MAKERERE UNIVERSITY

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DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING

EMT 1201: ENGINEERING MATHEMATICS II LECTURE NOTES 2017/2018

CHAPTER FOUR: NUMERICAL ANALYSIS

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4. NUMERICAL ANALYSIS

Many of the problems that occur in engineering and physics have no analytical solution, and even when one can be found it is frequently the case that the form in which it arises is difficult to use directly if numerical results are required. There are many reasons for such limitations, some typical ones being that the zeros of a function involved in the solution cannot be found analytically, a definite integral that arises cannot be evaluated analytically, an analytical solution of a nonlinear differential equation cannot be found, or a large system of linear simultaneous equations must be solved. A situation of a different type arises when an analytical solution is known, but its application in specific cases leads to a prohibitive amount of calculation, so a more efficient numerical method becomes necessary.

4.1 Decimal places and significant figures

Most numerical results can only be approximate, such as calculations involving$\sqrt{2}$, e or π it is necessary to have a simple way of indicating their accuracy. This is accomplished either by stating that a result is accurate to *n decimal places*, or that it is accurate to a given number of *significant digits (figures)*. For example, when approximating a number such as 17.213622, to *three* decimal places, the *fourth* digit after the decimal point is examined, and if the digit is 5 or more the preceding digit is increased by one and the result truncated to three places after the decimal point. However, if the *fourth* digit is 4 or less, the previous digit is left unchanged and the result is truncated to the existing three digits that follow the decimal point. When this process is applied to the above number to approximate it to an accuracy of three decimal places it becomes 17.214, whereas if it is approximated to an accuracy of four decimal places it becomes 17.2136.

4.2 Roots of non – linear functions

Let *f(x)* be a real valued function on the interval$a \leq x \leq b$. A number, x_0, is called a *root* of the function f(x) in this interval if $f(x_0) = 0$ and correspondingly a number, $x = x_0$, is called a *zero* of the function f(x).

The need to find roots of functions is fundamental to the development and application of mathematics, and only in simple cases can the roots be determined analytically, so in all other cases it is necessary to find them numerically.

Numerical determination of the roots of functions

4.2.1 The Bisection method

This method applies to roots of functions $f(x)$ with the property that $f(x)$ changes sign when x crosses a root. This method can be easily programmed.

Consider a continuous function *f(x)* and numbers $\alpha < \beta$ such that *f(α)* and *f(β)* have opposite signs. Then by the intermediate value theorem, the function *f(x)* must varnish at least once (must have at least one root, x_0) in the interval $\alpha < x < \beta$ as shown in the proceeding figures:

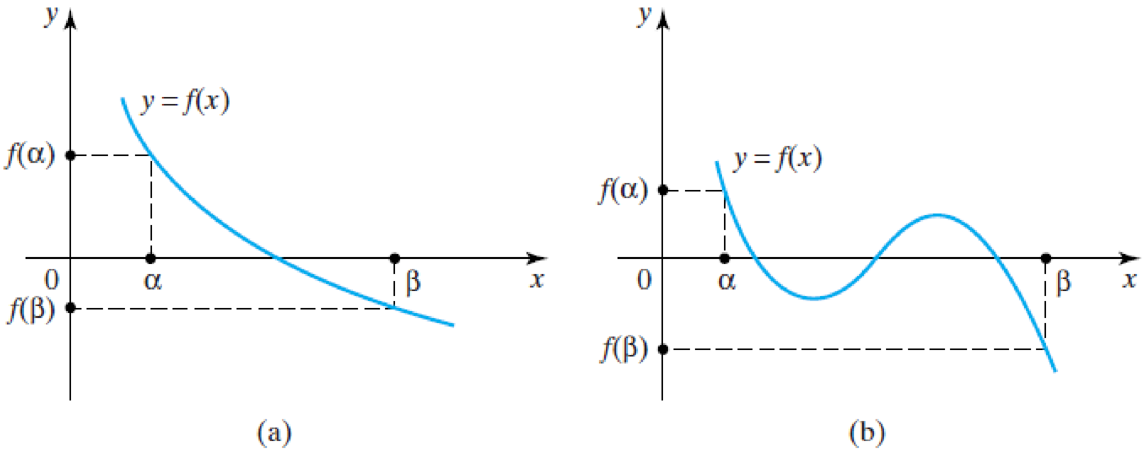


Figure 4.1 Roots of a function y = f(x)

If *f(α)* and *f(β)*, have the same sign, nothing can be deduced about the existence of a root in the interval. Figs c – e illustrate situations in which there is a double root, two roots and no root respectively.

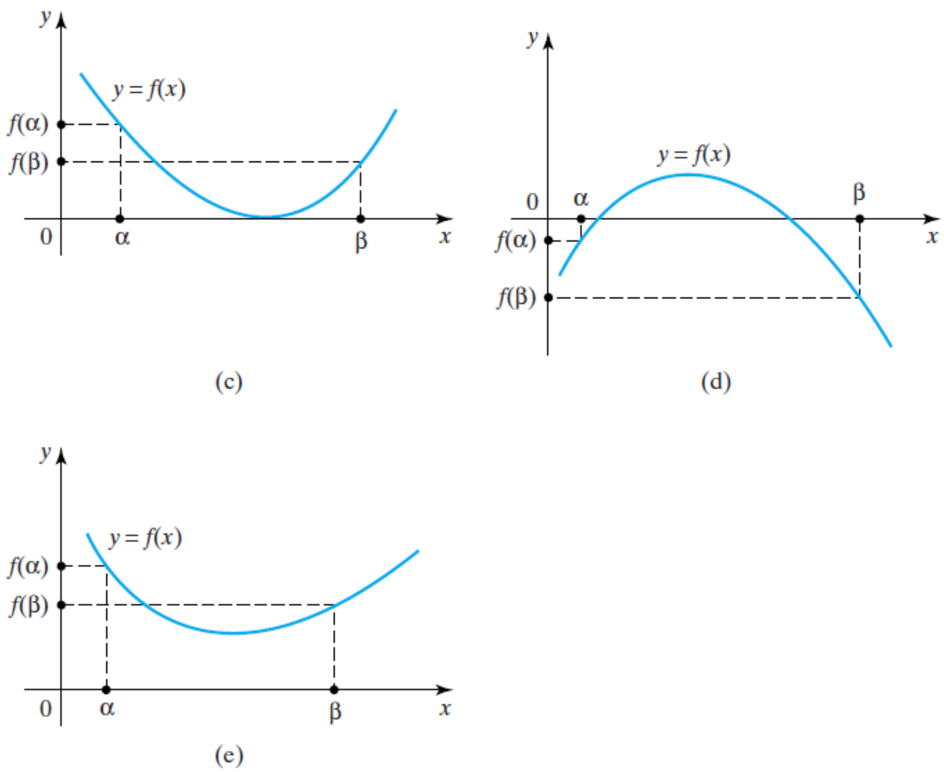


Figure 4.2 Existence of a root(s) in the interval (α, β)

Steps in the bisection method

- If the product *f(α)f(β)* is negative, it indicates that the function has opposite signs at the extremes of the interval, $\alpha \leq x \leq \beta$ but when the product is positive there is no such change in sign.
- The first step in the bisection method involves dividing (bisecting) the interval, $\alpha \leq x \leq \beta$ into the subinterval $\alpha \leq x \leq x_1$ and $x_1 \leq x \leq \beta$, where $x_1 = \frac{\alpha+\beta}{2}$.
- If the product, $f(\alpha)f(x_1) > 0$ the next subinterval to be considered in the proceeding step is$x_1 \leq x \leq \beta$, obtained by replacing α by x_1 because in this case, $f(x)$ changes sign in the subinterval $x_1 < x < \beta$ so this interval must contain the root of f(x).

