Numerical Analysis

Junior Students Course – Mechanical Engineering

Dr. Wail Sami Sarsam 2020-2021 University of Baghdad

Numerical Analysis

Junior Students Course

Mechanical Engineering Department

College of Engineering

University of Baghdad

by

Dr. Wail Sami Sarsam

2020-2021

Table of Contents

Chapter One - Numerical Errors and Roots of Equations

1.1. Introduction

Nowadays, computers and numerical methods provide an alternative for such complicated calculations. Using computer power to obtain solutions directly, you can approach these calculations without recourse to simplifying assumptions or time-intensive techniques. Although analytical solutions are still extremely valuable both for problem solving and for providing insight, numerical methods represent alternatives that greatly enlarge your capabilities to confront and solve problems. As a result, more time is available for the use of your creative skills.

There are several reasons why you should study numerical methods:

1. Numerical methods are extremely powerful problem-solving tools. They are capable of handling large systems of equations, nonlinearities, and complicated geometries that are familiar in engineering practice and that are often impossible to solve analytically. As such, they greatly enhance your problem-solving skills.
2. During your careers, you may often have occasion to use commercially available prepackaged, or "canned," computer programs that involve numerical methods. The intelligent use of these programs is often predicated on knowledge of the basic theory underlying the methods.
3. Many problems cannot be approached using canned programs. If you are familiar with numerical methods and are proficient in computer programming, you can design your own programs to solve problems without having to buy expensive software.
4. Numerical methods are an efficient medium for learning to use computers. It is well known that an effective way to learn programming is to write computer programs. Because numerical methods are for the most part designed for implementation on computers, they are ideal for this purpose.
5. Numerical methods provide a means for you to reinforce your understanding of mathematics. Because one function of numerical methods is to reduce higher mathematics to basic arithmetic operations.

1.2. Significant Figures (Digits)

This course deals extensively with approximations connected with the manipulation of numbers. Consequently, before discussing the errors associated with numerical methods, it is useful to review basic concepts related to approximate representation of the numbers themselves. Whenever we employ a number in a computation, we must have assurance that it can be used with confidence. For example, **Fig. 1.1** shows a speedometer and odometer from an automobile. Visual inspection of the speedometer indicates that the car is traveling between **48 and 49 km/h**. Because the indicator is

higher than the midpoint between the markers on the gauge, we can say with confidence that the car is traveling at approximately 49 km/h. However, let us say that we insist that the **speed be estimated to one decimal place**. For this case, one person might say **48.8**, whereas another might say **48.9** km/h. Therefore, because of the limits of this instrument, only the first two digits can be used with confidence. Estimates of the third digit (or higher) must be viewed as approximations. Based on this speedometer, it would be ridiculous to claim that the automobile is traveling at **48.8642138** km/h. In contrast, the odometer provides up to six certain digits. From **Fig. 1.1**, we can conclude that the car has traveled slightly less than 87,324.5 km during its lifetime. In this case, the seventh digit (and higher) is uncertain.

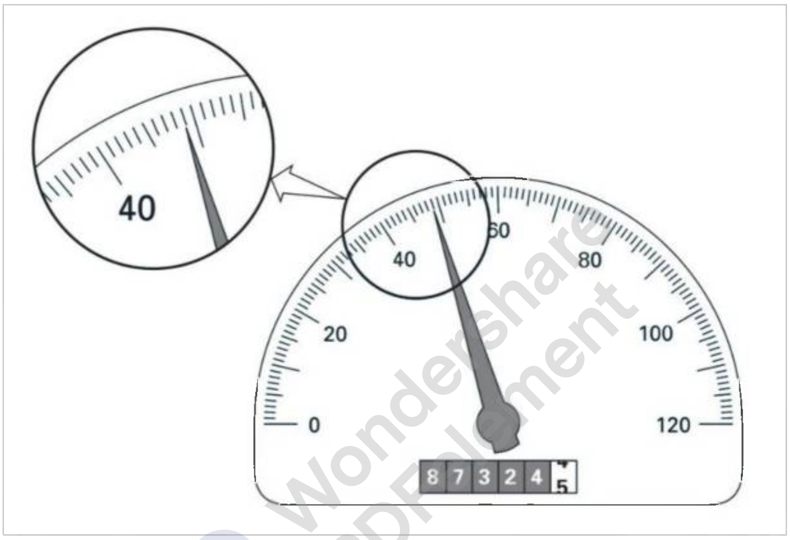


Fig. 1.1 An automobile speedometer and odometer illustrating the concept of a significant figure.

The concept of a ***significant figure***, or ***digit***, has been developed to specify the reliability of a numerical value. ***The significant digits of a number are those that can be used with confidence. They correspond to the number of certain digits and one estimated digit***. For example, the speedometer and the odometer in **Fig. 1.1** yield readings of **three** and **seven significant figures**, respectively. For the speedometer, the two certain digits are 48. It is conventional to set the estimated digit at one-half of the smallest scale division on the measurement device. Thus, the speedometer reading would consist of the three significant figures: **48.5**. In a similar fashion, the odometer would yield a seven-significant-figure reading of **87,324.45**.

The rules for identifying significant figures when writing or interpreting numbers can be summarized as follows;

- Leading zeros that come before the first nonzero number are not significant figures, for example, "013", "0.13' and "0.0013' have two significant figures: "1" and "3".
- Trailing zeros (zeros after non-zero numbers) in a number without a decimal are not significant

figures, for example, "130" has two significant figures: “1” and “3”.

- Leading zeros before the first nonzero digit in decimal fractions (i.e., in the presence of decimal point) are not significant figures because they are necessary just to locate a decimal point. For example, the numbers 0.00001845, 0.0001845, 0.001845, and 0.01845 all have four significant figures.
- Trailing zeros used in decimal fractions (i.e., in the presence of decimal point) are significant digits. For example, the numbers 4.53, 4.530, and 4.5300 have three, four, and five significant figures, respectively.

An example explaining these rules can be seen in the following table;

Number	Decimal Places	Significant Figures (Digits)
1725	0	4
0725	0	3
07250.0	1	5
7250	0	3
25.870	3	5
0.7013	4	4
1.7013	4	5
0.00215	5	3
0.01230	5	4
0.0123	4	3
1.0123	4	5
01.01230	5	6

1.3. Fixed Point and Floating Point Numbers Representation

The real numbers include all the rational numbers (which are the numbers that can be expressed as fractions of two integers), such as the integer −5 and the fraction 4/3, and all the irrational numbers (which are all the real numbers which are not rational numbers), such as the square root of √2 (1.41421356). There are two major approaches to store real numbers in in digital computers. These are (a) ***fixed point notation*** and (b) ***floating point notation***. In ***fixed-point notation***, there are a fixed number of digits after the decimal point (such as 70.825, 7.000, 0001, and 0.015). While ***floating-point numbers*** are represented with a fixed number of significant digits and scaled using an exponent in some fixed base; the base for the scaling is normally two, ten, or sixteen (such as 72.056×10^{1}, 72056×10^{-2}, or 0.72056×10^{3}).

1.4. Accuracy and Precision

The errors associated with both calculations and measurements can be characterized with regard to their ***accuracy*** and ***precision***. ***Accuracy*** refers to how closely a computed or measured value agrees with the true value. ***Precision*** refers to how closely individual computed or measured values agree with each other.

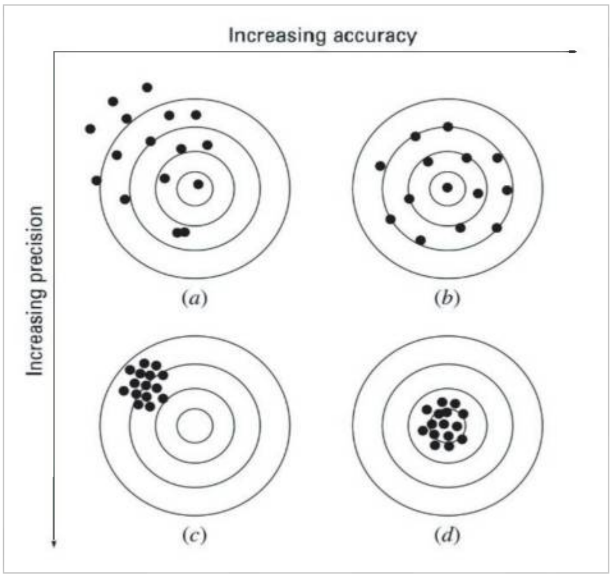


Fig. 1.2 An example from marksmanship illustrating the concepts of accuracy and precision. (a) Inaccurate & imprecise; (b) Accurate & imprecise; (c) Inaccurate & precise; (d) Accurate & precise.

1.5. Numerical Errors

Numerical errors arise from the use of approximations to represent exact mathematical operations and quantities. These include ***truncation errors***, which result when approximations are used to represent exact mathematical procedures, and ***round-off errors***, which result when numbers having limited significant figures are used to represent exact numbers. For both types, the relationship between the exact, or true, result and the approximation can be formulated as

$$Error = True\ value - Approximation \qquad (1.1)$$

1.6. Roots of Equations

Although they arise in other problem contexts, roots of equations frequently occur in the area of engineering design. You have previously learned to use the quadratic formula

$$x = \frac{-b \mp \sqrt{b^2 - 4\,a\,c}}{2\,a} \qquad (1.2)$$

to solve
$$f(x) = a\,x^2 + b\,x + c = 0 \qquad (1.3)$$

The values calculated with Eq. (1.2) are called the "roots" of Eq. (1.3). They represent the values of x that make Eq. (1.3) equal to zero. Thus, we can define the root of an equation as the value of x that makes $f(x) = 0$. For this reason, roots are sometimes called the zeros of the equation.

Although the quadratic formula is handy for solving Eq. (1.3), there are many other functions for which the roots cannot be determined easily. For these cases, the numerical methods provide efficient means to obtain the answer. The following sections of this chapter deal with a variety of numerical methods for determining roots of relationships. These methods can be divided into two groups; the ***bracketing methods*** with initial guesses that bracket or contain the root and ***open methods*** that do not require initial guesses to bracket the root.

1.6.1. Bracketing Methods

This group of methods for finding roots of equations is based on the fact that a function typically changes sign in the vicinity of a root. These techniques are called bracketing methods because two initial guesses for the root are required. As the name implies, these guesses must "bracket," or be on either side of, the root. The particular methods described herein employ different strategies to systematically reduce the width of the bracket and, hence, home in on the correct answer.

The roots can occur (or be absent) in an interval prescribed by a lower bound (x_l) and an upper bound (x_u). **Fig. 1.3b** represents the case where a single root is bracketed by negative and positive values of $f(x)$. However, **Fig. 1.3d**, where $f(x_l)$ and $f(x_u)$ are also on opposite sides of the x axis, shows three roots occurring within the interval. In general, if $f(x_l)$ and $f(x_u)$ have opposite signs, there are an odd number of roots in the interval. If $f(x_l)$ and $f(x_u)$ have the same sign, as indicated by **Fig. 1.3a and c**, there are either no roots or an even number of roots between the values.

Graphical method is a simple method for obtaining an estimate for the root of the equation by plotting the function and observing where it crosses the *x* axis. However, it is of limited practical use because it is not precise and can only be utilized to obtain rough estimates of roots. These estimates can be employed as starting guesses for numerical methods discussed in this chapter. Two specific methods are covered: ***bisection*** and ***false position***.

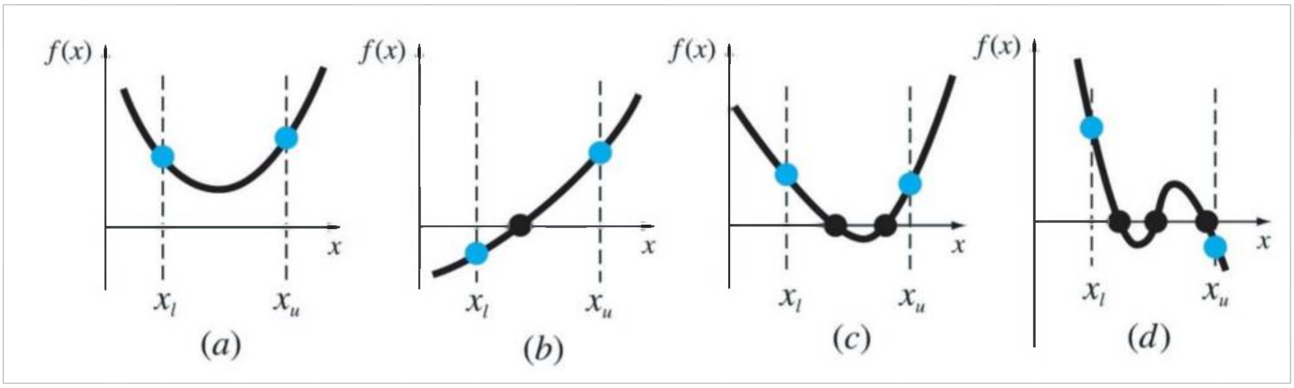


Fig. 1.3 Illustration of a number of general ways that a root may occur in an interval prescribed by a lower bound (x_l) and an upper bound (x_u). Parts **(a)** and **(c)** indicate that if both $f(x_l)$and $f(x_u)$ have the same sign, either there will be no roots or there will be an even number of roots within the interval. Parts **(b)** and **(d)** indicate that if the function has different signs at the end points, there will be an odd number of roots in the interval.

1.6.1.1. The Bisection Method

We have previously observed that $f(x)$ changed sign on opposite sides of the root. In general, if $f(x)$ is real and continuous in the interval from x_l to x_u and $f(x_l)$and $f(x_u)$ have opposite signs, that is,

$$f(x_l)\, f(x_u) < 0 \tag{1.4}$$

then there is at least one real root between x_l to x_u. A simple algorithm for the bisection calculation can be listed as;

Step 1: Choose lower x_l and upper x_u guesses for the root such that the function changes sign over the interval. This can be checked by ensuring that $f(x_l)\, f(x_u) < 0$

Step 2: An estimate of the root (x_r) is determined by

$$\text{Estimate of the root} = x_r = \frac{x_l + x_u}{2} \tag{1.5}$$

Step 3: Make the following evaluations to determine in which subinterval the root lies:

(a) If $f(x_l)\, f(x_r) < 0$, the root lies in the lower subinterval. Therefore, set $x_u = x_r$ and return to ***Step 2***.

(b) If $f(x_l)\, f(x_r) > 0$, the root lies in the upper subinterval. Therefore, set $x_l = x_r$ and return to ***Step 2***.

(c) If $f(x_l)\, f(x_r) = 0$, the root equals x_r; terminate the computation.

Step 3: Iterations continued until the percent relative error (ε), defined in the equation below, becomes less than a pre-specified stopping criterion.

$$\varepsilon = \left| \frac{x_r^{new} - x_r^{old}}{x_r^{new}} \right| * 100\% \tag{1.6}$$

<u>Example (1.1)</u>: Using the bisection method with initial guesses of $x_l = 5$ and $x_u = 7$, find the root of the equation $0.6x^2 = 2.4x + 5.5$. Iterate until the error falls below 3%.

<u>Solution</u>:

With $x_l = 5,\ x_u = 7$, the initial guess of the root using the bisection method $x_r = \frac{x_l + x_u}{2} = \frac{5+7}{2} = 6$

Iteration	x_l	x_u	x_r	$f(x_l)$	$f(x_u)$	$f(x_r)$	ε (%)
1	5	7	6	2.5	-7.1	-1.7	/
2	5	6	5.5	2.5	-1.7	0.55	9.091
3	5.5	6	5.75	0.55	-1.7	-0.54	4.348
4	5.5	5.75	5.625	0.55	-0.538	0.0156	2.222

Example (1.2): The relation between the velocity, mass, time, acceleration, and drag coefficient for a parachutist is presented in the following equation

$$f(c) = \frac{g\,m}{c}\left(1 - e^{-(c/m)t}\right) - v$$

Using the bisection method with initial guesses of (12) and (16), determine the drag coefficient (c) needed for a parachutist of mass (m) = 68.1 kg to have a velocity (v) of 40 m/s after free-falling for time t = 10 s. Take the acceleration due to gravity (g) = 9.81 m/s^2 and iterate until the error falls below a stopping criterion of 2%

Solution:

Using the bisection method, the initial estimate of the root x_r lies at the midpoint of the interval

$$x_l = 12, \; x_u = 16, \qquad \rightarrow x_r = \frac{x_l + x_u}{2} = \frac{12+16}{2} = 14$$

$$f(x_l) = \frac{g\,m}{c}\left(1 - e^{-(c/m)t}\right) - v = \frac{9.81 * 68.1}{12}\left(1 - e^{-(12/68.1)*10}\right) - 40 = 6.1139$$

$$f(x_u) = \frac{g\,m}{c}\left(1 - e^{-(c/m)t}\right) - v = \frac{9.81 * 68.1}{16}\left(1 - e^{-(16/68.1)*10}\right) - 40 = -2.2303$$

Iteration	x_l	x_u	x_r	$f(x_l)$	$f(x_u)$	$f(x_r)$	ε (%)
1	12	16	14	6.114	-2.230	1.611	/
2	14	16	15	1.611	-2.230	-0.384	6.667
3	14	15	14.5	1.611	-0.384	0.594	3.448
4	14.5	15	14.75	0.594	-0.384	0.100	1.695

Exercise (1.1):

a) Using the bisection method with initial guesses of $x_l = -1$ and $x_u = 0$, find the roots of the equation $f(x) = -13 - 20x + 19x^2 - 3x^3$. Iterate until the error falls below 10%.

b) Use the bisection method to find the root of the equation $e^x = \sin x$ located between -4 and -3. Note that x is in radians.

c) Use the bisection method to locate the root of the equation $f(x) = x^{10} - 1$ lying between x = 0 and 1.3. Use four decimal digits during the computation and iterate until the error falls below 10%.

1.6.1.2. The False-Position Method

Although the bisection method is a perfectly valid technique for locating the roots of equations, it has a shortcoming in dividing the interval from x_l to x_u into equal halves with no account for the magnitudes of $f(x_l)$ and $f(x_u)$. For example, if $f(x_l)$ is much closer to zero than $f(x_u)$, it is likely that the root is closer to xl than to xu (**Fig. 1.4**). An alternative method that utilizes this graphical insight is to join $f(x_l)$ and $f(x_u)$ by a straight line. The intersection of this line with the x-axis represents an improved estimate of the root. The fact that the replacement of the curve by a straight line gives a "***false position***" of the root is the origin of the name, ***method of false position***. It is also called the ***linear interpolation method***.

From (**Fig. 1.4**) and using similar triangles, the intersection of the straight line with the x axis can be estimated as

$$\frac{f(x_l)}{x_r - x_l} = \frac{f(x_u)}{x_r - x_u} \qquad (1.7)$$

which can be solved, after some algebraic manipulations, to give

$$x_r = x_u - \frac{f(x_u)(x_l - x_u)}{f(x_l) - f(x_u)} \qquad (1.8)$$

The calculation procedure for the root and the stopping criterion for iterations are the same as the bisection method.

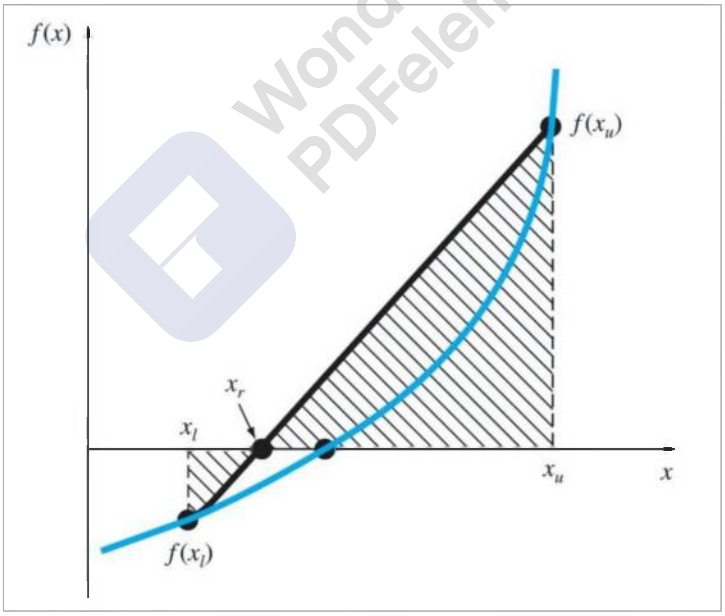


Fig. 1.4 A graphical representation of the false position method. The similar triangles used to derive the formula for the method are shaded.

Example (1.3): Repeat Example (1.2) using the false-position method to determine the root of the same equation investigated.

Solution:

Using the false-position method with $x_l = 12,\ x_u = 16,\ f(x_l) = 6.1139\ ,\ f(x_u) = -2.2303$

$$\rightarrow x_r = x_u - \frac{f(x_u)(x_l - x_u)}{f(x_l) - f(x_u)} = 14.9309$$

Iteration	x_l	x_u	x_r	$f(x_l)$	$f(x_u)$	$f(x_r)$	ε (%)
1	12	16	14.9309	6.1139	-2.2303	-0.2515	/
2	12	14.9309	14.8151	6.1139	-0.2515	-0.0271	0.782

Exercise (1.2):

a) Determine the root of $f(x) = -25 + 82x - 90x^2 + 44x^3 - 8x^4 + 0.7x^5$ using the false position method. Employ initial guesses of $x_l = 0.5$ and $x_u = 1.0$ and iterate until the error falls below 1%.

b) Using the false position method with initial guesses of $x_l = -1$ and $x_u = 0$, find the roots of the equation $f(x) = -13 - 20x + 19x^2 - 3x^3$. Iterate until the error falls below 10%.

c) Find the root of the equation x tan x = -1 located between 2.5 and 3 using the false position method.

d) Using the false position method with two iterations, locate the root of the equation $x^2 + x - 1 = 0$ lying between x = 0 and 1.

1.6.2. Open Methods

In the ***bracketing methods***, the root is located within an interval prescribed by a lower and an upper bound. Repeated application of these methods always results in closer estimates of the root. Such methods are said to be convergent because they move closer to the truth as the computation progresses (**Fig. 1.5a**). In contrast, the ***open methods*** are based on formulas that require only a ***single starting value of x*** or ***two starting values that do not necessarily bracket the root***. As such, they sometimes ***diverge*** or move away from the true root as the computation progresses (**Fig. 1.5b**). However, when the open methods converge (**Fig. 1.5c**), they usually do so much more quickly than the bracketing methods.

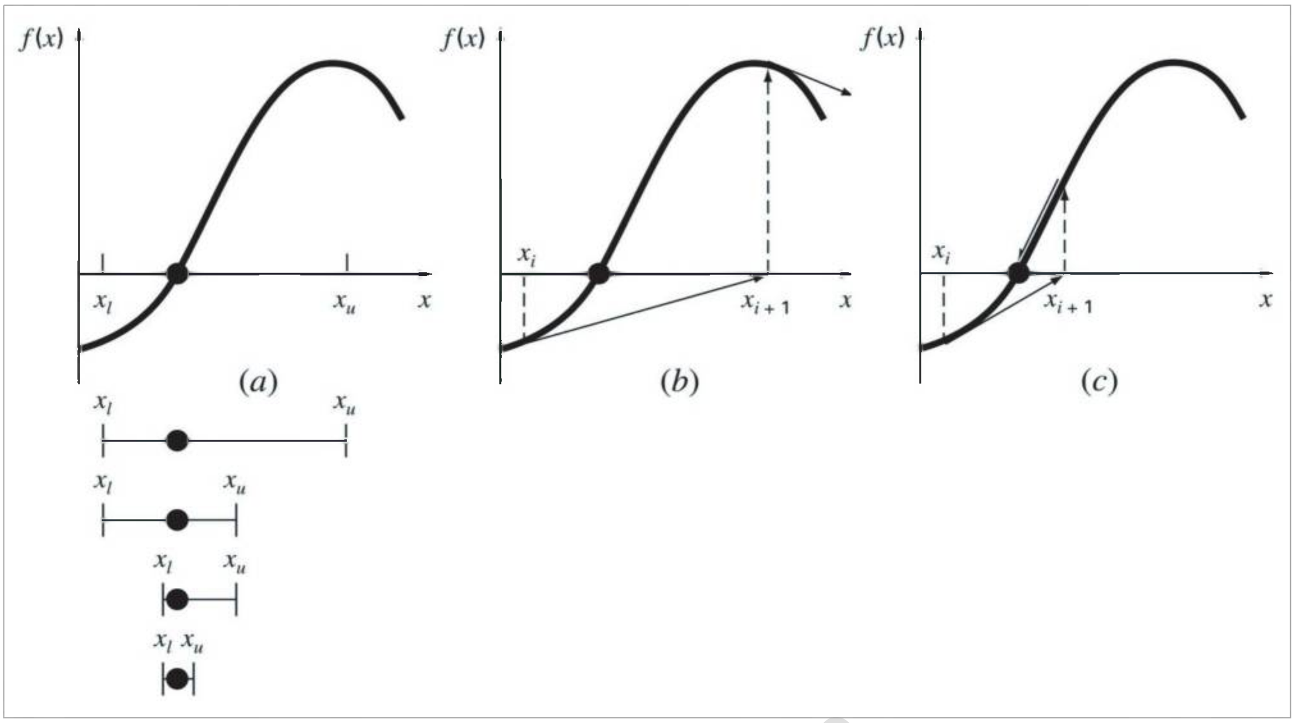


Fig. 1.5 Graphical depiction of the fundamental difference between the (*a*) bracketing and (*b*) and (*c*) open methods for root location. In (*a*), which is the bisection method, the root is constrained within the interval prescribed by x_l and x_u. In contrast, for the open method depicted in (*b*) and (*c*), a formula is used to project from x_i to x_{i+1} in an iterative fashion. Thus, the method can either (*b*) diverge or (*c*) converge rapidly, depending on the value of the initial guess.

1.6.2.1. Simple Fixed-Point Iteration

This method to predict the root of an equation employs a formula that can be developed by rearranging the function $f(x) = 0$ so that x is on the left-hand side of the equation. This transformation can be accomplished either by algebraic manipulation or by simply adding x to both sides of the original equation

$$x = g(x) \tag{1.9}$$

For example,

$f(x) = 0$	$x = g(x)$
$f(x) = x^2 - 2x + 3 = 0$	$x = \dfrac{x^2 + 3}{2}$
$f(x) = \sin x = 0$	$x = \sin x + x$

The utility of Eq. (1.9) is that it provides a formula to predict a new value of x as a function of an old value of x. Thus, given an initial guess at the root x_i, Eq. (1.9) can be used to compute a new estimate x_{i+1} as expressed by the iterative formula

$$x_{i+1} = g(x_i) \tag{1.10}$$

As with other iterative methods in this chapter, iterations continued until the percent relative error, defined in the equation below, becomes less than a pre-specified stopping criterion.

$$\varepsilon = \left|\frac{x_{i+1} - x_i}{x_{i+1}}\right| * 100\% \tag{1.11}$$

Example (1.4): Use simple fixed-point iteration to locate the root of $f(x) = e^{-x} - x$. Start with an initial guess of $x = 0$ and iterate until the error falls below 10%.

Solution: The function can be separated directly and expressed in the form of Eq. (1.10) as

$$x_{i+1} = e^{-x_i}$$

Iteration	x_i	ε (%)
0	0	/
1	1.000000	100.0
2	0.367879	171.8
3	0.692201	46.9
4	0.500473	38.3
5	0.606244	17.4
6	0.545396	11.2
7	0.579612	5.90

Exercise (1.3):

a) Use simple fixed-point iteration to locate the root of $f(x) = \sin(\sqrt{x}) - x$. Use an initial guess of $x_0 = 0.5$ and iterate until error falls below 2%.

b) Determine the root of $f(x) = 2x^3 - 11.7x^2 + 17.7x - 5$ using simple fixed-point iteration method. Make three iterations and start with an initial guess of $x_0 = 3$.

c) Consider the equation $f(x) = 5x^3 - 20x + 3$. Use simple fixed-point iteration to locate the root using an initial estimate of $x_0 = 0$ with three iterations.

1.6.2.2. The Newton-Raphson Method

Perhaps the most widely used of all root-locating formulas is the Newton-Raphson equation (**Fig. 1.6**). If the initial guess at the root is x_i, a tangent can be extended from the point $[x_i, f(x_i)]$. The point where this tangent crosses the x axis usually represents an improved estimate of the root. As in **Fig. 1.6**, the first derivative at x_i is equivalent to the slope:

$$f'(x_i) = \frac{f(x_i) - 0}{x_i - x_{i+1}} \tag{1.12}$$

which can be rearranged to yield the following equation called the ***Newton-Raphson formula***. Iterations continued until the percent relative error, defined in the simple fixed-point iteration method, becomes less than a pre-specified stopping criterion.

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \tag{1.13}$$

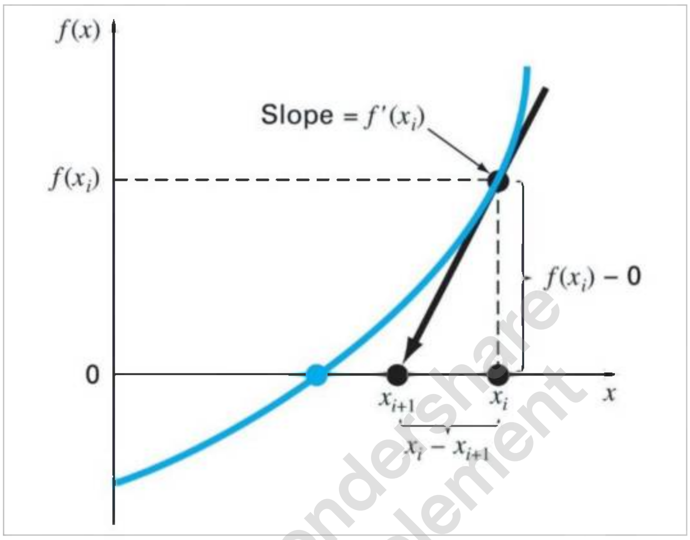


Fig. 1.6 Graphical depiction of the Newton-Raphson method. A tangent to the function of x_i [that is, f' (xi)] is extrapolated down to the x-axis to provide an estimate of the root at x_{i+1}.

<u>Example (1.5)</u>: Use the Newton-Raphson method to estimate the root of $f(x) = e^{-x} - x$, employing an initial guess of $x_0 = 0$ with four iterations.

<u>Solution</u>: The first derivative of the function can be evaluated as

$$f'(x) = -e^{-x} - 1$$

which can be substituted along with the original function into Eq. (1.13) to give

$$x_{i+1} = x_i - \frac{e^{-x_i} - x_i}{-e^{-x_i} - 1}$$

Starting with an initial guess of $x_0 = 0$, this iterative equation can be applied to compute

Iteration	x_i	ε (%)
0	0	/
1	0.500000000	100.00
2	0.566311003	11.709
3	0.567143165	0.1467
4	0.567143290	2.204E-5

Thus, the approach rapidly converges on the true root. Notice that the percent relative error at each iteration decreases much faster than it does in simple fixed-point iteration method.

Exercise (1.4):

a) Determine the root of $f(x) = 2x^3 - 11.7x^2 + 17.7x - 5$ using Newton-Raphson method. Make three iterations and start with an initial guess of $x_0 = 3$.

b) Use Newton-Raphson method to locate the root of $f(x) = -0.9\,x^2 + 1.7\,x + 2.5$. Use an initial guess of $x_0 = 5$ and iterate until the error falls below 0.1%.

c) Employ the Newton-Raphson method with initial guesses of **(a)** 4.52 and **(b)** 4.54 to determine the root for $f(x) = -1 + 5.5\,x - 4\,x^2 + 0.5\,x^3$. Iterate until the error falls below 10%.

1.6.2.3. The Secant Method

The existence of certain functions whose derivatives may be extremely difficult or inconvenient to evaluate represents a potential problem in implementing the Newton-Raphson method, which requires the evaluation of the derivative for its use. For these cases, the derivative can be approximated by a backward finite divided difference, as in (**Fig. 1.7**)

$$f'(x_i) \cong \frac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i} \qquad (1.14)$$

This approximation can be substituted into Eq. (1.13) to yield the following iterative equation:

$$x_{i+1} = x_i - \frac{f(x_i)\,(x_{i-1} - x_i)}{f(x_{i-1}) - f(x_i)} \qquad (1.15)$$

Equation (1.15) is the formula for the ***secant method***. Notice that the approach requires ***two initial estimates of x***. However, because *f*(x) is not required to change signs between the estimates, it is not classified as a bracketing method. Iterations continued until the percent relative error becomes less than a pre-specified stopping criterion.

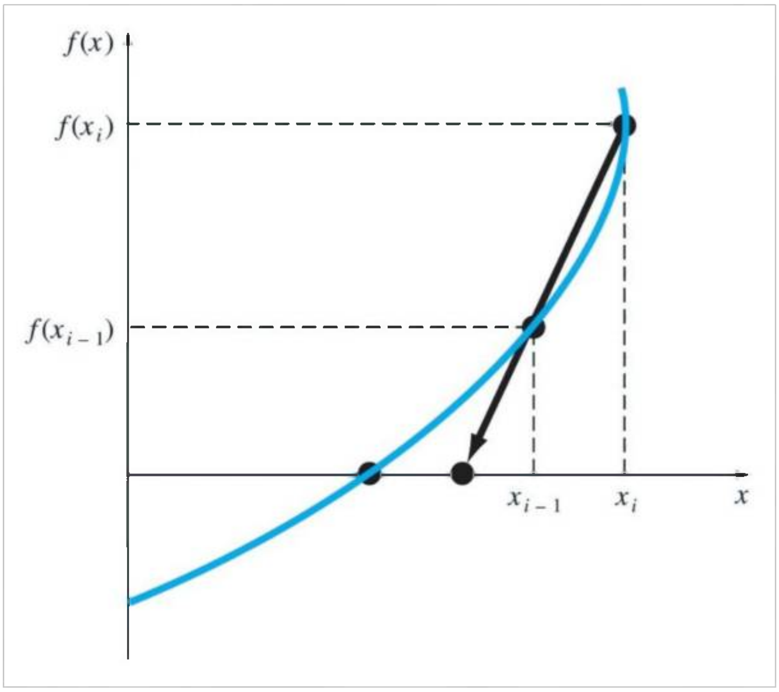


Fig. 1.7 Graphical depiction of the secant method. This technique is similar to the Newton-Raphson technique in the sense that an estimate of the root is predicted by extrapolating a tangent of the function to the x-axis. However, the secant method uses a difference rather than a derivative to estimate the slope.

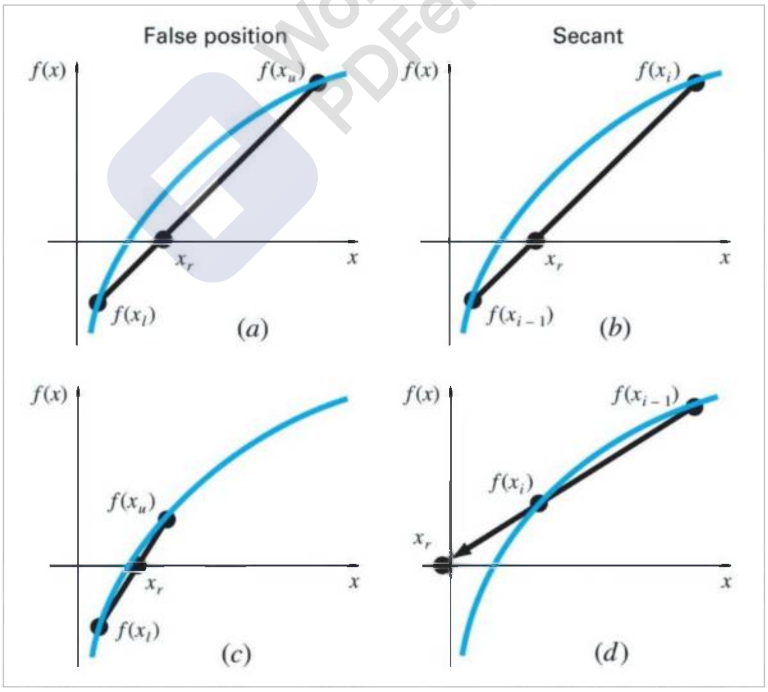


Fig. 1.8 Comparison of the false-position and the secant methods. The first iterations (a) and (b) for both techniques are identical. However, for the second iterations (c) and (d), the points used differ. Consequently, the secant method can diverge, as indicated in (d).

Example (1.6): Use the secant method to estimate the root of $f(x) = e^{-x} - x$. Start with initial estimates of $x_{-1} = 0$ and $x_0 = 1.0$. Iterate until the error falls below 1%.

Solution: Remember that the true root is 0.56714329.

First iteration:

$$x_{-1} = 0 \qquad f(x_{-1}) = 1.00000$$

$$x_0 = 1 \qquad f(x_0) = -0.63212$$

$$x_1 = x_0 - \frac{f(x_0)\,(x_{-1} - x_0)}{f(x_{-1}) - f(x_0)} = 1 - \frac{(-0.63212)\,(0-1)}{1-(-0.63212)} = 0.61270$$

Second iteration:

$$x_0 = 1 \qquad f(x_0) = -0.63212$$

$$x_1 = 0.61270 \qquad f(x_1) = -0.07081$$

(Note that both estimates are now on the same side of the root.)

$$x_2 = x_1 - \frac{f(x_1)\,(x_0 - x_1)}{f(x_0) - f(x_1)} = 0.61270 - \frac{(-0.07081)\,(1-0.61270)}{(-0.63212)-(-0.07081)} = 0.56384$$

$$\varepsilon = \left|\frac{x_{i+1} - x_i}{x_{i+1}}\right| * 100\% = \left|\frac{0.56384 - 0.61270}{0.56384}\right| * 100\% = 8.666\%$$

Third iteration:

$$x_1 = 0.61270 \qquad f(x_1) = -0.07081$$

$$x_2 = 0.56384 \qquad f(x_1) = 0.00518$$

$$x_3 = x_2 - \frac{f(x_2)\,(x_1 - x_2)}{f(x_1) - f(x_2)} = 0.56384 - \frac{0.00518\,(0.61270 - 0.56384)}{(-0.07081) - 0.00518} = 0.56717$$

$$\varepsilon = \left|\frac{x_{i+1} - x_i}{x_{i+1}}\right| * 100\% = \left|\frac{0.56717 - 0.56384}{0.0.56717}\right| * 100\% = 0.587\%$$

Exercise (1.5):

a) Determine the root of $f(x) = 2x^3 - 11.7x^2 + 17.7x - 5$ using Secant method. Make three iterations and start with an initial estimates of $x_{-1} = 3$, $x_0 = 4$.

b) Determine the root of $f(x) = 7(\sin x)e^{-x} - 1$. Using the secant method with five iterations and initial guesses of $x_{i-1} = 0.5$ and $x_i = 0.4$.

c) Locate the root of $f(x) = \sin x + \cos(1 + x^2) - 1$ where x is in radians. Use four iterations of the secant method with initial guesses of **(a)** $x_{i-1} = 1.0$ and $x_i = 3.0$; **(b)** $x_{i-1} = 1.5$ and $x_i = 2.5$, and **(c)** $x_{i-1} = 1.5$ and $x_i = 2.25$ to locate the root. Use the graphical method to explain your results.

