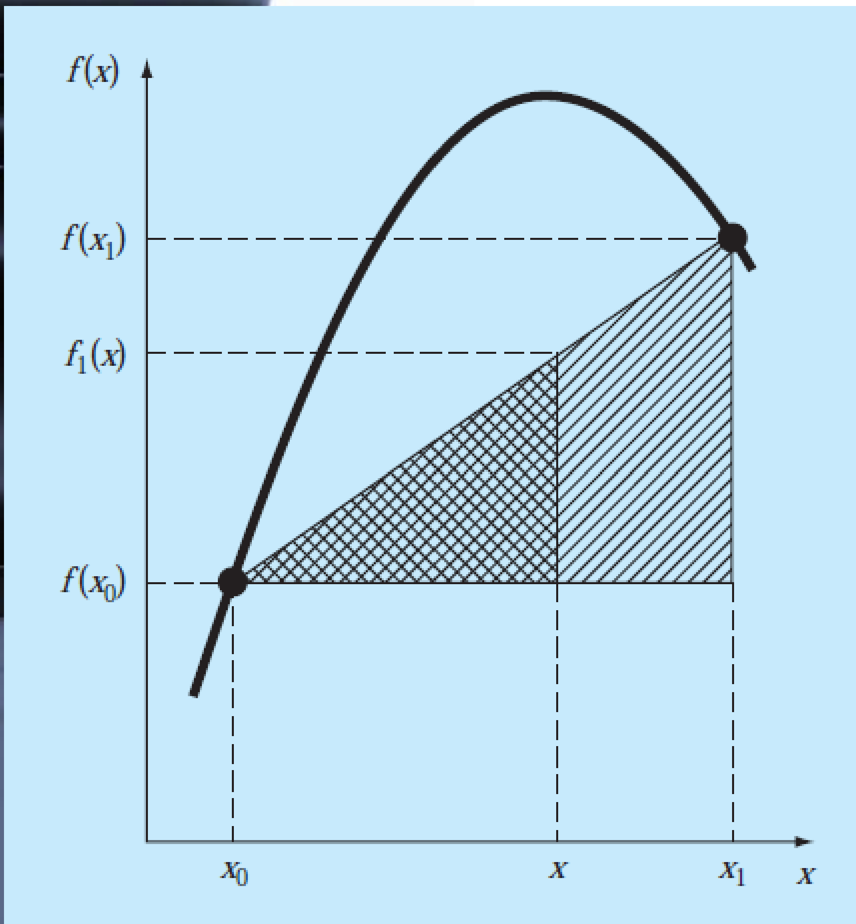
The *Trapezoidal rule* is the first of the Newton-Cotes closed integration formulas, corresponding to the case where the polynomial is first order:

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

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

$$I = (b-a)\frac{f(a)+f(b)}{2} \quad \Big\} \ \textit{Trapezoidal rule}$$

Recall from Linear Interpolation



$$\frac{f_1(x) - f(x_0)}{x - x_0} = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$f_1(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0)$$

Derivation of Trapezoidal Rule

Before integration, Eq. (21.2) can be expressed as

$$f_1(x) = \frac{f(b) - f(a)}{b - a} x + f(a) - \frac{a\,f(b) - a\,f(a)}{b - a}$$

Grouping the last two terms gives

$$f_1(x) = \frac{f(b) - f(a)}{b - a} x + \frac{b f(a) - a f(a) - a f(b) + a f(a)}{b - a}$$

or

$$f_1(x) = \frac{f(b) - f(a)}{b - a} x + \frac{b f(a) - a f(b)}{b - a}$$

which can be integrated between $x = a$ and $x = b$ to yield

$$I = \frac{f(b) - f(a)}{b - a} \frac{x^2}{2} + \frac{b f(a) - a f(b)}{b - a} x \Big|_a^b$$

This result can be evaluated to give

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

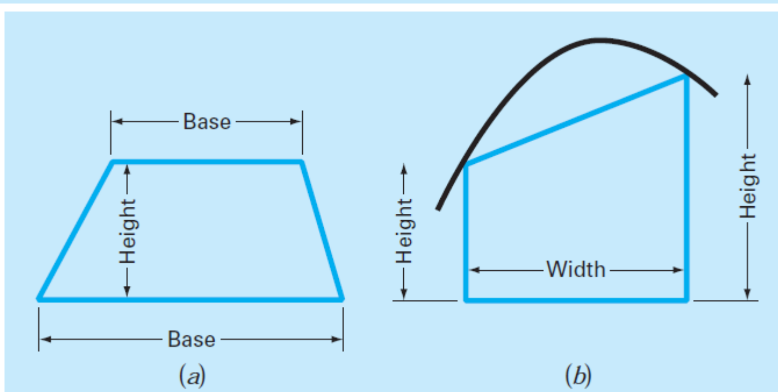
Now, since $b^2 - a^2 = (b - a)(b + a)$,

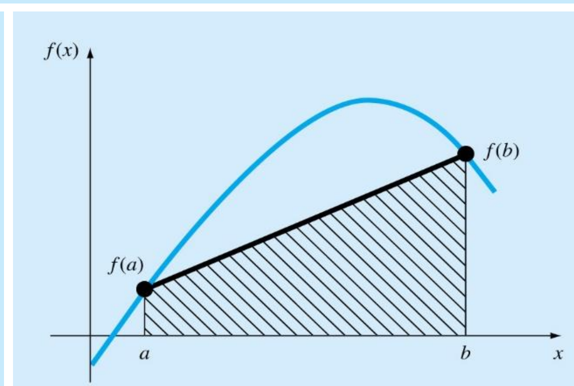
$$I = [f(b) - f(a)] \frac{b + a}{2} + b f(a) - a f(b)$$

Multiplying and collecting terms yields

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

which is the formula for the trapezoidal rule.