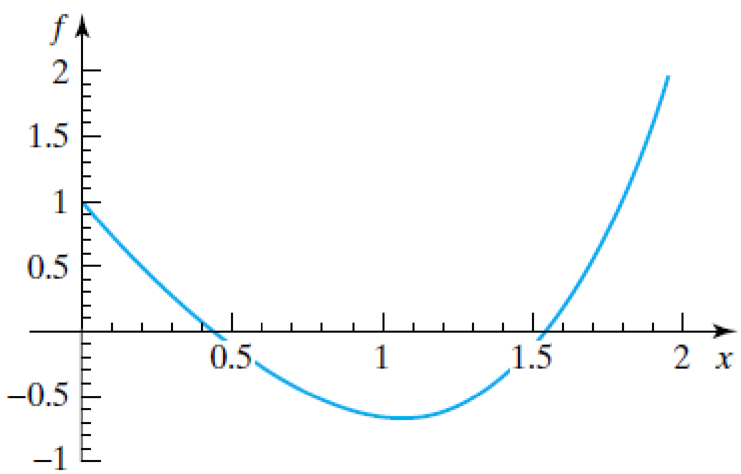
  If $f(\alpha)f(x_1) < 0$ the subinterval to be used in the next step is obtained by replacing β by x_1 because in this case f(x) experiences a change of sign in the interval, $\alpha \leq x \leq x_1$ and this interval must contain the required root.
- The bisection method involves a repetition of this procedure each time using the smaller subinterval found at the previous stage of the calculation, until a required degree of accuracy is achieved.

Example 4.2.1

Use the bisection method to find the smallest root of the function $f(x) = 1 - 3x + \frac{1}{2}xe^x$ correct to 2 decimal places.

Solution

The function in question can be represented in the figure below:



From the figure it is clear that $f(x) = 0$ for values$x \approx 0.45$. Suitable values for α and β are $\alpha = 0.43$ and $\beta = 0.47$ because $f(\alpha) = 0.0405$ and $f(\beta) = -0.0340$.We wish to approximate the root approximate to 2 dps hence our error should be within 0.005. x_l and x_r denote the x – value at the extreme left and right of the given subinterval respectively.

n	x_l	x_r	x_n	$f(x_l)$	$f(x_r)$	$f(x_l)f(x_r)$	New interval	$\|x_{n+1} - x_n\|$
1	0.43	0.47	0.45	0.0405	0.0029	> 0	$0.45 < x < 0.47$	
2	0.45	0.47	0.46	0.0029	-0.0157	< 0	$0.45<x<0.46$	0.01
3	0.45	0.460	0.455	0.0029	-0.0064	< 0	$0.45<x<0.455$	0.005
4	0.45	0.455	0.4525	0.0029	-0.0018	< 0	$0.45<x<0.4525$	0.0025

Therefore, the root of the equation in question is 0.45 (2dps)

4.2.2 Fixed point iteration

This method is well suited to machine computation provided numerical values of the function involved are easily calculated, and a good approximation to the root is used to start the iteration process. The method involves first writing the given function *f(x)*, in the form;

$$f(x) = x - g(x) \quad \text{.......... (1)}$$

Then if $x = x_0$ makes the expression on the right vanish, it follows that x_0 is a root of *f(x)*.

The expression of the function, *f(x)*, is however, not unique because g(x) can be written in more than one way.

If we now consider the function $g(x)$ to *map* a point x into a point $g(x)$, then a root $x = x_0$ of equation (1) has the property that $g(x)$ maps the point x_0 into itself, and for this reason x_0 is called a *fixed point* of the equation;

$$x = g(x) \quad \text{.......... (2)}$$

The fixed point iteration scheme follows from (2) by writing it as;

$$x_{n+1} = g(x_n) \quad \text{.......... (3)}$$

Example 4.2.2

Find a fixed point iteration scheme for determining $\sqrt{a}$ when $a > 0$, and use it to determine $\sqrt{2}$ to an accuracy of six decimal places.

Solution

We need to determine x such that, $x = \sqrt{a} \Rightarrow x^2 = a$

Therefore, $f(x) = x^2 - a = 0$

This can be written as, $2x^2 = x^2 + a$, dividing through by 2x we get;

$$x = \frac{x}{2} + \frac{a}{2x} = \frac{1}{2}\left(x + \frac{a}{x}\right)$$

So, in the notation of (2), $g(x) = \frac{1}{2}\left(x + \frac{a}{x}\right)$

The fixed point iteration scheme is;

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right)$$

To compute$\sqrt{2}$, it is evident that, $a = 2$

$$\Rightarrow x_{n+1} = \frac{1}{2}\left(x_n + \frac{2}{x_n}\right)$$

For simplicity, we can take $x_0 = 1$; then the results of the calculation are;

$x_0 = 1$, $x_1 = 1.5$, $x_2 = 1.41666667$, $x_3 = 1.41421569$, $x_4 = 1.41421356$, $x_4 = 1.41421356$.

Point x_4 and x_5 are identical and the difference$|x_5 - x_4| < 0.5 \times 10^{-6}$, hence the required root is 1.414214 (correct to 6 dps)

Example 4.2.3

Devise fixed point iteration schemes to find the roots of the quadratic equation; $2x^2 - 24x + 41 = 0$ and test them numerically

Solution

The fixed iterative schemes of the equation can be obtained by either writing it in the forms;

$x = \frac{1}{24}(2x^2 + 41)$ or $x = 12 - \frac{41}{2x}$

Hence the two possible schemes are;

Scheme A: $x_{n+1} = \frac{1}{24}(2{x_n}^2 + 41)$ or

Scheme B: $x_{n+1} = 12 - \frac{41}{2x_n}$

Investigation of the quadratic shows that the quadratic has roots close to $x_0 = 2$ and $x_0 = 10$

Using scheme A:

$x_0 = 2$	$x_0 = 10$
$x_1 = 2.0417$	$x_1 = 10.0417$
$x_2 = 2.0557$	$x_2 = 10.1113$
$x_3 = 2.0605$	.
$x_4 = 2.0621$	.
$x_5 = 2.0627$	$x_8 = 12.4801$
$x_6 = 2.0630$	$x_9 = 14.6877$
.	.
.	.
$x_\infty = 2.0630$	$x_\infty = \infty$

Clearly scheme A is only partially successful, although when started at $x_0 = 2$ it converges to a zero close to 2 but it diverges when started at $x_0 = 10$ and unsuccessful to determine the zero close to 10.

Using Scheme B:

$$
\begin{array}{ll}
x_0 = \ \ 2 & x_0 = 10 \\
x_1 = \ \ 1.75 & x_1 = \ 9.7222 \\
x_2 = \ \ 0.2857 & x_2 = \ 9.8914 \\
x_3 = -59.7500 & x_3 = \ 9.9275 \\
x_4 = \ \ 12.3431 & x_4 = \ 9.9350 \\
x_5 = \ \ 10.3392 & x_5 = \ 9.9370 \\
x_6 = \ \ 10.0172 & x_6 = \ 9.9370 \\
x_7 = \ \ 9.9535 & \quad \vdots \\
\quad \vdots & x_\infty = \ 9.9370 \\
x_\infty = \ \ 9.9370. &
\end{array}
$$

Here the scheme is also partially successful; although it can be successfully be used to determine the zero close to 10, it can't be used for that close to 2.

Convergence of a fixed point iterative scheme

Let $g(x)$ be defined in the interval $a \le x \le b$ in which it has a fixed point x_0, and let g(x) be continuous throughout this interval with a continuous derivative, $g'(x)$ such that $|g'(x)| \le k < 1$. Then the equation $x = g(x)$ has a unique fixed point x_0 in the interval and if $a \le x_0 \le b$ the iterative scheme;

$x_{n+1} = g(x_n)$ will converge to x_0.

4.2.3 Newton's method

The *Newton's method* for determining the zero of the differentiable function $f(x) = 0$ is also known as the *Newton Raphson method*. The method is commonly used because of its simplicity.