Chapter Two - System of Linear Algebraic Equations

2.1. Introduction

In chapter one, we determined the value x that satisfied a single equation, f (x) = 0. In this chapter, we deal with the case of determining the values of ***n unknowns*** $x_1, x_2, \ldots, x_n$ that simultaneously satisfy a set of ***n linear algebraic equations***. Linear systems of equations are associated with many problems in engineering and science. A system of algebraic equations has the form

$$
\begin{aligned}
f_1(x_1, x_2, \dots, x_n) &= 0 \\
f_2(x_1, x_2, \dots, x_n) &= 0 \\
&\vdots \\
f_n(x_1, x_2, \dots, x_n) &= 0
\end{aligned}
$$

Such systems can be either linear or nonlinear. In this chapter, we deal with linear algebraic equations that are of the general form

$$
\begin{aligned}
a_{11}\, x_1 + a_{12}\, x_2 + \cdots + a_{1n}\, x_n &= b_1 \\
a_{21}\, x_1 + a_{22}\, x_2 + \cdots + a_{2n}\, x_n &= b_2 \\
&\vdots \\
a_{n1}\, x_1 + a_{n2}\, x_2 + \cdots + a_{nn}\, x_n &= b_n
\end{aligned} \tag{2.1}
$$

where the ***a's*** are ***constant coefficients***, the ***b's*** are ***constants***, and ***n*** is the number of equations. All other equations are nonlinear. In matrix notation, the equations are written as

$$
\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} \tag{2.2}
$$

or simply, $A\,x = b$ (2.3)

A ***system of linear equations*** in ***n unknowns*** has a ***unique solution***, provided that the ***determinant of the coefficient matrix (A)*** is ***non-singular*** (a non-singular matrix is a square one whose determinant is not zero), i.e., if $|A| \neq 0$. There are ***two classes of methods*** for solving system of linear algebraic equations: ***direct and iterative methods***.

2.2. Direct Methods for Solving System of Linear Algebraic Equations

The common characteristics of direct methods are that they transform the original equation into equivalent equations (equations that have the same solution) that can be solved more easily. The transformation is carried out by applying certain operations. In this section, we will present two direct methods: Gauss Elimination Method and Gauss-Jordan Method.

2.2.1. Gauss Elimination Method

Consider the following system of linear simultaneous equations:

$$a_{11}\,x_1 + a_{12}\,x_2 + a_{13}\,x_3 = b_1 \tag{2.4}$$

$$a_{21}\,x_1 + a_{22}\,x_2 + a_{23}\,x_3 = b_2 \tag{2.5}$$

$$a_{31}\,x_1 + a_{32}\,x_2 + a_{33}\,x_3 = b_3 \tag{2.6}$$

Gauss elimination reduces the coefficient matrix *(A)* into an upper triangular matrix through a sequence of operations carried out on the matrix. The constants vector ***(b)*** is also modified in the process. The solution vector $\{x\}$ is obtained from a backward substitution procedure. The method can be described by the following steps:

Step 1: Eliminate x_1 from the second and third equations. Using the first Equation (2.4) and assuming that $a_{11} \neq 0$, the following operations are performed:

$$\text{Equation (2.5)} - \left(\frac{a_{21}}{a_{11}}\right) \times \text{Equation (2.4)} \quad \textit{and} \quad \text{Equation (2.6)} - \left(\frac{a_{31}}{a_{11}}\right) \times \text{Equation (2.4)}$$

gives

$$a_{11}\,x_1 + a_{12}\,x_2 + a_{13}\,x_3 = b_1 \tag{2.7}$$

$$a'_{22}\,x_2 + a'_{23}\,x_3 = b'_2 \tag{2.8}$$

$$a'_{32}\,x_2 + a'_{33}\,x_3 = b'_3 \tag{2.9}$$

Equation (2.7) is called the ***pivotal equation*** and the coefficient a_{11} is the ***pivot***.

Step 2: Eliminate x_2 from Equation (2.9) using Equation (2.8) by assuming that $a_{22} \neq 0$. We perform the following operation:

$$\text{Equation (2.9)} - \left(\frac{a'_{32}}{a'_{22}}\right) \times \text{Equation (2.8)}$$

to obtain

$$a_{11}\,x_1 + a_{12}\,x_2 + a_{13}\,x_3 = b_1 \tag{2.10}$$

$$a'_{22}\,x_2 + a'_{23}\,x_3 = b'_2 \tag{2.11}$$

$$a''_{33}\,x_3 = b''_3 \tag{2.12}$$

Here Eq. (2.11) is called the ***pivotal equation*** and the coefficient a'_{22} is the ***pivot***.

Step 3: To find x_1, x_2 and x_3, we apply back substitution starting from Equation (2.12) giving x_3, then x_2 from Equation (2.11) and x_1 from Equation (2.10).

2.2.1.1. Pivoting

Gauss elimination method fails if any one of the pivots in the above equations (2.4) to (2.12) becomes zero. To overcome this difficulty, the equations are to be rewritten in a slightly different order such that the pivots are not zero.

a) Partial pivoting method

Step 1: The numerically largest coefficient of x_1 is selected from all the equations as pivot and the corresponding equation becomes the first equation (2.4).

Step 2: The numerically largest coefficient of x_2 is selected from all the remaining equations as pivot and the corresponding equation becomes the second equation (2.8). This process is repeated until an equation into a single variable is obtained.

b) Complete pivoting method

In this method, we select at each stage the numerically largest coefficient of the complete matrix of coefficients. This procedure leads to an interchange of the equations as well as interchange of the position of variables.

Example (2.1): Solve the following equations by Gauss elimination method:

$$2x + 4y - 6z = -4$$
$$x + 5y + 3z = 10$$
$$x + 3y + 2z = 5$$

Solution: Forward elimination is the first part of the procedure.

$$2x + 4y - 6z = -4 \qquad \text{Eq. 1}$$
$$x + 5y + 3z = 10 \qquad \text{Eq. 2}$$
$$x + 3y + 2z = 5 \qquad \text{Eq. 3}$$

To eliminate x from (Eq.2) and (Eq.3) using (Eq.1):

$$2x + 4y - 6z = -4$$

Eq. 1 + (–2) * Eq. 2 → $\quad -6y - 12z = -24 \qquad$ Eq. 4

Eq. 1 + (–2) * Eq. 3 → $\quad -2y - 10z = -14 \qquad$ Eq. 5

To eliminate y from (Eq.5) using (Eq.4):

$$2x + 4y - 6z = -4$$

$$-6y - 12z = -24$$

Eq. 4 + (–3) * Eq. 5 → $18z = 18$ → $z = 1$

Evaluation of the unknowns by back substitution:

$-6y - 12z = -24 \rightarrow -6y - 12 \times 1 = -24 \rightarrow y = 2$

$2x + 4y - 6z = -4 \rightarrow 2x + 4 \times 2 - 6 \times 1 = -4 \rightarrow x = -3$

<u>Example (2.2)</u>: Use Gauss elimination to solve

$$3x - 0.1y - 0.2z = 7.85$$

$$0.1x + 7y - 0.3z = -19.3$$

$$0.3x - 0.2y + 10z = 71.4$$

Carry six significant figures during the computation. Verify the solution.

<u>Solution:</u> The first part of the procedure is forward elimination.

$3x - 0.1y - 0.2z = 7.85$ Eq. 1

$0.1x + 7y - 0.3z = -19.3$ Eq. 2

$0.3x - 0.2y + 10z = 71.4$ Eq. 3

To eliminate x from (Eq.2) and (Eq.3) using (Eq.1):

$$3x - 0.1y - 0.2z = 7.85$$

Eq. 2 + (–0.1/3) * Eq. 1 → $7.00333y - 0.293333z = -19.5617$ Eq. 4

Eq. 3 + (–0.3/3) * Eq. 1 → $-0.190000y + 10.0200z = 70.6150$ Eq. 5

To complete the forward elimination, y must be removed from (Eq.5) using (Eq.4):

$$3x - 0.1y - 0.2z = 7.85$$

$$7.00333y - 0.293333z = -19.5617$$

Eq. 5 + $\left(\frac{0.190000}{7.00333}\right)$ * Eq. 4 → $10.0120z = 70.0843$ Eq. 6

From Eq. 6 → $z = 70.0843 / 10.0120 = 7.00000$

This result can be back-substituted into Eq. 5:

$7.00333y - 0.293333\,(7.00000) = -19.5617 \rightarrow y = -2.50000$

Finally, from Eq. 1:

$3x - 0.1\,(-2.50000) - 0.2\,(7.00000) = 7.85 \rightarrow x = 3.00000$

The solution can be verified by substituting the results into the original equation set

$\rightarrow$ $3\,(3) - 0.1\,(-2.5) - 0.2\,(7) = 7.85$

$\rightarrow$ $0.1\,(3) + 7\,(-2.5) - 0.3\,(7) = -19.3$

$\rightarrow$ $0.3\,(3) - 0.2\,(-2.5) + 10\,(7) = 71.4$

Example (2.3): Using Gaussian elimination method with pivoting, solve the following system of linear equations:

$$x_1 + x_2 + x_3 - x_4 = 2$$
$$4\,x_1 + 4\,x_2 + x_3 + x_4 = 11$$
$$x_1 - x_2 - x_3 + 2\,x_4 = 0$$
$$2\,x_1 + x_2 + 2\,x_3 - 2\,x_4 = 2$$

Solution:

$x_1 + x_2 + x_3 - x_4 = 2$ Eq. 1

$4\,x_1 + 4\,x_2 + x_3 + x_4 = 11$ Eq. 2

$x_1 - x_2 - x_3 + 2\,x_4 = 0$ Eq. 3

$2\,x_1 + x_2 + 2\,x_3 - 2\,x_4 = 2$ Eq. 4

In the first step, eliminate x_1 terms from second, third, and fourth equations of the set of equations to obtain:

$x_1 + x_2 + x_3 - x_4 = 2$

Eq. 2 + (–4/1) * Eq. 1 $\rightarrow$ $-3x_3 + 5x_4 = 3$ Eq. 5

Eq. 3 + (–1/1) * Eq. 1 $\rightarrow$ $-2x_2 - 2x_3 + 3x_4 = -2$ Eq. 6

Eq. 4 + (–2/1) * Eq. 1 $\rightarrow$ $-x_2 = -2$ Eq. 7

Exchanging columns in the above equations by putting the variables in the order x_1, x_4, x_3 and x_2 as

$x_1 - x_4 + x_3 + x_2 = 2$ Eq. 8

$+ 5x_4 - 3x_3 = 3$ Eq. 9

$+ 3x_4 - 2x_3 - 2x_2 = -2$ Eq. 10

$-x_2 = -2$ Eq. 11

In the second step, eliminate x_4 term in third equation using (Eq. 9):

$x_1 - x_4 + x_3 + x_2 = 2$

$+ 5x_4 - 3x_3 = 3$

Eq. 10 + (–3/5) * Eq. 9 $\rightarrow$ $-(1/5)x_3 - 2x_2 = -19/5$ Eq. 12

$-x_2 = -2$

Now, by the process of back substitution, we have

$\rightarrow$ $x_2 = 2$, $x_3 = -1$, $x_4 = 0$, and $x_1 = 1$.

2.2.2. Gauss-Jordan Method

Gauss-Jordan method is an extension of the Gauss elimination method. The major difference is that when an unknown is eliminated in the Gauss-Jordan method, it is eliminated from all other equations rather than just the subsequent ones. In addition, all rows are normalized by dividing them by their pivot elements. The set of equations $\boldsymbol{Ax = b}$ is reduced to a diagonal set $\boldsymbol{Ix = b'}$, where $\boldsymbol{I}$ is an identity (also called unit) matrix. Thus, the elimination step results in an identity matrix rather than a triangular matrix. The identity matrix (sometimes called a unit matrix) of size n is the n × n square matrix with ones on the main diagonal and zeros elsewhere. Therefore, the diagonal set $\boldsymbol{Ix = b'}$ is equivalent to $\boldsymbol{x = b'}$, i.e., it is not necessary to employ back substitution to obtain the solution.

Example (2.4): Carrying six significant figures during the computation, use the Gauss-Jordan technique to solve the same system as in Example (2.2):

$$3x - 0.1y - 0.2z = 7.85$$
$$0.1x + 7y - 0.3z = -19.3$$
$$0.3x - 0.2y + 10z = 71.4$$

Solution: First, express the coefficients and the right-hand side as an ***augmented matrix*** (which is a ***matrix*** obtained by ***adding*** the columns of two given ***matrices***).

$$\begin{bmatrix} 3 & -0.1 & -0.2 & : & 7.85 \\ 0.1 & 7 & -0.3 & : & -19.3 \\ 0.3 & -0.2 & 10 & : & 71.4 \end{bmatrix}$$

Then, normalize the first row by dividing it by the pivot element, 3, to yield

$$\begin{bmatrix} 1 & -0.0333333 & -0.066667 & : & 2.61667 \\ 0.1 & 7 & -0.3 & : & -19.3 \\ 0.3 & -0.2 & 10 & : & 71.4 \end{bmatrix}$$

The x_1 term can be eliminated from the ***second row*** by ***subtracting 0.1 times the first row*** from the ***second row***. Similarly, ***subtracting 0.3 times the first row*** from the ***third row*** will eliminate the x_1 term from the ***third row***:

$$\begin{bmatrix} 1 & -0.0333333 & -0.066667 & : & 2.61667 \\ 0 & 7.00333 & -0.293333 & : & -19.5617 \\ 0 & -0.190000 & 10.0200 & : & 70.6150 \end{bmatrix}$$

Next, normalize the second row by dividing it by 7.00333:

$$\begin{bmatrix} 1 & -0.0333333 & -0.066667 & : & 2.61667 \\ 0 & 1 & -0.0418848 & : & -2.79320 \\ 0 & -0.190000 & 10.0200 & : & 70.6150 \end{bmatrix}$$

Reduction of the x_2 terms from the first and third equations gives

$$\begin{bmatrix} 1 & 0 & -0.0680629 & : & 2.52356 \\ 0 & 1 & -0.0418848 & : & -2.79320 \\ 0 & 0 & 10.01200 & : & 70.0843 \end{bmatrix}$$

The third row is then normalized by dividing it by 10.0120:

$$\begin{bmatrix} 1 & 0 & -0.0680629 & : & 2.52356 \\ 0 & 1 & -0.0418848 & : & -2.79320 \\ 0 & 0 & 1 & : & 7.0000 \end{bmatrix}$$

Finally, the x_3 terms can be reduced from the first and the second equations to give

$$\begin{bmatrix} 1 & 0 & 0 & : & 3.00000 \\ 0 & 1 & 0 & : & -2.50000 \\ 0 & 0 & 1 & : & 7.00000 \end{bmatrix}$$

Thus, the coefficient matrix has been transformed to the identity matrix, and the solution is obtained in the right-hand-side vector. Notice that no back substitution was required to obtain the solution.

Example (2.5): Solve the following system of equations by Gauss-Jordan method.

$$x + 3y + 2z = 17$$

$$x + 2y + 3z = 16$$

$$2x - y + 4z = 13$$

Solution:

$$\begin{bmatrix} 1 & 3 & 2 & : & 17 \\ 1 & 2 & 3 & : & 16 \\ 2 & -1 & 4 & : & 13 \end{bmatrix}$$

Eliminate x term from the second (Row 2 + (–1) Row 1) and third (Row 3 + (–2) Row 1) rows as

$$\begin{bmatrix} 1 & 3 & 2 & : & 17 \\ 0 & -1 & 1 & : & -1 \\ 0 & -7 & 0 & : & -21 \end{bmatrix}$$

Next, normalize the second row by dividing it by –1:

$$\begin{bmatrix} 1 & 3 & 2 & : & 17 \\ 0 & 1 & -1 & : & 1 \\ 0 & -7 & 0 & : & -21 \end{bmatrix}$$

Eliminate y term from the first (Row 1 + (–3) Row 2) and third (Row 3 + (7) Row 2) rows as

$$\begin{bmatrix} 1 & 0 & 5 & : & 14 \\ 0 & 1 & -1 & : & 1 \\ 0 & 0 & -7 & : & -14 \end{bmatrix}$$

Next, normalize the third row by dividing it by –7:

$$\begin{bmatrix} 1 & 0 & 5 & : & 14 \\ 0 & 1 & -1 & : & 1 \\ 0 & 0 & 1 & : & 2 \end{bmatrix}$$

Eliminate z term from the first (Row 1 + (–5) Row 3) and second (Row 2 + (1) Row 3) rows as

$$\begin{bmatrix} 1 & 0 & 0 & : & 4 \\ 0 & 1 & 0 & : & 3 \\ 0 & 0 & 1 & : & 2 \end{bmatrix}$$

$\rightarrow$ x = 4, y = 3, and z = 2

Example (2.6): Using the Gauss-Jordan method, solve the following system of equations.

$$x - 2y = -4$$
$$-5y + z = -9$$
$$4x - 3z = -10$$

Solution: Expressing the coefficients and the right-hand side as an augmented matrix

$$\begin{bmatrix} 1 & -2 & 0 & : & -4 \\ 0 & -5 & 1 & : & -9 \\ 4 & 0 & -3 & : & -10 \end{bmatrix}$$

Eliminate x term from the third row as (Row 3 + (–4) Row 1)

$$\begin{bmatrix} 1 & -2 & 0 & : & -4 \\ 0 & -5 & 1 & : & -9 \\ 0 & 8 & -3 & : & 6 \end{bmatrix}$$

Next, normalize the second row by dividing it by –5:

$$\begin{bmatrix} 1 & -2 & 0 & : & -4 \\ 0 & 1 & -1/5 & : & 9/5 \\ 0 & 8 & -3 & : & 6 \end{bmatrix}$$

Eliminate y term from the first (Row 1 + (2) Row 2) and third (Row 3 + (–8) Row 2) rows as

$$\begin{bmatrix} 1 & 0 & -2/5 & : & -2/5 \\ 0 & 1 & -1/5 & : & 9/5 \\ 0 & 0 & -7/5 & : & -42/5 \end{bmatrix}$$

Next, normalize the third row by dividing it by –7/5:

$$\begin{bmatrix} 1 & 0 & -2/5 & : & -2/5 \\ 0 & 1 & -1/5 & : & 9/5 \\ 0 & 0 & 1 & : & 6 \end{bmatrix}$$

Eliminate z term from the first (Row 1 + (2/5) Row 3) and second (Row 2 + (1/5) Row 3) rows as

$$\begin{bmatrix} 1 & 0 & 0 & : & 2 \\ 0 & 1 & 0 & : & 3 \\ 0 & 0 & 1 & : & 6 \end{bmatrix}$$

$\rightarrow$ x = 2, y = 3, and z = 6

2.3. Iterative Methods for Solving System of Linear Algebraic Equations

Iterative or indirect methods, start with a guess of the solution x, and then repeatedly refine the solution until a certain convergence criterion is reached. Iterative methods are generally less efficient than direct methods due to the large number of operations or iterations required. The initial guess affects only the number of iterations that are required for convergence. In this section, we will present two iterative methods; ***Jacobi's Iteration Method*** and ***Gauss-Seidel Iteration Method***.

2.3.1. Jacobi's Iteration Method

This method is also known as the ***method of simultaneous displacements***. Consider the system of linear equations

$$\begin{aligned} a_{11}\,x_1 + a_{12}\,x_2 + a_{13}\,x_3 &= b_1 \\ a_{21}\,x_1 + a_{22}\,x_2 + a_{23}\,x_3 &= b_2 \\ a_{31}\,x_1 + a_{32}\,x_2 + a_{33}\,x_3 &= b_3 \end{aligned} \tag{2.13}$$

Here, we assume that the coefficients a_{11}, a_{22} and a_{33} are the ***largest coefficients*** in the respective equations so that

$$\begin{aligned} |a_{11}| &> |a_{12}| + |a_{13}| \\ |a_{22}| &> |a_{21}| + |a_{23}| \\ |a_{33}| &> |a_{31}| + |a_{32}| \end{aligned} \tag{2.14}$$

Jacobi's iteration method is applicable only if the conditions given in Eq. (2.14) are satisfied. Now, using Eq. (2.13) we can write

$$\begin{aligned} x_1 &= \frac{1}{a_{11}}(b_1 - a_{12}\,x_2 - a_{13}\,x_3) \\ x_2 &= \frac{1}{a_{22}}(b_2 - a_{21}\,x_1 - a_{23}\,x_3) \\ x_3 &= \frac{1}{a_{33}}(b_3 - a_{31}\,x_1 - a_{32}\,x_2) \end{aligned} \tag{2.15}$$

Let the initial approximations for $x_1, x_2,$ and x_3 be abbreviated as $x_1^{(0)}, x_2^{(0)},$ and $x_3^{(0)}$, respectively. The following iterations are then carried out.

Iteration 1: The first improvements are found as

$$\begin{aligned} x_1^{(1)} &= \frac{1}{a_{11}}\left(b_1 - a_{12}\,x_2^{(0)} - a_{13}\,x_3^{(0)}\right) \\ x_2^{(1)} &= \frac{1}{a_{22}}\left(b_2 - a_{21}\,x_1^{(0)} - a_{23}\,x_3^{(0)}\right) \\ x_3^{(1)} &= \frac{1}{a_{33}}\left(b_3 - a_{31}\,x_1^{(0)} - a_{32}\,x_2^{(0)}\right) \end{aligned} \tag{2.16}$$

Iteration 2: The second improvements are obtained as

$$x_1^{(2)} = \frac{1}{a_{11}}\left(b_1 - a_{12}\, x_2^{(1)} - a_{13}\, x_3^{(1)}\right)$$
$$x_2^{(2)} = \frac{1}{a_{22}}\left(b_2 - a_{21}\, x_1^{(1)} - a_{23}\, x_3^{(1)}\right) \qquad (2.17)$$
$$x_3^{(2)} = \frac{1}{a_{33}}\left(b_3 - a_{31}\, x_1^{(1)} - a_{32}\, x_2^{(1)}\right)$$

The above iteration procedure for x_1, x_2, and x_3 is continued until the relative error between two consecutive iterations falls below a pre-assigned degree of accuracy. Convergence error can be estimated using the following relation

$$Error\ \% = \left|\frac{x_i^{(j)} - x_i^{(j-1)}}{x_i^{(j)}}\right| \times 100 \qquad (2.18)$$

for all *i*, where *(j)* and *(j – 1)* are the present and previous iterations, respectively. In Jacobi's method, it is a general practice to assume that $x_1^{(0)} = x_2^{(0)} = x_3^{(0)} = 0$. The method can be extended to a system of ***n linear simultaneous equations*** in ***n unknowns***.

Example (2.7): Solve the following equations by Jacobi's method with seven iterations.

15x + 3y – 2z = 85

2x + 10y + z = 51

x – 2y + 8z = 5

Solution: In the above equations:

$$|a_{11}| > |a_{12}| + |a_{13}| \quad \rightarrow \quad |15| > |3| + |-2|$$
$$|a_{22}| > |a_{21}| + |a_{23}| \quad \rightarrow \quad |10| > |2| + |1|$$
$$|a_{33}| > |a_{31}| + |a_{32}| \quad \rightarrow \quad |8| > |1| + |-2|$$

Therefore, Jacobi's method is applicable. We rewrite the given equations as follows:

$$x^{(1)} = \frac{1}{15}\left(85 - 3\, y^{(0)} + 2\, z^{(0)}\right)$$
$$y^{(1)} = \frac{1}{10}\left(51 - 2\, x^{(0)} - z^{(0)}\right)$$
$$z^{(1)} = \frac{1}{8}\left(5 - x^{(0)} + 2\, y^{(0)}\right)$$

Let the initial approximations be $x^{(0)} = y^{(0)} = z^{(0)} = 0$

Iteration 1: Now $x^{(0)} = 0, \quad y^{(0)} = 0, \quad \text{and} \quad z^{(0)} = 0$

$$x^{(1)} = \frac{1}{15}(85) = \frac{17}{3}$$

$$y^{(1)} = \frac{1}{10}(51) = \frac{51}{10}$$

$$z^{(1)} = \frac{1}{8}(5) = \frac{5}{8}$$

Iteration 2: Now $x^{(1)} = \frac{17}{3}, \quad y^{(1)} = \frac{51}{10}, \quad \text{and} \quad z^{(1)} = \frac{5}{8}$

$$x^{(2)} = \frac{1}{15}\left(85 - 3\left(\frac{51}{10}\right) + 2\left(\frac{5}{8}\right)\right) = 4.73$$

$$y^{(2)} = \frac{1}{10}\left(51 - 2\left(\frac{17}{3}\right) - \left(\frac{5}{8}\right)\right) = 3.904$$

$$z^{(2)} = \frac{1}{8}\left(5 - \left(\frac{17}{3}\right) + 2\left(\frac{51}{10}\right)\right) = 1.192$$

Result for subsequent iterations are presented in the following table:

Variable	Iteration							
	0	**1**	**2**	**3**	**4**	**5**	**6**	**7**
x	0	17/3	4.73	5.045	4.994	5.002	5.0	5.0
y	0	51/10	3.904	4.035	3.99	4.001	4.0	4.0
z	0	5/8	1.192	1.010	1.003	0.998	1.0	1.0

2.3.2. Gauss-Seidel Iteration Method

The Gauss-Seidel method is an additional iterative method for solving system of linear algebraic equations. It is an improved version of Jacobi's method and it also known as the ***method of successive approximations***. Consider the system of linear simultaneous equations

$$\begin{aligned} a_{11}\,x_1 + a_{12}\,x_2 + a_{13}\,x_3 &= b_1 \\ a_{21}\,x_1 + a_{22}\,x_2 + a_{23}\,x_3 &= b_2 \\ a_{31}\,x_1 + a_{32}\,x_2 + a_{33}\,x_3 &= b_3 \end{aligned} \qquad (2.19)$$

The Gauss-Seidel method is applicable if the coefficients a_{11}, a_{22} and a_{33} are the ***largest coefficients*** in the respective equations so that

$$\begin{aligned} |a_{11}| &> |a_{12}| + |a_{13}| \\ |a_{22}| &> |a_{21}| + |a_{23}| \\ |a_{33}| &> |a_{31}| + |a_{32}| \end{aligned} \qquad (2.20)$$

Now, using Eq. (2.19) we can write

$$x_1 = \frac{1}{a_{11}}(b_1 - a_{12}\,x_2 - a_{13}\,x_3)$$
$$x_2 = \frac{1}{a_{22}}(b_2 - a_{21}\,x_1 - a_{23}\,x_3) \qquad (2.21)$$
$$x_3 = \frac{1}{a_{33}}(b_3 - a_{31}\,x_1 - a_{32}\,x_2)$$

Let the initial approximations for $x_1, x_2,$ and x_3 be abbreviated as $x_1^{(0)}, x_2^{(0)},$ and $x_3^{(0)}$, respectively. The following iterations are then carried out.

Iteration 1: The first improvements are found as

$$x_1^{(1)} = \frac{1}{a_{11}}\left(b_1 - a_{12}\,x_2^{(0)} - a_{13}\,x_3^{(0)}\right)$$
$$x_2^{(1)} = \frac{1}{a_{22}}\left(b_2 - a_{21}\,x_1^{(1)} - a_{23}\,x_3^{(0)}\right) \qquad (2.22)$$
$$x_3^{(1)} = \frac{1}{a_{33}}\left(b_3 - a_{31}\,x_1^{(1)} - a_{32}\,x_2^{(1)}\right)$$

Iteration 2: The second improvements are obtained as

$$x_1^{(2)} = \frac{1}{a_{11}}\left(b_1 - a_{12}\,x_2^{(1)} - a_{13}\,x_3^{(1)}\right)$$
$$x_2^{(2)} = \frac{1}{a_{22}}\left(b_2 - a_{21}\,x_1^{(2)} - a_{23}\,x_3^{(1)}\right) \qquad (2.23)$$
$$x_3^{(2)} = \frac{1}{a_{33}}\left(b_3 - a_{31}\,x_1^{(2)} - a_{32}\,x_2^{(2)}\right)$$

Since the most recent approximations of the variables are used while proceeding to the next step, the convergence of the Gauss-Seidel method is twice as fast as in Jacobi's method. The above iteration process is continued until the values of x_1, x_2, and x_3 are obtained to a pre-assigned or desired degree of accuracy.

In general, the initial approximations are assumed as $x_1^{(0)} = x_2^{(0)} = x_3^{(0)} = 0$. Like the Jacobi's method, Gauss-Seidel method can also be extended to *n linear simultaneous algebraic equations* in *n unknowns*.

Example (2.8): Solve the following equations by Gauss-Seidel method with three iterations.

15x + 3y – 2z = 85

2x + 10y + z = 51

x – 2y + 8z = 5

Solution: In the above equations:

$$|a_{11}| > |a_{12}| + |a_{13}| \quad \rightarrow \quad |15| > |3| + |-2|$$
$$|a_{22}| > |a_{21}| + |a_{23}| \quad \rightarrow \quad |10| > |2| + |1|$$
$$|a_{33}| > |a_{31}| + |a_{32}| \quad \rightarrow \quad |8| > |1| + |-2|$$

Therefore, Gauss-Seidel method is applicable. We rewrite the given equations as follows:

$$x^{(1)} = \frac{1}{15}\left(85 - 3\,y^{(0)} + 2\,z^{(0)}\right)$$
$$y^{(1)} = \frac{1}{10}\left(51 - 2\,x^{(0)} - z^{(0)}\right)$$
$$z^{(1)} = \frac{1}{8}\left(5 - x^{(0)} + 2\,y^{(0)}\right)$$

Let the initial approximations be $x^{(0)} = y^{(0)} = z^{(0)} = 0$

Iteration 1: Now $x^{(0)} = 0$, $y^{(0)} = 0$, and $z^{(0)} = 0$

$$x^{(1)} = \frac{1}{15}\left(85 - 3\,y^{(0)} + 2\,z^{(0)}\right) = \frac{85}{15}$$
$$y^{(1)} = \frac{1}{10}\left(51 - 2\,x^{(1)} - z^{(0)}\right) = \frac{1}{10}\left(51 - 2\,\frac{85}{15} - 0\right) = 3.96667$$
$$z^{(1)} = \frac{1}{8}\left(5 - x^{(1)} + 2\,y^{(1)}\right) = \frac{1}{8}\left(5 - \frac{85}{15} + 2(3.96667)\right) = 0.908334$$

Iteration 2: Now $x^{(1)} = \frac{85}{15}$, $y^{(1)} = 3.96667$, and $z^{(1)} = 0.908334$

$$x^{(2)} = \frac{1}{15}\left(85 - 3\,y^{(1)} + 2\,z^{(1)}\right) = \frac{1}{15}\left(85 - 3(3.96667) + 2\,(0.908334)\right) = 4.994443$$
$$y^{(2)} = \frac{1}{10}\left(51 - 2\,x^{(2)} - z^{(1)}\right) = \frac{1}{10}\left(51 - 2\,(4.994443) - 0.908334\right) = 4.010278$$
$$z^{(2)} = \frac{1}{8}\left(5 - x^{(2)} + 2\,y^{(2)}\right) = \frac{1}{8}\left(5 - (4.994443) + 2(4.010278)\right) = 1.003264$$

Iteration 3: Now $x^{(2)} = 4.994443$, $y^{(2)} = 4.010278$, and $z^{(2)} = 1.003264$

$$x^{(3)} = \frac{1}{15}\left(85 - 3\,y^{(2)} + 2\,z^{(2)}\right) = \frac{1}{15}\left(85 - 3(4.010278) + 2\,(1.003264)\right) = 5.0$$
$$y^{(3)} = \frac{1}{10}\left(51 - 2\,x^{(3)} - z^{(2)}\right) = \frac{1}{10}\left(51 - 2\,(5.0) - 1.003264\right) = 4.0$$
$$z^{(3)} = \frac{1}{8}\left(5 - x^{(3)} + 2\,y^{(3)}\right) = \frac{1}{8}\left(5 - (5.0) + 2(4.0)\right) = 1.0$$

It is proved that with three iterations, the convergence of the Gauss-Seidel method is twice as fast as in Jacobi's method, which required six iterations to reach convergence.

Exercise (2.1):

a) Using the methods of (a) Gauss elimination and (b) Gauss-Jordan, solve the following system of equations.

$$2x + 2y + 4z = 18$$
$$x + 3y + 2z = 13$$
$$3x + y + 3z = 14$$

b) Using partial pivoting, solve the following system of equations by (a) Gauss elimination method and (b) Gauss-Jordan method.

$$y + 2z = 5$$
$$x + 2y + 4z = 11$$
$$-3x + y - 5z = -12$$

c) Using (a) Gauss elimination method and (b) Gauss-Jordan method, solve the following system of equations.

$$2x + y + z = 4$$
$$x - y + 2z = 2$$
$$2x + 2y - z = 3$$

d) Solve the system of equations below using the following methods: (a) Gauss elimination, (b) Gauss-Jordan, (c) Jacobi's Iteration, and (d) Gauss-Seidel.

$$5x + 2y + z = 12$$
$$x + 4y + 2z = 15$$
$$x + 2y + 5z = 20$$

e) Using the methods of (a) Jacobi's Iteration and (b) Gauss-Seidel, solve the following system of equations.

$$5x - 2y + z = 4$$
$$x + 4y - 2z = 3$$
$$x + 2y + 4z = 17$$

f) Solve the following system of equations using (a) Jacobi's Iteration method and (b) Gauss-Seidel Iteration method.

$$10x + y + z = 12$$
$$2x + 10y + z = 13$$
$$2x + 2y + 10z = 14$$

Chapter Three - Curve Fitting

3.1. Introduction

Data are often given for discrete values along a continuum. However, you may require estimates at points between the discrete values. The present chapter describes techniques to fit curves to such data to obtain intermediate estimates. Furthermore, you may require a simplified version of a complicated function. One way to do this is to compute values of the function at a number of discrete values along the range of interest. Then, a simpler function may be derived to fi t these values. Both of these applications are known as curve fitting.

There are **two general approaches for curve fitting** that are distinguished from each other based on the amount of error associated with these data.

- **First**, where these data exhibit a significant degree of error or "noise," the strategy is to derive a single curve that represents the general trend of these data. One method of this approach is called ***least-squares regression*** (**Fig. 3.1a**).
- **Second**, where these data are known to be very precise, the basic approach is to fit a curve or a series of curves that pass directly through each of the points. Such data usually originate from tables. Examples are values for the density of water or for the heat capacity of gases as a function of temperature. The estimation of values between well-known discrete points is called **interpolation** (**Fig. 3.1b and c**).

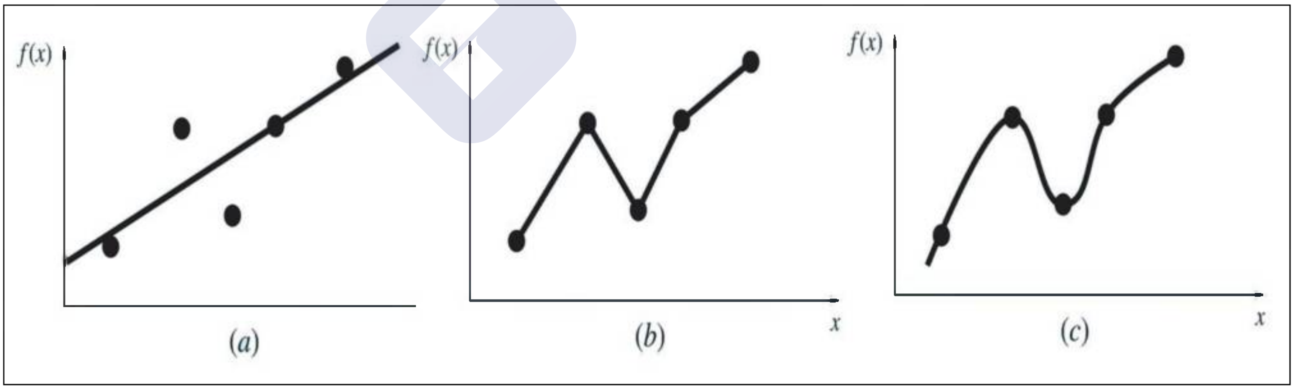


Fig. 3.1 Three attempts to fit a "best" curve through five data points. (a) Least-squares regression, (b) linear interpolation, and (c) curvilinear interpolation.

3.2. Linear Regression

Where substantial error is associated with data, polynomial interpolation is inappropriate and may yield unsatisfactory results when used to predict intermediate values. Experimental data are often of this type. A more appropriate strategy for such cases is to derive an approximating function that fits the shape or general trend of the data without necessarily matching the individual points. The simplest example of a least-squares approximation is fitting a straight line to a set of paired observations: $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$. The mathematical expression for the straight line is;

$$y = a_0 + a_1 x + e \tag{3.1}$$

where a_0 and a_1 are coefficients representing the intercept and the slope, respectively, and e is the error, or residual, between the true value of y and the estimated value from the above linear mathematical expression, which can be represented by rearranging as (**Fig. 3.2**);

$$e = y - a_0 - a_1 x \tag{3.2}$$

One strategy for fitting a "best" line through the data would be to minimize the sum of the residual errors (e) for all the available data, as in

$$\sum_{i=1}^{n} e_i = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i) \tag{3.3}$$

where n is total number of points. However, this is an inadequate criterion, as illustrated by **Fig. 3.3a**, which depicts the fit of a straight line to two points. Obviously, the best fit is the line connecting the points. However, any straight line passing through the midpoint of the connecting line (except a vertical line) results in a minimum value. Therefore, ***another logical criterion*** might be to minimize the sum of the absolute values of the discrepancies, as in

$$\sum_{i=1}^{n} |e_i| = \sum_{i=1}^{n} |y_i - a_0 - a_1 x_i| \tag{3.4}$$

Fig. 3.3b demonstrates why this criterion is also. For the four points shown, any straight line falling within the dashed lines will minimize the sum of the absolute values. Thus, this criterion also does not yield a unique best fit. ***A third strategy*** for fitting a best line is the ***minimax criterion***. In this technique, the line is chosen that minimizes the maximum distance that an individual point falls from the line. As depicted in **Fig. 3.3c**, this strategy is inappropriate for regression because it gives excessive influence to an outlier, that is, a single point with a large error.