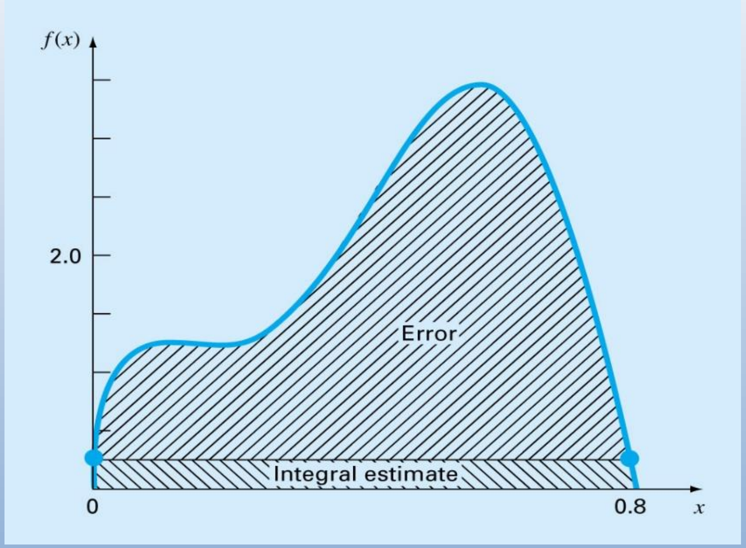


Error of the Trapezoidal Rule

When we employ the integral under a straight line segment to approximate the integral under a curve, error may be substantial:

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

where x lies somewhere in the interval from *a* to *b*.



Example #1

Integrate the following equation

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

from a = 0 to b = 0.8.

The function values

f(0) = 0.2

f(0.8) = 0.232

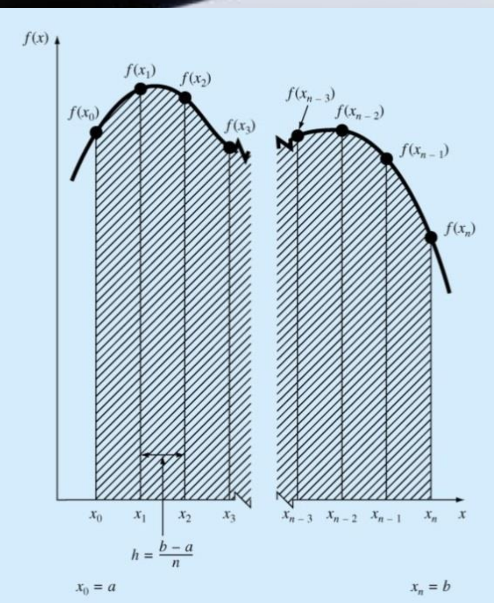
$$I \cong 0.8\frac{0.2 + 0.232}{2} = 0.1728$$

$f''(x) = -400 + 4050x - 10{,}800x^2 + 8000x^3$

$$\bar{f}''(x) = \frac{\int_0^{0.8} (-400 + 4050x - 10{,}800x^2 + 8000x^3)\,dx}{0.8 - 0} = -60$$

$$E_a = -\frac{1}{12}(-60)(0.8)^3 = 2.56$$

The Multiple Application Trapezoidal Rule



One way to improve the accuracy of the trapezoidal rule is to divide the integration interval from a to b into a number of segments and apply the method to each segment.

The areas of individual segments can then be added to yield the integral for the entire interval.

$$h = \frac{b-a}{n} \qquad a = x_0 \quad b = x_n$$

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

Substituting the trapezoidal rule for each integral yields:

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

The Multiple Application Trapezoidal Rule

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

$$I = \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}}_{\text{Average height}}$$

$$E_a = -\frac{(b-a)^3}{12n^2} \sum_{i=1}^{n} f''(\xi_i)$$

$$\bar{f}'' \cong \frac{\sum_{i=1}^{n} f''(\xi_i)}{n}$$

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

Example #2

Use the two-segment trapezoidal rule to estimate the integral of

$$f(x) = 0.2 + 25x - 200x2 + 675x3 - 900x4 + 400x5$$

from a = 0 to b = 0.8. Recall that the correct value for the integral is 1.640533.

Solution. $n = 2\ (h = 0.4)$:

$f(0) = 0.2 \qquad f(0.4) = 2.456 \qquad f(0.8) = 0.232$

$$I = 0.8\frac{0.2 + 2(2.456) + 0.232}{4} = 1.0688$$

$E_t = 1.640533 - 1.0688 = 0.57173 \qquad \varepsilon_t = 34.9\%$

$$\bar{f}''(x) = \frac{\int_0^{0.8}(-400 + 4050x - 100800x^2 + 8000x^3)dx}{0.8 - 0} = -60$$