The idea in this method is that we approximate the graph of the function f by suitable tangents. Consider Figure 4.3 below:

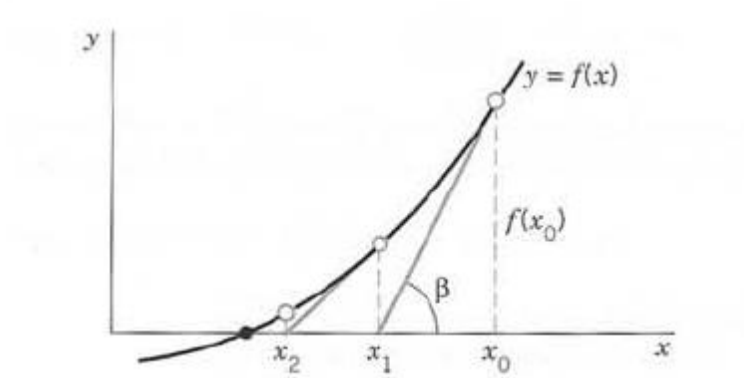


Figure 1.3 Newton's method

Using an approximate value x_0 obtained from the graph of f, we let x_1 be the point of intersection of the x – axis and the tangent to the curve at x_0, then;

$$\tan\beta = f'(x_0) = \frac{f(x_0)}{x_0 - x_1} \text{ hence, } x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

In the second step we compute $x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$, in the third step we compute x_3 from x_2 using the same formula, so generally; $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$.

The following Algorithm therefore, describes the steps taken in finding the zero of the equation *f(x) = 0*:

Newton Raphson Algorithm

INPUT: *f, f'*, initial approximation x_0, tolerance (acceptable error), $\varepsilon > 0$ or maximum number of iterations, *N*.

OUTPUT: Approximate solution, x_n $(n \leq N)$, or message of failure.

For *n = 0, 1, 2, ……N-1*, the following is done:

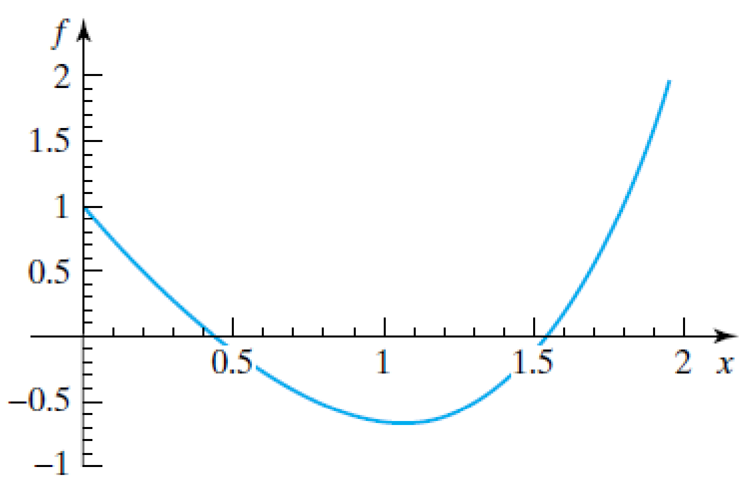
1. Compute $f'(x_n)$.
2. If, $f'(x_n) = 0$, then OUTPUT "Failure". Stop. [Procedure completed unsuccessfully]
3. Else compute, $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$.
4. If $|x_{n+1} - x_n| \leq \varepsilon$ then OUTPUT x_{n+1}. Stop.

Example 4.2.4

Use Newton's method to find the zeros of $f(x) = 1 - 3x + \frac{1}{2}xe^x$ accurate to five decimal places.

Solution

The function f(x) in question can be sketched as shown in the figure below:



The graph shows that the function has two zeros, one close to 0.5 and the other close to 1.6.

$f'(x) = \frac{1}{2}(1 + x)e^x - 3$. Newton's method becomes;

$$x_{n+1} = x_n - \left(1 - 3x_n + \frac{1}{2}x_n e^{x_n}\right) / \left(\frac{1}{2}(1 + x_n)e^{x_n} - 2\right)$$

This problem requires determining the zero of the given function to 5 dps. Hence the tolerance, of the problem is $\varepsilon \leq 0.000005$

For $x_0 = 0.5$;

n	x_n	$\lvert x_{n+1} - x_n \rvert$
0	0.500000	
1	0.450200	0.0498
2	0.451541	0.001341
3	0.451542	0.000001
4	0.451542	0.000000

Hence the zero of the function close to 0.5 is 0.45154 (to 5 dps)

For $x_0 = 1.6$

n	x_n	$\lvert x_{n+1} - x_n \rvert$
0	1.600000	
1	1.552769	0.047231
2	1.549552	0.003231
3	1.549538	0.000014
4	1.549538	0.000000

Hence the zero of the function close to 1.60 is 1.54954 (to 5 decimal places)

This example illustrates how fast the Newton's method can converge if a good initial approximation is used.

4.2.4 The secant method

Newton's method is very powerful but it has a disadvantage that it requires determination of the derivative *f'* that sometimes may be a far more difficult expression to determine and its evaluation is therefore, computationally expensive. This situation suggests the idea of replacing the derivative with the difference quotient;

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

Then instead of the Newton's method formula, we have the popular secant method as;

$$x_{n+1} = x_n - f(x_n)\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}$$

Example 4.2.5

Find the positive solution of $f(x) = x - sinx = 0$ by the secant method, starting with $x_0 = 2$ and $x_1 = 1.9$.

Solution

We have that;

$$x_{n+1} = x_n - \frac{(x_n - 2sinx_n)(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})} = x_n - \frac{N_n}{D_n}$$

Substituting numeric values, we get results in table below;

n	x_{n-1}	x_n	N_n	***Dn***	$\lvert x_{n+1} - x_n \rvert$
1	2.000000	1.900000	-0.000740	-0.174005	0.004253
2	1.900000	1.895747	-0.000002	-0.0006986	0.000252
3	1.895747	1.895494	0	0	0

Hence the root is 1.895494 (correct to 6 Dps)

Exercise 4.1

a) Use the bisection method to determine the required root:

-The root of $sinx - \frac{1}{3}x = 0$ close to $x = 2.2$

-The largest possible root of $x^3 - 1.9x^2 - 2.3x + 3.7 = 0$

-The root of $\frac{1}{2}\sqrt{1 - x^2} - x^2 = 0$

b) Use a fixed point iteration scheme to determine the required roots:

-Determine $a^{1/n}$ where $a > 0$ and n is an integer. Check the result by finding $4^{1/3}$

-Find the positive root of $sinx - \frac{1}{2}x = 0$

-Find the roots of $x^2 + 4x + 1 = 0$ and check the results by using the quadratic formula.

c) Use Newton's method to determine the required root:

-Find the root of $3x - e^{-x} = 0$

-Find the smallest root of $tanx + 2tanhx = 0$

-Find the largest root of $x^4 - 4x^3 + x^2 + 1.2 = 0$

4.3 Interpolation and extrapolation

Sometimes a function $f(x)$ that is assumed to be smooth is only known in the form of a set of discrete values $y_i = f(x_i)$ at a set of arguments $x_1, x_2, \ldots, x_n$ such that $x_1 < x_2 < \cdots \ldots \ldots < x_n$.

When this occurs it often becomes necessary to estimate the value $f(\alpha)$ when α lies between two of the known arguments xi . This process is called the *interpolation* of the function $f(x)$ between its known values.

Various interpolation methods exist with different errors committed in using each. Some of the factors to be taken into account when choosing an interpolation method are whether $f(x)$ appears to be convex or concave for$x_1 < x_2 < x_n$, whether it is oscillatory, and whether it exhibits sharp curvature at a point or points belonging to the interval.

The estimation of $f(\alpha)$ when α lies outside the interval, either to the left of x_1 or to the right of x_n, is called *extrapolation* of the function $f(x)$, and as the process can be liable to considerable error it should be used with care.

4.3.1 Linear interpolation

Let the data points $(x_1, y_1), (x_2, y_2), \ldots \ldots \ldots (x_n, y_n)$ belonging to an unknown smooth function $y = f(x)$ be plotted on a graph. Then the simplest way to estimate the value of $y(x)$ when x lies in the interval $x_i < x < x_{i+1}$ is to join the points (x_i, y_i) and (x_{i+1}, y_{i+1}) by a straight line and then use the point on the line with argument x as the approximation of $y(x)$. This process is called linear interpolation and it is illustrated in Figure 4.4.