A strategy that overcomes the shortcomings of the aforementioned approaches is to minimize the sum of the squares of the residuals between the measured y and the y calculated with the linear model. This criterion has a number of advantages, including the fact that it yields a unique line for a given set of data.

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left(y_{i_{\text{measured}}} - y_{i_{\text{model}}}\right)^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2 \tag{3.5}$$

To determine values for a_0 and a_1, S_r is differentiated with respect to each coefficient.

$$\frac{\partial S_r}{\partial a_0} = -2 \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i) \quad (3.6)$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum_{i=1}^{n} [(y_i - a_0 - a_1 x_i) x_i] \quad (3.7)$$

Now, setting these derivatives equal to zero will result in a minimum value of S_r. Then, the final equations for a_0 and a_1 can be expressed as;

$$a_1 = \frac{n \sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n \sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2} \quad (3.8)$$

$$a_0 = \bar{y} - a_1 \bar{x} \quad (3.9)$$

where $\bar{y}$ and $\bar{x}$ are the mean values of y and x, respectively. Therefore, the least-squares fit line is

$$y = a_0 + a_1 x \quad (3.10)$$

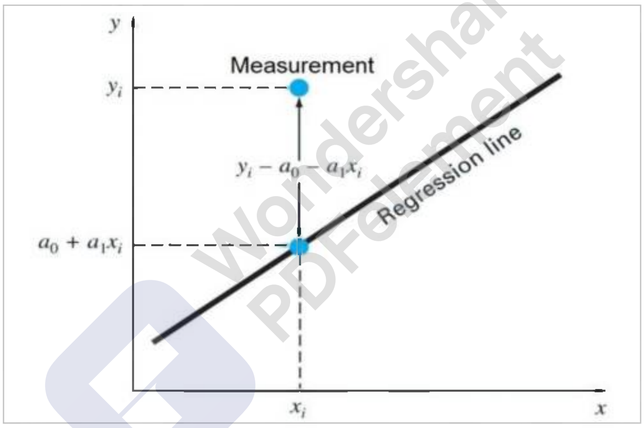


Fig. 3.2 The residual in linear regression represents the vertical distance between a data point and the straight regression line.

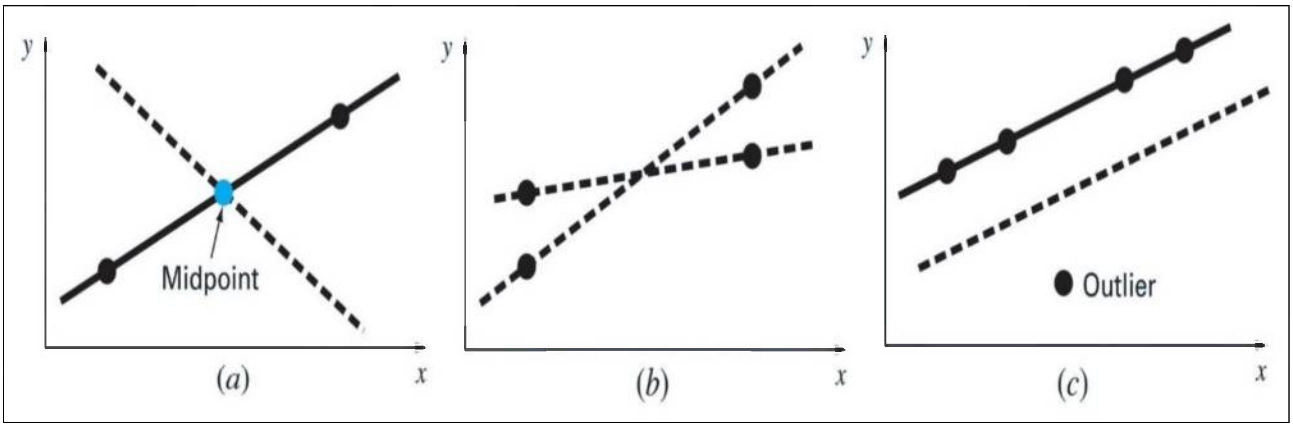


Fig. 3.3 Examples of some criteria for "best fit" that are inadequate for regression: (a) minimizes the sum of the residuals, (b) minimizes the sum of the absolute values of the residuals, and (c) minimizes the maximum error of any individual point.

Example (3.1): Fit a straight line to the x and y values presented in the following table.

x	1	2	3	4	5	6	7
y	0.5	2.5	2.0	4.0	3.5	6.0	5.5

Solution:

The following quantities can be computed:

n = 7, $\sum x_i = 28$, $\sum y_i = 24$, $\sum x_i\, y_i = 119.5$, $\sum x_i^2 = 140$,

$\bar{x} = \frac{28}{7} = 4$, $\bar{y} = \frac{24}{7} = 3.428571$

$$a_1 = \frac{7(119.5) - 28(24)}{7(140) - (28)^2} = 0.8392857$$

a_0 = 3.428571 - 0.8392857(4) = 0.07142857

Therefore, the least-squares fit line is; y = 0.07142857 + 0.8392857 x

Example (3.2): The experimental data for the force (F) and velocity (V) for an object suspended in a wind tunnel are given in the table below. Fit a straight line to the data using the least-square regression method and then use it to calculate the force when the velocity is 55 m/s.

Velocity, V (m/s)	10	20	30	40	50	60	70	80
Force, F (N)	24	68	378	552	608	1218	831	1452

Solution:

From the data presented, the following quantities can be calculated:

n	x_i	y_i	$(x_i)^2$	$x_i\, y_i$
1	10	24	100	240
2	20	68	400	1360
3	30	378	900	11340
4	40	552	1600	22080
5	50	608	2500	30400
6	60	1218	3600	73080
7	70	831	4900	58170
8	80	1452	6400	116160
$\sum$	360	5131	20400	312830

n = 8, $\sum x_i = 360$, $\sum y_i = 5131$, $\sum x_i\, y_i = 312830$, $\sum x_i^2 = 20400$,

$\bar{x} = \frac{360}{8} = 45$, $\bar{y} = \frac{5131}{8} = 641.375$

$a_1 = \frac{8(312830) - 360(5131)}{8(20400) - (360)^2} = 19.5083$

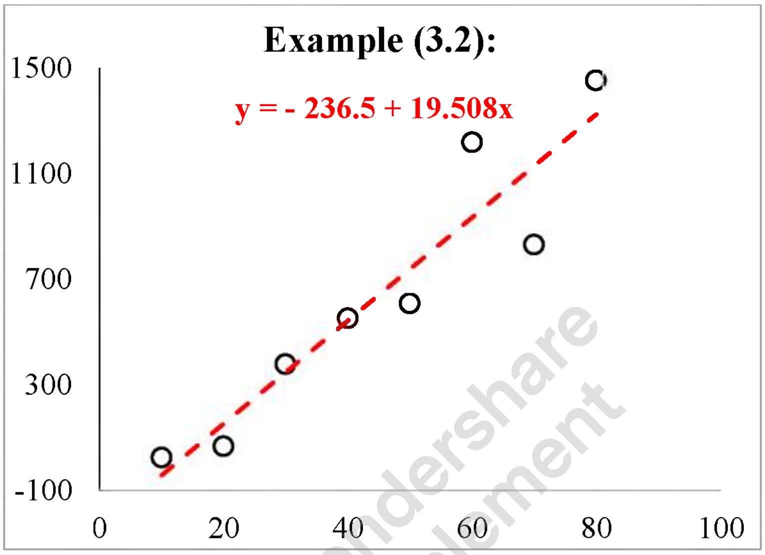
a_0 = 641.375 - (19.5083 x 45) = -236.5

Then the equation for the straight line is $y = a_0 + a_1 x = -236.5 + 19.5083\ x$

Or, $F = a_0 + a_1 V = -236.5 + 19.5083\ V$

Then, the predicted value of force at a velocity of 55 m/s is

$$F = a_0 + a_1 V = -236.5 + 19.5083\ V = -236.5 + 19.5083\ (55) = 836.4583\ N$$



Exercise (3.1):

a) Fit a straight line for the data points (-1, 10), (0, 9), (1, 7), (2, 5), (3, 4), (4, 3), (5, 0), and (6, -1).

b) Using the following data (-2, 1), (-1, 2), (0, 3), (1, 3), and (2, 4), find the least square line.

c) Using the least-square regression method, fit a straight line for the following data points (-4, 1.2), (-2, 2.8), (0, 6.2), (2, 7.8), and (4, 13.2).

d) The daily income for a worker is presented in the table below with the corresponding daily food expenditure. Using the least squares regression method, fit a line to the data presented considering the income as the independent variable and food expenditure as the dependent variable.

Daily income (USD)	35	50	22	40	16	30	25
Daily food expense (USD)	9	15	6	11	5	8	9

e) The monthly income in hundreds of dollars with the corresponding monthly internet bills in dollars for a random sample of 10 households is presented in the table below. Fit a line to the data using the least squares regression method considering the income as the independent variable and internet bill as the dependent variable.

Monthly income * 100 (USD)	16	45	35	31	30	14	40	15	36	40
Monthly internet bill (USD)	36	140	171	70	94	25	159	41	78	98

3.3. Interpolation

You will frequently have occasion to estimate intermediate values between precise data points. ***Interpolation*** is used in such occasions as an alternative curve-fitting technique and the most common method used for this purpose is ***polynomial interpolation***. Recall that the general formula for an nth-order polynomial is

$$f(x) = a_0 + a_1\, x + a_2\, x^2 + \cdots + a_n\, x^n \qquad (3.11)$$

Polynomial interpolation consists of determining the unique **nth-order polynomial** that passes the **n + 1 data points**. This polynomial then provides a formula to compute the intermediate values. Although there is one and **only one nth-order polynomial** that fits **n + 1 points**, there are a variety of mathematical formats in which this polynomial can be expressed. In this chapter, we will describe two alternatives: the ***Newton*** and the ***Lagrange*** **polynomials**.

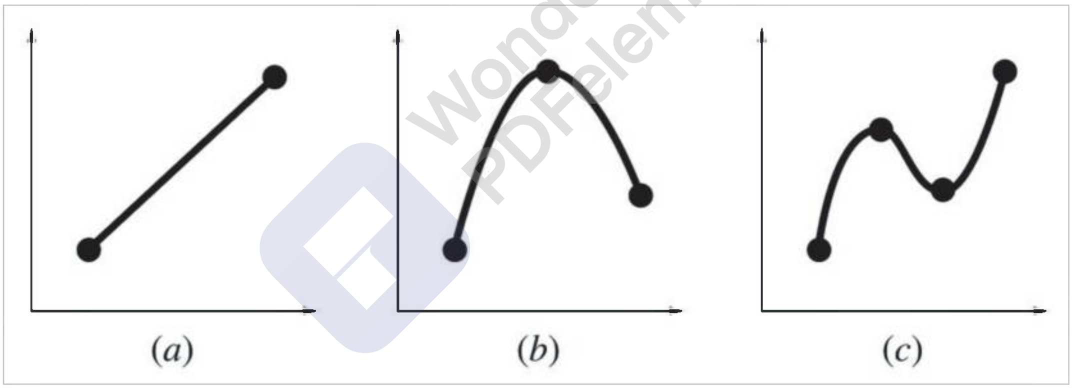


Fig. 3.4 Examples of interpolating polynomials: **(a)** first-order (linear) connecting two points, **(b)** second order (quadratic or parabolic) connecting three points, and **(c)** third-order (cubic) connecting four points.

3.3.1. Newton's Divided-Difference Interpolating Polynomials

Newton's divided-difference interpolating polynomial is among the most popular and useful forms. Before presenting the general equation, we will introduce the first- and second-order versions because of their simple visual interpretation.

3.3.1.1. Linear Interpolation

The simplest form of interpolation is to connect **two data points** with a **straight line**. This technique, called ***linear interpolation***, is illustrated graphically in **Fig. 3.5**. Using similar triangles,

$$\frac{f_1(x) - f(x_0)}{x - x_0} = \frac{f(x_1) - f(x_0)}{x_1 - x_0} \tag{3.12}$$

which can be rearranged to yield;

$$f_1(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0) \tag{3.13}$$

which is a linear-interpolation formula. The ***notation $f_1(x)$*** designates that this is a ***first order interpolating polynomial***. Notice that the term $[f(x_1) - f(x_0)]/(x_1 - x_0)$ is a ***finite-divided-difference*** approximation of the first derivative besides representing the slope of the line connecting the points. In general, **the smaller the interval between the data points**, the better the approximation. This is because, as the interval decreases, a continuous function will be better approximated by a straight line. This characteristic is demonstrated in the following example.

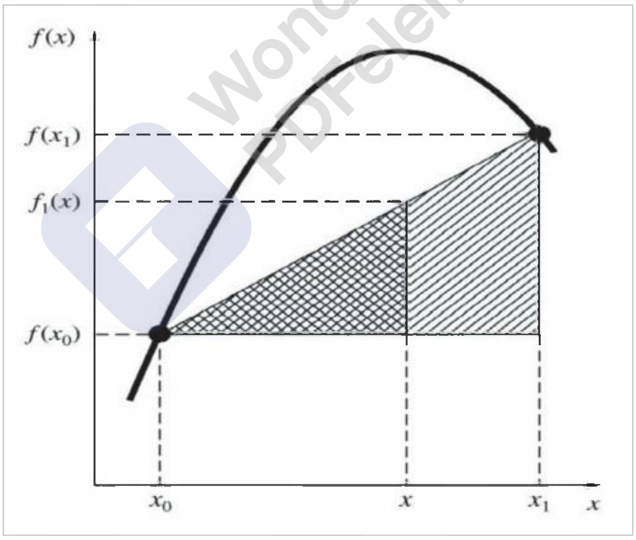


Fig. 3.5 Graphical depiction of linear interpolation. The shaded areas indicate the similar triangles used to derive the linear-interpolation formula

<u>**Example (3.3)**</u>: Estimate the natural logarithm of 2 using linear interpolation. First, perform the computation by interpolating between ln 1 = 0 and ln 6 = 1.791759. Then, repeat the procedure, but use a smaller interval from ln 1 to ln 4 = 1.386294. Note that the true value of ln 2 is 0.6931472.

Solution:

Using linear interpolation for In 2 from $x_0 = 1$ to $x_1 = 6$ will give:

$$f_1(2) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0) = 0 + \frac{1.791759 - 0}{6 - 1}(2 - 1) = 0.3583519$$

which represents an error of $\left|\frac{0.3583519 - 0.6931472}{0.6931472}\right| \times 100 = 48.3\%$.

Using the smaller interval from $x_0 = 1$ to $x_1 = 4$ yields

$$f_1(2) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0) = 0 + \frac{1.386294 - 0}{4 - 1}(2 - 1) = 0.4620981$$

Thus, using the smaller interval reduces the percent relative error to 33.3%.

Exercise (3.2): Estimate the common logarithm of 10 using linear interpolation

a) Interpolate between log 8 = 0.9030900 and log 12 = 1.0791812.

b) Interpolate between log 9 = 0.9542425 and log 11 = 1.0413927.

For each of the interpolations, compute the percent error based on the true value (log 10 = 1).

3.3.1.2. Newton's Second-Order Polynomial (Quadratic Interpolation)

The error in previous example resulted from approximating a curve with a straight line. Consequently, a strategy for improving the estimate is to introduce some curvature into the line connecting the points. If three data points are available, this can be accomplished with a second-order polynomial (also called a quadratic polynomial or a parabola). A particularly convenient form for this purpose is

$$f_2(x) = b_0 + b_1\,(x - x_0) + b_2\,(x - x_0)(x - x_1) \qquad (3.14)$$

A simple procedure can be used to determine the values of the coefficients. For (b_0), the above equation can be used with $x = x_0$ to compute

$$b_0 = f(x_0) \qquad (3.15)$$

For (b_1), equation (3.15) for (b_0) can be substituted into equation (3.14), which can be evaluated at $x = x_1$ to calculate

$$b_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0} \qquad (3.16)$$

Finally for (b_2), equations (3.15) and (3.16) can be substituted into equation (3.14), which can be evaluated at $x = x_2$ and solved (after some algebraic manipulations) to compute

$$b_2 = \frac{\frac{f(x_2) - f(x_1)}{x_2 - x_1} - \frac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0} \qquad (3.17)$$

Notice that, as was the case with linear interpolation, b_1 still represents the slope of the line connecting points x_0 and x_1. Thus, the first two terms of equation (3.14) are equivalent to linear interpolation from x_0 to x_1, as specified previously in equation (3.13). The last term, $b_2\,(x - x_0)(x - x_1)$, introduces the second-order curvature into the formula.

Example (3.4): Fit a second-order Newton's polynomial to the three points used in Example (3.3) and use it to evaluate ln 2. Note that the true value of ln 2 is 0.6931472.

$x_0 = 1$ $\quad f(x_0) = 0$

$x_1 = 4$ $\quad f(x_1) = 1.386294$

$x_2 = 6$ $\quad f(x_2) = 1.791759$

Solution:

$$b_0 = f(x_0) = 0$$

$$b_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{1.386294 - 0}{4 - 1} = 0.4620981$$

$$b_2 = \frac{\frac{f(x_2) - f(x_1)}{x_2 - x_1} - \frac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0} = \frac{\frac{1.791759 - 1.386294}{6 - 4} - 0.4620981}{6 - 1} = -0.0518731$$

$$f_2(x) = b_0 + b_1\,(x - x_0) + b_2\,(x - x_0)(x - x_1)$$

$$= 0 + 0.4620981(x - 1) - 0.0518731(x - 1)(x - 4)$$

At x = 2 we have $\quad f_2(2) = 0.4620981(2 - 1) - 0.0518731(2 - 1)(2 - 4) = 0.5658444$

which represents a relative error of $\left|\frac{0.5658444 - 0.6931472}{0.6931472}\right| \times 100 = 18.4\%$.

Thus, the curvature introduced by the quadratic formula improves the interpolation compared with the result obtained using straight lines.

Exercise (3.3): Fit a second order Newton's interpolating polynomial to estimate log 10 using the following data from exercise (3.2):

$x_0 = 8$ $\quad f(x_0) = 0.9030900$

$x_1 = 9$ $\quad f(x_1) = 0.9542425$

$x_2 = 11$ $\quad f(x_2) = 1.0413927.$

3.3.1.3. General Form of Newton's Interpolating Polynomials

The preceding analysis can be generalized to fit an **nth-order polynomial** to **n + 1 data points**. The nth-order polynomial is

$$f_n(x) = b_0 + b_1\,(x - x_0) + \cdots + b_n\,(x - x_0)\,(x - x_1)\,...\,(x - x_{n-1}) \tag{3.18}$$

As was done previously with the linear and quadratic interpolations, data points can be used to evaluate the coefficients b_0, b_1, ... , b_n. For an nth-order polynomial, n + 1 data points are required: $[x_0, f(x_0)]$, $[x_1, f(x_1)]$, ... , $[x_n, f(x_n)]$. These data points and the following equations are used to evaluate the coefficients:

$$b_0 = f(x_0) \tag{3.19}$$

$$b_1 = f[x_1,\ x_0] \tag{3.20}$$

$$b_2 = f[x_2,\ x_1,\ x_0] \tag{3.21}$$

.
.
.

$$b_n = f[x_n,\ x_{n-1},\ ...\ ,\ x_1,\ \ x_0] \tag{3.22}$$

where the bracketed function evaluations are finite divided differences. For example, the ***first finite divided difference*** is represented generally as

$$f[x_i,\ x_j] = \frac{f(x_i) - f(x_j)}{x_i - x_j} \tag{3.23}$$

The ***second finite divided difference***, which represents the difference of two first divided differences, is expressed generally as

$$f[x_i,\ x_j,\ x_k] = \frac{f[x_i,\ x_j] - f[x_j,\ x_k]}{x_i - x_k} \tag{3.24}$$

Similarly, the ***nth finite divided difference*** is

$$f[x_n,\ x_{n-1},\ ...\ ,x_1,\ x_0] = \frac{f[x_n,\ x_{n-1},...\ ,x_1] - f[x_{n-1},\ x_{n-2},...\ ,x_0]}{x_n - x_0} \tag{3.25}$$

These differences can be used to evaluate the coefficients in equations (3.19) through (3.22), which can then be substituted into equation (3.18) to yield the interpolating polynomial, which is called ***Newton's divided-difference interpolating polynomial***.

$$f_n(x) = f(x_0) + (x - x_0) f[x_1, x_0] + (x - x_0)(x - x_1) f[x_2, x_1, x_0] + \cdots + (x - x_0)(x - x_1) \ldots (x - x_{n-1}) f[x_n, x_{n-1}, \ldots, x_0] \quad (3.26)$$

It should be noted that it is **not necessary** for the data points used to be **equally spaced** or that the **abscissa values** necessarily be in **ascending order**, as illustrated in the following example.

Example (3.5): In Example (3.4), data points at $x_0 = 1$, $x_1 = 4$, and $x_2 = 6$ were used to estimate ln 2 with a parabola. Now, adding a fourth point [$x_3 = 5$; $f(x_3) = 1.609438$], estimate ln 2 with a third-order Newton's interpolating polynomial. Note that the true value of ln 2 is 0.6931472.

Solution: The third-order polynomial, equation (3.18) with n = 3, is

$$f_3(x) = b_0 + b_1 (x - x_0) + b_2 (x - x_0)(x - x_1) + b_3 (x - x_0)(x - x_1)(x - x_2)$$

$x_0 = 1$ $f(x_0) = 0$

$x_1 = 4$ $f(x_1) = 1.386294$

$x_2 = 6$ $f(x_2) = 1.791759$

$x_3 = 5;$ $f(x_3) = 1.609438$

$f(x_0) = 0 \quad = \mathbf{b_0}$

The first divided differences for the problem are

$$f[x_1, x_0] = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{1.386294 - 0}{4 - 0} = 0.4620981 \quad = \mathbf{b_1}$$

$$f[x_2, x_1] = \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{1.791759 - 1.386294}{6 - 4} = 0.2027326$$

$$f[x_3, x_2] = \frac{f(x_3) - f(x_2)}{x_3 - x_2} = \frac{1.609438 - 1.791759}{5 - 6} = 0.1823216$$

The second divided differences are

$$f[x_2, x_1, x_0] = \frac{f[x_2, x_1] - f[x_1, x_0]}{x_2 - x_0} = \frac{0.2027326 - 0.4620981}{6 - 1} = -0.05187311 \quad = \mathbf{b_2}$$

$$f[x_3, x_2, x_1] = \frac{f[x_3, x_2] - f[x_2, x_1]}{x_3 - x_1} = \frac{0.1823216 - 0.2027326}{5 - 4} = -0.02041100$$

The third divided difference is

$$f[x_3, x_2, x_1, x_0] = \frac{f[x_3, x_2, x_1] - f[x_2, x_1, x_0]}{x_3 - x_0} = \frac{-0.02041100 - (-0.05187311)}{5 - 1}$$

$$= 0.007865529 \quad = \mathbf{b_3}$$

$$\rightarrow f_3(x) = 0 + 0.4620981\,(x-1) - 0.05187311\,(x-1)(x-4) + 0.007865529\,(x-1)\,(x-4)\,(x-6)$$

Now, we can evaluate $f_3(x)$ at $x = 2 \quad \rightarrow \quad f_3(2) = 0.6287686$,

which represents a relative error of $\left|\frac{0.6287686 - 0.6931472}{0.6931472}\right| \times 100 = 9.3\%$.

Thus, adding a fourth point improves the interpolation.

Example (3.6): The upward velocity of a rocket is given as a function of time in the table below. Determine the value of the velocity at t = 16 seconds using third order Newton's divided difference interpolating polynomial method.

t (s)	0	10	15	20	22.5	30
V (m/s)	0	227.04	362.78	517.35	602.97	901.67

Solution:

Procedure 1

Since we want to find the rocket velocity at t = 16 and we are using a third order interpolating polynomial, we need to choose the four data points that are closest to t = 16 that also bracket t = 16 to evaluate it. The four data points that are selected to be the most appropriate are

$t_0 = 10 \qquad f(t_0) = 227.04$
$t_1 = 15 \qquad f(t_1) = 362.78$
$t_2 = 20 \qquad f(t_2) = 517.35$
$t_3 = 22.5 \qquad f(t_3) = 602.97$

$$V = f_3(t) = b_0 + b_1\,(t-t_0) + b_2\,(t-t_0)(t-t_1) + b_3\,(t-t_0)\,(t-t_1)\,(t-t_2)$$

$f(t_0) = 227.04 \quad = \mathbf{b_0}$

The first divided differences for the problem are

$$f[t_1,\ t_0] = \frac{f(t_1) - f(t_0)}{t_1 - t_0} = \frac{362.78 - 227.04}{15 - 10} = 27.148 \quad = \mathbf{b_1}$$

$$f[t_2,\ t_1] = \frac{f(t_2) - f(t_1)}{t_2 - t_1} = \frac{517.35 - 362.78}{20 - 15} = 30.914$$

$$f[t_3,\ t_2] = \frac{f(t_3) - f(t_2)}{t_3 - t_2} = \frac{602.97 - 517.35}{22.5 - 20} = 34.248$$

The second divided differences are

$$f[t_2,\ t_1,\ t_0] = \frac{f[t_2,\ t_1] - f[t_1,\ t_0]}{t_2 - t_0} = \frac{30.914 - 27.148}{20 - 10} = 0.37660 \quad = \mathbf{b_2}$$

$$f[t_3,\ t_2,\ t_1] = \frac{f[t_3,\ t_2] - f[t_2,\ t_1]}{t_3 - t_1} = \frac{34.248 - 30.914}{22.5 - 15} = 0.44453$$

The third divided difference is

$$f[t_3,\ t_2,\ t_1,\ t_0] = \frac{f[t_3,\ t_2,\ t_1] - f[t_2,\ t_1,\ t_0]}{t_3 - t_0} = \frac{0.44453 - 0.37660}{22.5 - 10} = 0.0054344 \quad = \mathbf{b_3}$$

$$\rightarrow V = f_3(t) = 227.04 + 27.148\,(t-10) + 0.37660\,(t-10)(t-15)$$
$$+\, 0.0054344\,(t-10)\,(t-15)\,(t-20)$$

which can be used to evaluate the rocket velocity at t = 16 as

$$\rightarrow V_{(\text{at } t=16\text{ s})} = f_3(16) = 227.04 + 27.148\,(16-10) + 0.37660\,(16-10)(16-15) +$$
$$0.0054344\,(16-10)\,(16-15)\,(16-20) = 392.06 \text{ m/s}$$

Procedure 2

To find the rocket velocity at t = 16, the four data points that were previously selected are

$t_0 = 10$ $f(t_0) = 227.04$
$t_1 = 15$ $f(t_1) = 362.78$
$t_2 = 20$ $f(t_2) = 517.35$
$t_3 = 22.5$ $f(t_3) = 602.97$

The following table can be used as an alternative procedure to find the third order Newton's divided difference interpolating polynomial.

t_i	$f(t_i)$	*First divided differences*	*Second divided differences*	*Third divided difference*
$t_0 = 10$	$f(t_0) = 227.04$ $= \mathbf{b_0}$			
		$f[t_1,\ t_0] = 27.148$ $= \mathbf{b_1}$		
$t_1 = 15$	$f(t_1) = 362.78$		$f[t_2,\ t_1,\ t_0] = 0.37660$ $= \mathbf{b_2}$	
		$f[t_2,\ t_1] = 30.914$		$f[t_3,\ t_2,\ t_1,\ t_0] = 0.0054344$ $= \mathbf{b_3}$
$t_2 = 20$	$f(t_2) = 517.35$		$f[t_3,\ t_2,\ t_1] = 0.44453$	
		$f[t_3,\ t_2] = 34.248$		
$t_3 = 22.5$	$f(t_3) = 602.97$			

Exercise (3.4):

a) Given these data in the table below, calculate *f*(2.8) using Newton's interpolating polynomials of order 1 through 3. Choose the sequence of the points to attain the best possible accuracy.

x	1.6	2	2.5	3.2	4	4.5
***f*(x)**	2	8	14	15	8	2

b) Using the data presented in the table below, evaluate *f*(6) using Newton's divided difference formula with a suitable order.

x	5	7	11	13	21
***f*(x)**	150	392	1452	2366	9702

c) Calculate *f*(4) using Newton's interpolating polynomials of order 1 through 4. Choose your base points to attain good accuracy.

x	1	2	3	5	7	8
***f*(x)**	3	6	19	99	291	444

3.3.2. Lagrange Interpolation Polynomials

The ***Lagrange interpolating polynomial*** is simply a reformulation of the ***Newton polynomial*** that avoids the computation of divided differences. It can be represented concisely as

$$f_n(x) = \sum_{i=0}^{n} L_i(x)\ f(x_i) \tag{3.27}$$

where

$$L_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j} \tag{3.28}$$

where $\prod$ designates the "product of". For example, the ***linear version (n = 1)*** is

$$f_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) \tag{3.29}$$

and the ***second-order version (n = 2)*** is

$$f_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2) \tag{3.30}$$

Note that each term $L_i(x)$ will be equal to 1 at $x = x_i$ and equal to 0 at all other sample points. Thus, each product $L_i(x)\, f(x_i)$ takes on the value of $f(x_i)$ at the sample point x_i, For more details we have

$$f_2(x)\ at\ x = x_0 \rightarrow L_0(x_0) = 1, L_1(x_0) = 0, L_2(x_0) = 0 \rightarrow f_2(x_0) = f(x_0) + 0 + 0 = f(x_0)$$

$$f_2(x)\ at\ x = x_1 \rightarrow L_0(x_1) = 0, L_1(x_1) = 1, L_2(x_1) = 0 \rightarrow f_2(x_1) = 0 + f(x_1) + 0 = f(x_1)$$

$$f_2(x)\ at\ x = x_2 \rightarrow L_0(x_2) = 0, L_1(x_2) = 0, L_2(x_2) = 1 \rightarrow f_2(x_2) = 0 + 0 + f(x_2) = f(x_2)$$

Example (3.7): Use a Lagrange interpolating polynomial of the first and second order to evaluate ln 2 based on the data given in Example (3.4):

$x_0 = 1$ $f(x_0) = 0$
$x_1 = 4$ $f(x_1) = 1.386294$
$x_2 = 6$ $f(x_2) = 1.791759$

Solution:

The first-order polynomial at x = 2 (using $x_0 = 1$ and $x_1 = 4$)

$$f_1(2) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) = \frac{2-4}{1-4}\, 0 + \frac{2-1}{4-1} 1.386294 = 0.4620981$$

In a similar way, the second-order polynomial is developed as

$$f_2(2) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

$$= \frac{(2-4)(2-6)}{(1-4)(1-6)}\, 0 + \frac{(2-1)(2-6)}{(4-1)(4-6)} 1.386294 + \frac{(2-1)(2-4)}{(6-1)(6-4)} 1.791759$$

$$= 0.5658444$$

As expected, both these results agree with those previously obtained using Newton's interpolating polynomial.

Example (3.8): Find a polynomial which passes the points (0, -12), (1, 0), (3, 6), (4, 12) using a suitable order of Lagrange's interpolation polynomial formula.

Solution:

$x_0 = 0$ $f(x_0) = -12$
$x_1 = 1$ $f(x_1) = 0$
$x_2 = 3$ $f(x_2) = 6$
$x_3 = 4$ $f(x_3) = 12$

We have n = 4 data points, thus, we should use 3^{rd} order Lagrange's interpolation polynomial (n-1).

$$f_3(x) = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} f(x_0) + \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} f(x_1) + \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} f(x_2) + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} f(x_3)$$

$$f_3(x) = \frac{(x-1)(x-3)(x-4)}{(0-1)(0-3)(0-4)}(-12) + \frac{(x-0)(x-3)(x-4)}{(x_1-0)(x_1-3)(x_1-4)}\,0 + \frac{(x-0)(x-1)(x-4)}{(3-0)(3-1)(3-4)}\,6 + \frac{(x-0)(x-1)(x-3)}{(4-0)(4-1)(4-3)}\,12$$

$$f_3(x) = \frac{x^3-8x^2+19x-12}{-12}(-12) + \frac{x^3-5x^2+4x}{-6}\,6 + \frac{x^3-4x^2+3x}{12}\,12$$

$$f_3(x) = x^3-8x^2+19x-12-x^3+5x^2-4x+x^3-4x^2+3x$$

The required 3rd order Lagrange's interpolation formula is

$$f_3(x) = x^3-7x^2+18x-12$$

Exercise (3.5):

a) Find the value of y corresponding to x = 10 using Lagrange interpolating polynomial and the following data for (x, y): (5, 12), (6, 13), (9, 14), and (11, 16).

b) Repeat problems (a) and (b) in Exercise (3.4) using Lagrange interpolating polynomials.

c) Repeat problem (c) in Exercise (3.4) using Lagrange polynomials of order 1 through 3.

Chapter Four - Numerical Integration and Differentiation

4.1. Introduction

Calculus is the mathematics of change. Because engineers must continuously deal with systems and processes that change, calculus is an essential tool of our profession. Standing at the heart of calculus are the related mathematical concepts of differentiation and integration. According to the dictionary definition, to ***differentiate*** means "to mark off by differences; distinguish; . . . to perceive the difference in or between." Mathematically, the ***derivative*** represents ***the rate of change of a dependent variable with respect to an independent variable***. As depicted in **Fig. 4.1**, the mathematical definition of the derivative begins with a difference approximation:

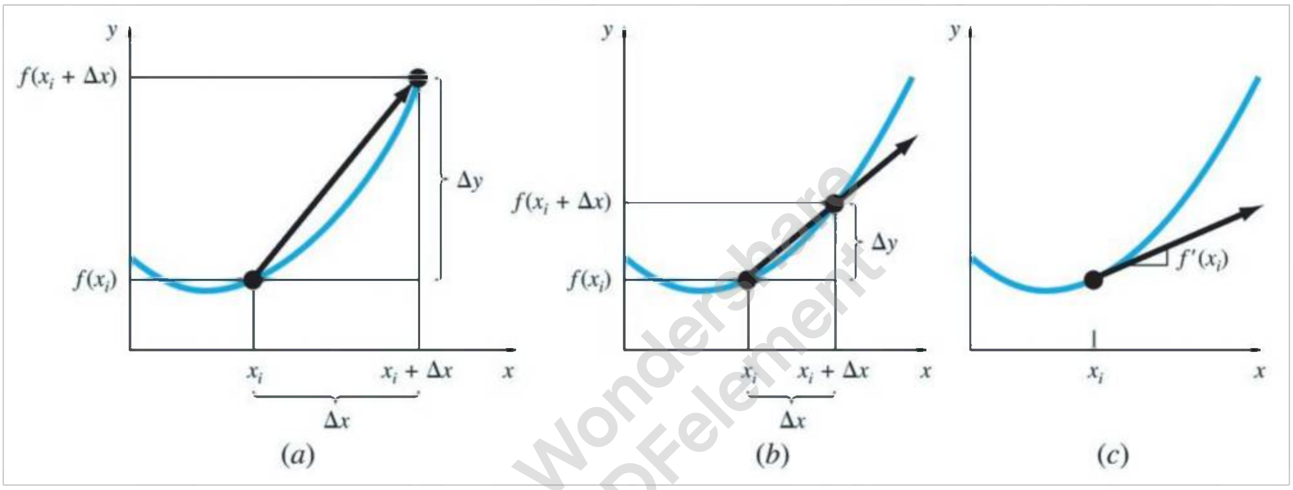


Fig. 4.1 The graphical definition of a derivative: as Δx approaches zero in going from (*a*) to (*c*), the difference approximation becomes a derivative.

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} \tag{4.1}$$

where ***y and f(x)*** are alternative representatives for the ***dependent variable*** and ***x*** is the ***independent variable***. If Δx is allowed to approach zero, as occurs in moving from **Fig. 4.1a to c**, the difference becomes a derivative

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} \tag{4.2}$$

where *dy/dx* [which can also be designated as y' or $f'(x_i)$] is the first derivative of y with respect to x evaluated at x_i. As seen in the visual depiction of **Fig. 4.1c**, ***the derivative*** is the ***slope of the tangent to the curve at*** x_i.

The ***second derivative*** represents the ***derivative of the first derivative***,

$$\frac{d^2y}{dx^2} = \frac{d}{dx}\left(\frac{dy}{dx}\right) \tag{4.3}$$

Thus, the ***second derivative*** tells us how fast the slope is changing. It is commonly referred to as the ***curvature***, because a high value for the second derivative means high curvature.

Finally, ***partial derivatives*** are used for ***functions that depend on more than one variable***. Partial derivatives can be thought of as taking the derivative of the function at a point with all but one variable held constant. For example, given a function f that depends on both x and y, the partial derivative of f with respect to x at an arbitrary point (x, y) is defined as

$$\frac{\partial f}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x,\ y) - f(x,\ y)}{\Delta x} \tag{4.4}$$

Similarly, the partial derivative of f with respect to y is defined as

$$\frac{\partial f}{\partial y} = \lim_{\Delta y \to 0} \frac{f(x,\ y + \Delta y) - f(x,\ y)}{\Delta y} \tag{4.5}$$

For further understanding of ***partial derivatives***, recognize that a ***function that depends on two variables*** is a ***surface rather than a curve***. Suppose you are mountain climbing and have access to a function (f) that yields elevation as a function of longitude (the east-west oriented x-axis) and latitude (the north-south oriented y-axis). If you stop at a particular point, (x_0, y_0), the slope to the east would be $\partial f(x_0, y_0)/\partial x$ and the slope to the north would be $\partial f(x_0, y_0)/\partial y$.

The inverse process to differentiation in calculus is ***integration***. According to the definition of dictionary, "***to integrate***" means "***to bring parts together into a whole***"; "***to unite***"; or "***to indicate the total amount***". Mathematically, ***integration*** is represented by

$$I = \int_a^b f(x)\, dx \tag{4.6}$$

which stands for the integral of the function $f(x)$ with respect to the independent variable x, evaluated between the limits x = a to x = b. The function $f(x)$ in Eq. (4.6) is referred to as the ***integrand*** (i.e., the function that is to be integrated).