$$E_a = -\frac{0.8^3}{12(2)^2}(-60) = 0.64$$

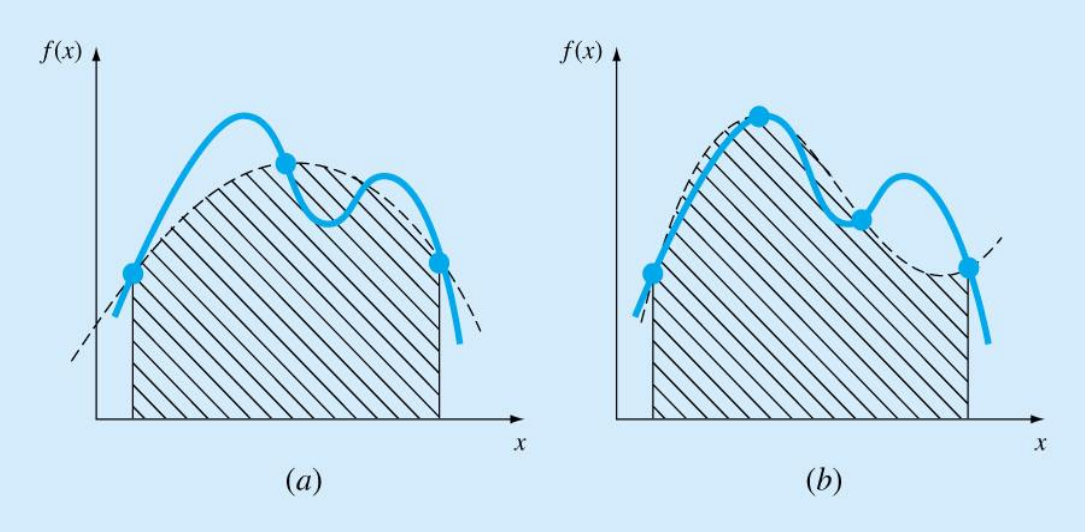
Example #3

Results for multiple-application trapezoidal rule to estimate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from x = 0 to 0.8. The exact value is 1.640533.

n	h	I	ε_t (%)
2	0.4	1.0688	34.9
3	0.2667	1.3695	16.5
4	0.2	1.4848	9.5
5	0.16	1.5399	6.1
6	0.1333	1.5703	4.3
7	0.1143	1.5887	3.2
8	0.1	1.6008	2.4
9	0.0889	1.6091	1.9
10	0.08	1.6150	1.6

Simpson’s Rules

More accurate estimate of an integral is obtained if a high-order polynomial is used to connect the points. The formulas that result from taking the integrals under such polynomials are called *Simpson’s rules*.



(a) Graphical depiction of Simpson’s 1/3 rule: It consists of taking the area under a parabola connecting three points.
(b) Graphical depiction of Simpson’s 3/8 rule: It consists of taking the area under a cubic equation connecting four points.

Simpson's 1/3 Rule

$$I = \int_a^b f(x)dx \cong \int_a^b f_2(x)dx$$

$$a = x_0 \quad b = x_2$$

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

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

Single segment application of Simpson's 1/3 rule has a truncation error of:

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi) \qquad a \prec \xi \prec b$$

Simpson's 1/3 rule is more accurate than trapezoidal rule.

Recall from Lagrange Interpolation Polynomials

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

$$f_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

$$f_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

Example #4

Use Simpson’s 1/3 Rule to integrate

$$f(x) = 0.2 + 25x - 200x2 + 675x3 - 900x4 + 400x5$$

from a = 0 to b = 0.8. Recall that the exact integral is 1.640533

f (0) = 0.2 f (0.4) = 2.456 f (0.8) = 0.232

$$I \cong 0.8\frac{0.2 + 4(2.456) + 0.232}{6} = 1.367467$$

$$E_t = 1.640533 - 1.367467 = 0.2730667 \qquad \varepsilon_t = 16.6\%$$

$$E_a = -\frac{(0.8)^5}{2880}(-2400) = 0.2730667$$

The Multiple-Application Simpson’s 1/3 Rule

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

The total integral can be represented as

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

Substituting Simpson’s 1/3 rule for the individual integral yields

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

or, combining terms

$$I \cong \underbrace{(b-a)}_{\text{Width}}\ \underbrace{\frac{f(x_0) + 4\displaystyle\sum_{i=1,3,5}^{n-1} f(x_i) + 2\displaystyle\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}}_{\text{Average height}}$$

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

Example #5

Use Eq. (21.18) with n = 4 to estimate the integral of

$$f(x) = 0.2 + 25x - 200x2 + 675x3 - 900x4 + 400x5$$

from a = 0 to b = 0.8. Recall that the exact integral is 1.640533.

Solution. $n = 4\ (h = 0.2)$:

$$f(0) = 0.2 \qquad f(0.2) = 1.288$$
$$f(0.4) = 2.456 \qquad f(0.6) = 3.464$$
$$f(0.8) = 0.232$$

$$I = 0.8\,\frac{0.2 + 4(1.288 + 3.464) + 2(2.456) + 0.232}{12} = 1.623467$$

$$E_t = 1.640533 - 1.623467 = 0.017067 \qquad \varepsilon_t = 1.04\%$$

$$E_a = -\frac{(0.8)^5}{180(4)^4}(-2400) = 0.017067$$

Simpson's 3/8 Rule

An odd-segment-even-point formula used in conjunction with the 1/3 rule to permit evaluation of both even and odd numbers of segments.

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

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

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

$$E_t = -\frac{(b-a)^5}{6480} f^{(4)}(\xi)$$

Example #6

(a) Use Simpson's 3/8 rule to integrate

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

from a = 0 to b = 0.8.

(b) Use it in conjunction with Simpson's 1/3 rule to integrate the same function for five segments.

(a) A single application of Simpson's 3/8 rule requires four equally spaced points:

$$f(0) = 0.2 \qquad f(0.2667) = 1.432724$$

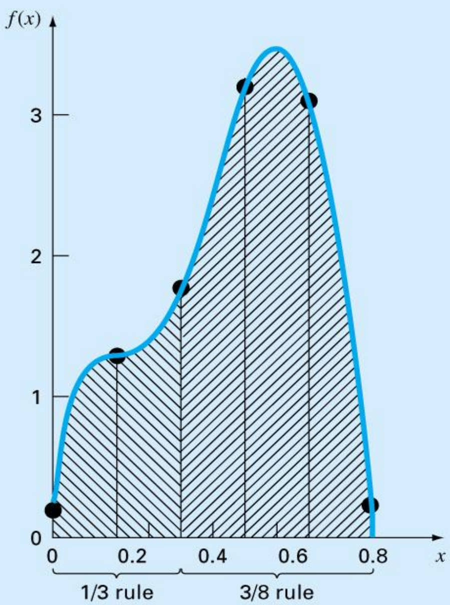
$$f(0.5333) = 3.487177 \qquad f(0.8) = 0.232$$

Using Eq. (21.20),

$$I \cong 0.8\,\frac{0.2 + 3(1.432724 + 3.487177) + 0.232}{8} = 1.519170$$

$$E_t = 1.640533 - 1.519170 = 0.1213630 \qquad \varepsilon_t = 7.4\%$$

$$E_a = -\frac{(0.8)^5}{6480}(-2400) = 0.1213630$$



(b) The data needed for a five-segment application ($h = 0.16$) is

$$f(0) = 0.2 \qquad f(0.16) = 1.296919$$
$$f(0.32) = 1.743393 \qquad f(0.48) = 3.186015$$
$$f(0.64) = 3.181929 \qquad f(0.80) = 0.232$$

The integral for the first two segments is obtained using Simpson's 1/3 rule:

$$I \cong 0.32\,\frac{0.2 + 4(1.296919) + 1.743393}{6} = 0.3803237$$

For the last three segments, the 3/8 rule can be used to obtain

$$I \cong 0.48\,\frac{1.743393 + 3(3.186015 + 3.181929) + 0.232}{8} = 1.264754$$

The total integral is computed by summing the two results:

$$I = 0.3803237 + 1.264753 = 1.645077$$
$$E_t = 1.640533 - 1.645077 = -0.00454383 \qquad \varepsilon_t = -0.28\%$$

Newton-Cotes closed integration formulas

Segments (n)	Points	Name	Formula	Truncation Error
1	2	Trapezoidal rule	$(b-a)\dfrac{f(x_0)+f(x_1)}{2}$	$-(1/12)h^3f''(\xi)$
2	3	Simpson's 1/3 rule	$(b-a)\dfrac{f(x_0)+4f(x_1)+f(x_2)}{6}$	$-(1/90)h^5f^{(4)}(\xi)$
3	4	Simpson's 3/8 rule	$(b-a)\dfrac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}$	$-(3/80)h^5f^{(4)}(\xi)$
4	5	Boole's rule	$(b-a)\dfrac{7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)}{90}$	$-(8/945)h^7f^{(6)}(\xi)$
5	6		$(b-a)\dfrac{19f(x_0)+75f(x_1)+50f(x_2)+50f(x_3)+75f(x_4)+19f(x_5)}{288}$	$-(275/12{,}096)h^7f^{(6)}(\xi)$

INTEGRATION WITH UNEQUAL SEGMENTS

In practice, there are many situations where this assumption does not hold and we must deal with unequal-sized segments.

For these cases, one method is to apply the trapezoidal rule to each segment and sum the results:

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

where hi = the width of segment i

Example #7

Use Trapezoidal Rule with Unequal Segments to determine the integral for the data in the following table. Recall that the correct answer is 1.640533.

x	f(x)	x	f(x)
0.0	0.200000	0.44	2.842985
0.12	1.309729	0.54	3.507297
0.22	1.305241	0.64	3.181929
0.32	1.743393	0.70	2.363000
0.36	2.074903	0.80	0.232000
0.40	2.456000		

(Data for f(x) = 0.2 + 25x − 200x2 + 675x3 −900x4 + 400x5, with unequally spaced values of x.)

$$I = 0.12\frac{1.309729 + 0.2}{2} + 0.10\frac{1.305241 + 1.309729}{2} + \cdots + 0.10\frac{0.232 + 2.363}{2}$$

$$= 0.090584 + 0.130749 + \cdots + 0.12975 = 1.594801$$

which represents an absolute percent relative error of $\varepsilon_t = 2.8\%$.

Part B

INTEGRATION OF EQUATIONS

Integration of Equations

Functions to be integrated numerically are in two forms:

A table of values. We are limited by the number of points that are given.

A function. We can generate as many values of *f(x)* as needed to attain acceptable accuracy.

Will focus on two techniques that are designed to analyze functions:

Romberg integration

Gauss quadrature

Romberg Integration

Is based on successive application of the trapezoidal rule to attain efficient numerical integrals of functions.

Richardson's Extrapolation

Uses two estimates of an integral to compute a third and more accurate approximation.

The estimate and error associated with a multiple-application trapezoidal rule can be represented generally as

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

$$h = (b-a)/n$$

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

$$n = (b-a)/h$$

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

Assumed constant regardless of step size

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

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

I =exact value of integral

I(h) =the approximation from an n segment application of trapezoidal rule with step size h

E(h) =the truncation error

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

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

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

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

	$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
(a)	0.172800	1.367467		
	1.068800			
(b)	0.172800	1.367467	1.640533	
	1.068800	1.623467		
	1.484800			
(c)	0.172800	1.367467	1.640533	1.640533
	1.068800	1.623467	1.640533	
	1.484800	1.639467		
	1.600800			

Example #8

For example, single and multiple applications of the trapezoidal rule yielded the following results:

Segments	h	Integral	ε_t, %
1	0.8	0.1728	89.5
2	0.4	1.0688	34.9
4	0.2	1.4848	9.5

Use Error Corrections of the Trapezoidal Rule to compute improved estimates of the integral. (f(x) = 0.2 + 25x −200x2 + 675x3 − 900x4 + 400x5 from a = 0 to b = 0.8.)

For the special case where the interval is halved (h2 = h1/2), this equation becomes

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

or, collecting terms,

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

The estimates for one and two segments can be combined to yield

$$I \cong \frac{4}{3}(1.0688) - \frac{1}{3}(0.1728) = 1.367467$$

The error of the improved integral is $E_t = 1.640533 - 1.367467 = 0.273067 (\varepsilon_t = 16.6\%)$, which is superior to the estimates upon which it was based.

In the same manner, the estimates for two and four segments can be combined to give

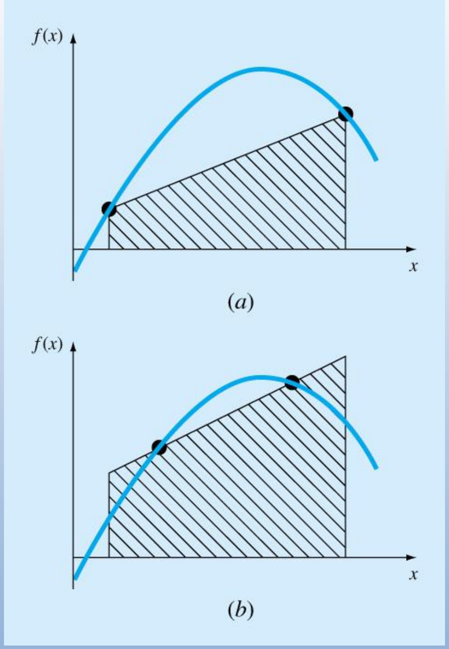
$$I \cong \frac{4}{3}(1.4848) - \frac{1}{3}(1.0688) = 1.623467$$

which represents an error of $E_t = 1.640533 - 1.623467 = 0.017067$ ($\varepsilon_t = 1.0\%$).

Gauss Quadrature

Gauss quadrature implements a strategy of positioning any two points on a curve to define a straight line that would balance the positive and negative errors.

Hence the area evaluated under this straight line provides an improved estimate of the integral.

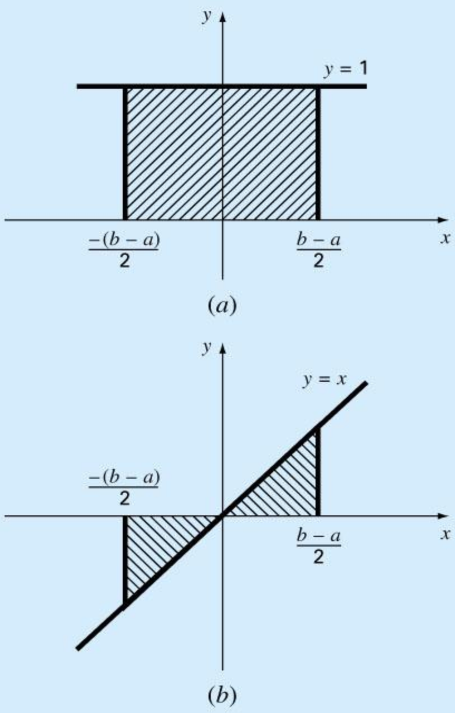


(a) Graphical depiction of the trapezoidal rule as the area under the straight line joining fixed end points.

(b) An improved integral estimate obtained by taking the area under the straight line passing through two intermediate points.

By positioning these points wisely, the positive and negative errors are balanced, and an improved integral estimate results.

Method of Undetermined Coefficients



The trapezoidal rule yields exact results when the function being integrated is a constant or a straight line, such as *y*=1 and *y*=*x*: $I \cong c_0 f(a) + c_1 f(b)$

$$c0 + c1 = \int_{-(b-a)/2}^{(b-a)/2} 1\,dx$$

$$-c_0 \frac{b-a}{2} + c_1 \frac{b-a}{2} = \int_{-(b-a)/2}^{(b-a)/2} x\,dx$$

$$c_0 + c_1 = b - a$$

$$-c_0 \frac{b-a}{2} + c_1 \frac{b-a}{2} = 0$$

$$c_0 = c_1 = \frac{b-a}{2}$$

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

Trapezoidal rule

Derivation of the Two-Point Gauss-Legendre Formula

The object of Gauss quadrature is to determine the equations of the form

$$I \cong c_0 f(x_0) + c_1 f(x_1)$$

However, in contrast to trapezoidal rule that uses fixed end points a and b, the function arguments x_0 and x_1 are not fixed end points but unknowns.

Thus, *four unknowns* to be evaluated require *four conditions*.

First two conditions are obtained by assuming that the above equation fits the integral of a constant and a linear function exactly.

The other two conditions are obtained by extending this reasoning to *a parabolic* and *a cubic* functions.

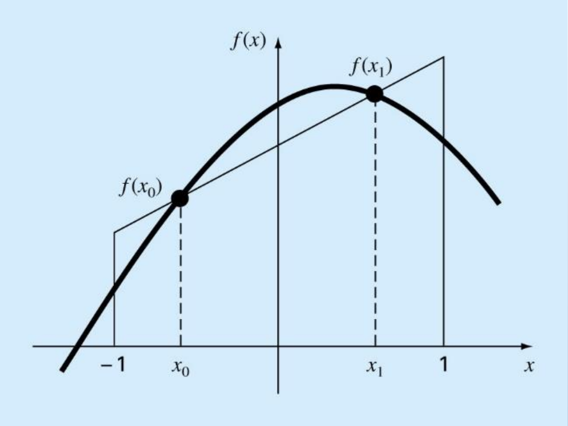
$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} 1\, dx = 2$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x\, dx = 0$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x^2\, dx = \frac{2}{3}$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x^3\, dx = 0$$

Solved simultaneously



$$c_0 = c_1 = 1$$

$$x_0 = -\frac{1}{\sqrt{3}} = -0.5773503\ldots$$

$$x_1 = \frac{1}{\sqrt{3}} = -0.5773503\ldots$$

$$\boxed{I \cong f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)}$$

Yields an integral estimate that is third order accurate

Notice that the integration limits are from -1 to 1. This was done for simplicity and make the formulation as general as possible.

This is accomplished by assuming that a new variable xd is related to the original variable x in a linear fashion, as in

x = a0 + a1xd (22.24)

If the lower limit, x = a, corresponds to xd =−1, these values can be substituted to yield

a = a0 + a1(−1) (22.25)

Similarly, the upper limit, x = b, corresponds to xd = 1, to give

b = a0 + a1(1)

So,

$$a_0 = \frac{b+a}{2}$$

and

$$a_1 = \frac{b-a}{2}$$

$$x = \frac{(b+a) + (b-a)x_d}{2}$$

This equation can be differentiated to give

$$dx = \frac{b-a}{2}\, dx_d$$

Example #9

Use Two-Point Gauss-Legendre Formula to evaluate the integral of

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

between the limits x = 0 to 0.8. Recall that the exact value of the integral is 1.640533.

Before integrating the function, we must perform a change of variable so that the limits are from −1 to +1. To do this, we substitute a = 0 and b = 0.8 to yield

x = 0.4 + 0.4xd

The derivative of this relationship is

dx = 0.4 dxd

Both of these can be substituted into the original equation to yield

$$\int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5)\, dx$$

$$= \int_{-1}^{1} \big[0.2 + 25(0.4 + 0.4x_d) - 200(0.4 + 0.4x_d)^2 + 675(0.4 + 0.4x_d)^3$$

$$- 900(0.4 + 0.4x_d)^4 + 400(0.4 + 0.4x_d)^5\big]0.4\, dx_d$$

The transformed function can be evaluated at $-1/\sqrt{3}$ to be equal to 0.516741 and at $1/\sqrt{3}$ to be equal to 1.305837.

I = 0.516741 + 1.305837 = 1.822578

Higher-Point Formulas

Beyond the two-point formula described in the previous section, higher-point versions can be developed in the general form

$I := c_0 f(x_0) + c_1 f(x_1) + \cdots + c_{n-1} f(x_{n-1})$

where n = the number of points.

Points	Weighting Factors	Function Arguments	Truncation Error
2	$c_0 = 1.0000000$ $c_1 = 1.0000000$	$x_0 = -0.577350269$ $x_1 = 0.577350269$	$\cong f^{(4)}(\xi)$
3	$c_0 = 0.5555556$ $c_1 = 0.8888889$ $c_2 = 0.5555556$	$x_0 = -0.774596669$ $x_1 = 0.0$ $x_2 = 0.774596669$	$\cong f^{(6)}(\xi)$
4	$c_0 = 0.3478548$ $c_1 = 0.6521452$ $c_2 = 0.6521452$ $c_3 = 0.3478548$	$x_0 = -0.861136312$ $x_1 = -0.339981044$ $x_2 = 0.339981044$ $x_3 = 0.861136312$	$\cong f^{(8)}(\xi)$
5	$c_0 = 0.2369269$ $c_1 = 0.4786287$ $c_2 = 0.5688889$ $c_3 = 0.4786287$ $c_4 = 0.2369269$	$x_0 = -0.906179846$ $x_1 = -0.538469310$ $x_2 = 0.0$ $x_3 = 0.538469310$ $x_4 = 0.906179846$	$\cong f^{(10)}(\xi)$
6	$c_0 = 0.1713245$ $c_1 = 0.3607616$ $c_2 = 0.4679139$ $c_3 = 0.4679139$ $c_4 = 0.3607616$ $c_5 = 0.1713245$	$x_0 = -0.932469514$ $x_1 = -0.661209386$ $x_2 = -0.238619186$ $x_3 = 0.238619186$ $x_4 = 0.661209386$ $x_5 = 0.932469514$	$\cong f^{(12)}(\xi)$

Example #10

Use the three-point formula to estimate the integral for the same function as in the previous example.