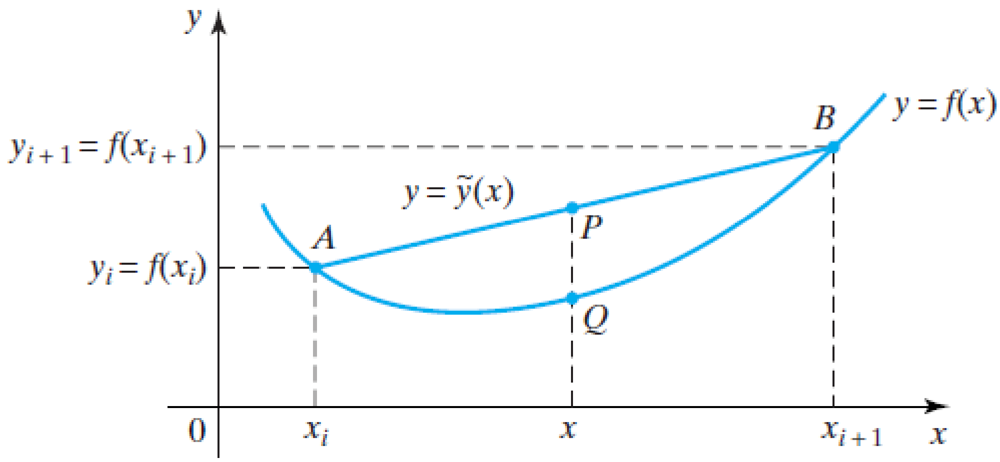


Figure 4.4 Linear interpolation

A simple calculation shows that the straight line segment $y = \tilde{y}(x)$ representing the *linear interpolation function* between the points (x_i, y_i) and (x_{i+1}, y_{i+1}) is given by;

$$\tilde{y}(x) = \left(\frac{y_{i+1} - y_i}{x_{i+1} - x_i}\right)(x - x_i) + y_i; \qquad for\ x_i < x < x_{i+1} \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

If x is chosen so that either $x < x_1$ or $x > x_n$, result (1) becomes a linear extrapolation formula for $y = y(x)$ outside the interval $x_1 < x < x_n$.

Result (1) is useful for interpolation when the variation of x_i and y_i between adjacent data points is small, but as the formula introduces an error due to its failure to cater for the curvature of the curve, the error can become large when the result is used for extrapolation.

4.3.2 Lagrange interpolation

Instead of using linear interpolation to join successive pairs of data points; $(x_1, y_1), (x_2, y_2) \ldots\ldots\ldots (x_n, y_n)$, it is possible that a better result can be obtained by constructing a polynomial $y = P(x)$ that passes through each data point. As a polynomial is a smooth curve, it is to be hoped that it will take some account of the curvature of the function to which the data points belong, as exhibited by a set of data points, and so provide a better interpolation formula.

The polynomial used in this equation is given by;

$P(x) = \sum_{k=1}^{n} L_k(x) y_k$, where;

$$L_k(x) = \frac{(x-x_1)(x-x_2)\ldots(x-x_{k-1})(x-x_{k+1})\ldots(x-x_n)}{(x_k-x_1)(x_k-x_2)\ldots(x_k-x_{k-1})(x_k-x_{k+1})\ldots(x_k-x_n)} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

Therefore,

- For a curve that passes through the points, $(x_1, y_1), (x_2, y_2)\ and\ (x_3, y_3)$ can be approximated by the polynomial, $y(x) = a_0 + a_1 x + a_2 x^2$. This can be re – written (using result 2) as;

$$y(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)} y_1 + \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)} y_2 + \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)} y_3$$

- For data 4 data points, $(x_1, y_1), (x_2, y_2), (x_3, y_3)\ and\ (x_4, y_4)$, the Lagrange polynomial is $y(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$ which can be obtained from result 2 as;

$$y(x) = \frac{(x-x_2)(x-x_3)(x-x_4)}{(x_1-x_2)(x_1-x_3)(x_1-x_4)} y_1 + \frac{(x-x_1)(x-x_3)(x-x_4)}{(x_2-x_1)(x_2-x_3)(x_2-x_4)} y_2 + \frac{(x-x_1)(x-x_2)(x-x_4)}{(x_3-x_1)(x_3-x_2)(x_3-x_4)} y_3 + \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_4-x_1)(x_4-x_2)(x_4-x_3)} y_4$$

- Other higher order Lagrange polynomials for more than four data pairs are determined in a similar way.

Note

(i) The polynomial has a highest degree of *n -1*, i.e. the degree of the polynomial has a degree which is 1 less than the number of data points; 3 data points lead to a second degree polynomial, 4 data points lead to a third degree polynomial, 5 data points lead to a forth degree polynomial etc.

(ii) When $n = 2$, the result (2) reduces to a result of linear interpolation.

Example 4.3.1

Given a certain unknown function, f(x), has the following values at the corresponding x – values:

x	***f(x)***
1.5	0.405
2.1	0.742
3	1.099

Use Lagrange interpolation to find *f(1.8)*.

Solution

From result,

$$y(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)}y_1 + \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)}y_2 + \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)}y_3$$

$$= \frac{(x-2.1)(x-3)}{(1.5-2.1)(1.5-3)}.0.405 + \frac{(x-1.5)(x-3)}{(2.1-1.5)(2.1-3)}.0.742 + \frac{(x-1.5)(x-2.1)}{(3-1.5)(3-2.1)}.1.099$$

$$= \frac{(x^2-5.1x+6.3)}{0.9}.0.405 + \frac{(x^2-4.5x+4.5)}{-0.54}.0.742 + \frac{(x^2-3.6x+3.15)}{1.35}.1.099$$

$$= -0.11x^2 + 0.958x - 0.784$$

Hence, $f(x) \approx y(x) = -0.11(1.8)^2 + 0.958(1.8) - 0.784 = 0.58$ (2 dps)

Example 4.3.2

Given a certain unknown function, f(x), has the following values at the cor-3.5responding x – values:

x	***f(x)***
1	0.368
1.2	0.301
1.3	0.273
1.5	0.223

Use Lagrange interpolation to find *f(1.4)*.

Solution

$$y(x) = \frac{(x-1.2)(x-1.3)(x-1.5)}{(1-1.2)(1-1.3)(1-1.5)}.0.368 + \frac{(x-1)(x-1.3)(x-1.5)}{(1.2-1)(1.2-1.3)(1.2-1.5)}.0.301$$

$$+ \frac{(x-1)(x-1.2)(x-1.5)}{(1.3-1)(1.3-1.2)(1.3-1.5)}.0.273$$

$$+ \frac{(x-1)(x-1.2)(x-1.3)}{(1.5-1)(1.5-1.2)(1.5-1.3)}.0.223$$

$$y(x)=\frac{(x^3-4x^2+5.31x-2.34)}{-0.03}.0.368+\frac{(x^3-3.8x^2+4.75x-1.95)}{0.006}.0.301$$
$$+\frac{(x^3-3.7x^2+4.5x-1.8)}{-0.006}.0.273+\frac{(x^3-3.5x^2+4.06x-1.56)}{0.03}.0.223$$

$$y(x)=-0.167x^3+0.767x^2-1.415x+1.183$$

$$\Rightarrow f(1.4)\approx y(1.4)=0.25$$

Another type of interpolation is the cubic spline interpolation method. You may read about this method from reference books numbers 4 and 6.

Exercise 4.2

1. Graph the function $f(x)=x/(1+x^2)$ in the interval $0\le x\le 3$. Select four points on the graph and after constructing a polynomial that passes through each of the points graph the polynomial and compare the result with the original graph.
2. Graph the function $f(x)=sinx/(1+x^2)$ in the interval $0\le x\le \pi$. Select five points on the graph and after constructing a polynomial that passes through each of the points graph the polynomial and compare the results with the original graph.

4.4 Numerical integration

The need for *numerical integration*, also called *numerical quadrature*, arises when either a definite integral that is required cannot be evaluated analytically, or when special functions involved in an analytical solution are too complicated to be of direct use. A typical definite integral that can only be evaluated numerically is;

$\int_0^5 \frac{\sin 3x}{\sqrt{x^2+x+1}}dx$, whose value can be determined to be 0.364873

4.4.1 The trapezoidal rule

The basis of this simple rule can be understood by Figure 4.5, in which the integral $\int_a^b f(x)dx$ is approximated by the area the *trapezoid* PQRS shown as the shaded area in the interval $a\le x\le b$.