The "***meaning***" of Eq. (4.6) is the ***total value***, or ***summation***, of ***f(x) dx*** over the range ***x = a to b***. In fact, the symbol $\int$ is actually a ***stylized capital S*** that is intended to signify the close connection between integration and summation. **Fig. 4.2** represents a graphical demonstration of ***definite integration***. For functions lying above the x axis, the integral expressed by Eq. (4.6) corresponds to the area under the curve of $f(x)$ between x = a and b.

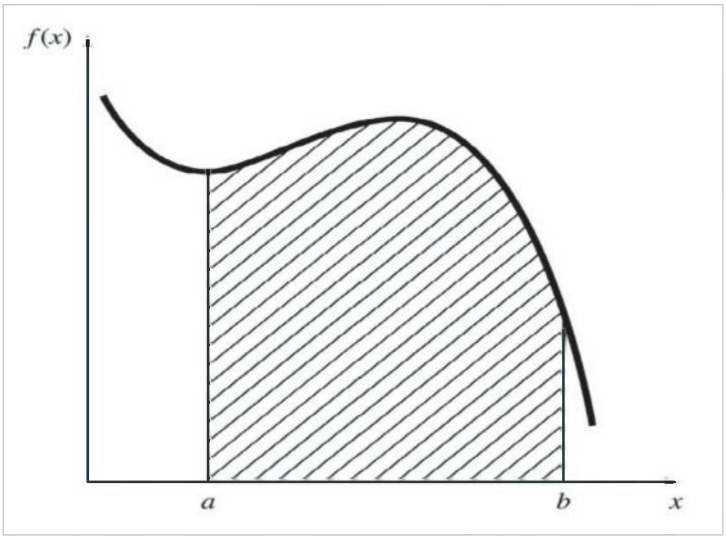


Fig. 4.2 Graphical representation of the integral of $f(x)$ between the limits x = a to b. The integral is equivalent to the area under the curve.

The ***differentiation*** and ***integration*** are closely related processes that are, in fact, inversely related (**Fig. 4.3**). For example, if we are given a function y(t) that specifies an ***object's position as a function of time***, ***differentiation*** provides a means to determine its ***velocity***, as in (**Fig. 4.3a**).

$$v(t) = \frac{d}{dt}\, y(t)$$

Conversely, if we are provided with ***velocity as a function of time***, ***integration*** can be used to determine its ***position*** (**Fig. 4.3b**),

$$y(t) = \int_0^t v(t)\, dt$$

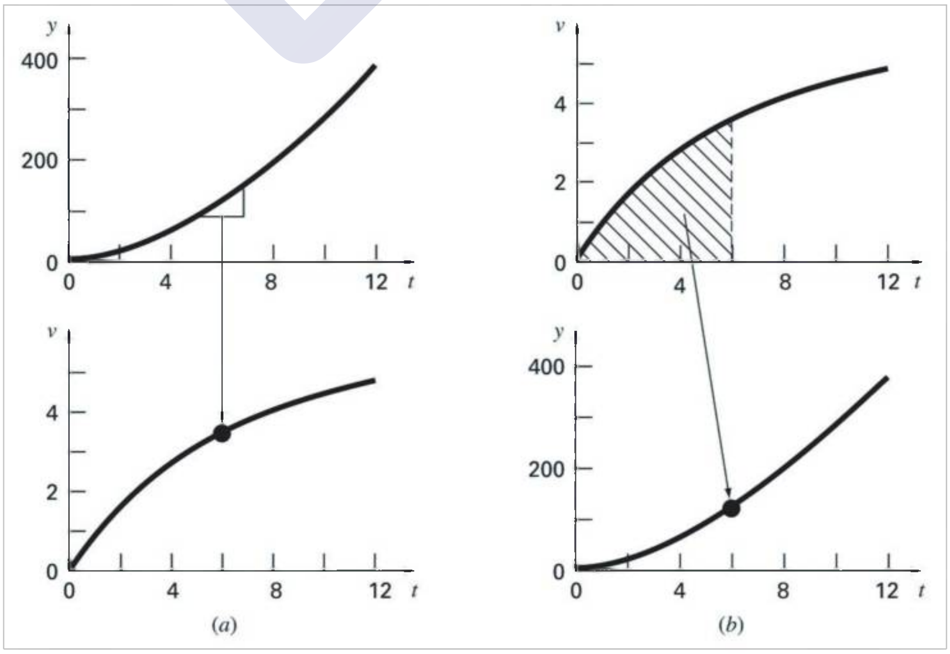


Fig. 4.3 The contrast between (a) differentiation and (b) integration.

4.2. Numerical Integration: Newton-Cotes Integration Formulas

The calculation of integrals is important in engineering applications. A number of examples relate directly to the idea of the integral as the area under a curve are presented in **Fig. 4.4**. The most common approaches for numerical integration is the ***Newton-Cotes formulas***.

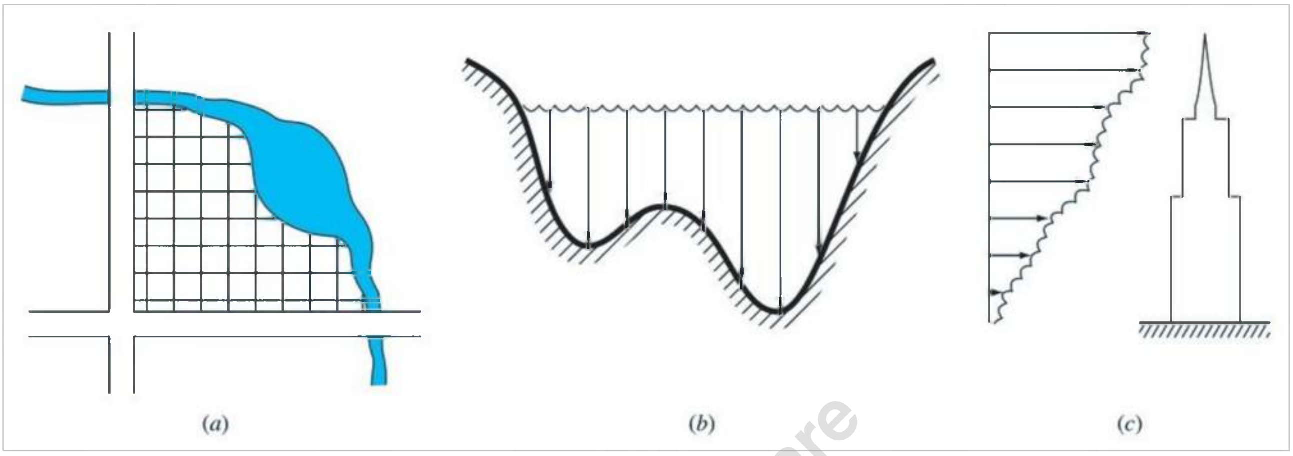


Fig. 4.4 Examples of how integration is used to evaluate areas in engineering applications. (a) A surveyor might need to know the area of a field bounded by a meandering stream and two roads. (b) A water-resource engineer might need to know the cross-sectional area of a river. (c) A structural engineer might need to determine the net force due to a non-uniform wind blowing against the side of a skyscraper.

The ***Newton-Cotes Integration Formulas*** are based on the strategy of replacing a complicated function or tabulated data with an approximating function that is easy to integrate:

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_n(x)\,dx \tag{4.7}$$

where $f_n(x)$ = a polynomial of the form

$$f_n(x) = a_0 + a_1 x + \cdots + a_{n-1} x^{n-1} + a_n x^n \tag{4.8}$$

where n is the order of the polynomial. For example, in **Fig. 4.5a**, a ***first-order polynomial*** (a straight line) is used as an approximation. In **Fig. 4.5b**, a ***parabola*** is employed for the same purpose. The integral can also be approximated using a series of polynomials applied piecewise to the function or data over segments of constant length. For example, in **Fig. 4.5c**, three straight-line segments are used to approximate the integral. Higher-order polynomials can be utilized for the same purpose.

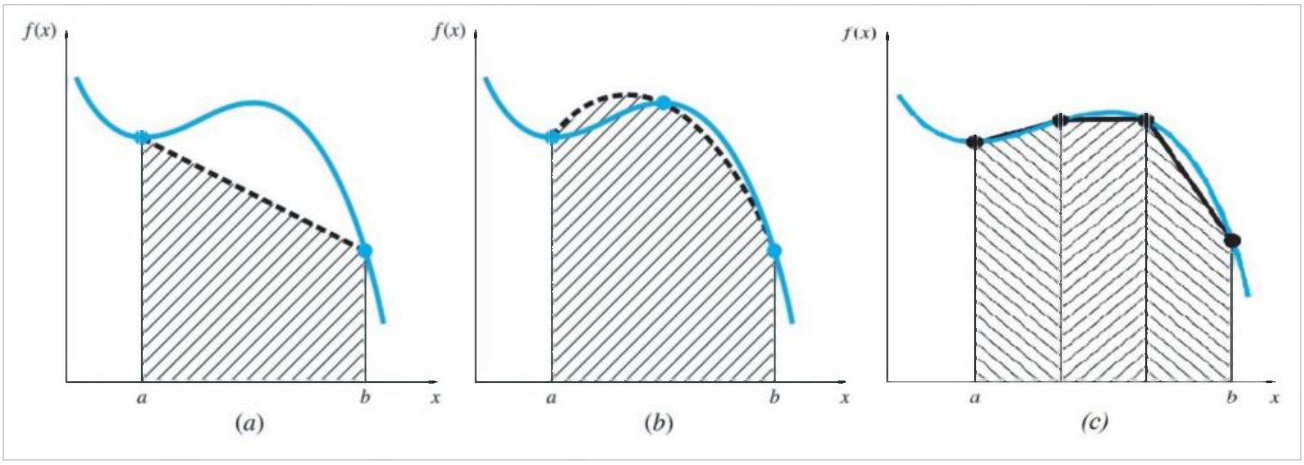


Fig. 4.5 The approximation of an integral by the area under (a) a single straight line and (b) a single parabola. (c) The approximation of an integral by the area under three straight-line segments.

Closed and ***open forms*** of the Newton-Cotes formulas are available. The ***closed forms*** are those where the data points at the beginning and end of the limits of integration are known (**Fig. 4.6a**). The ***open forms*** have integration limits that extend beyond the range of the data (**Fig. 4.6b**). In this sense, they are similar to extrapolation. Open Newton-Cotes formulas are not generally used for definite integration. This chapter deals with the ***closed forms*** of the ***Newton-Cotes integration formulas***.

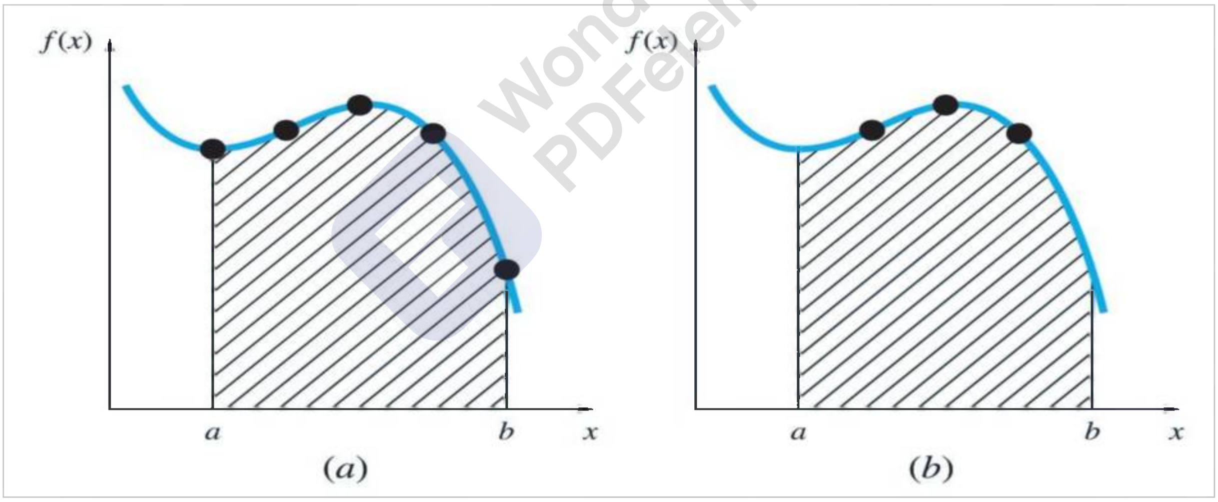


Fig. 4.6 The difference between (a) closed and (b) open integration formulas.

4.2.1. The Trapezoidal Rule

The ***trapezoidal rule*** is the first of the ***Newton-Cotes closed integration formulas***. It corresponds to the case where the polynomial in Eq. (4.7) is first order:

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_1(x)\,dx \quad (4.9)$$

Recall from linear interpolation in chapter three - curve fitting, the straight line can be represented as

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \tag{4.10}$$

The area under this straight line is an estimate of the integral of $f(x)$ between the limits a and b:

$$I = \int_a^b \left[f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right] dx \tag{4.11}$$

The result of the integration shown below is called the ***trapezoidal rule***.

$$I = (b - a)\,\frac{f(a) + f(b)}{2} \tag{4.12}$$

Geometrically, the trapezoidal rule is equivalent to approximating the area of the trapezoid under the straight line connecting $f(a)$ and $f(b)$ in **Fig. 4.7**. Therefore, the integral estimate can be represented as

$$I \cong \text{width} \times \text{average height} \cong (b - a) \times \text{average height} \tag{4.13}$$

All the ***Newton-Cotes closed formulas*** can be expressed in the general format of the above equation. In fact, ***they differ only*** with respect to the ***formulation of the average height***.

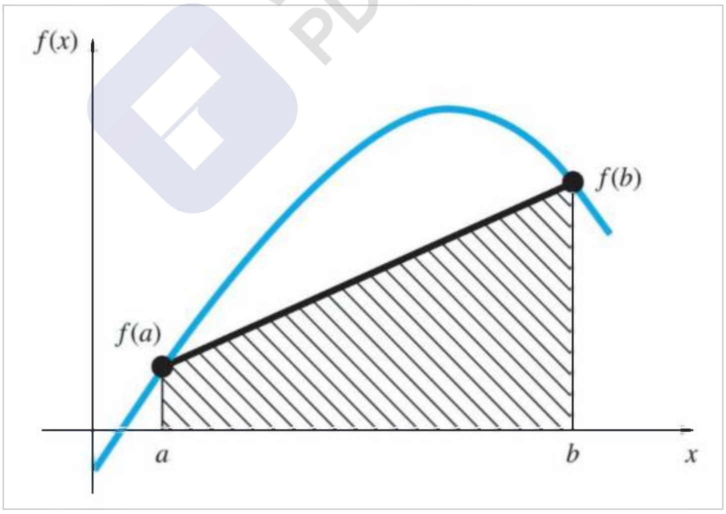


Fig. 4.7 Graphical depiction of the trapezoidal rule.

<u>Example (4.1)</u>: Use the trapezoidal rule to numerically integrate

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

from a = 0 to b = 0.8. Evaluate the error and note that the exact value of the integral is 1.640533.

Solution: The function values

At a = 0 $\rightarrow$ $f(a) = f(0) = 0.2$

At b = 0.8 $\rightarrow$ $f(b) = f(0.8) = 0.232$

can be substituted into Eq. (4.12) to yield

$$I = (b-a)\,\frac{f(a)+f(b)}{2} = (0.8-0)\,\frac{0.2+0.232}{2} = 0.1728$$

which represents an error of $\left|\frac{1.640533-0.1728}{1.640533}\right| \times 100 = 89.47\%$

Example (4.2): Evaluate the following integral using the trapezoidal rule. Estimate the error and note that x is in radians and the exact value of the integral is 12.4248.

$$I = \int_0^{\pi/2} (6+3\ \cos x)\ dx$$

Solution: Using $f(x) = 6+3\ \cos x$, the function values are

At a = 0 $\rightarrow$ $f(a) = f(0) = 9$

At b = $\pi/2 \rightarrow$ $f(b) = f(\pi/2) = 6$

$$I = (b-a)\,\frac{f(a)+f(b)}{2} = \left(\frac{\pi}{2}-0\right)\frac{9+6}{2} = 11.7809$$

which represents an error of $\left|\frac{12.4248-11.7809}{12.4248}\right| \times 100 = 5.18\%$

4.2.2. 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 (**Fig. 4.8**). The areas of individual segments can then be added to yield the integral for the entire interval. The resulting equations are called ***multiple-application***, or ***composite***, ***integration formulas***.

The general format and nomenclature we will use to characterize multiple-application integrals is shown in **Fig. 4.9**. There are ***n + 1 equally spaced base points*** ($x_0, x_1, x_2, \ldots, x_n$). Consequently, there are ***n segments*** of ***equal width (h)***:

$$h = \frac{b-a}{n} \tag{4.14}$$

If a and b are designated as x_0 and x_n, respectively, the total integral can be represented as

$$I = \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\,dx \tag{4.15}$$

Substituting the trapezoidal rule for each integral yields

$$I = h\frac{f(x_0)+f(x_1)}{2} + h\frac{f(x_1)+f(x_2)}{2} + \cdots + h\frac{f(x_{n-1})+f(x_n)}{2} \quad (4.16)$$

or, grouping terms,

$$I = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right] \quad (4.17)$$

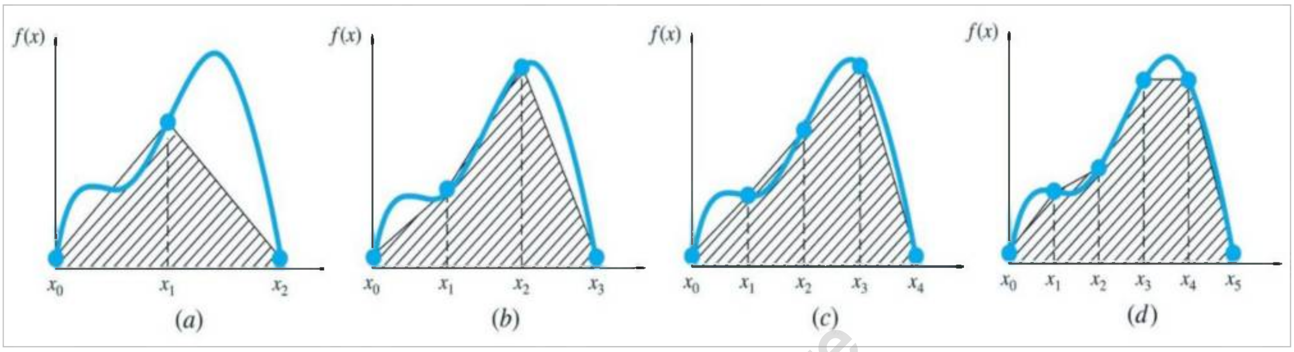


Fig. 4.8 Demonstration of the multiple-application trapezoidal rule. (a) Two segments, (b) three segments, (c) four segments, and (d) five segments.

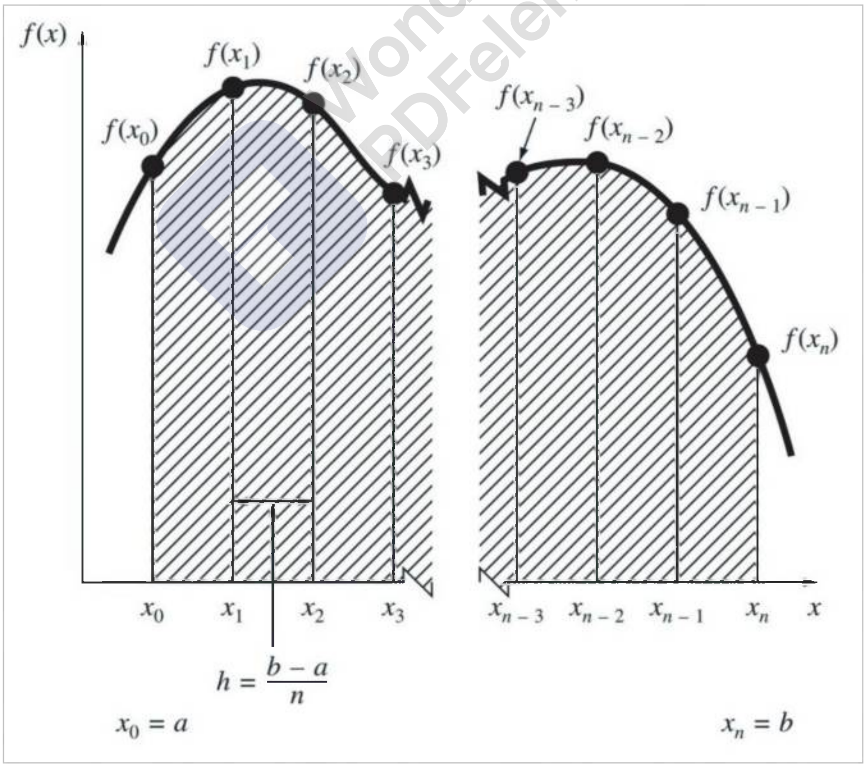


Fig. 4.9 The general format and nomenclature for multiple-application integrals.

or, using Eq. (4.14) to express Eq. (4.17) in the general form of Eq. (4.13),

$$I = \underbrace{(b-a)}_{Width} \underbrace{\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}}_{Average\ height} \tag{4.18}$$

Because the summation of the coefficients of $f(x)$ in the numerator divided by 2n is equal to 1, the ***average height*** represents a ***weighted average of the function values***. According to Eq. (4.18), the interior points are given twice the weight of the two end points $f(x_0)$ and $f(x_n)$.

Example (4.3): Use the two-segment trapezoidal rule to estimate the integral of

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

from a = 0 to b = 0.8. Estimate the error and note that the exact value of the integral is 1.640533.

Solution: With n = 2, (h = (b – a) /2 = (0.8 – 0) / 2 = 0.4) . The function values

At $x_0 = 0 \rightarrow f(x_0) = f(0) = 0.2$

At $x_1 = 0.4 \rightarrow f(x_1) = f(0.4) = 2.456$

At $x_2 = 0.8 \rightarrow f(x_2) = f(0.8) = 0.232$

can be substituted into Eq. (4.18) to yield

$$I = (b-a)\frac{f(x_0)+2\sum_{i=1}^{n-1} f(x_i)+f(x_n)}{2n} = (0.8)\frac{0.2 + 2\times(2.456) + 0.232}{2\times 2} = 1.0688$$

which represents an error of $\left|\frac{1.640533 - 1.0688}{1.640533}\right| \times 100 = 34.85\%$

The results of the previous example, along with three- through ten-segment applications of the trapezoidal rule, are summarized in the following table.

n	h	*I*	Error %
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	1.615	1.6

Example (4.4): Evaluate the following integral using multiple-application trapezoidal rule, with n = 2 and 4. Estimate the error in each stage and note that x is in radians and the exact value of the integral is 12.4248.

$$I = \int_0^{\pi/2} (6 + 3\ \cos x)\ dx$$

Solution:

Using $f(x) = 6 + 3\ \cos x$, the function values can be evaluated as follows;

(a) With n = 2, $h = \frac{b-a}{n} = \frac{\frac{\pi}{2} - 0}{2} = \frac{\pi}{4}$, the function values

$x_0 = 0 \quad \rightarrow \quad f(x_0) = f(0) = 9$

$x_1 = \frac{\pi}{4} \quad \rightarrow \quad f(x_1) = f(\frac{\pi}{4}) = 8.1213$

$x_2 = \frac{\pi}{2} \quad \rightarrow \quad f(x_2) = f(\frac{\pi}{2}) = 6$

can be substituted into Eq. (4.18) to yield

$$I = (b-a)\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n} = \left(\frac{\pi}{2}\right)\frac{9 + 2 \times (8.1213) + 6}{2 \times 2} = 12.2689$$

which represents an error of $\left|\frac{12.4248 - 12.2689}{12.4248}\right| \times 100 = 1.25\%$

(b) With n = 4, $h = \frac{b-a}{n} = \frac{\frac{\pi}{2} - 0}{4} = \frac{\pi}{8}$, the function values

$x_0 = 0 \quad \rightarrow \quad f(x_0) = f(0) = 9$

$x_1 = \frac{\pi}{8} \quad \rightarrow \quad f(x_1) = f(\frac{\pi}{8}) = 8.7716$

$x_2 = \frac{\pi}{4} \quad \rightarrow \quad f(x_2) = f(\frac{\pi}{4}) = 8.1213$

$x_3 = \frac{3\pi}{8} \quad \rightarrow \quad f(x_3) = f(\frac{3\pi}{8}) = 7.1481$

$x_4 = \frac{\pi}{2} \quad \rightarrow \quad f(x_4) = f(\frac{\pi}{2}) = 6$

can be substituted into Eq. (4.18) to yield

$$I = (b-a)\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n} = \left(\frac{\pi}{2}\right)\frac{9 + 2 \times (8.7716 + 8.1213 + 7.1481) + 6}{2 \times 4} = 12.3861$$

which represents an error of $\left|\frac{12.4248 - 12.3861}{12.4248}\right| \times 100 = 0.31\%$

Exercise (4.1):

a) Using the trapezoidal rule with **(a)** single application and **(b)** multiple-application, with n = 2 and 4, evaluate the following integral. Estimate the error in each stage and note that the exact value of the integral is 2.5012. $\int_0^3 (1 - e^{-2x})\ dx$

b) Evaluate the following integral using **(a)** single application of the trapezoidal rule and **(b)** multiple-application trapezoidal rule, with n = 2 and 4. Estimate the error in each stage and note that x is in radians and the exact value of the integral is 16.5664. $I = \int_0^{\pi/2}(8 + 4\cos x)\,dx$

c) Using the trapezoidal rule with n = 1, 2, 3, and 4, evaluate the following integral. Estimate the error in each stage and note that the exact value of the integral is 8.3333. $\int_1^2 \left(x + \frac{2}{x}\right)^2 dx$

4.2.3. Simpson's Rules

Aside from applying the trapezoidal rule with finer segmentation, another way to obtain a more accurate estimate of an integral is to use ***higher-order polynomials to connect the points***. For example, if there is an extra point midway between $f(a)$ and $f(b)$, the three points can be connected with a parabola (**Fig. 4.10a**). If there are two points equally spaced between $f(a)$ and $f(b)$, the four points can be connected with a third-order polynomial (**Fig. 4.10b**). The formulas that result from taking the integrals under these polynomials are called ***Simpson's rules***.

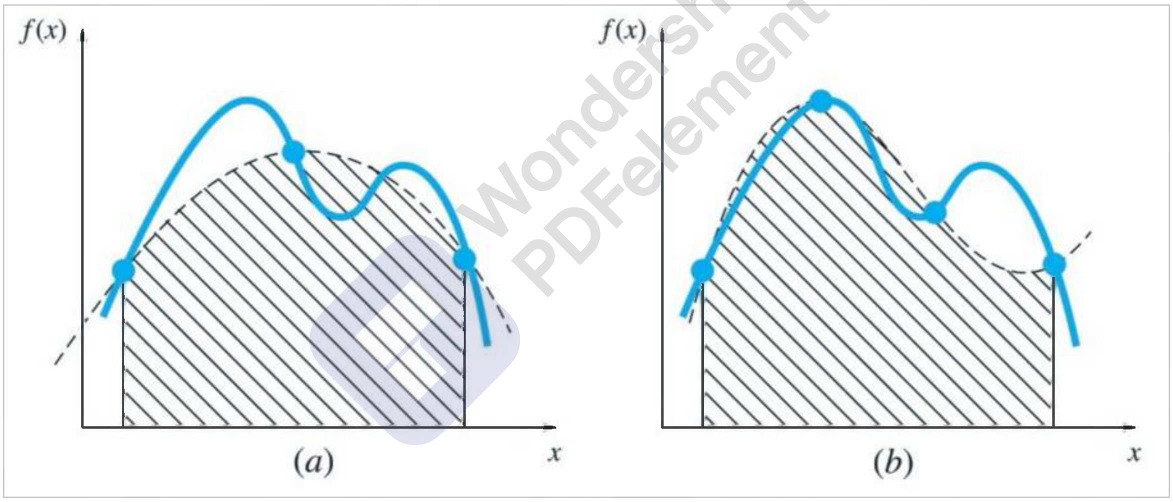


Fig. 4.10 (a) Graphical depiction of Simpson's 1/3 rule: It consists of taking the area under a parabola connecting three points. (b) Graphical depiction of Simpson's 3/8 rule: It consists of taking the area under a cubic (third-order) equation connecting four points.

4.2.3.1. Simpson's 1/3 Rule

Simpson's 1/3 rule results when a second-order interpolating polynomial (n = 2) is substituted into Eq. (4.7):

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_2(x)\,dx \qquad (4.19)$$

If a and b are designated as x_0 and x_2 and $f_2(x)$ is represented by a second-order Lagrange polynomial

[Eq. (3.30)], the integral becomes

$$I = \int_{x_o}^{x_2} \left[\frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2) \right] dx \qquad (4.20)$$

After integration and algebraic manipulation, the following formula results:

$$I \cong \frac{h}{3} \left[f(x_0) + 4 f(x_1) + f(x_2) \right] \qquad (4.21)$$

where, for this case, h = (b - a) / 2. This equation is known as ***Simpson's 1/3 rule***. It is ***the second Newton-Cotes closed integration formula***. The label "**1/3**" stems from the fact that ***h is divided by 3*** in Eq. (4.21). Simpson's 1y3 rule can also be expressed using the format of Eq. (4.13):

$$I \cong \underbrace{(b - a)}_{Width} \underbrace{\frac{f(x_0) + 4 f(x_1) + f(x_2)}{6}}_{Average\ height} \qquad (4.22)$$

where $a = x_0$, $b = x_2$, and x_1 = the point midway between a and b, which is given by (b + a) / 2. Notice that, according to Eq. (4.22), the ***middle point*** *is weighted by* ***two-thirds*** and the ***two end points*** *by* ***one-sixth***.

Example (4.5): Use Simpson's 1/3 rule to integrate the following equation from a = 0 to b = 0.8. Estimate the error and note that the exact value of the integral is 1.640533.

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

Solution: n = 2

With $x_0 = a = 0$ and $x_2 = b = 0.8$ → $h = \frac{b-a}{2} = \frac{0.8-0}{2} = 0.4$ ***or*** $x_1 = \frac{b+a}{2} = \frac{0.8+0}{2} = 0.4$

The function values $x_0 = 0$ → $f(x_0) = f(0) = 0.2$

$x_1 = 0.4$ → $f(x_1) = f(0.4) = 2.456$

$x_2 = 0.8$ → $f(x_2) = f(0.8) = 0.232$

Therefore, Eq. (4.22) can be used to compute

$$I \cong (b - a)\frac{f(x_0)+4 f(x_1)+f(x_2)}{6} = (0.8 - 0)\frac{0.2 + 4(2.456) + 0.232}{6} = 1.367467$$

which represents an error of $\left|\frac{1.640533 - 1.367467}{1.640533}\right| \times 100 = 16.64\%$

4.2.3.2. The Multiple-Application Simpson's 1/3 Rule

Just as with the trapezoidal rule, Simpson's rule can be improved by dividing the integration interval into a number of segments of equal width (**Fig. 4.11**):

$$h = \frac{b-a}{n} \tag{4.23}$$

The total integral can be represented as

$$I = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx \tag{4.24}$$

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

$$I \cong 2h\frac{f(x_0)+4f(x_1)+f(x_2)}{6} + 2h\frac{f(x_2)+4f(x_3)+f(x_4)}{6} + \cdots + 2h\frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6} \tag{4.25}$$

or, combining terms and using Eq. (4.23),

$$I \cong \underbrace{(b-a)}_{Width}\underbrace{\frac{f(x_0)+4\sum_{i=1,3,5}^{n-1}f(x_i)+2\sum_{j=2,4,6}^{n-2}f(x_j)+f(x_n)}{3n}}_{Average\ height} \tag{4.26}$$

Notice that, as illustrated in **Fig. 4.11**, an ***even number of segments*** must be utilized to implement the method. In addition, the coefficients "**4**" and "**2**" in Eq. (4.26) might seem strange at first glance. However, they follow naturally from Simpson's 1/3 rule. The ***odd points*** represent the middle term for each application and hence carry the ***weight of 4*** from Eq. (21.15). The ***even points*** are common to adjacent applications and hence are ***counted twice***.

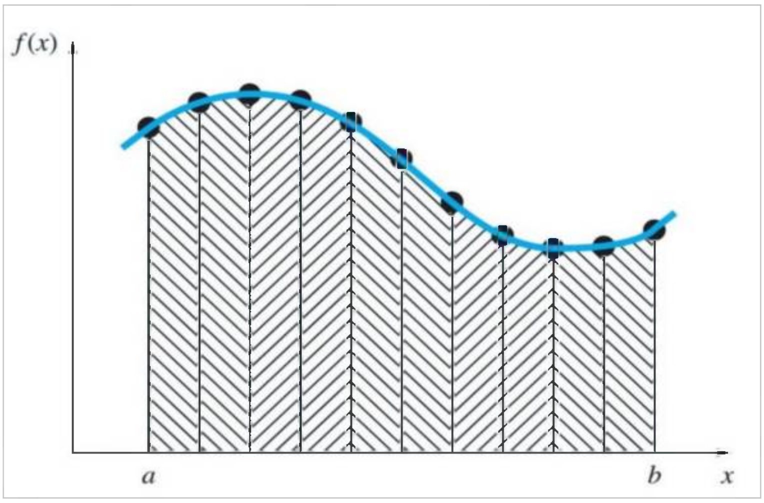


Fig. 4.11 Graphical representation of the multiple application of Simpson's 1/3 rule. Note that the method can be employed only if the ***number of segments is even***.

Example (4.6): Use Simpson's 1/3 rule with n = 4 to estimate the integral of

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

from a = 0 to b = 0.8. Estimate the error and note that the exact value of the integral is 1.640533.

Solution:

With a = 0 , b = 0.8 , and n = 4 $\rightarrow$ $h = \frac{b-a}{n} = \frac{0.8-0}{4} = 0.2$

The function values $x_0 = 0 \rightarrow f(x_0) = f(0) = 0.2$

$x_1 = 0.2 \rightarrow f(x_1) = f(0.2) = 1.288$

$x_2 = 0.4 \rightarrow f(x_2) = f(0.8) = 2.456$

$x_3 = 0.6 \rightarrow f(x_3) = f(0.6) = 3.464$

$x_4 = 0.8 \rightarrow f(x_4) = f(0.8) = 0.232$

Therefore, Eq. (4.26) can be used to compute

$$I \cong (b-a)\frac{f(x_0)+4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n} = (0.8 - 0)\frac{0.2 + 4\,(1,288+3.464) + 2\,(2.456) + 0.232}{3 \times 4} = 1.623467$$

which represents an error of $\left|\frac{1.640533 - 1.623467}{1.640533}\right| \times 100 = 1.04\%$

The previous example illustrates that the multiple-application version of Simpson's 1/3 rule yields very accurate results. For this reason, it is considered superior to the trapezoidal rule for most applications. However, as mentioned previously, ***it is limited*** to cases where ***the values are equispaced***. Further, ***it is limited*** to situations where there are an ***even number of segments*** and an ***odd number of points***.

Example (4.7): Calculate the total distance travelled in kilometers by a train from the time it starts moving from rest until it stops after 20 minutes using the data in the following table with Simpson's 1/3 rule.

Time (t) (minutes)	2	4	6	8	10	12	14	16	18
Velocity (v) (km/hr)	16	28.8	40	46.4	51.2	32.0	17.6	8	3.2

Solution:

The train starts moving from rest $\rightarrow$ at t = 0 (minutes), v = 0 (km/hr)

The train stops at t = 20 (minutes) $\rightarrow$ at t = 20 (minutes), v = 0 (km/hr)

$$v = \frac{ds}{dt} \rightarrow ds = v.dt \rightarrow \int ds = \int v.dt \rightarrow s = \int_0^{(20/60)\,hr} v.dt$$

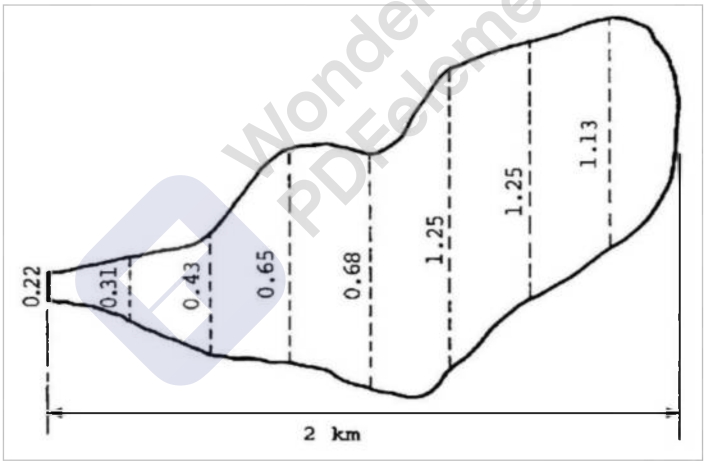
The two points in which the train starts and stops should be added to the given table to estimate the total distance travelled during 20 minutes from start to stop. Thus;

Time (t) (minutes)	0	2	4	6	8	10	12	14	16	18	20
t_i	t_0	t_1	t_2	t_3	t_4	t_5	t_6	t_7	t_8	t_9	t_{10}
Velocity (v) (km/hr)	0	16	28.8	40	46.4	51.2	32.0	17.6	8	3.2	0
$v_i = f(t_i)$	v_0	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8	v_9	v_{10}

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

$$= \frac{(20-0)}{60} \times \frac{0 + 4\,(16+40+51.2+17.6+3.2) + 2\,(28.8+46.4+32.0+8)+ 0}{3 \times 10} = 8.249 \text{ km}$$

Example (4.8): The dimensions (in km) of a dammed lake were measured from an aerial photograph with the results below in the figure. Estimate its area using the trapezoidal and Simpson's 1/3 rules.