The three-point formula is

I = 0.5555556 f(−0.7745967) + 0.8888889 f(0) + 0.5555556 f(0.7745967)

which is equal to

I = 0.2813013 + 0.8732444 + 0.4859876 = 1.640533

which is exact

Improper Integrals

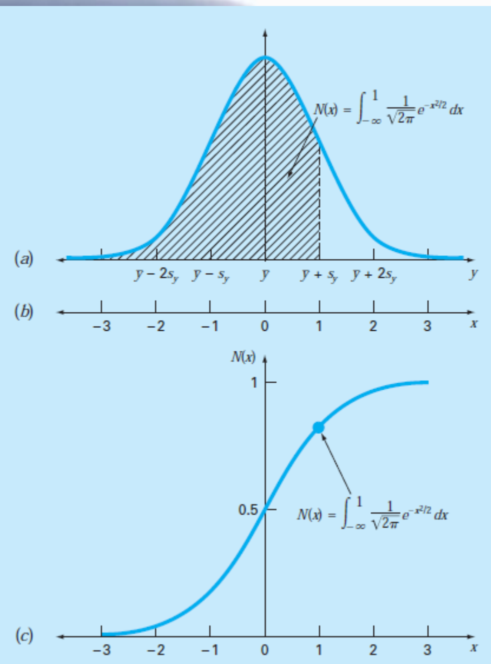
Improper integrals can be evaluated by making a change of variable that transforms the infinite range to one that is finite,

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

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

where –A is chosen as a sufficiently large negative value so that the function has begun to approach zero asymptotically at least as fast as $1/x^2$.

Example #11



The cumulative normal distribution is an important formula in statistics

$$N(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-x^2/2}\, dx$$

where $x = (y - \bar{y})/s_y$ is called the normalized standard deviate.

The equation can be reexpressed in terms as

$$N(x) = \frac{1}{\sqrt{2\pi}} \left(\int_{-\infty}^{-2} e^{-x^2/2}\, dx + \int_{-2}^{1} e^{-x^2/2}\, dx \right)$$

The first integral can be evaluated such as

$$\int_{-\infty}^{-2} e^{-x^2/2}\, dx = \int_{-1/2}^{0} \frac{1}{t^2} e^{-1/(2t^2)}\, dt$$

Then the extended midpoint rule with h = 1/8 can be employed to estimate

$$\int_{-1/2}^{0} \frac{1}{t^2} e^{-1/(2t^2)}\, dt \cong \frac{1}{8}[\, f(x_{-7/16}) + f(x_{-5/16}) + f(x_{-3/16}) + f(x_{-1/16})]$$

$$= \frac{1}{8}[0.3833 + 0.0612 + 0 + 0] = 0.0556$$

Simpson's 1/3 rule with $h = 0.5$ can be used to estimate the second integral as

$$\int_{-2}^{1} e^{-x^2/2}\,dx$$

$$= [1-(-2)]\frac{0.1353 + 4(0.3247 + 0.8825 + 0.8825) + 2(0.6065 + 1) + 0.6065}{3(6)}$$

$$= 2.0523$$

Therefore, the final result can be computed as

$$N(1) \cong \frac{1}{\sqrt{2\pi}}(0.0556 + 2.0523) = 0.8409$$

which represents an error of $\varepsilon_t = 0.046$ percent.

Part C

NUMERICAL DIFFERENTIATION

High Accuracy Differentiation Formulas

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

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

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

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

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

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

Forward finite-divided-difference formulas

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$	$O(h^2)$

Backward finite-divideddifference 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	
$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4}$	$O(h^2)$

Centered finite-divideddifference 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	
$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$O(h^2)$
$f''(x_i) = \dfrac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	$O(h^4)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3}$	$O(h^2)$
$f'''(x_i) = \dfrac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3}$	$O(h^4)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4}$	$O(h^2)$
$f''''(x_i) = \dfrac{-f(x_{i+3}) + 12f(x_{i+2}) + 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3})}{6h^4}$	$O(h^4)$

Example #12

Recall that we estimated the derivative of

f(x) = −0.1x4 − 0.15x3 − 0.5x2 − 0.25x + 1.2

at x = 0.5 using finite divided differences and a step size of h = 0.25,

	Forward $O(h)$	Backward $O(h)$	Centered $O(h^2)$
Estimate	−1.155	−0.714	−0.934
ε_t (%)	−26.5	21.7	−2.4

where the errors were computed on the basis of the true value of −0.9125.
Repeat this computation, but employ the high-accuracy formulas

Solution. The data needed for this example is

$$
\begin{aligned}
x_{i-2} &= 0 & f(x_{i-2}) &= 1.2 \\
x_{i-1} &= 0.25 & f(x_{i-1}) &= 1.1035156 \\
x_{i} &= 0.5 & f(x_{i}) &= 0.925 \\
x_{i+1} &= 0.75 & f(x_{i+1}) &= 0.6363281 \\
x_{i+2} &= 1 & f(x_{i+2}) &= 0.2
\end{aligned}
$$

The forward difference of accuracy $O(h^2)$ is computed as

$$f'(0.5) = \frac{-0.2 + 4(0.6363281) - 3(0.925)}{2(0.25)} = -0.859375 \qquad \varepsilon_t = 5.82\%$$

The backward difference of accuracy $O(h^2)$ is computed as

$$f'(0.5) = \frac{3(0.925) - 4(1.1035156) + 1.2}{2(0.25)} = -0.878125 \qquad \varepsilon_t = 3.77\%$$

The centered difference of accuracy $O(h^4)$ is computed as

$$f'(0.5) = \frac{-0.2 + 8(0.6363281) - 8(1.1035156) + 1.2}{12(0.25)} = -0.9125 \qquad \varepsilon_t = 0\%$$

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 t compute a third, more accurate approximation.

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

$$h_2 = h_1 / 2$$

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

$$\boxed{D \cong \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1)]}$$

For centered difference approximations with $O(h^2)$. The application of this formula yield a new derivative estimate of $O(h^4)$.