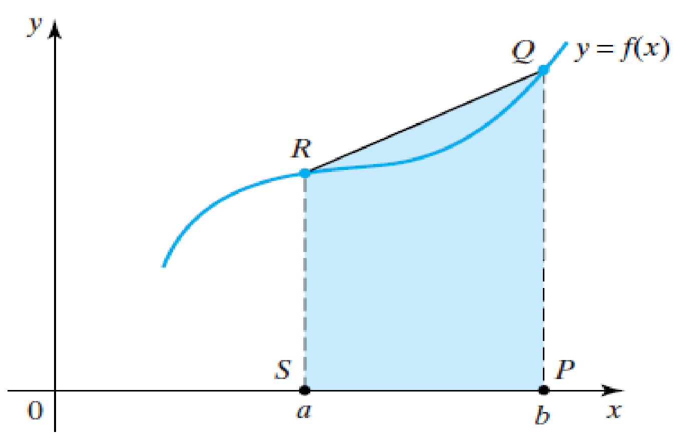


Figure4.2 The trapezoidal rule

Therefore, the approximation to the definite integral is;

$\int_a^b f(x)dx \approx \frac{1}{2}(b-a)[f(a)+f(b)]$……………………………………………………(1) In this case, $h = b - a$

If we denote the error in this approximation by *E(h)*, then;

$E(h) = \int_a^b f(x)dx - \frac{1}{2}(b-a)[f(a)+f(b)]$…………………………………………...(2)

A better estimate of the definite integral, $\int_a^b f(x)dx$ can be obtained by dividing $a \le x \le b$ into n subintervals, applying (1) to each of the n subintervals then summing the results. For simplicity, it is important that all the subintervals have the same length, $h = \frac{b-a}{n}$, where h is usually called the *step size*. It is clear that the error drastically reduces when the number of subintervals, n is made as big as possible and this is possibly done with the help of computer programs e.g. a spread sheet can greatly help.

Setting $x_i = x_0 + ih = a + ih$ for n =1, 2,3,…., we arrive at what is called the *composite trapezium rule*;

$$\int_a^b f(x)dx = \frac{1}{2}h\left[f(a) + 2\sum_{i=1}^{n-1} f(x_i) + f(b)\right]$$

$$= \frac{1}{2}h\left[f(a) + 2\big(f(x_1) + f(x_2) + \cdots + f(x_{n-1})\big) + f(b)\right]$$

Example 4.4.1

Use the composite trapezoidal rule with, n = 10, n = 30 and n = 50 subintervals to evaluate;

$$I = \int_0^5 \frac{\sin 3x}{\sqrt{x^2 + x + 1}}dx$$

Solution

For n = 10, $h = \frac{5-0}{10} = 0.5$

I	x_i	$f(x_i)$	$f(x_0)$, $f(x_n)$	$2f(x_i)$
0	0	0.00000	0.00000	
1	0.5	0.754035		1.50807
2	1	0.081476		0.162952
3	1.5	-0.44852		-0.89704
4	2	-0.10561		-0.21122
5	2.5	0.300400		0.6008
6	3	0.114301		0.228602
7	3.5	-0.21494		-0.42988
8	4	-0.11709		-0.23418
9	4.5	0.158398		0.316796
10	5	0.116795	0.116795	
		Sum	**0.116795**	**1.0449**

Therefore,

$$\int_0^5 \frac{\sin 3x}{\sqrt{x^2+x+1}}\,dx = \frac{1}{2}\times 0.5 \times [0.116795 + 1.0449] = 0.29042$$

Repeating the procedure for n = 30 and n = 50, using a computer we get $I = 0.356897$ and $I = 0.36201$ respectively.

4.4.2 Simpson's rule

In the trapezoidal rule, we approximate the function $y = f(x)$ for the interval $a \le x \le b$ by a straight line segment. A more accurate result would be expected if a point on the curve $y = f(x)$ is chosen inside the interval $a \le x \le b$ and f(x) is approximated by a parabola that passes through the two endpoints and the single internal point as shown in Figure 4.6.

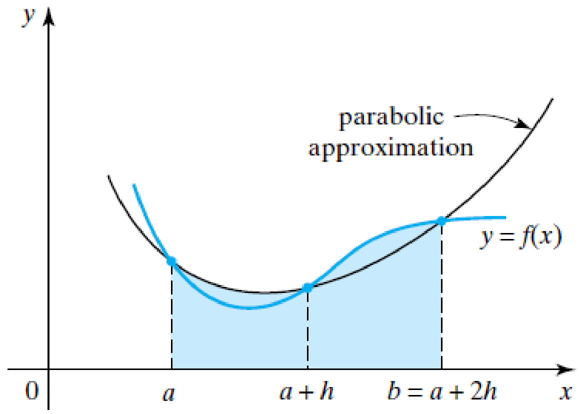


Figure4.3 Simpson's rule

Setting $b = a + 2h$, where h is the step size, and taking an additional point in the interval to be $x = a + h$ such that it is midway between a and b, the parabola must pass through the three consecutive points; $(a, f(a)), (a + h,\ f(a + h))\ and\ (a + 2h,\ f(a + 2h))$, by the Lagrange interpolation formula, this parabola is given by;

$$L(x) = \frac{1}{2}\frac{(x-a-h)(x-a-2h)}{h^2}f(a) - \frac{(x-a)(x-a-2h)}{h^2}f(a+h) + \frac{1}{2}\frac{(x-a)(x-a-h)}{h^2}f(a+2h)$$

Integrating *L(x)* over the interval $a \le x \le a + 2h$ and simplifying the result gives;

$$\int_a^{a+2h} f(x) \approx \frac{1}{3}h[f(a) + 4f(a+h) + f(a+2h)]\ldots\ldots\ldots(1)$$

Result (1) is known as the *Simpson's rule* or the *Simpson's 1/3 rule*. Equation (1) can also be re – written in the form;

$$\int_a^b f(x) \approx \frac{1}{6}(b-a)\left[f(a) + 4f\left(\frac{a+h}{2}\right) + f(b)\right]$$

The accuracy of the Simpson's rule can also be improved by increasing the number of subintervals, but because the rule involves constructing parabolas through three consecutive equidistant points, to use the rule for more than three points in the interval the number of points chosen must be *odd* so the number of intervals must be *even*.

Dividing the interval $a \le x \le b$ into 2n equal subintervals each of length $h = \frac{b-a}{2n}$, and adding the results gives the *composite Simpson's rule*;

$$\int_a^b f(x)dx = \frac{1}{3}h\left[f(a) + 4\sum_{i=1}^{n} f(a + (2i-1)h) + 2\sum_{i=1}^{n} f(a + 2ih) + f(b)\right]$$

This expression can be easily remembered from;

$$\int_a^b f(x)dx = \frac{h}{3}[(F + L) + 4E + 2R]$$

Where, h – step length i.e. the length of each strip

F+L – sum of the first and last ordinates

4E – 4 times the sum of the even positioned ordinates

2R – 2 times the sum of the remaining odd positioned ordinates.

Example 4.4.2

Use the composite Simpson's rule with, n = 10, n = 30 and n = 50 subintervals to evaluate;

$$I = \int_0^5 \frac{\sin 3x}{\sqrt{x^2 + x + 1}} dx$$

Solution

For n = 10

$h = \frac{5-0}{10} = 0.5$

xi	f(xi)	F+L	E	R
0	0	0		
0.5	0.754035		0.754035	
1	0.081476			0.081476
1.5	-0.44852		-0.44852	
2	-0.10561			-0.10561
2.5	0.3004		0.3004	
3	0.114301			0.114301
3.5	-0.21494		-0.21494	
4	-0.11709			-0.11709
4.5	0.158398		0.158398	
5	0.116795	0.116795		
	Sum	**0.116795**	**0.549369**	**-0.02692**

$$\int_0^5 \frac{sin3x}{\sqrt{x^2 + x + 1}} = \frac{h}{3}[(F + L) + 4E + 2R] = \frac{0.5}{3}(0.116795 + 4 \times 0.549369 - 2 \times 0.02692)$$
$$= 0.376738$$

Repeating the procedure using a spread sheet (on a computer) for n = 30 and n = 50, the integral is; $I = 0.365019$ and $I = 0.364892$ respectively.