Solution:

The dimensions of the dammed lake can be listed in the table below using n = 8 and including an end point of x_8 = 2 km and y_8 = 0 km

We have $n = 8$ *and* $h = \frac{b-a}{n} = \frac{2-0}{8} = 0.25\,km$

Length (x) (km)	0.00	0.25	0.50	0.75	1.00	1.25	1.50	1.75	2.00
x_i	x_0	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8
Width (y) (km)	0.22	0.31	0.43	0.65	0.68	1.25	1.25	1.13	0
$y_i = f(x_i)$	y_0	y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8

Using the trapezoidal rule with number of segments n = 8

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

$$= (2)\frac{0.22 + 2 \times (0.31 + 0.43 + 0.65 + 0.68 + 1.25 + 1.25 + 1.13) + 0}{2 \times 8}$$

$$= 1.453 \text{ km}^2$$

Using Simpson's 1/3 rule with n = 8

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

$$= (2) \times \frac{0.22 + 2 \times 4\,(0.31 + 0.65 + 1.25 + 1.13) + 2\,(0.43 + 0.68 + 1.25) + 0}{3 \times 8}$$

$$= 1.525 \text{ km}^2$$

Exercise (4.2):

a) Evaluate the integral $\int_1^4 \frac{1}{x} dx$ using **(a)** single application of Simpson's 1/3 rule and **(b)** multiple-application Simpson's 1/3 rule with n = 6. Estimate the error in each stage and note that the exact value of the integral is 1.3863.

b) Use Simpson's 1/3 Rule with n = 4 to find the approximate value of the integral $\int_0^1 \sqrt{1-x^2}\ dx$.

c) Using Simpson's 1/3 rule with **(a)** single application and **(b)** multiple-application with n = 4, evaluate the following integral. Estimate the error in each stage and note that the exact value of the integral is 2.5012. $\int_0^3 (1 - e^{-2x})\ dx$

d) Evaluate the following integral using **(a)** single application of Simpson's 1/3 rule and **(b)** multiple-application Simpson's 1/3 rule with n = 4. Estimate the error in each stage and note that x is in radians and the exact value of the integral is 16.5664. $I = \int_0^{\pi/2} (8 + 4\cos x)\ dx$

4.2.3.3. Simpson's 3/8 Rule

In a similar manner to the derivation of the trapezoidal and Simpson's 1/3 rule, a third-order Lagrange polynomial can be fitted to four points and integrated:

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_3(x)\,dx \qquad (4.27)$$

After integration and algebraic manipulation and if a and b are designated as x_0 and x_3 , the following formula results:

$$I \cong \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right] \qquad (4.28)$$

where h = (b - a) / 3. This equation is called ***Simpson's 3/8 rule*** because ***h is multiplied by 3/8***. It is the third Newton-Cotes closed integration formula. The 3/8 rule can also be expressed in the form of Eq. (4.13):

$$I \cong \underbrace{(b-a)}_{Width} \underbrace{\frac{f(x_0)+3\,f(x_1)+3\,f(x_2)+\,f(x_3)}{8}}_{Average\ height} \tag{4.29}$$

Thus, the two ***interior points*** *are given weights of* ***three-eighths***, whereas the ***end points*** *are weighted with* ***one-eighth***. Further, this formula is limited to situations where there are an ***odd number of segments*** and an ***even number of points***.

Example (4.9):

(a) Use Simpson's 3/8 rule to integrate the following equation from a = 0 to b = 0.8. Estimate the error and note that the exact value of the integral is 1.640533.

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

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

Solution:

(a) With n = 3, $x_0 = a = 0$ and $x_3 = b = 0.8 \rightarrow h = \frac{b-a}{3} = \frac{0.8-0}{3} = 0.2667$

The function values
$x_0 = 0 \rightarrow f(x_0) = f(0) = 0.2$
$x_1 = 0.2667 \rightarrow f(x_1) = f(0.2667) = 1.432724$
$x_2 = 0.5333 \rightarrow f(x_2) = f(0.5333) = 3.487177$
$x_3 = 0.8 \rightarrow f(x_3) = f(0.8) = 0.232$

Therefore, Eq. (4.22) can be used to compute

$$I \cong (b-a)\frac{f(x_0)+3\,f(x_1)+3\,f(x_2)+f(x_3)}{8} = (0.8)\frac{0.2+3\,(1.432724+3.487177)+0.232}{8} = 1.51917$$

which represents an error of $\left|\frac{1.640533-1.51917}{1.640533}\right| \times 100 = 7.39\%$

(b) The data needed for a five-segment application (n = 2 (Simpson's 1/3) + 3 (Simpson's 3/8) = 5)

With, n = 5, $x_0 = a = 0$ and $x_5 = b = 0.8 \rightarrow h = \frac{b-a}{n} = \frac{0.8-0}{5} = 0.16$

The function values
$x_0 = 0 \rightarrow f(x_0) = f(0) = 0.2$
$x_1 = 0.16 \rightarrow f(x_1) = f(0.16) = 1.296919$
$x_2 = 0.32 \rightarrow f(x_2) = f(0.32) = 1.743393$
$x_3 = 0.48 \rightarrow f(x_3) = f(0.48) = 3.186015$

$x_4 = 0.64 \quad \rightarrow \quad f(x_4) = f(0.64) = 3.181929$

$x_5 = 0.8 \quad \rightarrow \quad f(x_5) = f(0.8) = 0.232$

The integral (I_1) for the first two segments (from x_0 to x_2) is obtained using Simpson's 1/3 rule:

$$I_1 \cong (x_2 - x_0)\frac{f(x_0)+4f(x_1)+f(x_2)}{6} = (0.32-0)\frac{0.2+4(1.296919)+1.743393}{6} = 0.380324$$

The integral (I_2) for the last three segments (from x_2 to x_5) is obtained using Simpson's 3/8 rule:

$$I_2 \cong (x_5 - x_2)\frac{f(x_2)+3f(x_3)+3f(x_4)+f(x_5)}{8} = (0.8 - 0.32)\frac{1.743393+3(3.186015+3.181929)+0.232}{8} = 1.264754$$

The total integral is computed by summing the two results:

$$I = I_1 + I_2 = 0.3803237 + 1.264754 = 1.645078$$

which represents an error of $\left|\frac{1.640533-1.645078}{1.640533}\right| \times 100 = 0.28\%$

Example (4.10): Find the area beneath the curve $y = 1 - \sin x$ and the x-axis from $x = 0$ to $x = \pi$ using Simpson's 3/8 rule. Estimate the error and note that the exact value of the integral is 1.14159 and x in radians.

Solution: With $n = 3$, $x_0 = a = 0$ and $x_3 = b = \pi \rightarrow h = \frac{b-a}{3} = \frac{\pi - 0}{3} = \frac{\pi}{3}$

The function values $x_0 = 0 \quad \rightarrow \quad f(x_0) = f(0) = 1$

$x_1 = \frac{\pi}{3} \quad \rightarrow \quad f(x_1) = f(\frac{\pi}{3}) = 0.13397$

$x_2 = \frac{2\pi}{3} \quad \rightarrow \quad f(x_2) = f(\frac{2\pi}{3}) = 0.13397$

$x_3 = \pi \quad \rightarrow \quad f(x_3) = f(\pi) = 1$

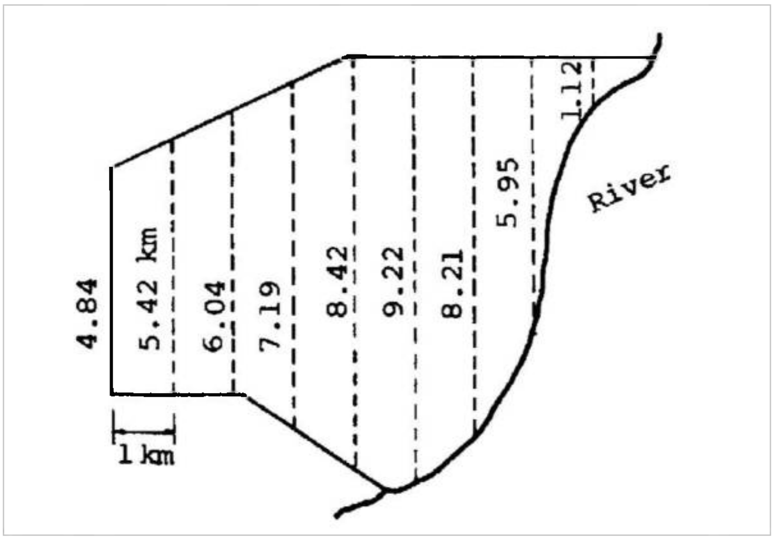
can be used to compute

$$I \cong (b-a)\frac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8} = (\pi)\frac{1+3(0.13397+0.13397)+1}{8} = 1.10106$$

which represents an error of $\left|\frac{1.14159-1.10106}{1.14159}\right| \times 100 = 3.55\%$

Exercise (4.3):

a) A farmer is planning to plant the palm plantation shown in the figure below. Using **(a)** multiple-application trapezoidal rule and **(b)** multiple-application Simpson's 3/8 rule, estimate the number of palm trees if a planting pattern of 16 trees per 1000 m^2 will to be used. All dimensions shown are in kilometers.



b) Evaluate the integral $\int_1^4 \frac{1}{x} dx$ using **(a)** single application of Simpson's 3/8 rule and **(b)** multiple-application Simpson's 3/8 rule with n = 6. Estimate the error in each stage and note that the exact value of the integral is 1.3863.

c) Use Simpson's 3/8 Rule to find the approximate value of the integral $\int_0^1 \sqrt{1-x^2}\ dx$.

d) Using Simpson's 3/8 rule with **(a)** single application and **(b)** multiple-application with n = 6, evaluate the following integral. Estimate the error in each stage and note that the exact value of the integral is 2.5012. $\int_0^3 (1 - e^{-2x})\ dx$

e) Evaluate the following integral using **(a)** single application of Simpson's 3/8 rule and **(b)** multiple-application Simpson's 3/8 rule with n = 6. Estimate the error in each stage and note that x is in radians and the exact value of the integral is 16.5664. $I = \int_0^{\pi/2} (8 + 4\ \cos x)\ dx$

4.2.3.4. Integration with Unequal Segments

All numerical integration formulas that have been presented in this chapter were based on ***equally spaced data points***. ***In practice***, there are many situations where this assumption does not hold and we must deal with ***unequal-sized segments***. For example, experimentally derived data are often of this type. For these cases, one method is to apply the trapezoidal rule to each segment and sum the results:

$$I = h_1 \frac{f(x_0) + f(x_1)}{2} + h_2 \frac{f(x_1) + f(x_2)}{2} + \cdots + h_n \frac{f(x_{n-1}) + f(x_n)}{2} \qquad (4.30)$$

where h_i = the width of ***segment i***. This was the same approach used for the multiple-application trapezoidal rule. The only difference between them is that the h's in the former are constant.

Example (4.11): Using the following polynomial function, the table below was generated with unequally spaced values of x. $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ Determine the integral for these data in the table using the trapezoidal rule. Estimate the error and note that the exact value of the integral is 1.640533.

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

Solution: From table, the number of segments n = 10

$$I = h_1 \frac{f(x_0)+f(x_1)}{2} + h_2 \frac{f(x_1)+f(x_2)}{2} + \cdots + h_9 \frac{f(x_8)+f(x_9)}{2} + h_{10} \frac{f(x_9)+f(x_{10})}{2}$$

$$I = 0.12 \frac{0.20+1.309729}{2} + 0.1 \frac{1.309729+1.305241}{2} + \cdots + 0.06 \frac{3.181929+2.363}{2} + 0.1 \frac{2.36+0.232}{2}$$

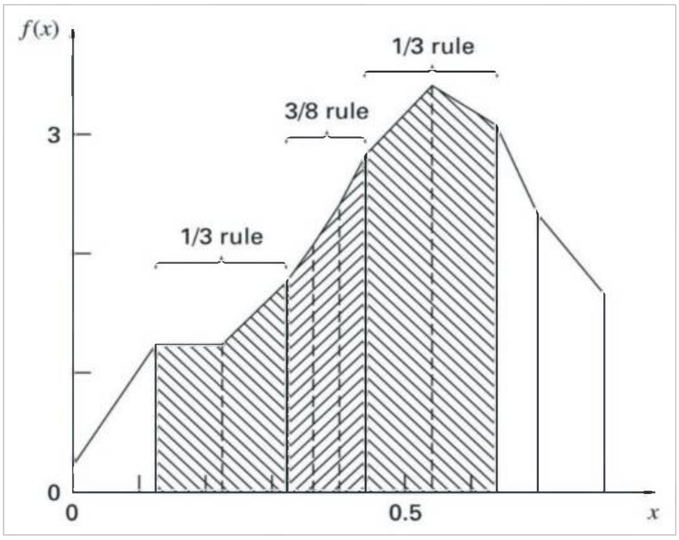
$$I = 1.594801$$

which represents an error of $\left|\frac{1.640533-1.594801}{1.640533}\right| \times 100 = 2.79\%$

Example (4.12): Resolve the previous example to compute the integral for the data in the table using the best combination of trapezoidal and Simpson's rules. Estimate the error and note that the exact value of the integral is 1.640533.

Solution:

The data in the table are depicted in the figure below. Notice that some adjacent segments are of equal width and, consequently, could have been evaluated using Simpson's rules. This usually leads to results that are more accurate.



From table, the best combination of trapezoidal and Simpson's rules are

x	0.0	0.12	0.22	0.32	0.36	0.40	0.44	0.54	0.64	0.70	0.80
***f* (x)**	0.200000	1.309729	1.305241	1.743393	2.074903	2.456000	2.842985	3.507297	3.181929	2.363000	0.232000
Method	Trapezoidal **h = 0.12**		Simpson's 1/3 rules **h = 0.1**		Simpson's 3/8 rules **h = 0.04**			Simpson's 1/3 rules **h = 0.1**		Trapezoidal **h = 0.06**	Trapezoidal **h = 0.1**

The first segment from x = 0.0 to 0.12 is evaluated with the ***trapezoidal rule***:

$$I_1 = (0.12 - 0)\ \frac{0.20+1.309729}{2} = 0.09058376$$

Because the next two segments from x = 0.12 to 0.32 are of equal length, their integral can be computed with ***Simpson's 1/3*** rule:

$$I_2 = (0.32 - 0.12)\ \frac{1.309729 + 4\ (1.305241) + 1.743393}{6} = 0.2758029$$

The next three segments from x = 0.32 to 0.44 are also equal and, as such, may be evaluated with the ***Simpson's 3/8*** rule to give:

$$I_3 = (0.44 - 0.32)\ \frac{1.743393 + 3\ (2.074903 + 2.4560) + 2.842985}{8} = 0.2726863$$

Similarly, the ***Simpson's 1/3*** rule can be applied to the two segments from x = 0.44 to 0.64 to yield:

$$I_4 = (0.64 - 0.44)\ \frac{2.842985 + 4\ (3.507297) + 3.181929}{6} = 0.6684701$$

Finally, the last two segments from x = 0.64 to 0.70 and from x = 0.70 to 0.80, which are of unequal length, can be evaluated with the ***trapezoidal rule*** to give:

$$I_5 = (0.7 - 0.64)\frac{3.181929 + 2.3630}{2} = 0.1663479$$

$$I_6 = (0.8 - 0.7)\frac{2.3630 + 0.232}{2} = 0.1297500$$

The area of these individual segments can be summed to yield a total integral of

$$I = I_1 + I_2 + I_3 + I_4 + I_5 + I_6 = \ 1.603641$$

which represents an error of $\left|\frac{1.640533 - 1.603641}{1.640533}\right| \times 100 = 2.25\%$

Exercise (4.4):

a) Using the unequally spaced data in the table below, evaluate the integral from x = 0 to 0.6 using **(a)** the trapezoidal rule and **(b)** the best combination of the trapezoidal and Simpson's rules to obtain the highest accuracy.

x	0	0.05	0.15	0.25	0.35	0.475	0.6
f(x)	2	1.8555	1.5970	1.3746	1.1831	0.9808	0.8131

b) The data in the table was collected for a cross-section of a river (y = distance from bank and H = depth). Compute the cross-sectional area of the river using numerical integration with **(a)** the trapezoidal rule and **(b)** the best combination of the trapezoidal and Simpson's rules.

y (m)	0	1	3	5	7	8	9	10
H (m)	0	1	1.5	3	3.5	3.2	2	0

c) The velocity of a bicycle versus time is presented in the table below. Using **(a)** the trapezoidal rule and **(b)** the best combination of the trapezoidal and Simpson's rules, estimate the distance traveled by the bicycle from rest in meters.

Time (min)	1	2	3.25	4.5	6	7	8	9	9.5	10
Velocity (m/s)	5	6	5.5	7	8.5	8	6	7	7	5

4.3. Numerical Differentiation

The ***Taylor series*** is of great value in the study of numerical methods. Essentially, the ***Taylor series*** provides a means to **predict** a **function value at one point** in terms of **the function value and its derivatives at another point**. In particular, the theorem states that **any smooth function can be approximated as a polynomial**.

A useful way to gain insight into the Taylor series is to build it term by term. For example, the first term in the series is

$$f(x_{i+1}) \cong f(x_i) \tag{4.31}$$

This relationship, called the ***zero-order approximation***, indicates that the value of f at the new point is the same as its value at the old point. This result makes intuitive sense because if x_i and x_{i+1} are close to each other, it is likely that the new value is probably similar to the old value.

Equation (4.31) provides a perfect estimate if the function being approximated is, in fact, **a constant**. However, if the function changes at all over the interval, additional terms of the Taylor series are required to provide a better estimate. For example, the ***first-order approximation*** is developed by adding another term to yield

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i) \tag{4.32}$$

The additional first-order term consists of a slope $f'(x_i)$ multiplied by the distance between x_i and x_{i+1}. Thus, the expression is now in the form of a straight line and is capable of predicting an increase or decrease of the function between x_i and x_{i+1}.

Although Equation (4.32) can predict a change, it is exact only for a straight-line, or ***linear,* trend**. Therefore, a ***second-order* term** is added to the series to capture some of the curvature that the function might exhibit:

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 \tag{4.33}$$

In a similar manner, additional terms can be included to develop the complete Taylor series expansion:

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \frac{f^{(3)}(x_i)}{3!}(x_{i+1} - x_i)^3 + \cdots + \frac{f^{(n)}(x_i)}{n!}(x_{i+1} - x_i)^n + R_n \tag{4.34}$$

where ***n!*** is the ***factorial of n***.

Note that because Equation (4.34) is an infinite series, an equal sign replaces the approximate sign that was used in Equations (4.31) through (4.33). A ***remainder*** term ($\boldsymbol{R_n}$) is included to account for all terms from $n + 1$ to infinity:

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x_{i+1} - x_i)^{n+1} \tag{4.35}$$

where the subscript n indicates that this is the remainder for the nth-order approximation and ξ is a value of x that lies somewhere between x_i and x_{i+1}. It is often convenient to simplify the Taylor series by defining a step size $h = x_{i+1} - x_i$ and expressing Equation (4.34) as

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n \qquad (4.36)$$

where the remainder term is now

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1} \qquad (4.37)$$

Example (4.13): Use zero- through fourth-order Taylor series expansions to approximate the function

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

from $x_i = 0$ with $h = 1$. That is, predict the function's value at $x_{i+1} = 1$.

Solution:

Because we are dealing with a known function, we can compute values for $f(x)$ between 0 and 1. The results (**Fig. 4.12**) indicate that the function starts at $f(0) = 1.2$ and then curves downward to $f(1) = 0.2$. Thus, the true value that we are trying to predict is 0.2.

The zero-order Taylor series approximation with $n = 0$ is [Eq. (4.31)]

$$f(x_{i+1}) \cong 1.2$$

Thus, as in **Fig. 4.12**, the zero-order approximation is a constant. Using this formulation results in a ***truncation error (E_r)*** of

$$\text{Truncation Error} = E_r = \text{true value} - \text{approximation} \qquad (4.38)$$

$$E_r = 0.2 - 1.2 = -1.0$$

Using the first-order Taylor series approximation with $n = 1$, the first derivative must be determined and evaluated at $x = 0$:

$$f'(0) = -0.4\,(0.0)^3 - 0.45\,(0.0)^2 - 1.0\,(0.0) - 0.25 = -0.25$$

Therefore, the first-order approximation is [Eq. (4.32)]

$$f(x_{i+1}) \cong 1.2 - 0.25\,h$$

which can be used to compute $f(1) = 0.95$. Consequently, the approximation begins to capture the downward trajectory of the function in the form of a sloping straight line (**Fig. 4.12**). This results in a reduction of the truncation error to

$E_r = 0.2 - 0.95 = -0.75$

For $n = 2$, the second-order Taylor series approximation requires the second derivative to be evaluated at $x = 0$:

$$f''(0) = -1.2\,(0.0)^2 - 0.9\,(0.0) - 1.0 = -1.0$$

Therefore, according to Eq. (4.33),

$$f(x_{i+1}) \cong 1.2 - 0.25\,h - 0.5\,h^2$$

and substituting $h = 1$, $f(1) = 0.45$. The inclusion of the second derivative now adds some downward curvature resulting in an improved estimate, as seen in Fig. 4.1. The truncation error is reduced further to

$E_r = 0.2 - 0.45 = -0.25$

Additional terms would improve the approximation even more. In fact, the inclusion of the third and the fourth derivatives results in exactly the same equation we started with (putting x = h):

$$f(x_{i+1}) = 1.2 - 0.25\,h - 0.5\,h^2 - 0.15\,h^3 - 0.1\,h^4$$

where the remainder term is

$$R_n = \frac{f^{(5)}(\xi)}{5!} h^5 = 0$$

because the fifth derivative of a fourth-order polynomial is zero. Consequently, the Taylor series expansion to the fourth derivative yields an exact estimate at $x_{i+1} = 1$:

$$f(1) = 1.2 - 0.25\,(1) - 0.5\,(1)^2 - 0.15\,(1)^3 - 0.1\,(1)^4 = 0.2$$

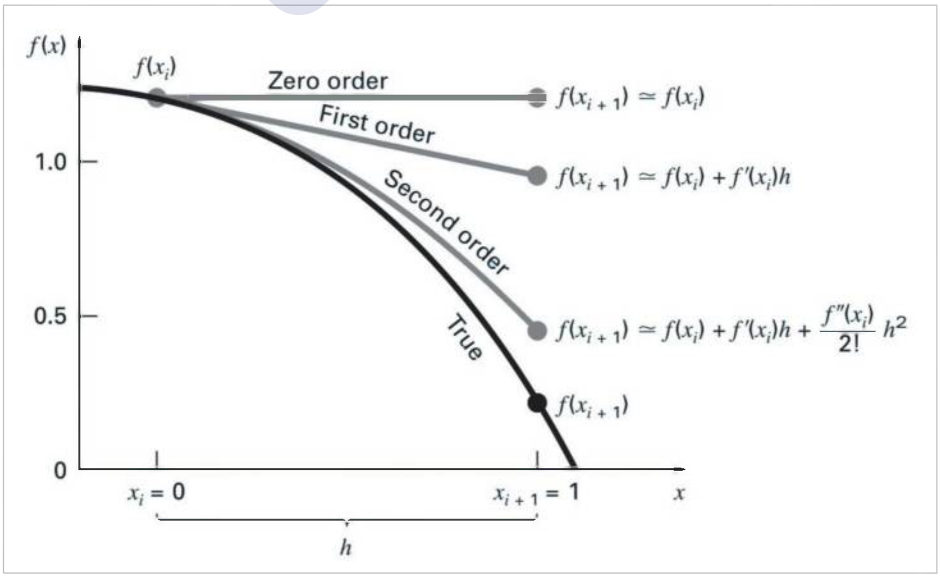


Fig. 4.12 The approximation using zero-order, first-order, and second-order Taylor series

In general, the ***n*th-order Taylor series expansion** will be **exact** for an ***n*th-order polynomial**. For other differentiable and continuous functions, such as exponentials and sinusoids, a finite number of terms will not yield an exact estimate. Each additional term will contribute some improvement, however slight, to the approximation.

The Taylor series can be used to estimate the value of derivatives in different forms, such as forward, backward, and centered divided difference approximations of the derivatives (**Fig. 4.13**).

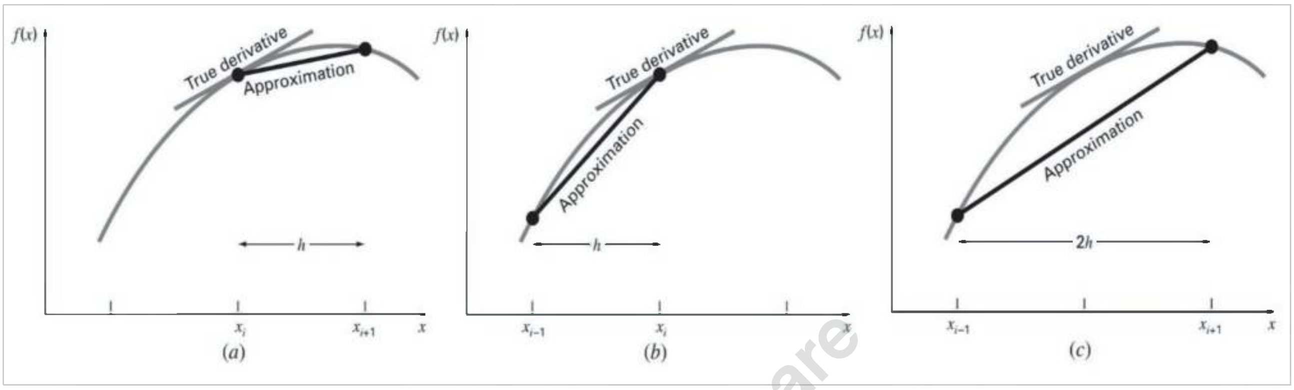


Fig. 4.13 Graphical depiction of (*a*) forward, (*b*) backward, and (*c*) centered finite-divided-difference approximations of the first derivative.

4.3.1. Forward Difference Approximation of the First Derivative

It is termed a "***forward***" difference because it utilizes data at ***i*** and ***i + 1*** to estimate the derivative. If the function *f* and its first $n+1$ derivatives are continuous on an interval containing x_i and x_{i+1}, then the value of the function at x_{i+1} is given by a ***forward Taylor series approximation*** as:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n \quad (4.39)$$

Equation (4.39) is called the ***forward Taylor series or Taylor's formula***. If the remainder R_n is omitted, the right side of Equation (4.39) is called the ***forward Taylor polynomial approximation*** to $f(x_{i+1})$. Truncating this equation after the first derivative and rearranging yields

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + R_1 \quad (4.40)$$

which can be solved for

$$f'(x_i) = \underbrace{\frac{f(x_{i+1}) - f(x_i)}{h}}_{\text{First-order approximation}} - \underbrace{\frac{R_1}{h}}_{\text{Truncation error}} \quad (4.41)$$

Using Eqs. (4.37) and (4.41) yields

$$\text{For } n = 1 \text{ and } R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!} h^{n+1} \rightarrow \frac{R_1}{h} = \frac{f''(\xi)}{2\,!}\frac{h^2}{h} = \frac{f''(\xi)}{2\,!} h \tag{4.42}$$

or

$$\frac{R_1}{h} = O(h) \tag{4.43}$$

Therefore, Equation (4.41) can be expressed as

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \tag{4.44}$$

Thus, the **estimate of the derivative** [the first part of Eq. (4.41) or (4.44)] has a truncation error of **order (h)**. In other words, the error of our derivative approximation should be proportional to the step size. Consequently, if we halve the step size, we would expect to halve the error of the derivative. Equation (4.44) is referred to as the ***forward finite divided difference*** of the ***first derivative***, ***h*** is called the step size, that is, the length of the interval over which the approximation is made, and ***O(h)*** is the error.

4.3.2. Backward Difference Approximation of the First Derivative

The Taylor series can be expanded "***backward***" to calculate a previous value ***i-1*** on the basis of a present value ***i***, as in

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \cdots \tag{4.45}$$

Truncating this equation after the first derivative and rearranging yields

$$f'(x_i) \cong \frac{f(x_i) - f(x_{i-1})}{h} \tag{4.46}$$

which is referred to as the ***backward finite divided difference*** of the ***first derivative*** with the **error** of ***O*(*h*)**.

4.3.3. Centered Difference Approximation of the First Derivative

A third way to approximate the first derivative is to subtract the backward from the forward Taylor series expansion to yield

$$f(x_{i+1}) = f(x_{i-1}) + 2\,f'(x_i)h + \frac{2\,f^{(3)}(x_i)}{3!}h^3 + \cdots \tag{4.47}$$

Truncating this equation after the first derivative, the above equation can be solved for

$$f'(x_i) \cong \frac{f(x_{i+1}) - f(x_{i-1})}{2\,h} - O(h^2) \qquad (4.48)$$

which is referred to as the ***centered finite divided difference*** of the ***first derivative*** with the **error** of ***O*(*h*²)**. Notice that the ***truncation error*** is of the order of ***h*²** in contrast to the ***forward*** and ***backward*** approximations that were of the order of ***h***. Consequently, the Taylor series analysis yields the practical information that the ***centered difference is a more accurate representation of the derivative***.

Example (4.14): Use forward and backward difference approximations of *O(h)* and a centered difference approximation of *O(h²)* to estimate the first derivative of

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

at x = 0.5 using a step size h = 0.5. Repeat the computation using h = 0.25. Note that the derivative can be calculated directly as

$$f'(x) = -0.4\,x^3 - 0.45\,x^2 - 1.0\,x - 0.25$$

and can be used to compute the true value as $f'(0.5) = -0.9125$.

Solution:

At x = 0.5 and h = 0.5, the function can be employed to determine

$x_{i-1} = 0 \quad \rightarrow \quad f(x_{i-1}) = f(0.0) = 1.2$

$x_i = 0.5 \quad \rightarrow \quad f(x_i) = f(0.5) = 0.925$

$x_{i+1} = 1.0 \quad \rightarrow \quad f(x_{i+1}) = f(1.0) = 0.2$

These values can be used to compute the forward divided difference,

$$f'(x_i) \cong \frac{f(x_{i+1}) - f(x_i)}{h} \rightarrow f'(0.5) \cong \frac{0.2 - 0.925}{0.5} = -1.45$$

which represents an error of $\left|\frac{-0.9125 - (-1.45)}{-0.9125}\right| \times 100 = 58.9\%$

The backward divided difference,

$$f'(x_i) \cong \frac{f(x_i) - f(x_{i-1})}{h} \rightarrow f'(0.5) \cong \frac{0.925 - 1.2}{0.5} = -0.55$$

which represents an error of $\left|\frac{-0.9125 - (-0.55)}{-0.9125}\right| \times 100 = 39.7\%$

The centered divided difference,

$$f'(x_i) \cong \frac{f(x_{i+1}) - f(x_{i-1})}{2\,h} \rightarrow f'(0.5) \cong \frac{0.2 - 1.2}{1.0} = -1.0$$

which represents an error of $\left|\frac{-0.9125 - (-1.0)}{-0.9125}\right| \times 100 = 9.6\%$

At x = 0.5 and h = 0.25, the function can be employed to determine

$x_{i-1} = 0.25 \quad \rightarrow \quad f(x_{i-1}) = f(0.25) = 1.10351563$

$x_i = 0.5 \quad \rightarrow \quad f(x_i) = f(0.5) = 0.925$

$x_{i+1} = 0.75 \quad \rightarrow \quad f(x_{i+1}) = f(0.75) = 0.63632813$

These values can be used to compute the forward divided difference,

$$f'(x_i) \cong \frac{f(x_{i+1}) - f(x_i)}{h} \rightarrow f'(0.5) \cong \frac{0.63632813 - 0.925}{0.25} = -1.155$$

which represents an error of $\left|\frac{-0.9125 - (-1.155)}{-0.9125}\right| \times 100 = 26.5\%$

The backward divided difference,

$$f'(x_i) \cong \frac{f(x_i) - f(x_{i-1})}{h} \rightarrow f'(0.5) \cong \frac{0.925 - 1.10351563}{0.25} = -0.714$$

which represents an error of $\left|\frac{-0.9125 - (-0.714)}{-0.9125}\right| \times 100 = 21.7\%$

The centered divided difference,

$$f'(x_i) \cong \frac{f(x_{i+1}) - f(x_{i-1})}{2\,h} \rightarrow f'(0.5) \cong \frac{0.63632813 - 1.10351563}{0.5} = -0.934$$

which represents an error of $\left|\frac{-0.9125 - (-0.934)}{-0.9125}\right| \times 100 = 2.4\%$

For both step sizes, the centered difference approximation is more accurate than forward or backward differences. Also, as predicted by the Taylor series analysis, halving the step size approximately halves the error of the backward and forward differences and quarters the error of the centered difference.

4.3.4. Finite Difference Approximations of Higher Derivatives.

Besides first derivatives, the Taylor series expansion can be used to derive numerical estimates of higher derivatives. To do this, we write a forward Taylor series expansion for $f(x_{i+2})$ in terms of $f(x_i)$:

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 + \cdots \qquad (4.49)$$

Equation (4.39) can be multiplied by 2 and subtracted from the above equation to give

$$f(x_{i+2}) - 2\,f(x_{i+1}) = -f(x_i) + f''(x_i)\,h^2 + \cdots \qquad (4.50)$$

which can be solved for

$$f''(x_i) \cong \frac{f(x_{i+2}) - 2\,f(x_{i+1}) + f(x_i)}{h^2} + O(h) \tag{4.51}$$

This relationship is called the ***forward finite divided difference*** approximations for ***the second derivative*** of the ***order of h***. Similar manipulations can be employed to derive a ***backward finite divided difference*** approximations for ***the second derivative*** of the ***order of h***

$$f''(x_i) \cong \frac{f(x_i) - 2\,f(x_{i-1}) + f(x_{i-2})}{h^2} + O(h) \tag{4.52}$$

and ***centered finite divided difference*** approximations for ***the second derivative*** of the ***order of h^2***

$$f''(x_i) \cong \frac{f(x_{i+1}) - 2\,f(x_i) + f(x_{i-1})}{h^2} + O(h^2) \tag{4.53}$$

As was the case with the first-derivative approximations, the ***centered case is more accurate***. Notice also that the centered version can be alternatively expressed as

$$f''(x_i) \cong \frac{\dfrac{f(x_{i+1}) - f(x_i)}{h} - \dfrac{f(x_i) - f(x_{i-1})}{h}}{h} = \frac{f(x_{i+1}) - 2\,f(x_i) + f(x_{i-1})}{h^2} \tag{4.54}$$

Thus, just as the second derivative is a derivative of a derivative, the second divided difference approximation is a difference of two first divided differences (using centered finite divided difference of the first derivative applied at $x_{i\pm h/2}$).

Example (4.15): Estimate the second derivative at x = 0.5 using a step size h = 0.25 of

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

using forward and backward difference approximations of *O(h)* and a centered difference approximation of *O(h^2)*. Note that the derivative can be calculated directly as

$$f''(x) = -1.2\,x^2 - 0.9\,x - 1.0$$

and can be used to compute the true value as $f''(0.5) = -1.75$.

Solution: **At x = 0.5 and h = 0.25**, the function can be employed to determine

$x_{i-2} = 0.0 \rightarrow f(x_{i-1}) = f(0.0) = 1.2$

$x_{i-1} = 0.25 \rightarrow f(x_{i-1}) = f(0.25) = 1.10351563$

$x_i = 0.5 \rightarrow f(x_i) = f(0.5) = 0.925$

$x_{i+1} = 0.75 \rightarrow f(x_{i+1}) = f(0.75) = 0.63632813$

$x_{i+2} = 1.0 \rightarrow f(x_{i+2}) = f(1.0) = 0.2$

These values can be used to compute the forward divided difference,

$$f''(x_i) \cong \frac{f(x_{i+2}) - 2\,f(x_{i+1}) + f(x_i)}{h^2} \rightarrow f''(0.5) \cong \frac{0.2 - 2\,(0.63632813) + 0.925}{0.25^2} = -2.3625$$

which represents an error of $\left|\frac{-1.75-(-2.3625)}{-1.75}\right| \times 100 = 35\%$

The backward divided difference,

$$f''(x_i) \cong \frac{f(x_i) - 2\,f(x_{i-1}) + f(x_{i-2})}{h^2} \rightarrow f''(0.5) \cong \frac{0.925 - 2\,(1.10351563) + 1.2}{0.25^2} = -1.3125$$

which represents an error of $\left|\frac{-1.75-(-1.3125)}{-1.75}\right| \times 100 = 25\%$

The centered divided difference,

$$f''(x_i) \cong \frac{f(x_{i+1}) - 2\,f(x_i) + f(x_{i-1})}{h^2} \rightarrow f''(0.5) \cong \frac{0.63632813 - 2\,(0.925) + 1.10351563}{0.25^2} = -1.7625$$

which represents an error of $\left|\frac{-1.75-(-1.7625)}{-1.75}\right| \times 100 = 0.71\%$

The centered difference approximation is more accurate than forward or backward differences.

<u>Exercise (4.5)</u>:

a) Use forward and backward difference approximations of $O(h)$ and a centered difference approximation of $O(h^2)$ to estimate the first derivative of the function below. Evaluate the derivative at $x = 2$ using a step size of $h = 0.2$. Compare your results with the true value of the derivative.

$$f(x) = 25\,x^3 - 6\,x^2 + 7\,x - 88$$

b) Estimate the second derivative of the same function examined in the previous problem. Use a centered difference approximation of $O(h^2)$. Perform the evaluation at $x = 2$ using step sizes of $h = 0.25$ and 0.125. Compare your estimates with the true value of the second derivative.

Chapter Five - Ordinary Differential Equations

5.1. Introduction

Numerical methods are becoming more and more important in engineering applications, not only because of the difficulties encountered in finding exact analytical solutions, but also due to the ease with which numerical techniques can be used in conjunction with modern high-speed digital computers. Several numerical procedures for solving initial value problems involving first-order ordinary differential equations are discussed in this chapter.

An ***ordinary differential equation*** is one in which an ***ordinary derivative of a dependent variable y*** with respect to an ***independent variable x*** is related in a prescribed manner to ***x, y and lower derivatives***. The most general form of an ***ordinary differential equation*** of ***nth order*** is given by

$$\frac{d^n y}{dx^n} = f\left(x, y, \frac{dy}{dx}, \frac{d^2y}{dx^2}, \cdots, \frac{d^{n-1}y}{dx^{n-1}}\right) \qquad (5.1)$$

The above equation is termed as ***ordinary*** (or ***ODE***) because there is only ***one independent variable***. This is in contrast to a ***partial differential equation*** (or ***PDE***) that involves ***two or more independent variables***. Differential equations are also classified as to their order. For example, the following equation, based on Newton's second law to compute the velocity y of a falling parachutist as a function of time *t*, is called a ***first-order equation*** because the ***highest derivative is a first derivative***.

$$\frac{dv}{dt} = g - \frac{c}{m}v \qquad (5.2)$$

where g is the gravitational constant, m is the mass, and c is a drag coefficient. A ***second-order equation*** would include a ***second derivative***. For example, the equation describing the position *x* of a mass-spring system with damping is the second-order equation,

$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + k\,x = 0 \qquad (5.3)$$

where c is a damping coefficient and k is a spring constant. Similarly, an ***nth-order equation*** would include an ***nth derivative***.

The ***degree of differential equation*** is represented by ***the power of the highest order derivative*** in the given differential equation. The ***differential equation*** must be a ***polynomial equation in derivatives*** for the degree to be defined. For example;

$$\frac{d^4y}{dx^4} + \left(\frac{d^2y}{dx^2}\right)^2 - 3\frac{dy}{dx} + y = 0 \quad \rightarrow \quad \text{Order: 4} \quad \text{Degree: 1}$$

$$x^2\frac{d^2y}{dx^2} + \frac{dy}{dx} + (x^2 - 4)y = 0 \quad \rightarrow \quad \text{Order: 2} \quad \text{Degree: 1}$$

$$\left(\frac{d^3y}{dx^3}\right)^2 + \left(\frac{d^2y}{dx^2}\right)^5 + \frac{y}{x^2+1} = e^x \quad \rightarrow \quad \text{Order: 3} \quad \text{Degree: 2}$$

The differential equations are also classified as ***Linear*** and ***non-Linear differential equations***. If a differential equation is of ***first degree*** in the ***dependent variable and its derivatives*** (accordingly, ***there cannot be*** any term involving the ***product of the dependent variable and its derivatives***) then it is called a ***linear differential equation*** otherwise it is non-linear.

$$\frac{d^2y}{dx^2} + 4x\frac{dy}{dx} + 2y = \cos x \quad \rightarrow \quad \text{Linear}$$

$$\frac{d^2y}{dx^2} + 4y\frac{dy}{dx} + 2y = \cos x \quad \rightarrow \quad \text{Non-Linear because of } \left(y\frac{dy}{dx}\right)$$

$$\frac{d^2y}{dx^2} + \sin y = 0 \quad \rightarrow \quad \text{Non-Linear because of } (\sin y)$$

To solve an ordinary differential equation of the type of equation (5.1), ***a set of conditions are required***. The ***number of conditions required*** is ***equal*** to the ***order of the differential equation***. When all the conditions are given at ***one value of the independent variable*** and the solution proceeds from that value of the independent variable, we have an ***initial-value problem***. When the conditions are given at ***different values of the independent variable***, we have a ***boundary-value problem***.

There are ***two broad categories*** of numerical methods to solve ***ordinary differential equations***: ***one-step*** or ***single-step methods*** **(Fig. 5.1a)**, which permit the calculation of y_{i+1}, given the differential equation and y_i. Moreover, ***multistep, step-by-step,*** or ***marching methods*** **(Fig. 5.1b)**, which require additional values of y other than at i.

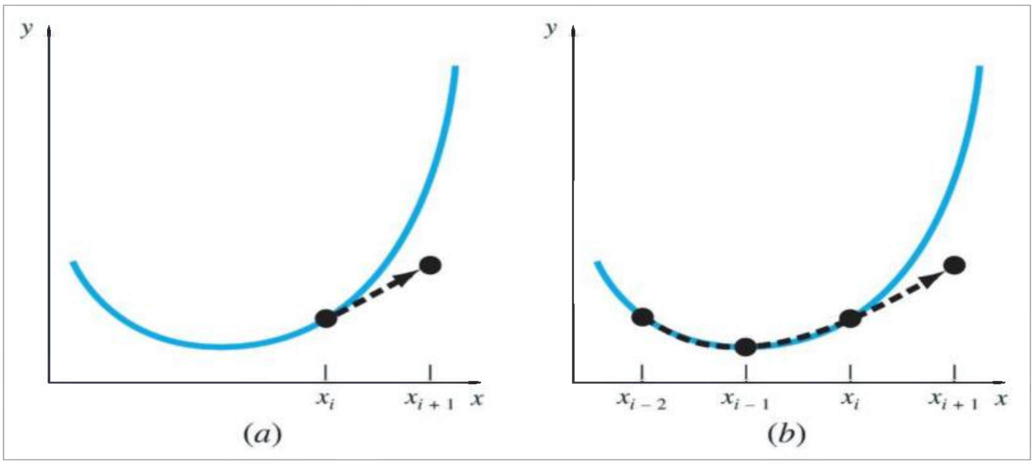


Fig. 5.1 Graphical depiction of the fundamental difference between (a) one-step and (b) multistep methods for solving ordinary differential equations (ODEs).

Higher-order differential equations can be reduced to a ***system of first-order equations***. For equation (5.3), this can be done by defining a new variable ***y***, where

$$y = \frac{dx}{dt} \tag{5.4}$$

which itself can be differentiated to yield

$$\frac{dy}{dt} = \frac{d^2x}{dt^2} \tag{5.5}$$

Equations (5.4) and (5.5) can then be substituted into equation (5.3) to give

$$m\frac{dy}{dt} + c\,y + k\,x = 0 \tag{5.6}$$

or

$$\frac{dy}{dt} = -\frac{c\,y + k\,x}{m} \tag{5.7}$$

Thus, equations (5.4) and (5.7) are a ***pair of first-order differential equations*** that are equivalent to the ***original second-order equation***. Because other ***nth-order differential equations*** can be similarly ***reduced***, ***this chapter*** focuses on the solution of ***initial value problems*** involving ***first-order differential equations*** and using ***one-step methods***.

5.2. One-Step or Single-Step Methods

This chapter is devoted to solving ordinary differential equations of the form $dy/dx = f(x, y)$. All ***one-step*** (also called ***single-step***) ***methods*** can be expressed in this ***general form below***, with the only difference being the manner in which the slope $\boldsymbol{\phi}$ is estimated.

New value = Old value + Slope × Step Size

or, in mathematical terms,

$$y_{i+1} = y_i + \emptyset\, h \tag{5.8}$$

According to this equation, the ***slope estimate*** of $\boldsymbol{\phi}$ is used to extrapolate from an ***old value*** $\boldsymbol{y_i}$ to a ***new value*** $\boldsymbol{y_{i+1}}$ over a ***distance*** or ***step size h*** (**Fig. 5.2**). This formula can be applied step-by-step to compute out into the future and, hence, trace out the trajectory of the solution. Several one-step methods will be studied in this chapter, which are Euler's method, modified Euler's method, and Runge-Kutta methods.

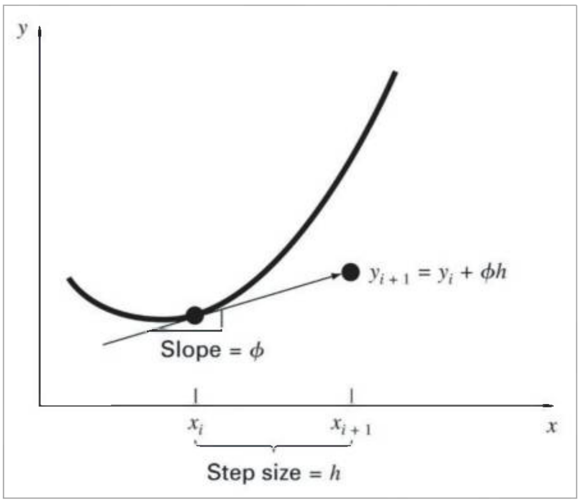


Fig. 5.2 Graphical depiction of a one-step method.

5.2.1. Euler's Method

Euler's method (also called the *forward Euler method*) is a single-step method for solving a first-order ordinary differential equation. The slope at the beginning of the interval is taken as an approximation of the average slope over the whole interval. The ***first derivative*** provides a direct estimate of the ***slope at*** x_i (**Fig. 5.3**):

$$\emptyset = f(x_i, y_i)$$

where $f(x_i, y_i)$ is the differential equation evaluated at x_i and y_i. This estimate can be substituted into equation (5.8):

$$y_{i+1} = y_i + f(x_i, y_i)\, h \quad (5.9)$$

This formula is referred to as ***Euler's*** (or the ***Euler-Cauchy*** or the ***point-slope***) ***method****.* A new value of *y* is predicted using the slope (equal to the first derivative at the original value of *x*) to extrapolate linearly over the step size *h* (**Fig. 5.3**).

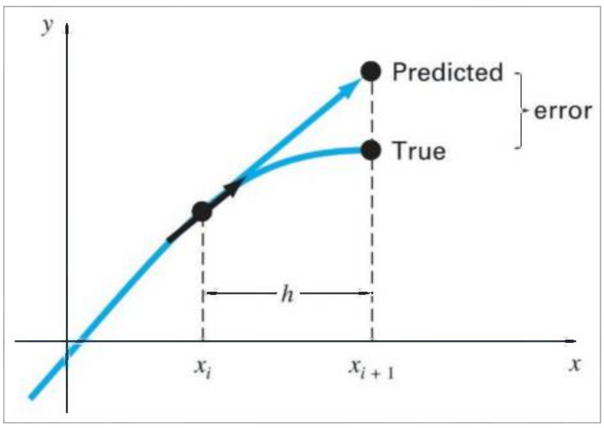


Fig. 5.3 Euler's method.

Example (5.1): Use Euler's method to solve the following differential equation

$$\frac{dy}{dx} = -x\,y^2 \ , \ y(2) = 1 \ \text{ and } \ 2 < x < 3 \ \text{ with } \ h = 0.1 \ \text{ and } \ 0.2$$

Find the relative error by comparing the results with exact solution from $y = \frac{2}{x^2-2}$

Solution:

At h = 0.1

Euler's formula given by Eq.(5.9) can be used the initial condition of $y_0 = 1$ at $x_0 = 2$

$$y_{i+1} = y_i + f(x_i, y_i)\,h = y_i - 0.1\,x_i\,y_i^2$$

$$y_1 = y(2.1) = y_0 - 0.1\,x_0\,y_0^2 = 1 - 0.1 \times 2 \times 1^2 = 0.8$$

$$y_2 = y(2.2) = y_1 - 0.1\,x_1\,y_1^2 = 0.8 - 0.1 \times 2.1 \times 0.8^2 = 0.6656$$

$$y_3 = y(2.3) = y_2 - 0.1\,x_2\,y_2^2 = 0.6656 - 0.1 \times 2.2 \times 0.6656^2 = 0.5681$$

The calculations continue until we reach $\mathbf{y_{10}}$. The predicted values of y for **x = 2, 2.1, 2.2, …., 3** with **h = 0.1** are presented in the table below in addition to the exact values.

x_i	y_i (Euler's method)	y_i (Exact values)	Relative Error % $\left\lvert (y_i^{Exact} - y_i^{Euler})/y_i^{Exact} \right\rvert \times 100$
$x_0 = 2.0$	$y_0 = 1$	$y_0 = 1$	0
2.1	0.8000	0.8299	3.60
2.2	0.6656	0.7042	5.48
2.3	0.5681	0.6079	6.55
2.4	0.4939	0.5319	7.14
2.5	0.4354	0.4706	7.48
2.6	0.3880	0.4202	7.66
2.7	0.3488	0.3781	7.75
2.8	0.3160	0.3425	7.74
2.9	0.2880	0.3120	7.69
$x_{10} = 3.0$	$y_{10} = 0.2640$	$y_{10} = 0.2857$	7.60

At h = 0.2

Euler's formula given by Eq.(5.9) can be used the initial condition of $y_0 = 1$ at $x_0 = 2$

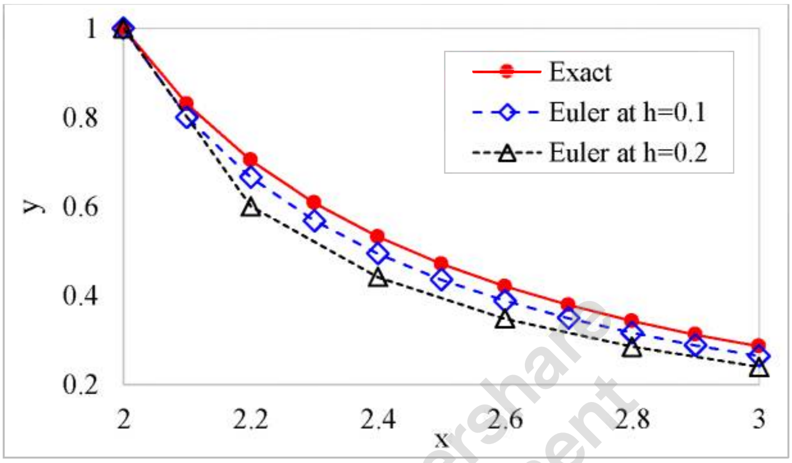
$$y_{i+1} = y_i + f(x_i, y_i)\,h = y_i - 0.2\,x_i\,y_i^2$$

$$y_1 = y(2.2) = y_0 - 0.2\,x_0\,y_0^2 = 1 - 0.2 \times 2 \times 1^2 = 0.6$$

$$y_2 = y(2.4) = y_1 - 0.2\,x_1\,y_1^2 = 0.6 - 0.2 \times 2.2 \times 0.6^2 = 0.4416$$

The calculations continue until we reach $\mathbf{y_5}$. The predicted values of y for **x = 2, 2.2, 2.4, …., 3** with **h = 0.2** are presented in the table below in addition to the exact values.

x_i	y_i (Euler's method)	y_i (Exact values)	Relative Error % $\lvert (y_i^{Exact} - y_i^{Euler})/y_i^{Exact} \rvert \times 100$
$x_0 = 2.0$	$y_0 = 1$	$y_0 = 1$	0
2.2	0.6000	0.7042	14.80
2.4	0.4416	0.5319	16.98
2.6	0.3480	0.4202	17.18
2.8	0.2850	0.3425	16.78
$x_5 = 3.0$	$y_5 = 0.2395$	$y_5 = 0.2857$	16.16



<u>Example (5.2)</u>: Use Euler's method to numerically integrate

$$\frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5$$

from $x = 0$ to $x = 4$ with a step size of 0.5 and 0.25. The initial condition at $x = 0$ is $y = 1$. Evaluate the relative error by comparing the results with exact solution given by

$$y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + 1$$

<u>Solution</u>:

<u>At h = 0.5</u>

Euler's formula given by Eq.(5.9) can be used the initial condition of $y_0 = 1$ at $x_0 = 0$

$$y_{i+1} = y_i + f(x_i, y_i)\, h = y_i - x_i^3 + 6x_i^2 - 10x_i + 4.25$$

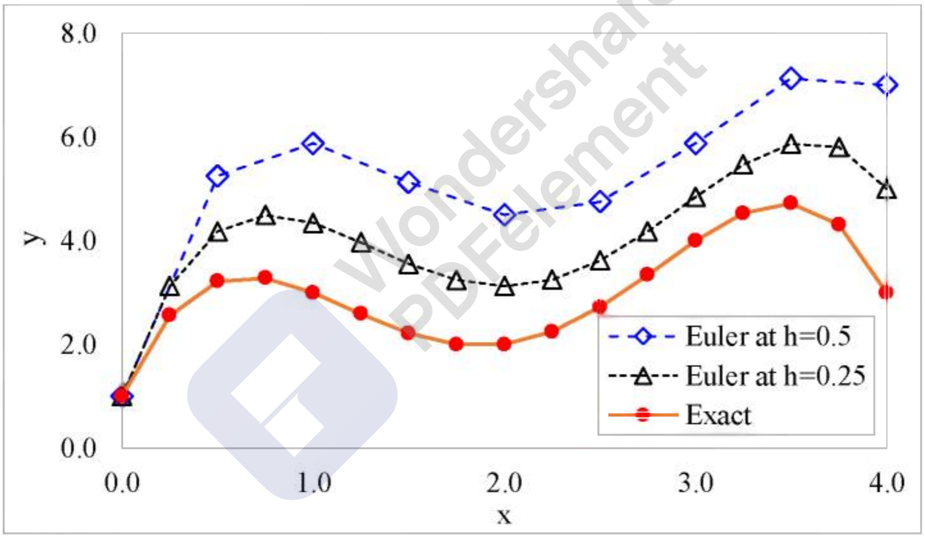
$$y_1 = y(0.5) = y_0 - x_0^3 + 6x_0^2 - 10x_0 + 4.25 = 1 - 0 + 0 - 0 + 4.25 = 5.25$$

$$y_2 = y(1.0) = y_1 - x_1^3 + 6x_1^2 - 10x_1 + 4.25 = 5.25 - (0.5)^3 + 6(0.5)^2 - 10(0.5) + 4.25 = 5.875$$

The calculations continue until we reach $\mathbf{y_8}$. The predicted values of y for **x = 0.0, 0.5, 1.0, …., 4** with **h = 0.5** are presented in the table below in addition to the exact values.

x_i	y_i (Euler's method)	y_i (Exact values)	Relative Error % $\lvert (y_i^{Exact} - y_i^{Euler})/y_i^{Exact} \rvert \times 100$
$x_0 = 0.0$	$y_0 = 1.0000$	$y_0 = 1.0000$	0.00
0.5	5.2500	3.2188	63.11
1.0	5.8750	3.0000	95.83
1.5	5.1250	2.2188	130.99
2.0	4.5000	2.0000	125.00
2.5	4.7500	2.7188	74.71
3.0	5.8750	4.0000	46.88
3.5	7.1250	4.7188	50.99
$x_8 = 4.0$	$y_8 = 7.0000$	$y_8 = 3.0000$	133.33

From the figure below, it can be noted that for h = 0.5, although the computation captures the general trend of the true solution, the error is considerable. This error can be reduced by using a smaller step size.



At h = 0.25

Euler's formula given by Eq.(5.9) can be used the initial condition of $y_0 = 1$ at $x_0 = 0$

$$y_{i+1} = y_i + f(x_i, y_i)\, h = y_i - 0.5x_i^3 + 3x_i^2 - 5x_i + 2.125$$

$$y_1 = y(0.25) = y_0 - 0.5x_0^3 + 3x_0^2 - 5x_0 + 2.125 = 1 - 0 + 0 - 0 + 2.125 = 3.125$$

$$y_2 = y(0.5) = y_1 - 0.5x_1^3 + 3x_1^2 - 5x_1 + 2.125 = 3.125 - 0.5\,(0.25)^3 + 3(0.25)^2 - 5(0.25) + 2.125 = 4.1797$$

The calculations continue until we reach $\mathbf{y_{16}}$. The predicted values of y for **x = 0.0, 0.25, 0.5, …., 4** with **h = 0.25** are presented in the table below in addition to the exact values. For h = 0.25 and from the figure above, it is clearly proved that a smaller step size reduced the relative error.

x_i	y_i (Euler's method)	y_i (Exact values)	Relative Error % $\lvert (y_i^{Exact} - y_i^{Euler}) / y_i^{Exact} \rvert \times 100$
$x_0 = 0.00$	$y_0 = 1.0000$	$y_0 = 1.0000$	0.00
0.25	3.1250	2.5605	22.04
0.50	4.1797	3.2188	29.85
0.75	4.4922	3.2793	36.99
1.00	4.3438	3.0000	44.79
1.25	3.9688	2.5918	53.13
1.50	3.5547	2.2188	60.21
1.75	3.2422	1.9980	62.27
2.00	3.1250	2.0000	56.25
2.25	3.2500	2.2480	44.57
2.50	3.6172	2.7188	33.05
2.75	4.1797	3.3418	25.07
3.00	4.8438	4.0000	21.09
3.25	5.4688	4.5293	20.74
3.50	5.8672	4.7188	24.34
3.75	5.8047	4.3105	34.66
$x_{16} = 4.00$	$y_{16} = 5.0000$	$y_{16} = 3.0000$	66.67

A fundamental source of error in Euler's method is that the derivative at the beginning of the interval is assumed to apply across the entire interval. A simple modification is available to help circumvent this shortcoming, which will be demonstrated in the next section. This modification actually belong to a larger class of solution techniques called Runge-Kutta methods. However, because they have a very straightforward graphical interpretation, we will present them prior to their formal derivation as Runge-Kutta methods.

5.2.2. Heun's Method

The ***Heun's method*** (also called ***modified Euler's method***) is a single-step numerical technique for solving a first-order ordinary differential equation. The method is a modification of Euler's method in which the slope or derivative in each interval is considered constant and equal to the slope of at the initial point.

One method to improve the estimate of the slope involves the determination of ***two derivatives for the interval***, one at the ***initial point*** and another at the **end point**. The ***two derivatives are then averaged*** to obtain an ***improved estimate of the slope*** for the entire interval. This approach, called ***modified Euler's method*** or ***Heun's method***, is depicted graphically in **Fig. 5.4**.

Recall that in Euler's method, the slope at the beginning of an interval

$$y_i' = f(x_i, y_i) \tag{5.10}$$

is used to extrapolate linearly to y_{i+1}:

$$y_{i+1}^0 = y_i + f(x_i, y_i)\, h \tag{5.11}$$

For the standard Euler method, we would stop at this point. However, in Heun's method the y_{i+1}^0 calculated in Eq. (5.11) is not the final answer, but an intermediate prediction. This is why we have distinguished it with a superscript 0. Equation (5.11) is called a ***predictor equation***. It provides an estimate of y_{i+1} that allows the calculation of an estimated slope at the end of the interval:

$$y_{i+1}' = f(x_{i+1}, y_{i+1}^0) \tag{5.12}$$

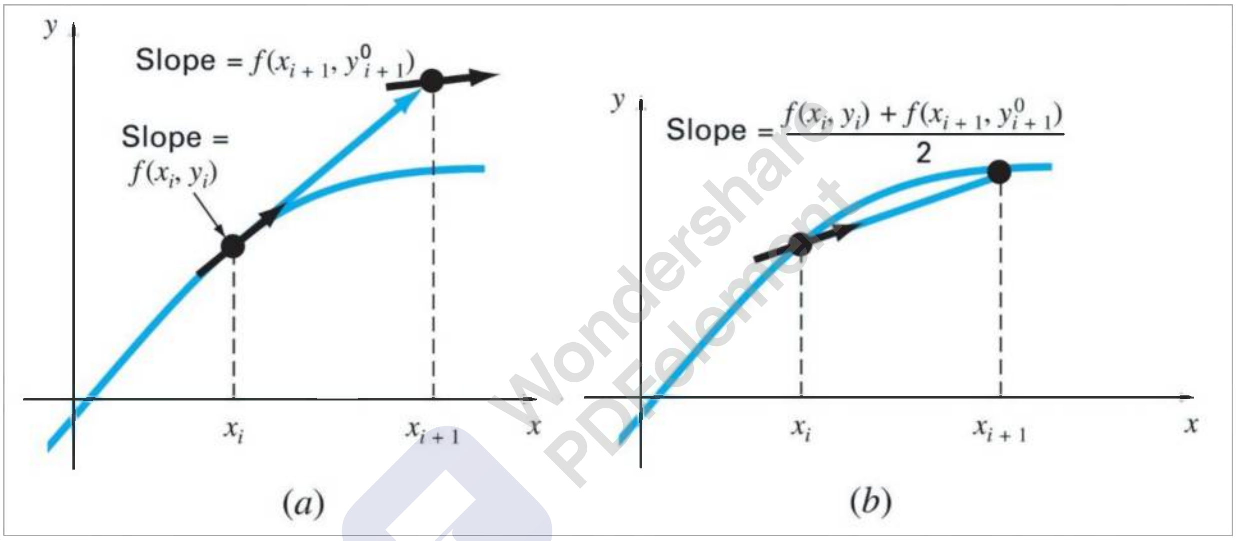


Fig. 5.4 Graphical depiction of Heun's method. (a) Predictor and (b) corrector.

Thus, the two slopes [Eqs. (5.10) and (5.12)] can be combined to obtain an average slope for the interval:

$$\bar{y}' = \frac{y_i' + y_{i+1}'}{2} = \frac{f(x_i, y_i) + f(x_{i+1}, y_{i+1}^0)}{2} \tag{5.13}$$

This average slope is then used to extrapolate linearly from y_i to y_{i+1} using Euler's method:

$$y_{i+1} = y_i + \bar{y}'\, h = y_i + \frac{f(x_i, y_i) + f(x_{i+1}, y_{i+1}^0)}{2}\, h \tag{5.14}$$

which is called a ***corrector equation***.

The ***Heun's method is a predictor-corrector approach***. All the multistep methods are of this type. The ***Heun's method is the only one-step predictor-corrector method described in this chapter***. As derived above, it can be expressed concisely as

Predictor (**Fig. 5.4a**): $y_{i+1}^0 = y_i + f(x_i, y_i)\, h$ (5.15)

Corrector (**Fig. 5.4b**): $y_{i+1} = y_i + \dfrac{f(x_i, y_i) + f(x_{i+1}, y_{i+1}^0)}{2}\, h$ (5.16)

Note that because Eq. (5.16) has y_{i+1} on both sides of the equal sign, it can be used in an iterative fashion. That is, an old estimate can be used repeatedly to provide an improved estimate of y_{i+1}.

Example (5.3): Use the modified Euler's method to solve the differential equation

$$\frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5$$

from $x = 0$ to $x = 4$ with a step size of 0.5. The initial condition at $x = 0$ is $y = 1$. Evaluate the relative error by comparing the results with exact solution given by

$$y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + 1$$

Solution:

To calculate y_1 using $x_0 = 0$, $y_0 = 1$, and $h = 0.5$

First, the slope at (x_0, y_0) is calculated as

$$f(x_0, y_0) = -2x_0^3 + 12x_0^2 - 20x_0 + 8.5$$

$$\rightarrow f(0,1) = -2x_0^3 + 12x_0^2 - 20x_0 + 8.5 = -0 + 0 - 0 + 8.5 = 8.5$$

From the predictor Eq. (5.15) $y_{i+1}^0 = y_i + f(x_i, y_i)h$ we have

$$y_1^0 = y_0 + f(x_0, y_0)h = 1 + (8.5)0.5 = 5.25$$

Note that this is the result that would be obtained by the standard Euler's method. Now, to improve the estimate for y_1, we use the value y_1^0 to predict the slope at the end of the interval (x_1, y_1^0). However, because the ODE is a function of x only, this result (y_1^0) has no effect on the second step to compute $f(x_1, y_1^0)$

$$f(x_1, y_1^0) = -2x_1^3 + 12x_1^2 - 20x_1 + 8.5$$

$$f(0.5, 5.25) = -2\,(0.5)^3 + 12\,(0.5)^2 - 20\,(0.5) + 8.5 = 1.25$$

Using the corrector Eq. (5.16) $y_1^1 = y_0 + \frac{f(x_0,y_0)+f(x_1,y_1^0)}{2}\, h = 1 + \frac{8.5+1.25}{2} 0.5 = 3.4375$

To calculate y_2 using $x_1 = 0.5$, $y_1 = 3.4375$, and $h = 0.5$

First, the slope at (x_1, y_1) is calculated as

$$f(x_1, y_1) = -2x_1^3 + 12x_1^2 - 20x_1 + 8.5$$

$$\rightarrow f(0.5, 3.4375) = -2(0.5)^3 + 12(0.5)^3 - 20(0.5) + 8.5 = 1.25$$

From the predictor Eq. (5.15) $y_{i+1}^0 = y_i + f(x_i, y_i)h$ we have

$$y_2^0 = y_1 + f(x_1, y_1)h = 3.4375 + (1.25)\ 0.5 = 4.0625$$

Now, to improve the estimate for y_2, we use the value y_2^0 to predict the slope at the end of the interval (x_2, y_2^0). However, because the ODE is a function of x only, this result (y_2^0) has no effect on the second step to compute $f(x_2, y_2^0)$

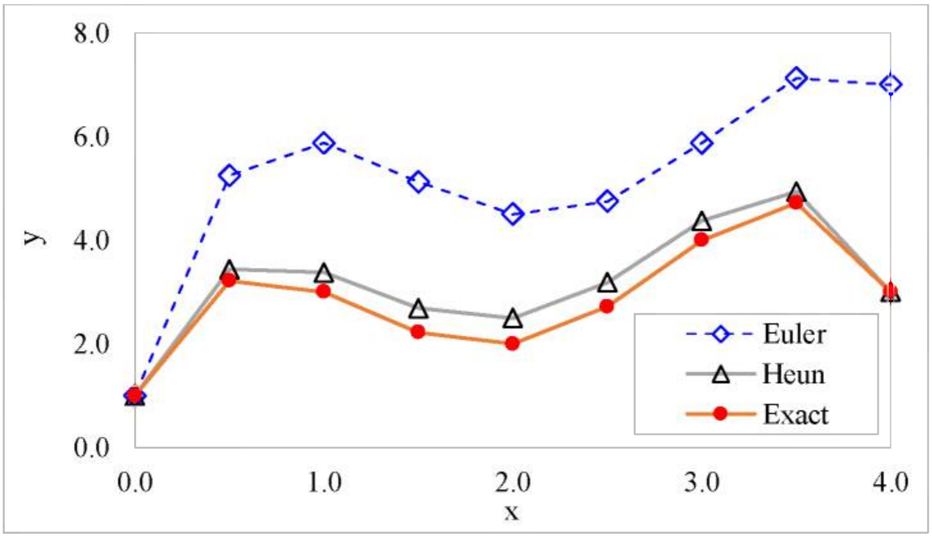
$$f(x_2, y_2^0) = -2x_2^3 + 12x_2^2 - 20x_2 + 8.5$$

$$f(1.0, 4.0625) = -2\,(1.0)^3 + 12\,(1.0)^2 - 20\,(1.0) + 8.5 = -1.5$$

Using Eq. (5.16) $y_2^1 = y_1 + \frac{f(x_1,y_1)+f(x_2,y_2^0)}{2}\,h = 3.4375 + \frac{1.25-1.5}{2}0.5 = 3.375$

The calculations continue until we reach y_8. The predicted values of y for **x = 0.0, 0.5, 1.0, …., 4** with **h = 0.5** using Heun's method are presented in the table below in addition to the exact values with the corresponding relative error and the values predicted by Euler's method in Example (5.2).

x_i	y_i (Euler's method)	y_i (Heun's method)	y_i (Exact values)	Relative Error % $\left\|(y_i^{Exact} - y_i^{Predicted})/y_i^{Exact}\right\| \times 100$	
				Euler's method	**Heun's method**
$x_0 = 0.0$	$y_0 = 1.0000$	$y_0 = 1.0000$	$y_0 = 1.0000$	0.00	0.00
0.5	5.2500	3.4375	3.2188	63.11	6.79
1.0	5.8750	3.3750	3.0000	95.83	12.5
1.5	5.1250	2.6875	2.2188	130.99	21.1
2.0	4.5000	2.5000	2.0000	125.00	25.0
2.5	4.7500	3.1875	2.7188	74.71	17.2
3.0	5.8750	4.3750	4.0000	46.88	9.40
3.5	7.1250	4.9375	4.7188	50.99	4.60
$x_8 = 4.0$	$y_8 = 7.0000$	$y_8 = 3.0000$	$y_8 = 3.0000$	133.33	0.00



Example (5.4): Use Heun's method to solve the differential equation $\frac{dy}{dx} = -2\,x\,y^2$ with $y(0) = 1$ and $0 < x < 0.5$ using step size $h = 0.1$. Compute the percentage relative error. Given the exact solution is given by $y = \frac{1}{1+x^2}$

Solution:

To calculate y_1 using $x_0 = 0,\ \ y_0 = 1,\ $ and $\ h = 0.1$

First, the slope at (x_0, y_0) is calculated as

$$f(x_0, y_0) = -2\,x_0\,y_0^2$$

$$\rightarrow f(0,1) = -2\,x_0\,y_0^2 = 0$$

From the predictor Eq. (5.15) we have

$$y_{i+1}^0 = y_i + f(x_i, y_i)h$$

$$\rightarrow \quad y_1^0 = y_0 + f(x_0, y_0)h = 1 + (0)\,0.1 = 1$$

Note that this is the result that would be obtained by the standard Euler's method. Now, to improve the estimate for y_1, we use the value y_1^0 to predict the slope at the end of the interval (x_1, y_1^0)

$$f(x_1, y_1^0) = -2\,x_1\,y_1^2$$

$$f(0.1, 1.0) = -2\,(0.1)\,(1.0)^2 = -0.2$$

Using the corrector Eq. (5.16) $\quad y_1^1 = y_0 + \frac{f(x_0,y_0)+f(x_1,y_1^0)}{2}\,h = 1 + \frac{0-0.2}{2}0.1 = 0.99$

The table below shows the remaining calculations using the modified Euler's method. It also shows the values obtained from the Euler's method, the exact values, and the percentage relative error for the both methods.

x_i	y_i (Euler's method)	y_i (Heun's method)	y_i (Exact values)	Relative Error % $\left\|(y_i^{Exact} - y_i^{Predicted})/y_i^{Exact}\right\| \times 100$	
				Euler's method	Heun's method
$x_0 = 0.0$	$y_0 = 1.0000$	$y_0 = 1.0000$	$y_0 = 1.0000$	0.00	0.00
0.1	1	0.9900	0.9901	0.9999	0.0101
0.2	0.9800	0.9614	0.9615	1.9241	0.0104
0.3	0.9416	0.9173	0.9174	2.6379	0.0109
0.4	0.8884	0.8620	0.8621	3.0507	0.0116
$x_5 = 0.5$	$y_5 = 0.8253$	$y_5 = 0.8001$	$y_5 = 0.8000$	3.1625	0.0125

5.2.3. Runge-Kutta Methods

Runge-Kutta (RK) methods are a family of ***single-step numerical techniques*** for solving a ***first-order ordinary differential equation***. Various types of ***Runge-Kutta methods are classified according to their order***. The ***order identifies the number of points within the subinterval*** that are utilized for finding the value of the slope in Eq. (5.8). For instance, ***second-order Runge-Kutta*** methods use the ***slope at two points; third-order methods*** use ***three-points;*** and so on. The ***classical Runge-Kutta method*** is of ***order four*** and uses ***four points***. ***Runge-Kutta methods*** give a more ***accurate solution compared to the simpler Euler's method***. The accuracy increases with increasing order of Runge-Kutta method.

Runge-Kutta (*RK*) methods achieve the accuracy of a Taylor series approach without requiring the calculation of higher derivatives. Many variations exist but all can be cast in the generalized form of Eq. (5.8):

$$y_{i+1} = y_i + \emptyset(x_i, y_i, h)\, h \tag{5.17}$$

Where $\boldsymbol{\emptyset(x_i, y_i, h)}$ is called an ***increment function***, which can be interpreted as a representative slope over the interval. The increment function can be written in general form as

$$\emptyset = a_1 k_1 + a_2 k_2 + \cdots + a_n k_n \tag{5.18}$$

where the ***a's*** are constants, ***n*** is ***the order*** of ***RK method***, and the ***k's*** are

$$\begin{aligned}
k_1 &= f(x_i, y_i) \\
k_2 &= f(x_i + p_1 h, y_i + q_{11} k_1 h) \\
k_3 &= f(x_i + p_2 h, y_i + q_{21} k_1 h + q_{22} k_2 h) \\
&\;\;\vdots \\
k_n &= f\left(x_i + p_{n-1} h, y_i + q_{n-1,1} k_1 h + q_{n-1,2} k_2 h + \cdots + q_{n-1,n-1} k_{n-1} h\right)
\end{aligned} \tag{5.19}$$

where the ***p's*** and ***q's*** are ***constants***. Notice that the ***k's*** are ***recurrence relationships***. That is, $\boldsymbol{k_1}$ appears in the equation for $\boldsymbol{k_2}$, which appears in the equation for $\boldsymbol{k_3}$, and so forth. Because each ***k*** is a functional evaluation, this recurrence makes RK methods efficient for computer calculations.

Various types of Runge-Kutta methods can be devised by employing different numbers of terms in the increment function $\boldsymbol{\emptyset(x_i, y_i, h)}$ as specified by ***n***. Note that the ***first-order Runge-Kutta (RK) method*** with ***n = 1*** is, in fact, ***Euler's method***. Once *n* is chosen, values for the ***a's, p's***, and ***q's*** are evaluated by setting Eq. (5.17) equal to terms in a Taylor series expansion.