Example #13

Using the same function as in the previous example, estimate the first derivative at x = 0.5 employing step sizes of h1 = 0.5 and h2 = 0.25. Then use Richardson Extrapolation to compute an improved estimate with Richardson extrapolation. Recall that the true value

is −0.9125.

Solution. The first-derivative estimates can be computed with centered differences as

$$D(0.5) = \frac{0.2 - 1.2}{1} = -1.0 \qquad \varepsilon_t = -9.6\%$$

and

$$D(0.25) = \frac{0.6363281 - 1.1035156}{0.5} = -0.934375 \qquad \varepsilon_t = -2.4\%$$

The improved estimate can be determined

$$D = \frac{4}{3}(-0.934375) - \frac{1}{3}(-1) = -0.9125$$

which for the present case is a perfect result.

Derivatives of Unequally Spaced Data

Data from experiments or field studies are often collected at unequal intervals. One way to handle such data is to fit a second-order Lagrange interpolating polynomial.

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

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

Where x is the value at which you want to estimate the derivative.

PARTIAL DERIVATIVES

Partial derivatives along a single dimension are computed in the same fashion as ordinary derivatives.

$$\frac{\partial f}{\partial x} = \frac{f(x+\Delta x, y) - f(x-\Delta x, y)}{2\Delta x}$$

$$\frac{\partial f}{\partial y} = \frac{f(x, y+\Delta y) - f(x, y-\Delta y)}{2\Delta y}$$

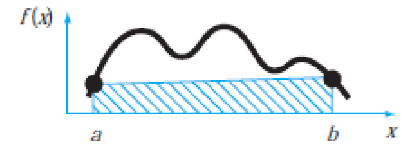
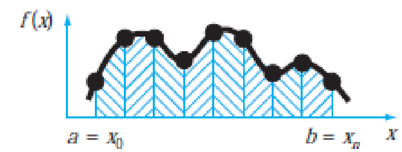
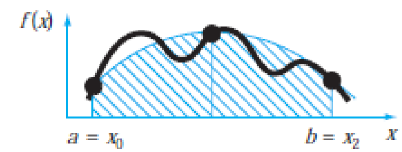
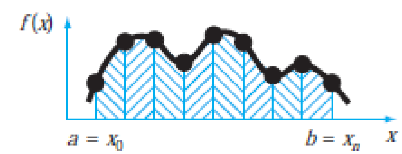
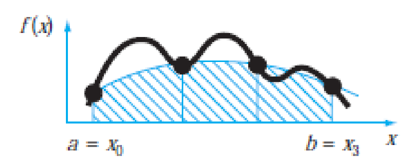
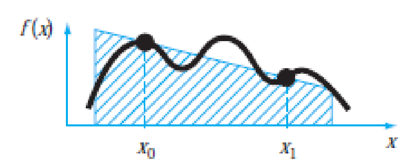
$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)$$

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\frac{\partial f}{\partial y}(x+\Delta x, y) - \frac{\partial f}{\partial y}(x-\Delta x, y)}{2\Delta x}$$

$$\frac{\frac{f(x+\Delta x, y+\Delta y) - f(x+\Delta x, y-\Delta y)}{2\Delta y} - \frac{f(x-\Delta x, y+\Delta y) - f(x-\Delta x, y-\Delta y)}{2\Delta y}}{2\Delta x}$$

$$\frac{f(x+\Delta x, y+\Delta y) - f(x+\Delta x, y-\Delta y) - f(x-\Delta x, y+\Delta y) + f(x-\Delta x, y-\Delta y)}{4\Delta x \Delta y}$$

Summary of important formulas

Method	Formulation	Graphic Interpretations	Error
Trapezoidal rule	$I \simeq (b-a)\dfrac{f(a)+f(b)}{2}$		$-\dfrac{(b-a)^3}{12}f''(\xi)$
Multiple-application trapezoidal rule	$I \simeq (b-a)\dfrac{f(x_0)+2\sum_{i=1}^{n-1}f(x_i)+f(x_n)}{2n}$		$-\dfrac{(b-a)^3}{12n^2}f''$
Simpson's 1/3 rule	$I \simeq (b-a)\dfrac{f(x_0)+4f(x_1)+f(x_2)}{6}$		$-\dfrac{(b-a)^5}{2880}f^{(4)}(\xi)$
Multiple-application Simpson's 1/3 rule	$I \simeq (b-a)\dfrac{f(x_0)+4\sum_{i=1,3}^{n-1}f(x_i)+2\sum_{j=2,4}^{n-2}f(x_j)+f(x_n)}{3n}$		$-\dfrac{(b-a)^5}{180n^4}f^{(4)}$
Simpson's 3/8 rule	$I \simeq (b-a)\dfrac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}$		$-\dfrac{(b-a)^5}{6480}f^{(4)}(\xi)$
Romberg integration	$I_{j,k} = \dfrac{4^{k-1}I_{j+1,k-1}-I_{j,k-1}}{4^{k-1}-1}$	$I_{j,k-1} \longrightarrow I_{j,k}$ $I_{j+1,k-1} \nearrow$	$O(h^{2k})$
Gauss quadrature	$I \simeq c_0f(x_0)+c_1f(x_1)+\cdots+c_{n-1}f(x_{n-1})$		$\simeq f^{(2n+2)}(\xi)$

Quiz #7

1. 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

2. Use Romberg integration to evaluate

$$I = \int_1^2 \left(2x + \frac{3}{x}\right)^2 dx$$

to an accuracy of $\varepsilon_s = 0.5\%$

Any Questions?

✉ hvusynh@hcmiu.edu.vn