4.4.3 Gaussian Quadrature

If when evaluating numerically an integral in the standard form, $\int_{-1}^{1} f(x)\, dx$, the points x_i at which the values of the integrand f (x) are sampled are chosen in a special way, then when n sample points are used the result can be made exact in the case that f (x) is an arbitrary polynomial of degree $2n-1$ or less. Unlike Simpson's rule, in this method the *n* sample points x_i are *non – uniformly* spaced throughout the interval of integration.

The sample points, or *nodes* as they are called, are chosen to get a formula that will integrate exactly polynomials of as high degree as possible. It turns out that the *n* sample points are real and lie in the open interval (−1, 1), and polynomials of degree $2n-1$ are integrated exactly.

Consider the simplest situation in which n = 2, so that only two sample points x_1 and x_2 are involved, with $-1 < x_1 < x_2 < 1$, the integration formula becomes;

$$\int_{-1}^{1} f(x)\,dx \approx w_1 f(x_1) + +w_2 f(x_2)$$

At this stage the values of the samples x_1 and x_2 and those of the *weights*, of the integration formula for the sample pints w_1 and w_2 are unknown. To determine the four numbers, we impose the requirement that this formula is exact if *f(x)* is an arbitrary polynomial of degree $2n-1=3$.

Hence we let $f(x) = c_0 + c_1x + c_2x^3 + c_3x^3$, in which c_0, c_1, c_2, c_3 are arbitrary.

Hence;

$\int_{-1}^{1}(c_0 + c_1x + c_2x^3 + c_3x^3)\,dx = w_1(c_0 + c_1x_1 + c_2{x_1}^3 + c_3{x_1}^3) + w_2(c_0 + c_1x_2 + c_2{x_2}^3 + c_3{x_2}^3)$

Evaluating the integral on the left, and equating the respective multipliers of the arbitrary coefficients c_0, c_1, c_2, and c_3 to make this result an identity, leads to;

- Coefficient c_0; $w_1 + w_2 = \int_{-1}^{1} dx = 2$
- Coefficient c_1; $w_1x_1 + w_2x_2 = \int_{-1}^{1} x dx = 0$
- Coefficient c_2; $w_1{x_1}^2 + w_2{x_2}^2 = \int_{-1}^{1} x^2 dx = \frac{2}{3}$
- Coefficient c_3; $w_1{x_1}^3 + w_2{x_2}^3 = \int_{-1}^{1} x^3 dx = 0$

This set of equations has a solution of; $x_1 = -\frac{1}{\sqrt{3}},\ x_2 = \frac{1}{\sqrt{3}},\ w_1 = 1\ and\ w_2 = 1$.

So the extremely simple two-point integration formula that gives exact results when f (*x*) is a polynomial of degree 3 or less is seen to be given by;

$$\int_{-1}^{1} f(x)\,dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

If this approach is extended to *n* points, an examination of the derivation of the formula shows that for the sample points, $x_1, x_2 \dots\dots x_n$ are simply the n roots of the Legendre polynomial $P_n(x) = 0$ of degree n with the corresponding weights w_i given by; $w_i = 2[P'(x_i)]^2/(1-{x_i}^2)$. The general integration formula involving n sample points becomes;

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

Generally, these results are called *Gaussian integration formulas* or *Gauss – Legendre integration formulas*.

Table 4.1 shows a list of Gaussian sampling points x_i and their associated weights for n = 2, 3, 4, 5, 10, and 16.

If the integral involved is $\int_a^b f(x)\,dx$ with $a \neq -1$ and $b \neq 1$ then it is necessary to change the variable, by;

$$x = \frac{1}{2}(b+a) + \frac{1}{2}(b-a)u$$

This converts the integral into the form; $I = \frac{b-a}{2}\int_{-1}^{1} F(u)du$

Table 4.1 Gaussian sampling points and weights

n	i	x_i	w_i
2	1	−0.57735 02692	1.00000 00000
	2	0.57735 02692	1.00000 00000
3	1	−0.77459 66692	0.55555 55556
	2	0.00000 00000	0.88888 88889
	3	0.77459 66692	0.55555 55556
4	1	−0.86113 63115	0.34785 48451
	2	−0.33998 10436	0.65214 51548
	3	0.33998 10436	0.65214 51548
	4	0.86113 63115	0.34785 48451
5	1	−0.90617 98459	0.23692 68851
	2	−0.53846 93101	0.47862 86705
	3	0.00000 00000	0.56888 88889
	4	0.53846 93101	0.47862 86705
	5	0.90617 98459	0.23692 68851
10	1	−0.97390 65285	0.06667 13443
	2	−0.86506 33667	0.14945 13492
	3	−0.67940 95683	0.21908 63625
	4	−0.43339 53941	0.26926 67193
	5	−0.14887 43390	0.29552 42247
	6	0.14887 43390	0.29552 42247
	7	0.43339 53941	0.26926 67193
	8	0.67940 95683	0.21908 63625
	9	0.86506 33667	0.14945 13492
	10	0.97390 65285	0.06667 13443
16	1	−0.98940 09350	0.02715 24594
	2	−0.94457 50231	0.06225 35230
	3	−0.86563 12024	0.09515 85117
	4	−0.75540 44084	0.12462 89713
	5	−0.61787 62444	0.14959 59888
	6	−0.45801 67777	0.16915 65194
	7	−0.28160 35508	0.18260 34150
	8	−0.09501 25098	0.18945 06105
	9	0.09501 25098	0.18945 06105
	10	0.28160 35508	0.18260 34150
	11	0.45801 67777	0.16915 65194
	12	0.61787 62444	0.14959 59888
	13	0.75540 44084	0.12462 89713
	14	0.86563 12024	0.09515 85117
	15	0.94457 50231	0.06225 35239
	16	0.98940 09350	0.02715 24594

Example 4.4.3

Use the five – point Gaussian formula to determine, $I = \int_0^{1/2} \frac{dx}{(1-x^2)^{1/2}}$. Compare the result with the analytical solution of the integral.

Solution

A change of variable $x = \frac{1}{4}(1+u)$ maps the interval $0 \le x \le \frac{1}{2}$ onto the interval $-1 \le x \le 1$.

$$\frac{dx}{du} = \frac{1}{4}$$

After changing variables, then;

$I = \int_{-1}^{1} \frac{du}{(15-2u-u^2)^{1/2}}$, setting $f(u) = 1/(15-2u-u^2)^{1/2}$ and applying the five – point Gaussian formula, gives;

u_i	$f(u_i)$	w_i	$w_i f(u_i)$
-0.906180	0.250069	0.236927	0.059248
-0.538469	0.251681	0.478629	0.120462
0	0.258199	0.568889	0.146887
0.538469	0.270834	0.478629	0.129629
0.906180	0.284366	0.236927	0.067374
		Sum	**0.52360**

$$I = 0.236927f(-0.906180) + 0.478629f(-0.538469) + 0.568889f(0) + 0.478629f(0.538469) + 0.236927f(0.906180) = 0.52360$$

Hence, $I = \int_0^{1/2} \frac{dx}{(1-x^2)^{1/2}} = 0.52360\ (5\ dps)$

The analytical solution is;

$$I = \int_0^{1/2} \frac{dx}{(1-x^2)^{1/2}} = Arcsin\left(\frac{1}{2}\right) = \frac{\pi}{6} = 0.523599$$

This clearly shows a negligible difference between the result from the Gaussian method and the analytical solution.

Exercise 4.3

1. Use the composite Simpson's rule with step length h = 0.5 to determine; $I = \int_1^3 (2x^3 - 3x^2 + 4x - 1)\, dx$ and verify that the rule integrates cubics exactly.