5.2.3.1. Second-Order Runge-Kutta Methods

The second-order version of Eq. (5.17) is

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)\, h \tag{5.20}$$

where

$$k_1 = f(x_i, y_i) \tag{5.21}$$

$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h) \tag{5.22}$$

In the Runge-Kutta methods of order two, we consider up to the second derivative term in the Taylor series expansion and then substitute the derivative terms with the appropriate function values in the interval. By doing this, the values of the four unknown constants a_1, a_2, p_1, and q_{11} can be evaluated using the following three equations

$$a_1 + a_2 = 1 \tag{5.23}$$

$$a_2\, p_1 = \frac{1}{2} \tag{5.24}$$

$$a_2\, q_{11} = \frac{1}{2} \tag{5.25}$$

Because we have three equations with four unknowns, we must assume a value of one of the unknowns to determine the other three. Suppose that we specify a value for a_2. Then Eqs. (5.23) through (5.25) can be solved simultaneously for

$$a_1 = 1 - a_2 \tag{5.26}$$

$$p_1 = q_{11} = \frac{1}{2\, a_2} \tag{5.27}$$

Because we can choose an ***infinite number of values for*** a_2, there are ***an infinite number of second-order RK methods***. Every version would yield exactly the same results if the solution to the ODE were quadratic, linear, or a constant. However, they yield different results when (as is typically the case) the solution is more complicated. We present ***three of the most commonly used and preferred versions of the second-order RK method***:

a) Heun's Method with a Single Corrector ($a_2 = 1/2$)

If ***a_2 is assumed to be 1/2***, Eqs. (5.26) and (5.27) can be solved for $a_1 = 1/2$ and $p_1 = q_{11} = 1$. These parameters, when substituted into Eq. (5.20), yield

$$y_{i+1} = y_i + \left(\frac{1}{2} k_1 + \frac{1}{2} k_2\right) h \tag{5.28}$$

where

$$k_1 = f(x_i, y_i) \tag{5.29}$$

$$k_2 = f(x_i + h, y_i + k_1 h) \tag{5.30}$$

Note that k_1 is the ***slope at the beginning of the interval*** and k_2 is the ***slope at the end of the interval***. Consequently, this ***second-order Runge-Kutta method*** is actually ***Heun's technique without iteration***.

b) The Midpoint Method ($a_2 = 1$)

If ***a_2 is assumed to be 1***, then **$a_1 = 0$, $p_1 = q_{11} = 1/2$**, and Eq. (5.20) becomes

$$y_{i+1} = y_i + k_2\, h \tag{5.31}$$

where

$$k_1 = f(x_i, y_i) \tag{5.32}$$

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) \tag{5.33}$$

This is the midpoint method.

c) Ralston's Method ($a_2 = 2/3$)

The value of ***$a_2 = 2/3$*** was chosen to provide a minimum bound on the truncation error for the second-order RK algorithms. For this version, **$a_1 = 1/3$** and **$p_1 = q_{11} = 3/4$**, and Eq. (5.20) yields

$$y_{i+1} = y_i + \left(\frac{1}{3}k_1 + \frac{2}{3}k_2\right)h \tag{5.34}$$

where

$$k_1 = f(x_i, y_i) \tag{5.35}$$

$$k_2 = f\left(x_i + \frac{3}{4}h, y_i + \frac{3}{4}k_1 h\right) \tag{5.36}$$

<u>Example (5.5)</u>: Use the midpoint method and Ralston's method to solve the differential equation

$$\frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5$$

from $x = 0$ to $x = 4$ with a step size of 0.5. The initial condition at $x = 0$ is $y = 1$. Compare the results with the values obtained in Example (5.3) using another second-order RK algorithm, which is the Heun's method without corrector iteration. Evaluate the relative error by comparing the results with exact solution given by $y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + 1$

Solution:

Midpoint method

The first step in the midpoint method is to use Eq. (5.32) with $x_0 = 0$, $y_0 = 1$, and h = 0.5 to compute

$$k_1 = f(x_i, y_i) = f(0,1) = -2(0)^3 + 12(0)^2 - 20(0) + 8.5 = 8.5$$

However, because the ODE is a function of x only, this result (k_1) has no effect on the second step to compute k_2 using Eq. (5.33)

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) = -2(0.25)^3 + 12(0.25)^2 - 20(0.25) + 8.5 = 4.21875$$

The slope at the midpoint can then be substituted into Eq. (5.31) to predict y at x = 0.5

$$y_{i+1} = y_i + k_2\, h \quad \rightarrow \quad y(0.5) = 1 + 4.21875\,(0.5) = 3.109375$$

The computation is repeated, and the results are summarized in the table below.

x_i	y_i					Relative Error % $\left|\left(y_i^{Exact} - y_i^{Predicted}\right)/y_i^{Exact}\right| \times 100$			
	Euler	Heun	Midpoint	Ralston	Exact values	Euler	Heun	Midpoint	Ralston
0.0	1.000	1.0000	1.00000	1.00000	1.0000	0.00	0.00	0.0	0
0.5	5.250	3.4375	3.10938	3.27734	3.2188	63.11	6.79	3.4	1.8
1.0	5.875	3.3750	2.81250	3.10156	3.0000	95.83	12.5	6.3	3.4
1.5	5.125	2.6875	1.98438	2.34766	2.2188	130.99	21.1	10.6	5.8
2.0	4.500	2.5000	1.75000	2.14063	2.0000	125.00	25.0	12.5	7.0
2.5	4.750	3.1875	2.48438	2.85547	2.7188	74.71	17.2	8.6	5.0
3.0	5.8750	4.3750	3.81250	4.11719	4.0000	46.88	9.40	4.7	2.9
3.5	7.1250	4.9375	4.60938	4.80078	4.7188	50.99	4.60	2.3	1.7
4.0	7.0000	3.0000	3.00000	3.03125	3.0000	133.33	0.00	0.0	1.0

Ralston's method

For Ralston's method, k_1 for the first interval from Eq. (5.35) equals 8.5 and to calculate k_2 using Eq. (5.36) with $x_0 = 0$, $y_0 = 1$, and h = 0.5

$$k_2 = f\left(x_i + \frac{3}{4}h, y_i + \frac{3}{4}k_1 h\right) = -2(0.375)^3 + 12(0.375)^2 - 20(0.375) + 8.5 = 2.58203125$$

which can be used to predict y at x = 0.5 using Eq. (5.34)

$$y_{i+1} = y_i + \left(\frac{1}{3}k_1 + \frac{2}{3}k_2\right)h \quad \rightarrow \quad y(0.5) = 1 + \left(\frac{1}{3}(8.5) + \frac{2}{3}(2.58203125)\right)(0.5) =$$

3.27734375

The computation is repeated, and the results are summarized in in the table above. ***Notice how all the second-order RK methods are superior to Euler's method***.

5.2.3.2. Third-Order Runge-Kutta Methods

For n = 3, a derivation similar to the one for the second-order method can be performed. The result of this derivation is six equations with eight unknowns. Therefore, values for two of the unknowns must be specified a priori in order to determine the remaining parameters. ***One common version*** that results is

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 4k_2 + k_3)h \tag{5.37}$$

where

$$k_1 = f(x_i, y_i) \tag{5.38}$$

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) \tag{5.39}$$

$$k_3 = f(x_i + h, y_i - k_1 h + 2k_2 h) \tag{5.40}$$

Note that if the derivative is a ***function of x only***, this ***third-order RK method reduces to Simpson's 1/3 rule.***

Example (5.6): Solve the following differential equation from $x = 0$ to $x = 1$ with a step size of 0.5 using the third-order RK method

$$\frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5$$

The initial condition at $x = 0$ is $y = 1$. Evaluate the relative error by comparing the results with exact solution given by $y = -0.5x^4 + 4x^3 - 10x^2 + 8.5x + 1$

Solution:

The first step to evaluate **y_1 at x = 0.5** in the third-order RK method is to use Eq. (5.38) with $x_0 = 0$, $y_0 = 1$, and h = 0.5 to compute

$$k_1 = f(x_i, y_i) = f(0, 1) = -2(0)^3 + 12(0)^2 - 20(0) + 8.5 = 8.5$$

However, because the ODE is a function of x only, this result (k_1) has no effect on the next steps to compute k_2 and k_3 using Equations (5.39) and (5.40), respectively.

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) = -2(0.25)^3 + 12(0.25)^2 - 20(0.25) + 8.5 = 4.21875$$

$$k_3 = f(x_i + h, y_i - k_1 h + 2k_2 h) = -2(0.5)^3 + 12(0.5)^2 - 20(0.5) + 8.5 = 1.25$$

Using Eq. (5.37) to predict y at x = 0.5, we have

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 4k_2 + k_3)h$$

$$\rightarrow \quad y(0.5) = 1 + \frac{1}{6}(8.5 + 4(4.21875) + 1.25)(0.5) = 3.21875$$

The exact value of $\mathbf{y_1}$ at x = 0.5

$$y_1 = y(0.5) = -0.5(0.5)^4 + 4(0.5)^3 - 10(0.5)^2 + 8.5(0.5) + 1 = 3.21875$$

It can be noticed that the predicted value of $\mathbf{y_1}$ by the third-order RK method and the exact value are equal. Thus, the relative error is zero.

To evaluate **$\mathbf{y_2}$ at x = 1.0** in the third-order RK method, we use Eq. (5.38) with $x_1 = 0.5$, $y_1 = 3.21875$, and h = 0.5 to compute

$$k_1 = f(x_i, y_i) = -2(0.5)^3 + 12(0.5)^2 - 20(0.5) + 8.5 = 1.25$$

However, because the ODE is a function of *x* only, this result (k_1) has no effect on the next steps to compute k_2 and k_3 using Equations (5.39) and (5.40), respectively.

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) = -2(0.75)^3 + 12(0.75)^2 - 20(0.75) + 8.5 = -0.59375$$

$$k_3 = f(x_i + h, y_i - k_1 h + 2k_2 h) = -2(1.0)^3 + 12(1.0)^2 - 20(1.0) + 8.5 = -1.50000$$

Using Eq. (5.37) to predict y at x = 1.0, we have

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 4k_2 + k_3)h$$

$$\rightarrow \quad y(1.0) = 3.21875 + \frac{1}{6}\big(1.25 + 4(-0.59375) + (-1.50000)\big)(0.5) = 3.0000$$

The exact value of $\mathbf{y_2}$ at x = 1.0

$$y_2 = y(1.0) = -0.5(1.0)^4 + 4(1.0)^3 - 10(1.0)^2 + 8.5(1.0) + 1 = 3.0000$$

Again, it can be observed that the predicted value of $\mathbf{y_2}$ by the third-order RK method and the exact value are equal. Thus, the relative error is zero. Consequently, ***the third-order RK method is superior to all the second-order RK methods***.

Example (5.7): Employ the third-order RK method to integrate $y' = 4\,e^{0.8\,t} - 0.5\,y$ from $t = 0$ to 1 using a step size of 1 with $y(0) = 2$. Evaluate the relative error by comparing the results with exact solution of 6.194631.

Solution:

The first step to evaluate **y_1 at t = 1.0** is to compute k_1, k_2, and k_3 using Equations (5.38) to (5.40), respectively, with $t_0 = 0$, $y_0 = 2$, and step size (h) = 1

$$k_1 = f(t_i, y_i) = f(0,2) = 4\,e^{0.8\,t_i} - 0.5\,y_i = 4\,e^{0.8\,(0)} - 0.5\,(2) = 3$$

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) = f(0.5, 3.5) = f(0,2) = 4\,e^{0.8\,(0.5)} - 0.5\,(3.5) = 4.217299$$

$$k_3 = f(x_i + h, y_i - k_1 h + 2k_2 h) = f(1.0, 7.4346) = 4e^{0.8\,(1)} - 0.5(7.4346) = 5.184864$$

Using Eq. (5.37) to predict y_1 at t = 1, we have

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 4k_2 + k_3)h$$

$$\rightarrow \quad y(1.0) = 2.0 + \frac{1}{6}(3 + 4(4.217299) + 5.184864)(1.0) = 6.175677$$

The relative error for y_1 can be calculated as

$$Relative\ Error\% = \left|\frac{y_i^{Exact} - y_i^{Predicted}}{y_i^{Exact}}\right| \times 100 = \left|\frac{6.194631 - 6.175677}{6.194631}\right| \times 100 = 0.306\%$$

5.2.3.3. Fourth-Order Runge-Kutta Methods

The ***most popular RK methods*** are ***fourth order***. As with the second-order approaches, there are an ***infinite number of versions***. The following is the ***most commonly used form***, and we therefore call it the ***classical fourth-order RK method:***

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h \tag{5.41}$$

where

$$k_1 = f(x_i, y_i) \tag{5.42}$$

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) \tag{5.43}$$

$$k_3 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h\right) \tag{5.44}$$

$$k_4 = f(x_i + h, y_i + k_3 h) \tag{5.45}$$

Notice that for ODEs that are a ***function of x alone***, the ***classical fourth-order RK method*** is

similar to Simpson's 1/3 rule. As depicted in **Fig. 5.5**, each of the ***k*'s** represents a ***slope***. Therefore, equation (5.41) represents a ***weighted average*** of these slopes to arrive at the improved slope.

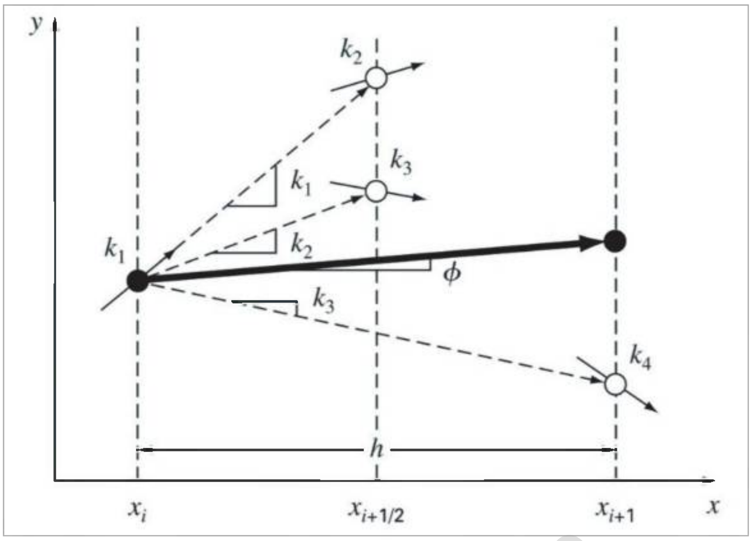


Fig. 5.5 Graphical depiction of the slope estimates comprising the fourth-order RK method.

Example (5.8): Using the classical fourth-order RK method with an initial condition of $y(0) = 2$, integrate $y' = 4\,e^{0.8\,t} - 0.5\,y$ from $t = 0$ to 1 with a step size of 1. Evaluate the relative error by comparing the results with exact solution of 6.194631.

Solution:

The first step to evaluate **y₁ at t = 1.0** is to compute k_1, k_2, k_3, and k_4 using Equations (5.42) to (5.45), respectively, with $t_0 = 0$, $y_0 = 2$, and step size (h) = 1

$$k_1 = f(t_i, y_i) = f(0,2) = 4\,e^{0.8\,t_i} - 0.5\,y_i = 4\,e^{0.8\,(0)} - 0.5\,(2) = 3$$

$$k_2 = f\left(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}k_1 h\right) = f(0.5, 3.5) = 4\,e^{0.8\,(0.5)} - 0.5\,(3.5) = 4.217299$$

$$k_3 = f\left(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}k_2 h\right) = f(0.5, 4.10865) = 4\,e^{0.8\,(0.5)} - 0.5\,(4.10865) = 3.912974$$

$$k_4 = f(x_i + h, y_i + k_3 h) = f(1.0, 5.912974) = 4\,e^{0.8\,(1.0)} - 0.5\,(4.10865) = 5.945677$$

Using Eq. (5.41) to predict y_1 at t = 1, we have

$$y_{i+1} = y_i + \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$$\rightarrow \quad y(1.0) = 2.0 + \tfrac{1}{6}(3 + 2(4.217299) + 2(3.912974) + 5.945677)(1.0) = 6.201037$$

The relative error for y_1 can be calculated as

$$\text{Relative Error \%} = \left|\frac{y_i^{Exact} - y_i^{Predicted}}{y_i^{Exact}}\right| \times 100 = \left|\frac{6.194631 - 6.201037}{6.194631}\right| \times 100 = 0.103\%$$

Accordingly, ***the classical fourth-order RK method is superior to the third-order RK method presented in the previous section of this chapter.***

Example (5.9): Solve the following differential equation from $x = 0$ to $x = 0.5$ with a step size of 0.5 using the classical fourth-order RK method.

$$\frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5$$

The initial condition at $x = 0$ is $y = 1$. Evaluate the relative error by comparing the result with the exact value of y(0.5) which is equal to (3.12875).

Solution:

The first step to evaluate y_1 at x = 0.5 in the classical fourth-order RK method is to use Eq. (5.42) with $x_0 = 0$, $y_0 = 1$, and h = 0.5 to compute

$$k_1 = f(x_i, y_i) = f(0,1) = -2(0)^3 + 12(0)^2 - 20(0) + 8.5 = 8.5$$

However, because the ODE is a function of x only, this result (k_1) has no effect on the next steps to calculate k_2, k_3, and k_4 using Equations (5.43), (5.44), and (5.45), respectively.

$$k_2 = f\left(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}k_1 h\right) = -2(0.25)^3 + 12(0.25)^2 - 20(0.25) + 8.5 = 4.21875$$

$$k_3 = f\left(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}k_2 h\right) = -2(0.25)^3 + 12(0.25)^2 - 20(0.25) + 8.5 = 4.21875$$

$$k_4 = f(x_i + h, y_i + k_3 h) = -2(0.5)^3 + 12(0.5)^2 - 20(0.5) + 8.5 = 1.25$$

Using Eq. (5.41) to predict y_1 at x = 0.5, we have

$$y_{i+1} = y_i + \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$$\rightarrow \quad y(0.5) = 1 + \tfrac{1}{6}(8.5 + 2(4.21875) + 2(4.21875) + 1.25)(0.5) = 3.21875$$

which is equal to the exact value and thus the relative error is zero.

Example (5.10): Use the classical fourth-order Runge-Kutta method with $h = 0.1$ for the solution of $\frac{dy}{dx} = 2xy$ to obtain an approximation to $y(1.5)$ with $y(1) = 1$. Determine the percentage relative error if the exact solution is given by $y = e^{x^2-1}$.

Solution:

With $x_0 = 1$, $y_0 = 1$, and h = 0.1, the first step to evaluate y_1 at x = 1.1 in the classical fourth-order RK method is to use Eq. (5.42) to compute k_1 as

$$k_1 = f(x_i, y_i) = f(1,1) = 2\,x_i\,y_i = 2(1)(1) = 2$$

The next steps are to calculate k_2, k_3, and k_4 using Equations (5.43), (5.44), and (5.45), respectively.

$$k_2 = f\left(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}k_1 h\right) = f(1.05, 1.1) = 2\,x_i\,y_i = 2(1.05)(1.1) = 2.31$$

$$k_3 = f\left(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}k_2 h\right) = f(1.05, 1.1155) = 2\,x_i\,y_i = 2(1.05)(1.1155) = 2.3426$$

$$k_4 = f(x_i + h, y_i + k_3 h) = f(1.1, 1.2343) = 2\,x_i\,y_i = 2(1.1)(1.2343) = 2.7154$$

Using Eq. (5.41) to predict y_1 at x = 1.1, we have

$$y_{i+1} = y_i + \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$$\rightarrow \quad y(1.1) = 1 + \tfrac{1}{6}(2 + 2(2.31) + 2(2.3426) + 2.7154)(0.1) = 1.2337$$

The exact value of y_1 at x = 1.1 is

$$y_{1\,\text{Exact}} = e^{x^2-1} = e^{1.1^2-1} = 1.2337$$

The predicted value for y_1 is equal to the exact value with zero error. The computation is repeated, and the results are summarized in in the table below.

x_i	y_i		Absolute error	Percentage relative error
	4th order RK	Exact values	$\lvert y_i^{Exact} - y_i^{Predicted}\rvert$	$\lvert(y_i^{Exact} - y_i^{Predicted})/y_i^{Exact}\rvert \times 100$
1	1	1	0	0
1.1	1.2337	1.2337	0	0
1.2	1.5527	1.5527	0	0
1.3	1.9937	1.9937	0	0
1.4	2.6116	2.6117	0.0001	0
1.5	3.4902	3.4904	0.0001	0

Example (5.11): Use the Runge-Kutta method of order four and with $h = 0.1$ to find an approximate solution of $\frac{dy}{dx} = f(x,y) = x^2 + y$ at x = 0.1. Given that y = –1 when x = 0. Compute the percentage relative error if the exact solution is given by $y = -x^2 - 2x + e^x - 2$.

Solution:

With $x_0 = 0$, $y_0 = -1$, and h = 0.1, the first step to evaluate y_1 at x = 0.1 in the fourth-order RK method is to use Eq. (5.42) to compute k_1 as

$$k_1 = f(x_i, y_i) = f(0, -1) = x_i^2 + y_i = (0)^2 + (-1) = -1$$

The next steps are to calculate k_2, k_3, and k_4 using Equations (5.43), (5.44), and (5.45), respectively.

$$k_2 = f\left(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}k_1 h\right) = f(0.05, -1.05) = (0.05)^2 - 1.05 = -1.0475$$

$$k_3 = f\left(x_i + \tfrac{1}{2}h, y_i + \tfrac{1}{2}k_2 h\right) = f(0.05, -1.0524) = (0.05)^2 - 1.0524 = -1.0549$$

$$k_4 = f(x_i + h, y_i + k_3 h) = f(0.1, -1.1055) = (0.1)^2 - 1..1055 = -1.0955$$

Using Eq. (5.41) to predict y_1 at x = 1.1, we have

$$y_{i+1} = y_i + \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$$\rightarrow \quad y(1.1) = -1 + \tfrac{1}{6}(-1 + 2(-1.0475) + 2(-1.0549) - 1.0955)(0.1) = -1.1050$$

The exact value of y_1 at x = 0.1 is

$$y_{1\,\text{Exact}} = -x^2 - 2x + e^x - 2 = -(0.1)^2 - 2(0.1) + e^{0.1} - 2 = -1.1049$$

The relative error for y_1 can be calculated as

$$\text{Relative Error }\% = \left|\frac{y_i^{Exact} - y_i^{Predicted}}{y_i^{Exact}}\right| \times 100 = \left|\frac{-1.1049 - (-1.1050)}{-1.1049}\right| \times 100 = 0.009\%$$

Exercise (5.1):

a) Use **(a)** Euler's method and **(b)** Heun's method to find y(4.4) from the ordinary differential equation $\frac{dy}{dx} = \frac{2-y^2}{5\,x}$ by taking h = 0.2. Take y = 1 at x = 4.

b) Using **(a)** Midpoint method, **(b)** Ralston's method, and **(d)** Third-order RK method, find the value of y at x = 0.1, 0.2, and 0.3 from the following differential equation $\frac{dy}{dx} = f(x, y) = x\,y + y^2$. Take the initial condition of $y(0) = 1$.

c) Solve the following initial value problem over the interval from $t = 0$ to 2 using **(a)** Euler's method, **(b)** Heun's method, **(c)** Midpoint method, and **(d)** Fourth-order RK method. Take the initial condition of $y(0) = 1$ and a step size (h) = 0.5. Compare all the results by presenting them on the same table.

$$\frac{dy}{dt} = f(t, y) = y\,t^2 - 1.1y$$

d) Using **(a)** Euler's method, **(b)** Heun's method, **(c)** Ralston's method, and **(d)** Third-order RK method, solve the following initial value problem over the interval from $x = 0$ to 0.5. Use a step size (h) = 0.1 and take the initial condition of $y(0) = 1$. Tabulate all the results for comparison.

$$\frac{dy}{dx} = \sin y$$

e) Solve the following problem over the interval from $x = 0$ to 1 using a step size (h) of 0.25 where $y(0) = 1$. Display all your results on the same table. Use **(a)** Euler's method, **(b)** Heun's method, **(c)** Ralston's method, **(d)** Third-order RK method, and **(e)** Fourth-order RK method

$$\frac{dy}{dx} = (1 + 4x)\sqrt{y}$$

Chapter Six - Partial Differential Equations

6.1. Introduction

Given a function u that depends on both x and y, the partial derivative of u with respect to x at an arbitrary point (x, y) is defined as

$$\frac{\partial u}{\partial x} = \lim_{\Delta x \to 0} \frac{u(x + \Delta x. y) - u(x. y)}{\Delta x} \tag{6.1}$$

Similarly, the partial derivative with respect to y is defined as

$$\frac{\partial u}{\partial y} = \lim_{\Delta y \to 0} \frac{u(x. y + \Delta y) - u(x. y)}{\Delta y} \tag{6.2}$$

An equation involving partial derivatives of an unknown function of two or more independent variables is called a **partial differential equation**, or **PDE**. The **order of a PDE** is that of the **highest-order partial derivative** appearing in the equation. For example, the following two equations are second- and third-order, respectively.

$$\frac{\partial^2 u}{\partial x^2} + 2xy \frac{\partial^2 u}{\partial y^2} + u = 1 \tag{6.3}$$

$$\frac{\partial^3 u}{\partial x^2\, \partial y} + x \frac{\partial^2 u}{\partial y^2} + 8u = 5y \tag{6.4}$$

A partial differential equation is said to be linear if it is linear in the unknown function and all its derivatives, with coefficients depending only on the independent variables. For example, the above two equations are linear, whereas the following two equations are not.

$$\left(\frac{\partial^2 u}{\partial x^2}\right)^3 + 6 \frac{\partial^3 u}{\partial x\, \partial y^2} = x \tag{6.5}$$

$$\frac{\partial^2 u}{\partial x^2} + xu \frac{\partial u}{\partial y} = x \tag{6.6}$$

Because of their widespread application in engineering, our treatment of PDEs will focus on linear, second-order equations. For two independent variables, such equations can be expressed in the following general form:

$$A \frac{\partial^2 u}{\partial x^2} + B \frac{\partial^2 u}{\partial x\, \partial y} + C \frac{\partial^2 u}{\partial y^2} + D = 0 \tag{6.7}$$

where A, B, and C are functions of x and y and D is a function of x, y, u, ∂u/∂x, and ∂u/∂y. Depending on the values of the coefficients of the second-derivative terms A, B, and C, Eq. (6.7) can be classified into one of three categories shown in **Table 6.1**. It should be noted that for cases where A, B, and C depend on x and y, the equation may actually fall into a different category, depending on the location in the domain for which the equation holds. For simplicity, we will limit the present discussion to PDEs that remain exclusively in one of the categories.

Table 6.1 Categories into which linear, second-order partial differential equations in two variables can be classified.

$B^2 - 4AC$	Category	Examples
< 0	Elliptic	Laplace equation (steady state with two spatial dimensions) $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$
= 0	Parabolic	Heat conduction equation (time variable with one spatial dimension) $\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t}$
> 0	Hyperbolic	Wave equation (time variable with one spatial dimension) $\frac{\partial^2 Y}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 Y}{\partial t^2}$

6.2. Partial differential equations (PDEs) and Engineering Practice

Each of the categories of partial differential equations in the above table conforms to specific kinds of engineering problems. The following sections in this chapter will be devoted to deriving each type of equation for a particular engineering problem context.

Elliptic equations are typically used to characterize steady-state systems. As in the Laplace equation in the above table, this is indicated by the absence of a time derivative. Thus, these equations are typically employed to determine the steady-state distribution of an unknown in two spatial dimensions.

A simple example is the heated plate in **Fig. 6.1 a**. For this case, the boundaries of the plate are held at different temperatures. Because heat flows from regions of high to low temperature, the boundary conditions set up a potential that leads to heat flow from the hot to the cool boundaries. If sufficient time elapses, such a system will eventually reach the stable or steady-state distribution of temperature depicted in **Fig. 6.1 a**. The Laplace equation, along with appropriate boundary conditions, provides a means to determine this distribution. By analogy, the same approach can be employed to tackle other problems involving potentials, such as seepage of water under a dam (**Fig. 6.1 b**) or the distribution of an electric field (**Fig. 6.1 c**).

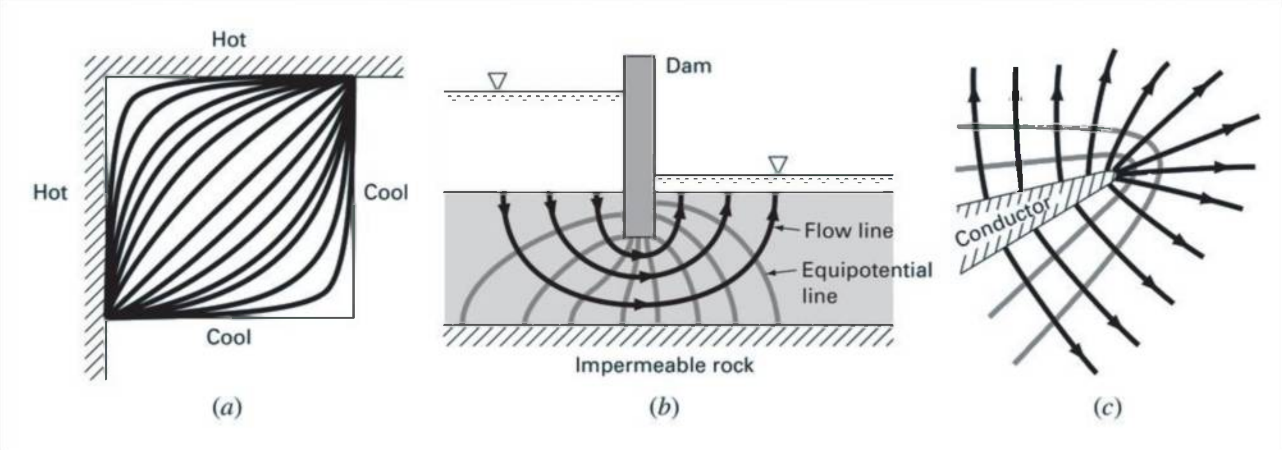


Fig. 6.1 Three steady-state distribution problems that can be characterized using elliptic partial differential equations (PDEs). **(a)** Temperature distribution on a heated plate, **(b)** seepage of water under a dam, and **(c)** the electric field near the point of a conductor.

In contrast to the elliptic category, ***parabolic equations*** determine how an unknown varies in both space and time. This is manifested by the presence of both spatial and temporal derivatives in the heat conduction equation from **Table 6.1**. Such cases are referred to as propagation problems because the solution "propagates,'' or changes, in time.

A simple example is a long, thin rod that is insulated everywhere except at its end (**Fig. 6.2 a**). The insulation is employed to avoid complications due to heat loss along the rod's length. As was the case for the heated plate in **Fig. 6.1 a**, the ends of the rod are set at fixed temperatures. However, in contrast to **Fig. 6.1 a**, the rod's thinness allows us to assume that heat is distributed evenly over its cross section, that is, laterally. Consequently, lateral heat flow is not an issue, and the problem reduces to studying the conduction of heat along the rod's longitudinal axis. Rather than focusing on the steady-state distribution in two spatial dimensions, the problem shifts to determining how the *one-dimensional spatial distribution changes as a function of time* (**Fig. 6.2 b**). Thus, the solution consists of a series of spatial distributions corresponding to the state of the rod at various times. Using an analogy from photography, the elliptic case yields a portrait of a system's stable state, whereas the parabolic case provides a motion picture of how it changes from one state to another. As with the other types of PDEs described herein, parabolic equations can be used to characterize a wide variety of other engineering problem contexts by analogy.

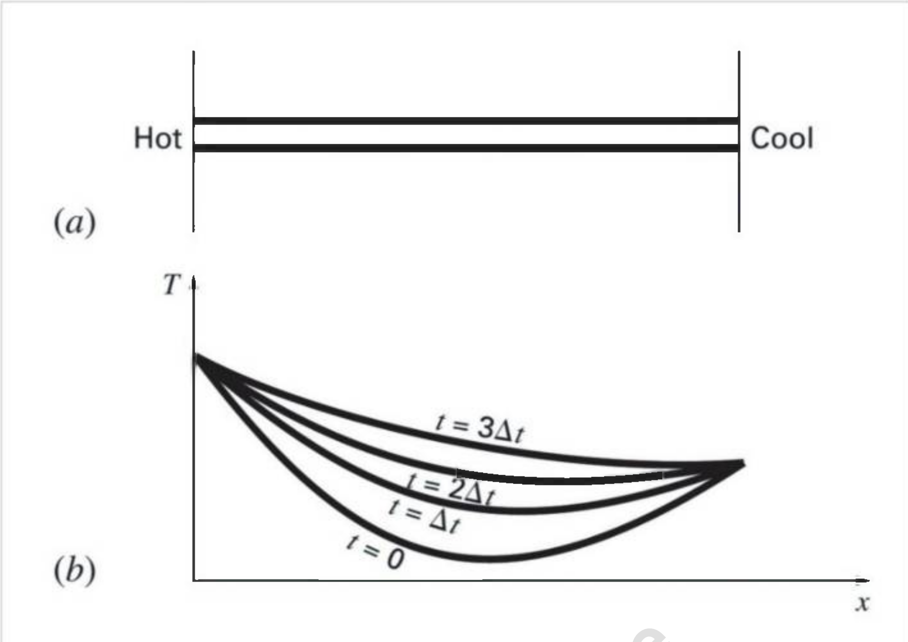


Fig. 6.2 (a) A long, thin rod that is insulated everywhere but at its end. The dynamics of the one-dimensional distribution of temperature along the rod's length can be described by a parabolic PDE. **(b)** The solution, consisting of distributions corresponding to the state of the rod at various times.

The final class of PDEs, **the hyperbolic category**, also deals with propagation problems. However, an important distinction manifested by the wave equation in **Table 6.1** is that the unknown is characterized by a ***second derivative with respect to time***. Consequently, the solution oscillates.

The vibrating string in **Fig. 6.3** is a simple physical model that can be described with the wave equation. The solution consists of a number of characteristic states with which the string oscillates. There are variety of engineering systems that can be characterized by this model such as vibrations of rods and beams, motion of fluid waves, and transmission of sound and electrical signals.

Fig. 6.3 A taut string vibrating at a low amplitude is a simple physical system that can be characterized by a hyperbolic PDE.

Prior to the advent of digital computers, engineers relied on analytical or exact solutions of partial differential equations. However, many physical systems could not be solved directly but had to be simplified. Although these solutions are elegant and yield insight, they are limited with respect to how faithfully they represent real systems, especially those that are highly nonlinear and irregularly shaped. Using numerical methods, partial differential equations PDEs can be solved with different categories of approaches such as finite-difference method and finite-element method. ***Finite-difference methods*** are based on approximating the solution at a finite number of points. In contrast, finite-element methods approximate the solution in pieces, or "elements." Various parameters are adjusted until these approximations conform to the underlying differential equation in an optimal sense. ***This chapter is devoted to the solution of partial differential equations PDEs using finite-difference methods.***

6.3. Finite-Difference Solutions of Elliptic Equations

Elliptic equations in engineering are typically used to characterize steady-state, boundary value problems. ***Laplace's equation*** and ***Poisson's equation*** are the simplest examples of elliptic partial differential equations and can be used to model a variety of problems. Because of its simplicity and general relevance to most areas of engineering, we will use a ***heated plate*** as our fundamental context for solving these elliptic PDEs. The plate is ***insulated everywhere*** but at its ***edges***, where the ***temperature*** can be set at a ***prescribed level***. The insulation and the thinness of the plate mean that heat transfer is limited to the x and y dimensions. At steady state, the flow of heat into the element over a unit time period Δt must equal the flow out. The two-dimensional steady-state temperature distribution in a heated plate can be represented by the ***Laplace equation*** as

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \qquad (6.8)$$

Note that for the case where there are ***sources*** or ***sinks*** of ***heat*** within the two-dimensional domain, the equation is referred to as the ***Poisson equation*** and can be represented as

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = f(x, y) \qquad (6.9)$$

where $f(x, y)$ is a function describing the sources or sinks of heat.

The ***finite-difference solution*** is based on treating the plate as a grid of discrete points (**Fig. 6.4**) and substituting the partial derivatives in **Eq. (6.8)** with finite-difference representations. The ***PDE*** is ***transformed*** into an ***algebraic difference equation***.

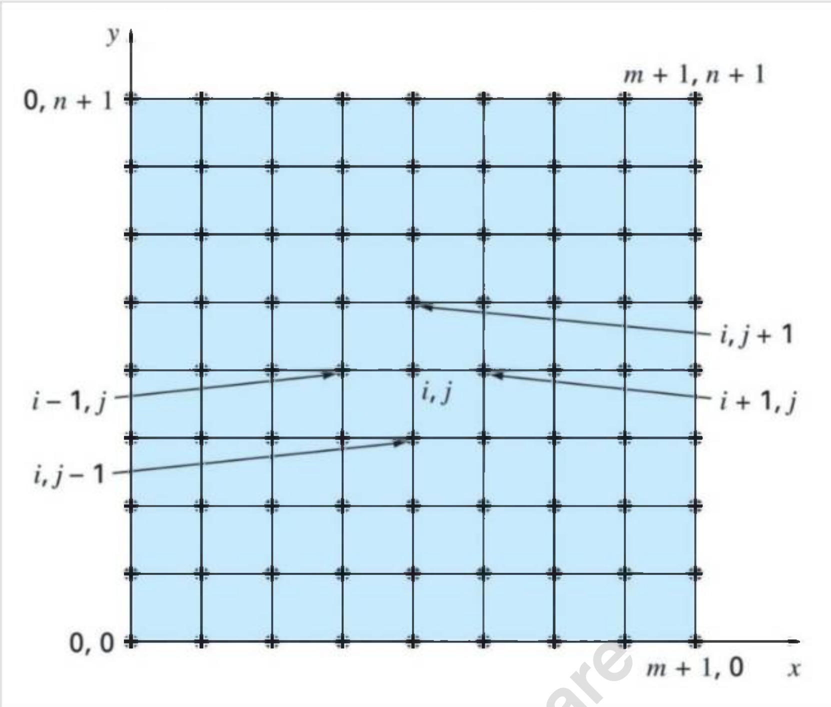


Fig. 6.4 A grid used for the finite-difference solution of elliptic PDEs in two independent variables such as the Laplace equation.

6.3.1. The Laplacian Difference Equation

Remembering "Numerical Differentiation" from "Chapter Four - Numerical Integration and Differentiation", the ***Central differences*** based on the grid scheme from **Fig. 6.4** are

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1,j} - 2\,T_{i,j} + T_{i-1,j}}{\Delta x^2} \tag{6.10}$$

and

$$\frac{\partial^2 T}{\partial y^2} = \frac{T_{i,j+1} - 2\,T_{i,j} + T_{i,j-1}}{\Delta y^2} \tag{6.11}$$

which have errors of $O[(\Delta(x)^2]$ and $O[(\Delta y)^2]$, respectively. Substituting these expressions into **Eq. (6.8)** gives

$$\frac{T_{i+1,j} - 2\,T_{i,j} + T_{i-1,j}}{\Delta x^2} + \frac{T_{i,j+1} - 2\,T_{i,j} + T_{i,j-1}}{\Delta y^2} = 0 \tag{6.12}$$

For the square grid in from **Fig. 6.4**, $\Delta x = \Delta y$, and by collection of terms, the equation becomes

$$T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4\,T_{i,j} = 0 \qquad (6.13)$$

This relationship, which holds for all ***interior points*** on the plate, is referred to as the ***Laplacian difference equation***.

In addition, ***boundary conditions along the edges of the plate*** must be specified to obtain a unique solution. The ***simplest case*** is where the ***temperature at the boundary is set at a fixed value***. This is called a ***Dirichlet boundary condition***. A common alternative boundary condition is the case where the ***derivative at the boundary*** is given. This is commonly referred to as a ***Neumann boundary condition***.

6.3.1.1. Dirichlet Boundary Condition

When the temperature at the boundary of a heated plate is set at a fixed value, this is called a ***Dirichlet boundary condition***. Such is the case for **Fig. 6.5**, where the edges are held at constant temperatures. For this case and according to **Eq. (6.13)**, a balance for ***node (1, 1)*** is,

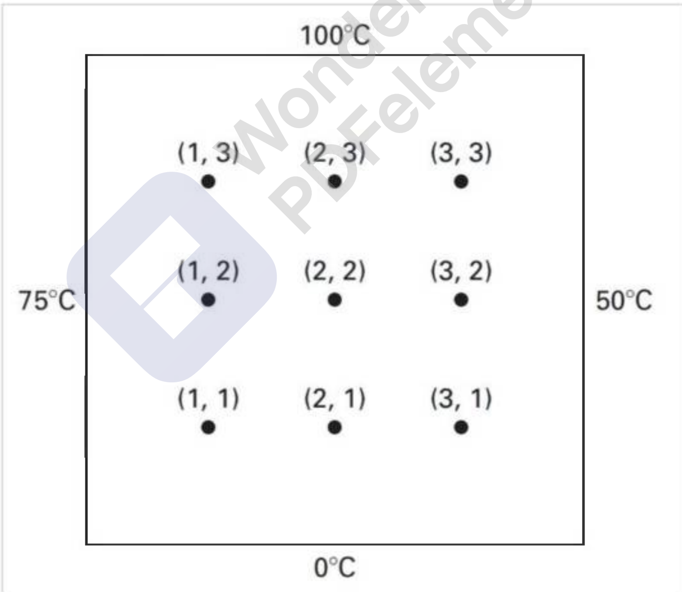


Fig. 6.5 A heated plate where boundary temperatures are held at constant levels. This case is called a ***Dirichlet boundary condition***.

$$T_{21} + T_{01} + T_{12} + T_{10} - 4\,T_{11} = 0 \qquad (6.14)$$

However, $T_{01} = 75$ and $T_{10} = 0$, and therefore, **Eq. (6.14)** can be expressed as

$$4\,T_{11} - T_{12} - T_{21} = 75 \qquad (6.15)$$

For the other ***interior points***, similar equations can be developed. The result is the following set of nine simultaneous equations with nine unknowns:

$$
\begin{array}{ccccccccccl}
4T_{11} & -T_{21} & & -T_{12} & & & & & & = & 75 \\
-T_{11} & +4T_{21} & -T_{31} & & -T_{22} & & & & & = & 0 \\
 & -T_{21} & +4T_{31} & & & -T_{32} & & & & = & 50 \\
-T_{11} & & & +4T_{12} & -T_{22} & & -T_{13} & & & = & 75 \\
 & -T_{21} & & -T_{12} & +4T_{22} & -T_{32} & & -T_{23} & & = & 0 \\
 & & -T_{31} & & -T_{22} & +4T_{32} & & & -T_{33} & = & 50 \\
 & & & -T_{12} & & & +4T_{13} & -T_{23} & & = & 175 \\
 & & & & -T_{22} & & -T_{13} & +4T_{23} & -T_{33} & = & 100 \\
 & & & & & -T_{32} & & -T_{23} & +4T_{33} & = & 150
\end{array}
\qquad (6.16)
$$

6.3.1.2. The Liebmann Method

Most numerical solutions of the Laplace equation involve systems that are much larger than **Eq. (6.16)**. For example, a 10-by-10 grid involves 100 linear algebraic equations. Notice that there are a ***maximum of five unknown terms per line*** in **Eq. (6.16)**. For larger-sized grids, this means that a significant number of the terms will be zero. When applied to such systems, ***full-matrix elimination methods*** waste great amounts of computer memory ***storing these zeros***. For this reason, approximate methods provide a possible approach for obtaining solutions for elliptical equations. The most commonly employed approach is ***Gauss-Seidel***, which ***when applied to PDEs*** is also referred to as ***Liebmann's method***. In this technique, **Eq. (6.13)** is solved iteratively for ***j = 1 to n*** and ***i = 1 to m*** and expressed as

$$T_{i,j} = \frac{T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1}}{4} \qquad (6.17)$$

Over-relaxation is sometimes employed to accelerate the rate of convergence by applying the following formula after each iteration:

$$T_{i,j}^{New} = \lambda\, T_{i,j}^{New} + (1-\lambda)\, T_{i,j}^{Old} \qquad (6.18)$$

where $T_{i,j}^{New}$ and $T_{i,j}^{Old}$ are the values of $T_{i,j}$ from the present and the previous iteration, respectively, and λ is a **weighting factor** that is set between **1** and **2**. As with the conventional Gauss-Seidel method, the iterations are repeated until the absolute values of all the percent relative errors ($\varepsilon_{i,j}$) fall below a pre-specified stopping criterion. These percent relative errors are estimated by

$$\varepsilon_{i,j} = \left|\frac{T_{i,j}^{New} - T_{i,j}^{Old}}{T_{i,j}^{New}}\right| * 100\% \qquad (6.19)$$

Example (6.1): Use Liebmann's method (Gauss-Seidel) to solve for the temperature of the heated plate in **Fig. 6.5**. Iterate until the **maximum error** falls below 1%.

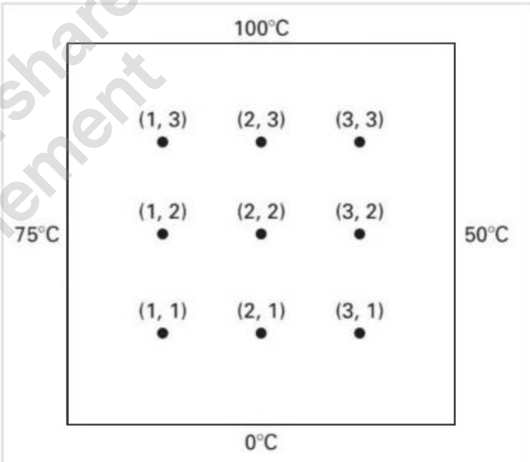
Solution:

For the first iteration, because all the $T_{i,j}$'s are initially zero, the values of error will be 100%.

Equation (6.17) at i = 1 and j = 1 is

$$T_{11} = \frac{0 + 75 + 0 + 0}{4} = 18.75$$

The computation is repeated for the values of i = 1 to 3 and j = 1 to 3 to give



$$T_{21} = \frac{0 + 18.75 + 0 + 0}{4} = 4.69$$

$$T_{31} = \frac{50 + 4.69 + 0 + 0}{4} = 13.67$$

$$T_{12} = \frac{0 + 75 + 0 + 18.75}{4} = 23.44$$

$$T_{22} = \frac{0 + 23.44 + 0 + 4.69}{4} = 7.03$$

$$T_{32} = \frac{50 + 7.03 + 0 + 13.67}{4} = 17.68$$

$$T_{13} = \frac{0 + 75 + 100 + 23.44}{4} = 49.61$$

$$T_{23} = \frac{0 + 49.61 + 100 + 7.03}{4} = 39.16$$

$$T_{33} = \frac{50 + 39.16 + 100 + 17.68}{4} = 51.71$$

49.61	39.16	51.71
23.44	7.03	17.68
18.75	4.69	13.67

For the second iteration the results are

63.38	60.51	61.91
39.36	26.96	37.13
25.78	11.62	19.83

The error for $T_{1,1}$ can be estimated as [Eq. (6.19)]

$$\varepsilon_{1,1} = \left|\frac{25.78 - 18.75}{25.78}\right| * 100\% = 27.27\%$$

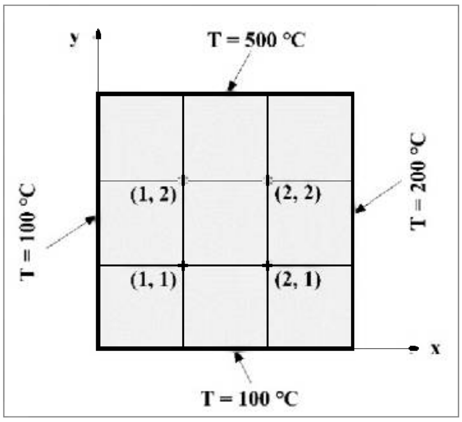
Because this value is above the stopping criterion of 1%, the computation is continued until a maximum error of 0.70% is reached after the ninth iteration; the results are presented in the following table,

Point	Number of Iteration																	
	1		2		3		4		5		6		7		8		9	
	T °C	ε%	T °C	ε%	T °C	ε%	T °C	ε%	T °C	ε%	T °C	ε%	T °C	ε%	T °C	ε%	T °C	ε%
1, 1	18.75	100.00	25.78	27.27	31.50	18.16	35.95	12.38	39.25	8.41	41.04	4.36	41.94	2.15	42.40	1.08	42.63	0.54
2, 1	4.69	100.00	11.62	59.64	19.57	40.62	26.06	24.90	29.62	12.02	31.43	5.76	32.35	2.84	32.80	1.37	33.03	0.70
3, 1	13.67	100.00	19.83	31.06	26.68	25.67	30.28	11.89	32.10	5.67	33.02	2.79	33.47	1.34	33.70	0.68	33.82	0.35
1, 2	23.44	100.00	39.36	40.45	49.21	20.02	55.94	12.03	59.52	6.01	61.34	2.97	62.26	1.48	62.72	0.73	62.95	0.37
2, 2	7.03	100.00	26.96	73.92	41.61	35.21	48.93	14.96	52.59	6.96	54.42	3.36	55.34	1.66	55.80	0.82	56.03	0.41
3, 2	17.68	100.00	37.13	52.38	45.05	17.58	48.79	7.67	50.63	3.63	51.54	1.77	52.00	0.88	52.23	0.44	52.35	0.23
1, 3	49.61	100.00	63.38	21.73	71.18	10.96	74.91	4.98	76.74	2.38	77.66	1.18	78.12	0.59	78.35	0.29	78.46	0.14
2, 3	39.16	100.00	60.51	35.28	68.68	11.90	72.44	5.19	74.29	2.49	75.20	1.21	75.66	0.61	75.89	0.30	76.01	0.16
3, 3	51.71	100.00	61.91	16.48	65.93	6.10	67.81	2.77	68.73	1.34	69.19	0.66	69.42	0.33	69.53	0.16	69.59	0.09

Exercise (6.1):

a. Repeat Example (6.1) using over-relaxation with a value of 1.5 for the weighting factor and iterate until the **maximum error** falls below 1%.

b. The four sides of the square plate shown in figure are kept at constant temperatures. Using finite difference method to solve the Laplace equation, find the temperature distribution at the four mesh points by applying Liebmann's (Gauss-Seidel) method. Make two iterations only.



6.3.1.3. Neumann Boundary Condition

The ***fixed*** or ***Dirichlet boundary condition*** discussed to this point is but one of several types that are used with partial differential equations. A common alternative is the case where the ***derivative is given***. This is commonly referred to as a ***Neumann boundary condition***. For the heated-plate problem, this amounts to specifying the ***heat flux rather than the temperature at the boundary***. One example is the situation where ***the edge is insulated***. In this case, the ***derivative is zero*** because insulating a boundary means that the heat flux (and consequently the gradient) must be zero.

Considering a node (0, j) at the left edge of a heated plate shown in Fig. 6.6 and applying Eq. (6.13) at the point gives

$$T_{1,j} + T_{-1,j} + T_{0,j+1} + T_{0,j-1} - 4\,T_{0,j} = 0 \qquad (6.20)$$

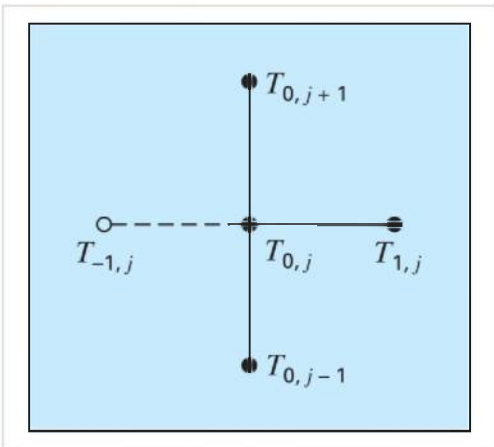


Fig. 6.6 A boundary node (0, j) on the left edge of a heated plate. To approximate the derivative normal to the edge (that is, the x derivative), an imaginary point (-1, j) is located a distance Δx beyond the edge.

Notice that an imaginary point (-1, j) lying outside the plate is required for this equation. Although this exterior fictitious point might seem to represent a problem, it actually serves as the vehicle for incorporating the derivative boundary condition into the problem. This is done by representing the first derivative in the x dimension at (0, j) by the finite divided difference

$$\frac{\partial T}{\partial x} \cong \frac{T_{1,j} - T_{-1,j}}{2\,\Delta x} \tag{6.21}$$

which can be solved for

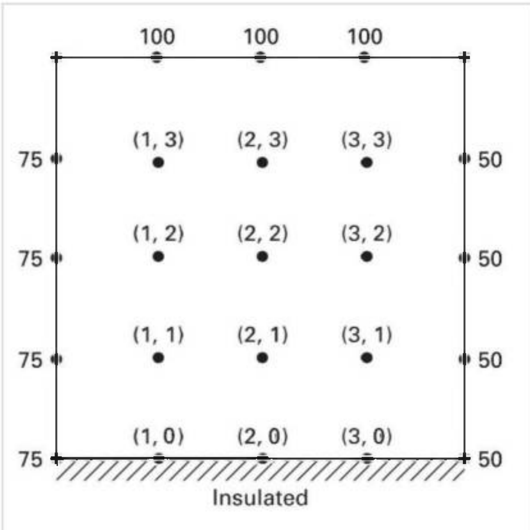
$$T_{-1,j} = T_{1,j} - 2\,\Delta x\,\frac{\partial T}{\partial x} \tag{6.22}$$

Now we have a relationship for $T_{-1,j}$ that actually includes the derivative. It can be substituted into Eq. (6.20) to give

$$2\,T_{1,j} - 2\,\Delta x\,\frac{\partial T}{\partial x} + T_{0,j+1} + T_{0,j-1} - 4\,T_{0,j} = 0 \tag{6.23}$$

Thus, we have incorporated the derivative into the balance. Similar relationships can be developed for derivative boundary conditions at the other edges. ***For an insulated edge, the derivative is zero***. The following example shows how this is done for the heated plate.

Example (6.2): Repeat the same problem as in Example (6.1), but with the lower edge insulated.



Solution:

The general equation to characterize a derivative at the lower edge (that is, at j = 0) of a heated plate is

$$T_{i+1,0} + T_{i-1,0} + 2\,T_{i,1} - 2\,\Delta y\,\frac{\partial T}{\partial y} - 4\,T_{i,0} = 0$$

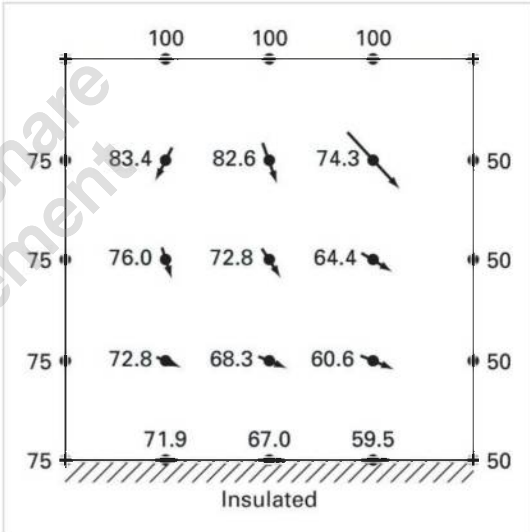
For an insulated edge, the derivative is zero and the equation becomes

$$T_{i+1,0} + T_{i-1,0} + 2\,T_{i,1} - 4\,T_{i,0} = 0$$

The simultaneous equations for temperature distribution on the plate, shown in the figure above, with an insulated lower edge can be written in matrix form as

$$
\begin{bmatrix}
4 & -1 & & -2 & & & & & & & & \\
-1 & 4 & -1 & & -2 & & & & & & & \\
& -1 & 4 & & & -2 & & & & & & \\
-1 & & & 4 & -1 & & -1 & & & & & \\
& -1 & & -1 & 4 & -1 & & -1 & & & & \\
& & -1 & & -1 & 4 & -1 & & -1 & & & \\
& & & -1 & & & 4 & -1 & & -1 & & \\
& & & & -1 & & -1 & 4 & -1 & & -1 & \\
& & & & & -1 & & -1 & 4 & & & -1 \\
& & & & & & -1 & & & 4 & -1 & \\
& & & & & & & -1 & & -1 & 4 & -1 \\
& & & & & & & & -1 & & -1 & 4
\end{bmatrix}
\begin{Bmatrix} T_{10} \\ T_{20} \\ T_{30} \\ T_{11} \\ T_{21} \\ T_{31} \\ T_{12} \\ T_{22} \\ T_{32} \\ T_{13} \\ T_{23} \\ T_{33} \end{Bmatrix}
=
\begin{Bmatrix} 75 \\ 0 \\ 50 \\ 75 \\ 0 \\ 50 \\ 75 \\ 0 \\ 50 \\ 175 \\ 100 \\ 150 \end{Bmatrix}
$$

Note that because of the derivative boundary condition, the matrix is increased to 12 × 12 in contrast to the 9 × 9 system in Eq. (6.16) to account for the three unknown temperatures along the plate's lower edge. These equations can be solved for



$T_{10} = 71.91$	$T_{20} = 67.01$	$T_{30} = 59.54$
$T_{11} = 72.81$	$T_{21} = 68.31$	$T_{31} = 60.57$
$T_{12} = 76.01$	$T_{22} = 72.84$	$T_{32} = 64.42$
$T_{13} = 83.41$	$T_{23} = 82.63$	$T_{33} = 74.26$

The temperatures and heat fluxes are displayed in in the figure above. Note that, because the lower edge is insulated, the plate's temperature is higher than that obtained in Example (6.1), where the bottom edge temperature is fixed at zero.

6.4. Finite-Difference Solutions of Parabolic Equations

The previous section dealt with steady-state PDEs. We now turn to the parabolic equations that are employed to characterize time-variable problems. In a fashion similar to the Laplace equation, which deals with the two-dimensional steady-state temperature distribution in a heated plate, conservation of heat can be used to develop a heat balance for the differential element in the ***long, thin insulated rod*** shown in Fig. 6.7. However, rather than examine the steady-state case, the present balance also considers the amount of heat stored in the element over a unit time period Δt. The resulting equation is the ***heat-conduction equation*** and it is an example of parabolic PDEs which is given as

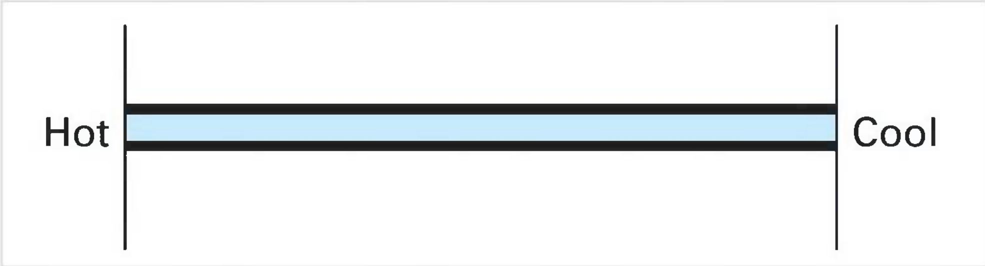


Fig. 6.7 A thin rod, insulated at all points except at its ends.

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t} \qquad (6.24)$$

knowing that, $$\alpha = \frac{k}{\rho\, C} \qquad (6.25)$$

where α is referred to as the coefficient of thermal diffusivity (cm^2/s), ρ is the density of the material (g/cm^3), **C** is the heat capacity of the material [cal/(g . °C)], **T** is the temperature (°C), and **k** is the coefficient of thermal conductivity [cal/(s . cm . °C)]. Both k and α are parameters that reflect how well the material conducts heat.

Just as with elliptic PDEs, parabolic equations can be solved by substituting finite divided differences for the partial derivatives. However, in contrast to elliptic PDEs, we must now consider changes in time as well as in space. Because of their time-variable nature, solutions to these equations involve a number of new issues, notably ***stability***. This, as well as other aspects of parabolic PDEs, will be examined in the following sections as we present two fundamental solution approaches, ***explicit and implicit schemes***.

The fundamental difference between explicit and implicit approximations is depicted In Fig. 6.8. For the ***explicit form***, we approximate the ***spatial derivative*** at ***time level l***. Recall that when we substituted this approximation into the partial differential equation, we obtained a difference equation with a single unknown T_i^{l+1}. Thus, we can solve "***explicitly***" for this unknown. In ***implicit methods***, the spatial derivative is approximated at an advanced time level ***l + 1***. The resulting difference equation contains ***several unknowns***. Thus, it cannot be solved explicitly by simple algebraic rearrangement as was done in explicit methods. Instead, the entire system of equations must be solved simultaneously. This is possible because, along with the boundary conditions, the implicit formulations result in a set of linear algebraic equations with the same number of unknowns. Thus, the method reduces to the solution of a set of simultaneous equations at each point in time.

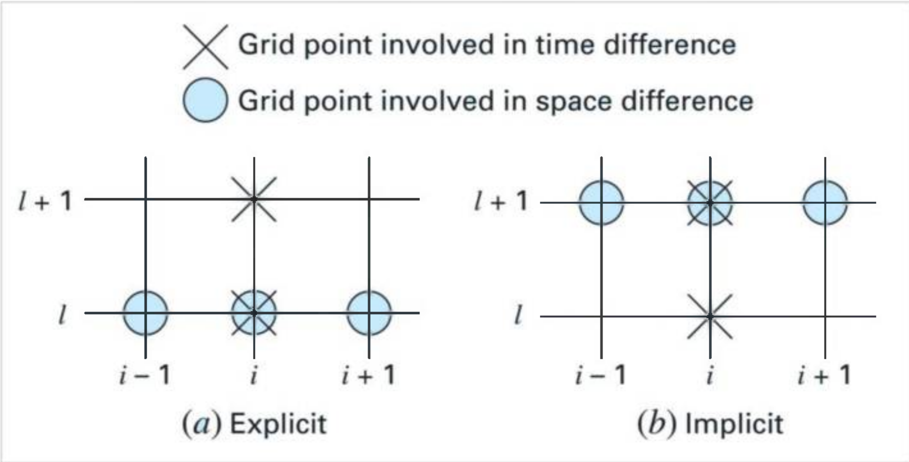


Fig. 6.8 Fundamental differences between (a) explicit and (b) implicit methods.

As noted previously, ***explicit finite-difference formulations*** have problems related to ***stability***. ***Implicit methods*** overcome both this difficulty at the expense of somewhat more complicated algorithms. Thus, the following sections in this chapter will be focused on the ***solution of parabolic PDEs*** using ***explicit scheme***.

6.4.1. Explicit Methods

The ***heat-conduction equation*** (**Eq. (6.24)**) requires ***approximations*** for the ***second derivative in space*** and the ***first derivative in time***. The ***second derivative in space*** is represented in the same fashion as for the Laplace equation by a ***centered finite-divided difference***:

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1}^{l} - 2\,T_i^l + T_{i-1}^l}{(\Delta x)^2} \tag{6.26}$$

which has an error of O[(Δx)^2]. Notice the slight change in ***notation of the superscripts*** is used to denote ***time***. This is done so that a second subscript can be used to designate a second spatial dimension when the approach is expanded to two spatial dimensions.

A ***forward finite-divided difference*** is used to approximate the ***time derivative***

$$\frac{\partial T}{\partial t} = \frac{T_i^{l+1} - T_i^l}{\Delta t} \tag{6.27}$$

which has an error of O(Δt).

Substituting Eqs. (6.26) and (6.27) into Eq. (6.24) yields

$$\alpha \frac{T_{i+1}^{l} - 2\,T_i^l + T_{i-1}^l}{(\Delta x)^2} = \frac{T_i^{l+1} - T_i^l}{\Delta t} \tag{6.28}$$

which can be solved for

$$T_i^{l+1} = T_i^l + \lambda\,(T_{i+1}^l - 2\,T_i^l + T_{i-1}^l) \tag{6.29}$$

where, $\lambda = \dfrac{\alpha\,\Delta t}{(\Delta x)^2}$

This equation can be written for ***all the interior nodes*** on the rod. It then provides an ***explicit means*** to compute values at ***each node for a future time*** based on the ***present values at the node and its neighbors***. Notice that this approach is actually a manifestation of Euler's method for solving ODEs. That is, if we know the temperature distribution as a function of position at an initial time, we can compute the distribution at a future time based on Eq. (6.29). A computational molecule for the explicit method is depicted in Fig. 6.8, showing the nodes that constitute the **spatial** and ***temporal (time-based)*** approximations.

Example (6.3): Use the explicit method to solve for the temperature distribution of a long, thin rod with a length of 10 cm and the following values: k = 0.49 cal/(s . cm . °C), Δx = 2 cm, and Δt = 0.1 s. At time t = 0, the temperature of the rod is zero and the boundary conditions are fixed for all times at T(0) = 100 °C and T(10) = 50 °C. Note that the rod is made of aluminum with C = 0.2174 cal/(g . °C) and ρ = 2.7 g/cm^3.

Solution:

We have $\alpha = \dfrac{k}{\rho\,C} = \dfrac{0.49}{2.7 \times 0.2174} = 0.835\ \text{cm}^2/\text{s}$

and $\lambda = \dfrac{\alpha\,\Delta t}{(\Delta x)^2} = \dfrac{0.835 \times 0{,}1}{(2)^2} = 0.020875$

At **t = 0.1 s** for the node at **x = 2 cm**, applying **Eq. (6.29)** gives the following value:

$$T_i^{l+1} = T_i^l + \lambda\,(T_{i+1}^l - 2\,T_i^l + T_{i-1}^l)$$

$$T_1^1 = 0 + 0.020875\,[0 - 2\,(0) + 100] = 2.0875$$

At the other interior points, **x = 4, 6, and 8 cm**, the results are

$$T_2^1 = 0 + 0.020875\,[0 - 2\,(0) + 0] = 0$$

$$T_3^1 = 0 + 0.020875\,[0 - 2\,(0) + 0] = 0$$

$$T_4^1 = 0 + 0.020875\,[\,50\ - 2\,(0) + 0] = 1.0438$$

At **t = 0.2 s**, the values at the four interior nodes are computed as

$$T_1^2 = 2.0875 + 0.020875\,[\,0\ - 2\,(2.0875) + 100] = 4.0878$$

$$T_2^2 = 0 + 0.020875\,[\,0\ - 2\,(0) + 2.0875] = 0.043577$$

$$T_3^2 = 0 + 0.020875\,[\,1.0438\ - 2\,(0) + 0] = 0.021788$$

$$T_4^2 = 1.0438 + 0.020875\,[\,50\ - 2\,(1.0438) + 0] = 2.0439$$

The computation is continued, and the results at 3-s intervals are depicted in Fig. 6.9. The general rise in temperature with time indicates that the computation captures the diffusion of heat from the boundaries into the aluminum rod.

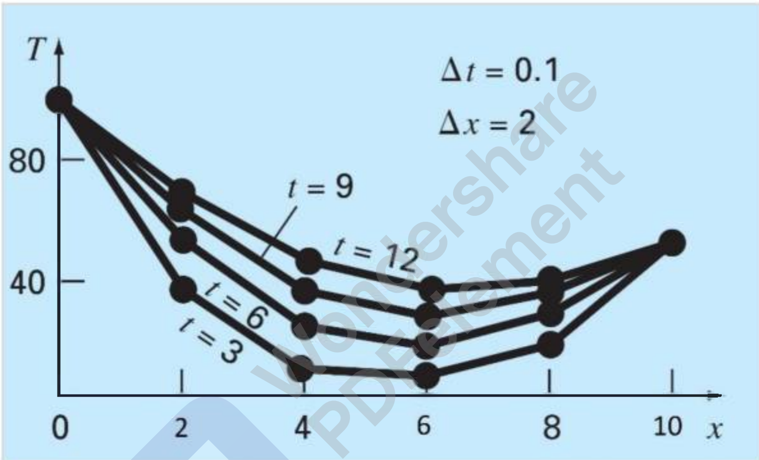


Fig. 6.9 Temperature distribution in a long, thin rod as computed with the explicit method**.**

6.4.1.1. Convergence and Stability

Convergence means that as Δx and Δt approach zero, the results of the finite-difference technique approach the true solution. ***Stability*** means that errors at any stage of the computation are not amplified but are attenuated as the computation progresses. It can be shown that the explicit method is both convergent and stable if

$$\lambda \le \frac{1}{2} \quad \text{where} \quad \lambda = \frac{\alpha\,\Delta t}{(\Delta x)^2} \quad \rightarrow \quad \Delta t \le \frac{1}{2}\,\frac{(\Delta x)^2}{\alpha} \qquad (6.30)$$

In addition, it should be noted that setting **λ ≤ 1/2** could result in a ***solution*** in which ***errors do not grow***, but ***oscillate***. Setting **λ ≤ 1/4** ensures that the ***solution will not oscillate***. It is also known that setting **λ = 1/6** tends to ***minimize truncation error***.

Fig. 6.10 is an example of instability caused by violating Eq. (6.30). This plot is for the same case as in Example 6.3 but with $\lambda = 0.735$, which is considerably greater than 0.5. As in Fig. 6.10, the solution undergoes progressively increasing oscillations. This situation will continue to deteriorate as the computation continues.

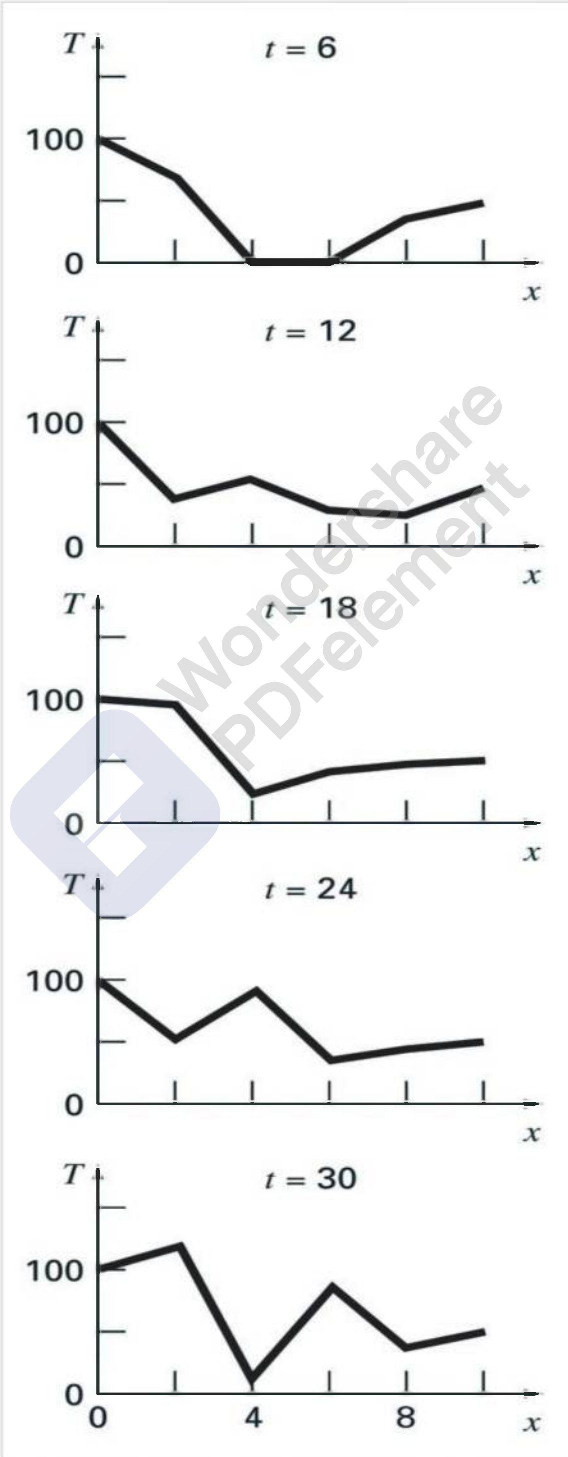


Fig. 6.10 An illustration of instability. Solution of Example 6.3 but with $\lambda = 0.735$.

Although satisfaction of Eq. (6.30) will alleviate the instabilities of the sort manifested in Fig. 6.10, it also places a strong limitation on the explicit method. For example, suppose that ***Δx is halved*** to ***improve the approximation of the spatial second derivative***. According to Eq. (6.30), the ***time step must be quartered*** (i.e., the number of time steps must be increased by a factor of 4) to maintain ***convergence and stability***. Furthermore, the computation for each of these time steps will take twice as long because halving Δx doubles the total number of nodes for which equations must be written. ***Consequently, for the one-dimensional case, halving Δx results in an eightfold increase in the number of calculations***. Thus, the computational load may be large to attain acceptable accuracy.

6.4.1.2. Derivative Boundary Conditions

As was the case for elliptic PDEs, derivative boundary conditions can be similarly incorporated into parabolic PDEs. For a one-dimensional rod, this necessitates adding two equations to characterize the heat balance at the end nodes. For example, ***the node at the left end (i = 0)*** would be represented by

$$T_0^{l+1} = T_0^l + \lambda\,(T_1^l - 2\,T_0^l + T_{-1}^l) \tag{6.31}$$

Thus, an imaginary point is introduced at i = -1 (recall Fig. 6.6). However, as with the elliptic case, this point provides a vehicle for incorporating the derivative boundary condition into the analysis. Using finite divided difference, the derivative boundary condition can be used to eliminate this imaginary node,

$$\left(\frac{\partial T}{\partial x}\right)_0^l \cong \frac{T_1^l - T_{-1}^l}{2\,\Delta x} \tag{6.32}$$

which can be solved for

$$T_{-1}^l = T_1^l - 2\,\Delta x \left(\frac{\partial T}{\partial x}\right)_0^l \tag{6.33}$$

Now we have a relationship for T_{-1}^l that actually includes the derivative. It can be substituted into Eq. (6.31) to give

$$T_0^{l+1} = T_0^l + \lambda\left(2\,T_1^l - 2\,T_0^l - 2\,\Delta x \left(\frac{\partial T}{\partial x}\right)_0^l\right) \tag{6.34}$$

For an ***insulated edge at i = 0***, the derivative $\left(\frac{\partial T}{\partial x}\right)_0^l = 0$ and equation (6.34) becomes

$$T_0^{l+1} = T_0^l + \lambda\,(\,2\,T_1^l \,-2\,T_0^l\,) \tag{6.35}$$

A similar analysis can be used to embed the ***derivative boundary condition*** in the equation for the ***fifth node (i = 5)*** (recall Fig. 6.9). The result is

$$T_5^{l+1} = T_5^l + \lambda\left(2\,T_4^l \,-2\,T_5^l \,-\,2\,\Delta x\left(\frac{\partial T}{\partial x}\right)_5^l\right) \tag{6.36}$$

For an ***insulated edge (zero derivative)*** for the ***fifth node (i = 5)*** (recall Fig. 6.9), equation (6.36) becomes

$$T_5^{l+1} = T_5^l + \lambda\,(\,2\,T_4^l \,-2\,T_5^l\,) \tag{6.37}$$

The equations for the derivative boundary condition and the interior nodes are used together and the entire system can be iterated with a specified time step.

<u>Example (6.4)</u>: Use the explicit method to solve for the temperature distribution of a long, thin rod with a length of 10 cm and the following values: k = 0.49 cal/(s . cm . °C), Δx = 2 cm, and Δt = 0.1 s. At time t = 0, the temperature of the rod is initially at 50 °C and the derivative boundary condition at x = 0 is equal to 1 and at x = 10 is equal to 0. Note that the rod is made of aluminum with C = 0.2174 cal/(g . °C) and ρ = 2.7 g/cm^3.

<u>Solution</u>:

We have $\alpha = \frac{k}{\rho\, C} = \frac{0.49}{2.7 \times 0.2174} = 0.835\ \text{cm}^2/\text{s}$

and $\lambda = \frac{\alpha\,\Delta t}{(\Delta x)^2} = \frac{0.835\ \times 0{,}1}{(2)^2} = 0.020875$

At **<u>t = 0.1 s</u>**

For the ***<u>node</u>*** at **<u>x = 0 cm</u>**, **<u>i = 0</u>**, applying **Eq. (6.34)** gives

$$T_0^{l+1} = T_0^l + \lambda\left(2\,T_1^l \,-2\,T_0^l -\,2\,\Delta x\left(\frac{\partial T}{\partial x}\right)_0^l\right)$$

and using $\Delta x = 2$ and $\left(\frac{\partial T}{\partial x}\right)_0^l = 1$, we have

$$\rightarrow \quad T_0^{l+1} = T_0^l + 0.020875\,(2\,T_1^l - 2\,T_0^l - 4)$$

For the ***interior nodes*** at **x = 2, 4, 6, and 8 cm**, **i = 1, 2, 3, and 4**, applying **Eq. (6.29)** gives

$$T_i^{l+1} = T_i^l + \lambda\,(T_{i+1}^l - 2\,T_i^l + T_{i-1}^l)$$

$$\rightarrow \quad T_i^{l+1} = T_i^l + 0.020875\,(T_{i+1}^l - 2\,T_i^l + T_{i-1}^l)$$

For the ***node*** at **x = 10 cm**, **i = 5**, applying **Eq. (6.37)** gives

$$T_5^{l+1} = T_5^l + \lambda\,(2\,T_4^l - 2\,T_5^l)$$

$$\rightarrow \quad T_5^{l+1} = T_5^l + 0.020875\,(2\,T_4^l - 2\,T_5^l)$$

The results for some of the early steps along with some later selected values are presented in the table below.

t	x = 0	x = 2	x = 4	x = 6	x = 8	x = 10
0	50	50	50	50	50	50
0.1	49.917	50	50	50	50	49.917
0.2	49.837	49.998	50	50	49.998	49.837
0.3	49.76	49.995	50	50	49.995	49.76
0.4	49.686	49.99	50	50	49.99	49.686
0.5	49.615	49.984	50	50	49.984	49.615
•	•	•	•	•	•	•
•	•	•	•	•	•	•
•	•	•	•	•	•	•
200	30	31.8	33.2	34.2	34.8	35
400	13.3	15.1	16.5	17.5	18.1	18.3
600	-3.401	-1.601	-0.201	0.7988	1.3988	1.5988
800	-20.11	-18.31	-16.91	-15.91	-15.31	-15.11
1000	-36.81	-35.01	-33.61	-32.61	-32.01	-31.81

Notice what is happening. The rod never reaches a steady state, because of the heat loss at the left end (unit gradient) and the insulated condition (zero gradient) at the right.

Exercise (6.2):

a. Repeat Example 6.3, but for a time step of $\Delta t = 0.05$ s.

b. Repeat Example 6.3, but for the case where the condition at $x = 10$ is a derivative boundary condition equal to zero.

c. Repeat Example 6.3, but for the case where the condition at $x = 0$ is a derivative boundary condition equal to zero.

d. A thin rod of 3 cm length having a thermal diffusivity coefficient (α) of 0.835 cm^2/s is initially kept at a temperature of 0 °C. The rod is insulated at all points except at its ends which are kept at all times at T(0) = 5 °C and T(3) = 10 °C. Use the explicit method to solve for the temperature distribution in the rod at t = 0.2 second using the following information; $\Delta x = 1$ cm, $\Delta t = 0.1$ second, and $\lambda = \alpha\, \Delta t/\Delta x^2$.

References

1. Chapra, S. C., & Canale, R. P. (2015). Numerical methods for engineers. New York: McGraw-Hill.
2. Dukkipati, R. V. (2010). Numerical methods. New Delhi: New Age International Ltd.
3. Chapra, S. C. (2018). Applied numerical methods with MATLAB for engineers and scientists. New York, N.Y: McGraw-Hill Education.
4. Bird, J. O. (2011). Basic engineering mathematics. Amsterdam: Elsevier.