2. Use the composite trapezoidal rule with step length h = 0.1 to determine; $I = \int_0^1 \frac{dx}{1+x^2}$, compare your result with the exact value $I = \frac{\pi}{4}$. Repeat the calculation with Simpson's rule with the same step length.
3. Use the composite trapezoidal and Simpson's rule each of 10 subintervals to evaluate,

$$I = \int_0^{\pi} \frac{sinx}{x} dx$$

   Compare your results with the exact solution $I = 1.851937$. which is the more accurate rule at computing the integral. *Ans: I_{trap} = 1.849317 and Isimp = 1.851944*
4. Use the 3 - , 5 - and 10 – point Gaussian formulas to compute the following integrals and compare the results with the given exactvalue:

   (i) $I = \int_0^{3\pi/2} cosx\, dx$. The exact value is, $I = -1$

   (ii) $I = \int_0^{1/2} \frac{dx}{(1-4x^2)^{1/2}}$. The exact value is, $I = \frac{\pi}{4}$

4.5 Numerical solution of Differential equations

Most differential equations have no known analytical solution, and even when one can be found it is often difficult to use. As a result, when solutions are required and an analytical solution either is not known or is inconvenient to use, it becomes necessary to use methods that produce a numerical solution directly. However, unlike the general analytical solution of an initial value problem that can be adapted to any appropriate initial conditions, a numerical solution is the solution of a specific initial value problem, so the calculation must be repeated if the initial conditions are changed.

4.5.1 Euler's method

The approximate numerical solution of the initial value problem;

$\frac{dy}{dx} = f(x, y)$ subject to the initial condition $y(x_0) = y_0$ generated by Euler's method with step size h is obtained from the algorithm ;

$y_{n+1} = y_n + hf(x_n, y_n)\ \ for\ \ n = 1,2,3, \dots \dots$

Where $x_n = x_0 + nh$.

Example 4.5.1

Use the Euler algorithm with a step size h = 0.2 to find an approximate solution of the first order initial value problem;

$$\frac{dy}{dx} = sinx - y \quad with\ y(0) = 1$$

in the interval $0 \le x \le 2$, and compare it with the exact solution;

$$y = \frac{1}{2}(sinx - cosx) + \frac{3}{2}e^{-x}$$

Solution

Setting h = 0.2, n = 10, and $f(x,y) = sinx - y$ in the Euler algorithm leads to the following results; the column y_{exact} contains the analytical solution.

n	x_n	y_n	$0.2 f(x_n, y_n)$	$y_{n+1} = y_n + 0.2 f(x_n, y_n)$	y_{exact}
0	0	1	−0.2	0.8	1
1	0.2	0.8	−0.1203	0.6797	0.8374
2	0.4	0.6797	−0.0581	0.6217	0.7397
3	0.6	0.6217	−0.0114	0.6103	0.6929
4	0.8	0.6103	0.0214	0.6317	0.6843
5	1	0.6317	0.0420	0.6736	0.7024
6	1.2	0.6736	0.0517	0.7253	0.7366
7	1.4	0.7253	0.0520	0.7773	0.7776
8	1.6	0.7773	0.0444	0.8218	0.8172
9	1.8	0.8218	0.0304	0.8522	0.8485
10	2	0.8522	0.0114	0.8636	0.8657

The error between y_{n+1} and y_{exact} can be reduced, but not limited, by choosing a smaller step size, though for significantly greater accuracy it is necessary to make use of a different method.

4.5.2 Heun's method: The modified Euler's method

A source of error in Euler's method is its failure to take account of the curvature of the solution curve at a point (x_i , y_i) when using the tangent line approximation to the curve to estimate y_{i+1}. An improvement can be obtained by using a two-stage process to arrive at a modified gradient $\tilde{f}(x_i, y_i)$ that can be used in Euler's method in place of $f(x_i , y_i)$.

The first step when finding the modified gradient involves computing the gradient $f(x_i , y_i)$ and then using it in Euler's method to compute the gradient $f(x_{i+1}, y_{i+1})$ at the point (x_{i+1}, y_{i+1}). The second and final step involves averaging these two gradients, to obtain the new gradient;

$$\tilde{f}(x_i, y_i) = \frac{1}{2}\{f(x_i, y_i) + f(x_{i+1}, y_{i+1})\}$$

and then using $\tilde{f}(x_i, y_i)$ in place of $f(x_i , y_i)$ in Euler's method at (x_i , y_i) to find an improved estimate $\tilde{y}_{i+1}$ at the point (x_{i+1}, y_{i+1}).

The modified Euler algorithm

The approximate numerical solution of the initial value problem;

$\frac{dy}{dx} = f(x, y)$ subject to the initial condition $y(x_0) = y_0$ generated by the modified Euler's method with step size h is obtained from the algorithm ;

$$y_{n+1} = y_n + \frac{1}{2}h[f(x_n, y_n) + f(x_n + h, y_n + hf(x_n, y_n))] \quad n = 1,2,3, \dots ..$$

Where $x_n = x_0 + nh$

Example 4.5.2

Use the Heun's algorithm with a step size h = 0.2 to find an approximate solution of the first order initial value problem;

$$\frac{dy}{dx} = sinx - y \quad with\, y(0) = 1$$

in the interval $0 \leq x \leq 2$, and compare it with the exact solution;

$y = \frac{1}{2}(sinx - cosx) + \frac{3}{2}e^{-x}$ and the results from Euler's method.

Solution

Setting h = 0.2, n = 10, and $f(x, y) = sinx - y$ in the Heun's algorithm leads to the following results;

n	***x_n***	***y_n***	***$f(x_n,y_n)$***	***$a=x_n+h$***	***$b = y_n + hf(x_n,y_n)$***	***$f(a,b)$***	***$y_{n+1} = y_n+0.5h[f(x_n,y_n)+f(a,b)]$***
0	0	1	-1.000000	0.2	0.8000	-0.6013	0.8399
1	0.2	0.8399	-0.641198	0.4	0.7116	-0.3222	0.7435
2	0.4	0.7435	-0.354108	0.6	0.6727	-0.1081	0.6973
3	0.6	0.6973	-0.132667	0.8	0.6708	0.0466	0.6887
4	0.8	0.6887	0.028656	1.0	0.6944	0.1470	0.7063
5	1	0.7063	0.135201	1.2	0.7333	0.1987	0.7397
6	1.2	0.7397	0.192376	1.4	0.7781	0.2073	0.7796
7	1.4	0.7796	0.205818	1.6	0.8208	0.1788	0.8181
8	1.6	0.8181	0.181482	1.8	0.8544	0.1195	0.8482
9	1.8	0.8482	0.125662	2.0	0.8733	0.0360	0.8643
10	2	0.8643	0.044948	2.2	0.8733	-0.0648	0.8624

The comparisons of the Heun's solution, $y_n^{(mod)}$ with the Euler's, $y_n^{(e)}$ and exact, y_{exact} solutions are as shown below:

n	0	1	2	3	4	5	6	7	8	9	10
x_n	0	0.2	0.4	0.6	0.8	1	1.2	1.4	1.6	1.8	2
$y_n^{(e)}$	1	0.8	0.6797	0.6217	0.6103	0.6317	0.6736	0.7253	0.7773	0.8212	0.8522
$y_n^{(mod)}$	1	0.8399	0.7435	0.6973	0.6887	0.7063	0.7397	0.7796	0.8181	0.8482	0.8643
y_{exact}	1	0.8374	0.7397	0.6929	0.6843	0.7024	0.7366	0.7776	0.8172	0.8485	0.8657

It is clear that there is an improvement in the accuracy when the modified Euler method is used.

4.5.3 The forth order Runge – Kutta method for a first order differential equation

This yet another modified method of determining the numerical solution of a first order differential equation.

The approximate numerical solution of the initial value problem;

$\frac{dy}{dx} = f(x, y)$ subject to the initial condition $y(x_0) = y_0$ with step size h can obtained from the following forth order Runge – Kutta algorithm, with $x_n = x_0 + nh$ and $y_n = y(x_n)$.

1. Calculate;

$$k_{1n} = hf(x_n, y_n)$$

$$k_{2n} = hf\left(x_n + \frac{1}{2}h,\ y_n + \frac{1}{2}k_{1n}\right)$$

$$k_{3n} = hf\left(x_n + \frac{1}{2}h,\ y_n + \frac{1}{2}k_{2n}\right)$$

$$k_{4n} = hf(x_n + h,\ y_n + k_{3n})$$

2. Calculate;

$$d_n = \frac{1}{6}(k_{1n} + 2k_{2n} + 2k_{3n} + k_{3n})$$

3. The numerical approximate y_{n+1} of the solution $y = y(x_{n+1})$ is given by;

   $y_{n+1} = y_n + d_n$ for n = 1,2,3…….

4.5.4 The Runge – Kutta algorithm for two first order simultaneous equations

The approximate numerical solution of the initial value problem for the simultaneous first order initial value problem;

$$\frac{dy}{dx} = f(x, y, z)\ and\ \frac{dz}{dx} = g(x, y, z)$$

Subject to the initial conditions, $y(x_0) = y_0\ \ and\ z(x_0) = z_0$ genereted by the forth order Runge – Kutta method with step size his obtained from the following algorithm in which $x_n = x_0 + nh$, $y(x_n) = y_n$ and $z(x_n) = z_n$.

1. Calculate the following order:

$k_{1n} = hf(x_n, y_n, z_n)$	$K_{1n} = hg(x_n, y_n, z_n)$
$k_{2n} = hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_{1n},\ z_n + \frac{1}{2}K_{1n}\right)$	$K_{2n} = hg\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_{1n},\ z_n + \frac{1}{2}K_{1n}\right)$
$k_{3n} = hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_{2n}, z_n + \frac{1}{2}K_{2n}\right)$	$K_{3n} = hg\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_{2n}, z_n + \frac{1}{2}K_{2n}\right)$
$k_{4n} = hf(x_n + h, y_n + k_{3n}, z_n + K_{3n})$	$K_{4n} = hg(x_n + h, y_n + k_{3n}, z_n + K_{3n})$

2. Calculate;

$$d_n = \frac{1}{6}(k_{1n} + 2k_{2n} + 2k_{3n} + k_{4n})$$ and

$$D_n = \frac{1}{6}(K_{1n} + 2K_{2n} + 2K_{3n} + K_{4n})$$

3. The numerical approximations of $y = y(x_{n+1})$ and $z = z(x_{n+1})$ are given by;

   $y_{n+1} = y_n + d_n$ and $z_{n+1} = z_n + D_n$

This forth order Runge – Kutta algorithm with step size h can be modified to find the solution of the following initial value problem for the single variable second order differential equation written in the standard form;

$\frac{d^2y}{d^2x} = g\left(x, y, \frac{dy}{dx}\right)$ with $y(x_0) = y_0 \ \ and \ \ y'(x_0) = z_0$

All that is necessary is to reduce the second order equation to a system of two simultaneous first order equations, by setting;

$\frac{dy}{dx} = z$ and $\frac{dz}{dx} = g(x, y, z)$

Example 4.5.3

Use the forth order Runge – Kutta algorithm with step size $h = 0.2$ to solve the initial value problem;

$\frac{dy}{dx} + 2y = sin3x \ with \ y(0) = 1$ in the interval $0 \le x \le 2.4$.

Example 4.5.4

Use the forth order Runge – Kutta algorithm with step size 0.1 to find a numerical solution of the initial value problem;

$y'' - 2xy' + 8y = 0$ with $y(0) = 12$ and $y'(0) = 0$ in the interval $0 \le x \le 1$

Solutions

Example 4.5.3

Setting h = 0.2 and $f(x,y) = sin3x - 2y$, the results of the spread sheet computations are;

n	xn	Yn	k1n	xn + (1/2)h	yn+(1/2)k1n	k2n	yn+(1/2)k2n	k3n	xn+h	yn+k3n	k4n	dn	yn+1
0	0	1	-0.4	0.1	0.8	-0.2609	0.86955202	-0.28872	0.2	0.711283	-0.17158	-0.27847	0.721532
1	0.2	0.721532	-0.17568	0.3	0.63368955	-0.09681	0.67312641	-0.11259	0.4	0.608946	-0.05717	-0.10861	0.612924
2	0.4	0.612924	-0.05876	0.5	0.58354306	-0.03392	0.59596482	-0.03889	0.6	0.574037	-0.03485	-0.03987	0.573054
3	0.6	0.573054	-0.03445	0.7	0.55582826	-0.04969	0.54820966	-0.04664	0.8	0.526412	-0.07547	-0.05043	0.522623
4	0.8	0.522623	-0.07396	0.9	0.48564483	-0.10878	0.46823217	-0.10182	1	0.420806	-0.1401	-0.10588	0.416748
5	1	0.416748	-0.13848	1.1	0.34751014	-0.17055	0.33147108	-0.16414	1.2	0.25261	-0.18955	-0.16623	0.250514
6	1.2	0.250514	-0.18871	1.3	0.1561588	-0.20002	0.15050518	-0.19776	1.4	0.052758	-0.19542	-0.19661	0.053902
7	1.4	0.053902	-0.19588	1.5	-0.0440363	-0.17789	-0.0350442	-0.18149	1.6	-0.12759	-0.1482	-0.17714	-0.12324
8	1.6	-0.12324	-0.14994	1.7	-0.1982064	-0.10588	-0.1761776	-0.11469	1.8	-0.23793	-0.05938	-0.10841	-0.23165
9	1.8	-0.23165	-0.06189	1.9	-0.2625949	-0.0051	-0.2341976	-0.01646	2	-0.24811	0.043359	-0.01027	-0.24192
10	2	-0.24192	0.040886	2.1	-0.2214798	0.091955	-0.1959455	0.081741	2.2	-0.16018	0.126381	0.085776	-0.15615
11	2.2	-0.15615	0.124767	2.3	-0.093763	0.153193	-0.0795498	0.147508	2.4	-0.00864	0.162189	0.14806	-0.00809
12	2.4	-0.00809	0.161968	2.5	0.07289737	0.158441	0.07113375	0.159146	2.6	0.15106	0.139285	0.156071	0.147985

Example 4.5.4

We set, $= \frac{dy}{dx} = f(x, y, z)$, hence;

From $y'' - 2xy' + 8y = 0 \Rightarrow \frac{dz}{dx} = 2xz - 8y = g(x, y, z)$

The initial conditions are, $y_0 = 12$ and $z_0 = y'(0) = 0$, with h = 0.1, the following are the results of the computations obtained using a spread sheet.

n	x_n	y_n	z_n	k_{1n}	K_{1n}	k_{2n}	K_{2n}	k_{3n}	K_{3n}	k_{4n}	K_{4n}	d_n	D_n	y_{n+1}	z_{n+1}
0	0.0	12.000	0.000	0.000	-9.600	-0.480	-9.648	-0.482	-9.456	-0.946	-9.403	-0.478	-9.535	11.522	-9.535
1	0.1	11.522	-9.535	-0.954	-9.408	-1.424	-9.263	-1.417	-9.073	-1.861	-8.828	-1.416	-9.151	10.106	-18.687
2	0.2	10.106	-18.687	-1.869	-8.832	-2.310	-8.492	-2.293	-8.307	-2.699	-7.870	-2.296	-8.383	7.810	-27.070
3	0.3	7.810	-27.070	-2.707	-7.872	-3.101	-7.335	-3.074	-7.159	-3.423	-6.527	-3.080	-7.231	4.730	-34.301
4	0.4	4.730	-34.301	-3.430	-6.528	-3.757	-5.793	-3.720	-5.629	-3.993	-4.801	-3.729	-5.696	1.001	-39.997
5	0.5	1.001	-39.997	-4.000	-4.800	-4.240	-3.864	-4.193	-3.717	-4.371	-2.692	-4.206	-3.776	-3.205	-43.773
6	0.6	-3.205	-43.773	-4.377	-2.688	-4.512	-1.550	-4.455	-1.422	-4.520	-0.199	-4.472	-1.472	-7.677	-45.245
7	0.7	-7.677	-45.245	-4.524	-0.193	-4.534	1.150	-4.467	1.255	-4.399	2.677	-4.488	1.216	-12.165	-44.029
8	0.8	-12.165	-44.029	-4.403	2.687	-4.269	4.236	-4.191	4.314	-3.972	5.936	-4.216	4.287	-16.380	-39.742
9	0.9	-16.380	-39.742	-3.974	5.951	-3.677	7.708	-3.589	7.756	-3.199	9.578	-3.617	7.743	-19.997	-31.999
10	1.0	-19.997	-31.999	-3.200	9.598	-2.720	11.566	-2.622	11.581	-2.042	13.603	-2.654	11.582	-22.652	-20.417

Plots of y_{n+1} and z_{n+1} versus x_n as shown in Figure below: