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Chapter 1: Solution of Nonlinear Equations

Introduction

Analysis versus Numerical Analysis

The word analysis in mathematics usually means to solve a problem through equations. The equations must then be reduced to an answer through procedures of algebra, calculus, differential equations, partial differential equations. Numerical analysis is similar in that prospect that the problems are solved but we only use simple arithmetic add, subtract, multiply, divide or compare only. Since these operations are exactly those that computers, so numerical analysis and computer are closely related

Example:

We need to find the cube root of 2 i.e. $\sqrt[3]{2}$ using only arithmetic operations. One way of solving this could be using trail and error method. We try choosing a value and multiply itself 3 times so that the value is close to 2. We take new approximation at get closer the number 2.

$1.2^3 = 1.728$ too small

$1.4^3 = 2.744$ too large

$$1.25^3 = 1.9531 \quad \text{pretty close}$$

$$1.26^3 = 2.0004 \quad \text{really close}$$

Now we can say that the cube root of 2 lies between 1.2-1.26, and we can choose the value according to our need, how accurate we need. Here in above example we calculated the cube root of 2 just by using simple arithmetic and compare.

Another difference between a numerical result and analytical result is that numerical result is always approximation. Analytical methods usually give the result in terms of mathematical function that can evaluate for specific instances. This also has the advantage that the behavior and properties of the function are often apparent, this is not the case for numerical answer, however numerical results can be plotted to show some of the behavior of the solution.

While the numerical results are an approximation this can usually be as accurate as needed. The necessary accuracy is of course determined by application and need. To achieve high accuracy many operations must be carried out, but as these operations are carried out the computer so that's not a big problem.

Solution by Taylor series

Taylor series is often used in determining the order of errors for methods and the series itself is the basic for some numerical procedures.

Let $y' = f(x, y), y(x_0) = y_0$ (1)

Be the differential equation to which the numerical solution is required. Expanding $y(x)$ about $x = x_0$ by Taylor Series we get

$$y(x) = y(x_0) + \frac{(x-x_0)y'(x_0)}{1!} + \frac{(x-x_0)^2 y''(x_0)}{2!} + \cdots \quad (2)$$

$$= y_0 + \frac{(x-x_0)y'_0}{1!} + \frac{(x-x_0)^2 y''_0}{2!} + \cdots \quad (3)$$

Putting$x = x_0 + h = x_1$, h=difference we have

$$y_1 = y(x_1) = y_0 + \frac{hy'_0}{1!} + \frac{h^2 y''_0}{2!} + \frac{h^3 y'''_0}{3!} \ldots \quad (4)$$

Here y'_0, y''_0, y'''_0 ... can be found using equation (1) and its successive differentiation at $x = x_0$. The series in (4) can be truncated at any stage if 'h' is small. Now having obtained $y_1$we can calculate y'_1, y''_1, y'''_1 from equation (1) at $x = x_0 + \mathrm{h}$

Now expanding $y(x)$ by Taylor series about $x = x_1$, we get

$$y_2 = y_1 + \frac{hy'_1}{1!} + \frac{h^2 y''_1}{2!} + \frac{h^3 y'''_1}{3!} \ldots \quad (5)$$

Proceeding further we get

$$y_n = y_{n-1} + \frac{hy'_{n-1}}{1!} + \frac{h^2 y''_{n-2}}{2!} + \frac{h^3 y'''_{n-3}}{3!} \dots \quad (6)$$

By taking sufficient number of terms in above series the value of y_n can be obtained without much error

If a Taylor series is truncated while there are still non-zero derivatives of higher order the truncated power series will not be exact. The error term for a truncated Taylor Series can be written in several ways but the most useful form when the series is truncated after n^{th} term is

Example:

Using Taylor series method solve $\frac{dy}{dx} = x^2 - y, y(0) = 1$ at $x =$ 0.1,0.2,0.3 &0.4. Compare the values with exact solution.

Solution

Given $y' = x^2 - y$,$y(0) = 1$,

$x_0 = 0, y_0 = 1,$ h $= 0.1, x = 0.1, x = 0.2, x = 0.3, x = 0.4$

Now

$y' = x^2 - y \qquad y'_0 = x_0^2 - y_0 = 0 - 1 = -1$

$y'' = 2x - y' \qquad y''_0 = 2x_0 - y'_0 = 2 * 0 - (-1) = 1$

$y''' = 2 - y'' \qquad y'''_0 = 2 - y''_0 = 1$

$y^{iv} = -y''' \qquad y_0^{iv} = -y'''_0 = -1$

By Taylor Series

$$y_1 = y_0 + \frac{hy'_0}{1!} + \frac{h^2 y''_0}{2!} + \frac{h^3 y'''_0}{3!} + \frac{h^4 y_0^{iv}}{4!} \dots$$

$y_1 = y(0.1)$

$= 1 + \frac{0.1(-1)}{1!} + \frac{(0.1)^2 * 1}{2!} + \frac{0.1^3 * 1}{3!} + \frac{0.1^4 * (-1)}{4!} \dots$

$= 1 - 0.1 + 0.005 + 0.0001667 - 0.00000417$

=0.90516

Now

$y_1' = x_1^2 - y_1 = (0.1)^2 - 0.90516$=-0.89516

$y_1'' = 2x_1 - y_1' = 2 * (0.1) - (-0.89516) = 1.09516$

$y_1''' = 2 - y_1'' = 2 - 1.0951 = 0.90484$

$y_1^{iv} = -y_1''' = -0.90484$

By Taylor Series

$$y_2 = y_1 + \frac{hy_1'}{1!} + \frac{h^2 y_1''}{2!} + \frac{h^3 y_1'''}{3!} + \frac{h^4 y_1^{iv}}{4!} \dots$$

$y_2 = y(0.2)$

= 0.90516+ $\frac{0.1*(-0.89516)}{1!} + \frac{(0.1)^2*1.09516}{2!} + \frac{0.1^3*0.90484}{3!} + \frac{0.1^4*(-)}{4!} \dots$

= $0.9051 - 0.089516 + 0.0054758 + 0.000150 - 0.00000377$

=0.821266

Now

$y_2' = x_2^2 - y_2 = (0.2)^2 - 0.8212352 = -0.7812352$

$y_2'' = 2x_2 - y_2' = 2 * (0.2) - (-0.7812352) = 1.1812352$

$y_2''' = 2 - y_2'' = 2 - 1.1812352 = 0.8187648$

$y_2^{iv} = -y_2''' = -0.8187648$

By Taylor Series

$$y_3 = y_2 + \frac{hy_2'}{1!} + \frac{h^2 y_2''}{2!} + \frac{h^3 y_2'''}{3!} + \frac{h^4 y_2^{iv}}{4!} \dots$$

$y_3 = y(0.3)$

$$= 0.8212352 + \frac{0.1 * (-0.7812352)}{1!} + \frac{(0.1)^2 * 1.1812352}{2!} + \frac{0.1^3 * 0.8187648}{3!} + \frac{0.1^4 * (-0.8187648)}{4!} \dots$$

$= 0.7491509$

Now

$y_3' = x_3^2 - y_3 = (0.3)^2 - 0.7491509 = -0.6591509$

$y_3'' = 2x_3 - y_3' = 2 * (0.3) - (-0.6591509) = 1.2591509$

$y_3''' = 2 - y_3'' = 2 - 1.2591509 = 0.740849$

$y_3^{iv} = -y_3''' = -0.740849$

By Taylor Series

$$y_4 = y_3 + \frac{hy_3'}{1!} + \frac{h^2y_3''}{2!} + \frac{h^3y_3'''}{3!} + \frac{h^4y_3^{iv}}{4!} \dots$$

$y_4 = y(0.4)$

$$= 0.7491509 + \frac{0.1 * (-0.6591509)}{1!} + \frac{(0.1)^2 * 1.2591509}{2!} + \frac{0.1^3 * 0.740849}{3!} + \cdots$$

$= 0.6896519$

Similarly we can find the values of y_n for n=5, 6, 7…..

Approximation and errors in Numerical Computation:

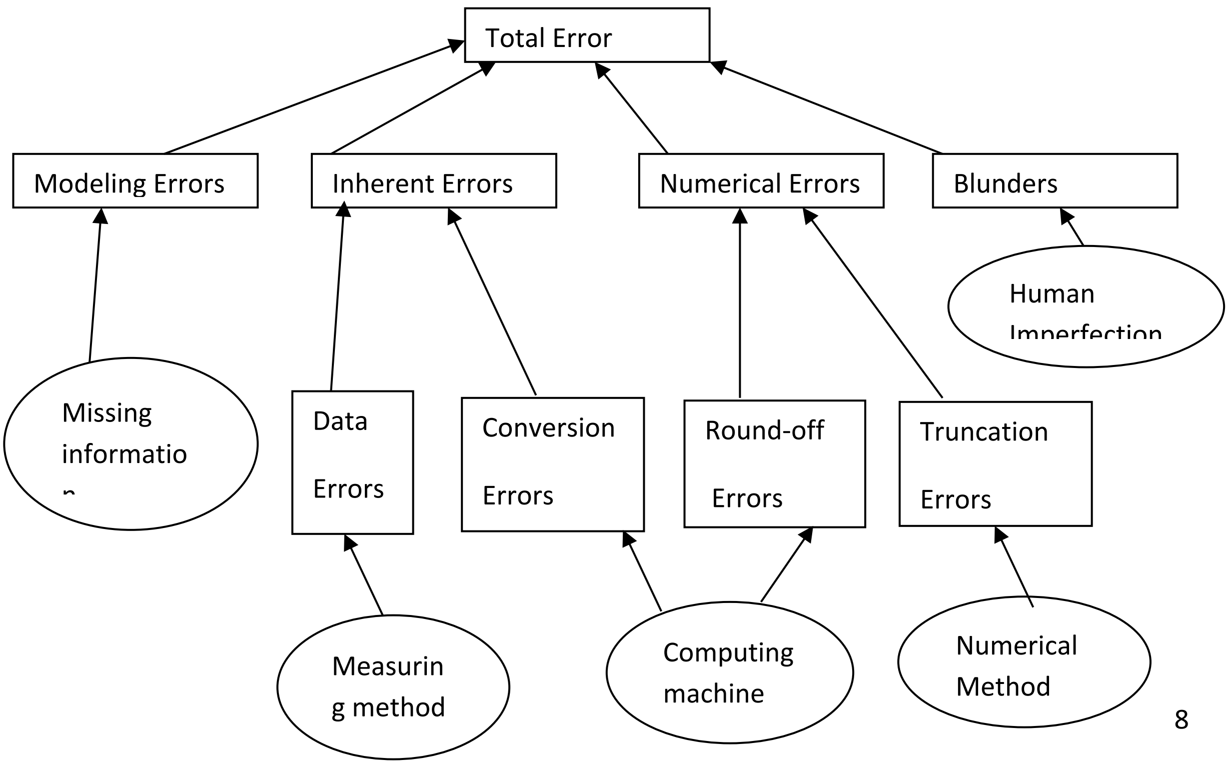


Figure: 1.1 (Taxonomy of Errors)

Modeling errors

Mathematical models are the basis for numerical solution. They are formulated to represent physical process using certain parameters involved in the situations. In many situations it is impractical or impossible to include all of the real problems, so we use certain assumptions for easy calculations. For example while developing a model for calculating the for acting on a falling body, we may not be able to estimate the air resistance coefficient properly or determine the direction and magnitude of wind force acting on the body and so on. To simply the model we may assume that the force due to the air resistance is linearly proportional to the velocity of the falling body or we assume that there is no wind force acting on the body. All such assumption certainly results in errors in the output from such models.

Inherent Errors

Inherent errors are those that are present in the data supplied to the model. Inherent error contains data errors and conversion error.

Data error

Data error (known as empirical errors) arises when data for a problem are obtained by some experimental mean and are therefore of limited accuracy and precision. This may be due to some limitations in instruments and reading and therefore may be unavoidable, for example there is no use in performing arithmetic operations to 4 decimal places when the original data themselves are correct up to 2 decimal places.

Conversion Error

Conversion errors (representation error) arise due to the limitations of the computer to store data exactly. We know that the floating point representation retains only a specific number of digits, that are not retained constitute round off error.

Example

0.1_{10}	=	0.00011001
0.4_{10}	=	0.01100110
Sum	=	0.01111111
0.5_{10}	=	0.25+0.125+0.0625+0.03125+0.015625+0.0078125+0.00390625
	=	0.49609373

Now from above example we can see that the addition of binary number conversion to decimal we do not get exact value as decimal number of 0.1 has non termination binary form 0.000110011001… and so on. The computer has fixed memory so it uses only certain number for digits after decimal so we get this type of errors which is caused by conversion.

Numerical Errors

Numerical errors (procedural errors) are introduced during the process of implementation of numerical methods. They come in two forms round off and truncation error.

Round off errors

Round off errors occurs when a fixed number of digits are used to represent exact number, since the number are stored at every stage of computation, round off error is introduced at the end of every arithmetic operations. Consequently even though an individual roundoff error could be very small the cumulative effect of a series of computation can be very significant.

Rounding a number can be done in two way, chopping and symmetric rounding.

Chopping

In chopping the extra digits are dropped, this is also called truncating a number. Suppose we are using a computer with a fixed word length of four digits then a number like 42.7893will be stored as 42.78 and the digit 93 will be dropped.

Symmetric round off

In symmetric round off method, the last retained significant digit is “rounded off” by 1 if the first discarded digit is larger or equal to 5, otherwise the last retained digit is unchanged. For example the number 42.7893 would become 42.79 and the number 76.5432 would become 76.54.

Sometimes a slightly more refined rule is used when the last the last number is 5, then the number is unchanged if the last digit is even and is increased by 1 it is odd.

Truncation error

Truncation error arises from using an approximation in place of an exact mathematical procedure. Typically it is the error resulting from the truncation of the numerical process. We often use some finite number of terms to eliminate the sum of an infinite series, for example

$s = \sum_{i=0}^{\infty} \mathrm{a_i x^i}$ is replaced by finite sum, the series is truncated as

$$\sin(\mathrm{x}) = x - \frac{\mathrm{x}^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} \dots$$

Truncation error can be reduced by using a better numerical model which usually increases the number of arithmetic operations. E.g. in numerical integration the truncation error can be reduced by increasing the number of points at which the function is integrated, but care should be exercised to see that the round off error which is bound to increase due to increased arithmetic operations does not offset the reduction in truncation error.

Blunders

Blunders are errors that are caused due to human imperfection. As the name indicated such errors may cause a very serious disaster in the result since these errors are due to human mistake. It should be possible to avoid them to a large extent by acquiring a sound knowledge of all aspect of the problem as well as numerical process.

Human errors can occur at any stage of the numerical processing cycle, some common types of errors are:

1. Lack of understanding of the problem.
2. Wrong assumption.
3. Overlooking of some basic assumption required for formulating the model.
4. Errors in deriving the mathematical equation or using model that does not describe adequately the physical system under study.

5. Selecting the wrong numerical method for solving the mathematical model.
6. Selecting a wrong algorithm for implementing the numerical method.
7. Making mistakes in the computer program, such as testing real number of zero, using <symbol in place of >.
8. Mistakes in date input such as misprints, giving values column wise instead of row wise to a matrix.
9. Wrong guessing of initial values.

Absolute and Relative Errors:

Some of the fundamental definition of errors analysis regardless of its source, an error is usually quantified in two different but related ways but are related in some ways, known as absolute error and relative error.

Let us suppose that true value of a date item is denoted by x_t and its approximated value is denoted byx_a, then they are related as True value, (x_t)=Approximate value(x_a)+error.

Error is given by error=x_t-x_a

The error may be negative or positive depending on the values of x_t and x_a. In error analysis what is important is magnitude of the error and not the sign and therefore we normally consider its absolute value, known as absolute error denoted by

$$error = |x_t - x_a|$$

In many case absolute error may not reflect its influence correctly as it does not take into account the order of magnitude of the value under study. For example an error of 1gm is much more significant in the weight of 10gm of gold than in weight of a bag of sugar of 1 kg. In view of this we introduce the concept of relative error which is nothing but the normalized value of absolute error. The relative error is defined as follows:

$$e_r = \frac{absolute\ error}{|true\ value|}$$

$$= \frac{|x_t - x_a|}{|x_t|}$$

$$= \left|1 - \frac{x_a}{x_t}\right|$$

Minimizing the total error

1. Increasing the significant figures of the computer.
2. Minimizing the number of arithmetic operations.
3. Avoiding subtractive cancellations
4. Choosing proper initial parameters.

Significant digits

We all know that all computers operate with fixed length so that all the floating point representation requires the mantissa to be specified number of digits. Some numbers such as the value of $\pi = 3.141592$ ..... we have to write as 3.14 or 3.14159 in all these cases we have omitted some digits. Now $2/_7 = 0.285714\ or\ \pi = 3.14159$ is said to have number containing 6 significant digits.

The concept of significant digit has been introduced primarily to indicate the accuracy if a numerical value. For example if the number y=23.40657 has correct value of only 23.406 then we may say that y has 5 significant digits and is correct up to 3 decimal places. The omission of certain digits from a number of results in roundoff error. The following statements describe the notion of significant digits.

1. All non zero digits are significant.
2. All zero occurring between non zero digit are significant digits.
3. Trailing zero following a decimal point are significant .e.g. 3.50, 65.0& 0.230 have three significant digits each.
4. Zeros between the decimal point and preceding non-zero digit are not significant e.g. following numbers have 4 significant digits.

$$0.0001234(1234x10^{-7})$$

$$0.001234(1234x10^{-6})$$

5. When the decimal point is not written trailing zeros are not considered to be significant. E.g. 4500 may be written as $45x10^2$ contains only two significant digits however.

$$4500.0 \quad 4\ significant\ digits$$
$$7.56x10^4 \quad 3\ significant\ digits$$
$$7.560x10^4 \quad 4\ significant\ digits$$
$$7.5600x10^4 \quad 5\ significant\ digits$$

The concept of accuracy and precision are closely related to significant digits. They are related as follows:

1. Accuracy refers to the number of significant digits in a value e.g. 57.396 is accurate to five significant digits.
2. Precision refers to the number of decimal position i.e. the order of magnitude if the last digit value. the number 57.396 has a precision of 0.001 or 10^{-3}

Iterative methods

There are number of iterative methods that have been tried and used successfully in various problem situations. All these methods typically generate a sequence of estimates of the solution which is expected to converge to the true solution. All iterative methods begin their process of solution with one or more guess of the solution and then using those guesses to find another better approximation and so on to get to required solution with desired accuracy. Iterative method can be grouped as:

1. Bracketing methods
2. Open end methods

Before we start to go further into the methods first we need to know about the starting and stopping criteria in an iterative process.

Starting criterion

Before an iterative process is initiated, we have to determine an interval that contains the roots of the equation. One method is to plot the curve and find the interval where the curve cuts the x-axis. Such that the interval that contains such point will contain roots. This gives us rough estimate of the roots, also helps to understand the properties of the function.

Stopping criterion

An iterative process must be terminated at some stage; we must have a criterion for deciding when to stop the process. We may use one or combination of following tests depending in the behavior of the function to terminate the process:

1. $|x_{i+1} - x_i| \leq E_a \; (absolute\ error\ in\ x)$
2. $\left|\frac{x_{i+1}-x_i}{x_{i+1}}\right| \leq E_r(relative\ error\ in\ x)x \neq 0$
3. $|f(x_{i+1})| \leq E \; (value\ of\ function\ at\ root\ )$
4. $|f(x_{i+1}) - f(x_i)| \leq E \; (difference\ in\ function\ value\ )$

x_i Represents the estimate of the root at i^{th} iteration and f (x_i) is the value of the function atx_i. There may be situations where these tests may fail when used alone so we use combination of many.

Bracketing method

This method starts with two initial guess that bracket the root and then systematically reduce the width of the bracket until the solution is reached. Two popular methods are:

1. Bisection method
2. False position method

Bisection method

The Bisection method is one of the simplest and most reliable method for solution of non-linear equations. This method relies on the fact that if $f(x)$ is real and continuous in the interval $a < x < b$ and $f(a)\&f(b)$ have opposite signs i.e $f(a) * f(b) < 0$ then there is at least one real root in the interval between a & b. let $x_1 = a\ and\ x_2 = b$. now determine another point x_3 to be mid point between a and b i.e $x_3 = \frac{x_1+x_2}{2}$ now there exists the following three conditions;

1. $f(x_3) = 0, then\ we\ have\ a\ root\ at\ x_3$
2. $if\ f(x_3) * f(x_1) < 0, then\ there\ is\ root\ in\ the\ interval\ \ x_1\& x_3$
3. $if\ f(x_3) * f(x_2) < 0, then\ there\ is\ root\ in\ the\ interval\ \ x_2\& x_3$

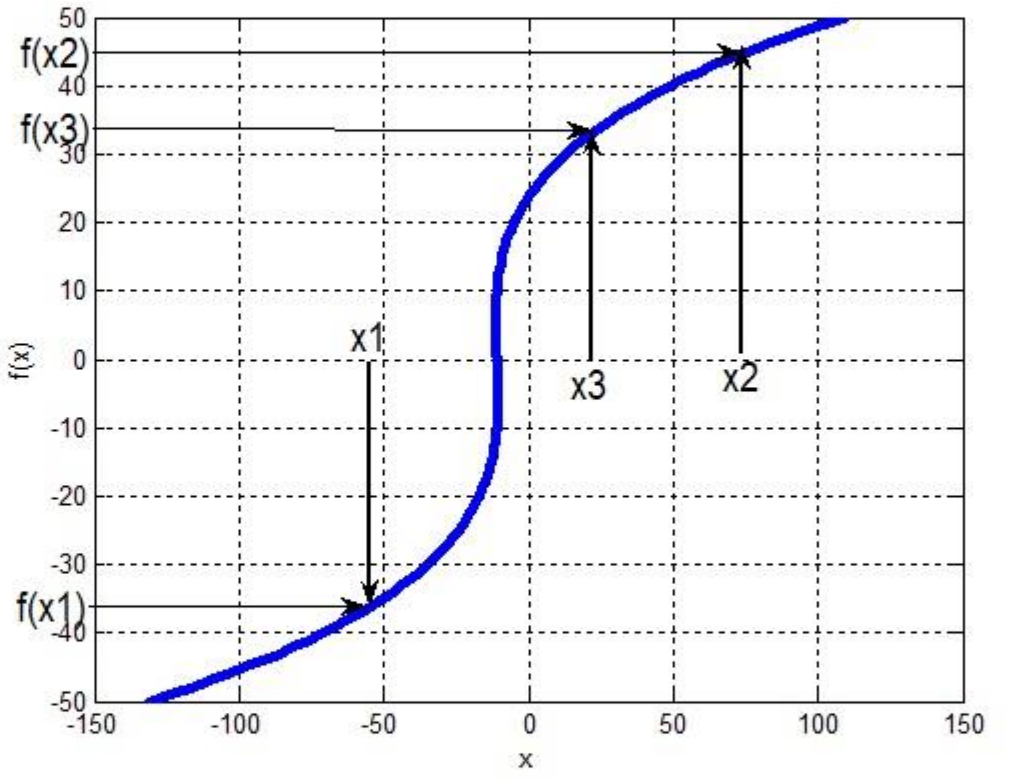


Figure 1.2: Illustration of Bisection method

Example 1: find a root of the equation $x^3 - x - 11 = 0$, correct up to 4 decimal place using bisection method.

Solution:$(x) = x^3 - x - 11 = 0$, *now we select the initial approximation, by selecting those values of x where their functional values have opposite sign.*

S.N	**x**	**f(x)**	
1	1	-11	
2	2	-5	
3	**3**	**13**	**sign changed**
4	4	49	
5	5	109	
6	6	199	
7	7	325	
8	8	493	

From above table we can that the values of f(x) changes at x=2 & x=3, we can randomly test for the values without creating the table but it will be easy to find out if we use table.

Now the initial approximation be$x_1 = 2$,$x_2 = 3$ then $f(2) = -5$ &$f(3) = 13$, where root lies in between 2 & 3, hence next approximation will be $x_3 = \frac{x_1+x_2}{2}$

e $x_3 = \frac{2+3}{2} = 2.5$, $f(2.5) = 2.125$. since $f(2)f(2.5) < 0$, a root lies in between 2 & 2.5, now proceeding further in tabular form we get.

Itr	**x1**	**f(x1)**	**x2**	**f(x2)**	**xm**	**f(xm)**	**error**
1	2.0000	-5.0000	3.0000	13.0000	2.5000	2.1250	1.0000
2	2.0000	-5.0000	2.5000	2.1250	2.2500	-1.8594	0.5000
3	2.2500	-1.8594	2.5000	2.1250	2.3750	0.0215	0.2500
4	2.2500	-1.8594	2.3750	0.0215	2.3125	-0.9460	0.1250
5	2.3125	-0.9460	2.3750	0.0215	2.3438	-0.4691	0.0625
6	2.3438	-0.4691	2.3750	0.0215	2.3594	-0.2256	0.0313
7	2.3594	-0.2256	2.3750	0.0215	2.3672	-0.1025	0.0156
8	2.3672	-0.1025	2.3750	0.0215	2.3711	-0.0406	0.0078
9	2.3711	-0.0406	2.3750	0.0215	2.3730	-0.0096	0.0039
10	2.3730	-0.0096	2.3750	0.0215	2.3740	0.0059	0.0020
11	2.3730	-0.0096	2.3740	0.0059	2.3735	-0.0018	0.0010
12	2.3735	-0.0018	2.3740	0.0059	2.3738	0.0021	0.0005
13	2.3735	-0.0018	2.3738	0.0021	2.3737	0.0001	0.0002
14	2.3735	-0.0018	2.3737	0.0001	2.3736	-0.0009	0.0001
15	2.3736	-0.0009	2.3737	0.0001	2.3736	-0.0004	0.0001
16	2.3736	-0.0004	2.3737	0.0001	2.3736	-0.0001	0.0000

Therefore, the root of the equation is 2.3737, since the value of error is 0.0000 or we can also say that the new root is same as old so this is the required roots for given stopping criteria.

Example 2: Find the root of the equation of $x^2 - 4x - 10 = 0$, correct upto 5 decimal places.

Solution:$f(x) = x^2 - 4x - 10 = 0$, let the initial approximation be -2& -1, chosen from table below .

S.N	x	f(x)
1	-3	11
2	-2	2
3	-1	-5
4	0	-10
5	1	-13
6	2	-14
7	3	-13

now the initial approximation be $x_1 = -2, x_2 = -1$, then $f(-2) = 2$ &$f(-1) = -5$, where root lies in between 2 & 3, hence next approximation will be $x_3 = \frac{x_1+x_2}{2}$

e $x_3 = \frac{-1-2}{2} = -1.5, f(-1.5) = -1.7500$, since $f(-2)f(-1.5) < 0$, a root lies in between -2 &-1.5, now proceeding further in tabular form we get.

Itr	x1	f(x1)	x2	f(x2)	xm	f(xm)	error
1	-2	2.0000	-1.0000	-5.0000	-1.5000	-1.7500	1.0000
2	-2	2.0000	-1.5000	-1.7500	-1.7500	0.0625	0.5000
3	-1.75	0.0625	-1.5000	-1.7500	-1.6250	-0.8594	0.2500
4	-1.75	0.0625	-1.6250	-0.8594	-1.6875	-0.4023	0.1250
5	-1.75	0.0625	-1.6875	-0.4023	-1.7188	-0.1709	0.0625
6	-1.75	0.0625	-1.7188	-0.1709	-1.7344	-0.0544	0.0313
7	-1.75	0.0625	-1.7344	-0.0544	-1.7422	0.0040	0.0156
8	-1.74219	0.0040	-1.7344	-0.0544	-1.7383	-0.0253	0.0078
9	-1.74219	0.0040	-1.7383	-0.0253	-1.7402	-0.0106	0.0039

10	-1.74219	0.0040	-1.7402	-0.0106	-1.7412	-0.0033	0.0020
11	-1.74219	0.0040	-1.7412	-0.0033	-1.7417	0.0003	0.0010
12	-1.7417	0.0003	-1.7412	-0.0033	-1.7415	-0.0015	0.0005
13	-1.7417	0.0003	-1.7415	-0.0015	-1.7416	-0.0006	0.0002
14	-1.7417	0.0003	-1.7416	-0.0006	-1.7416	-0.0001	0.0001
15	-1.7417	0.0003	-1.7416	-0.0001	-1.7417	0.0001	0.0001
16	-1.74167	0.0001	-1.7416	-0.0001	-1.7417	0.0000	0.0000

Therefore, the root of the equation is -1.7417, since the value of error is 0.0000.

Practice: find the roots of the equation for following equations, correct up to 5 decimal places.

1. $\boldsymbol{3x + \sin(x) - e^x = 0}$
2. $\boldsymbol{\sin(x) - 2x + 1 = 0}$
3. $\boldsymbol{e^x - x - 2 = 0}$
4. $\boldsymbol{x^3 - x - 3 = 0}$
5. $\boldsymbol{4x^3 - 2x - 6 = 0}$

NOTE: When there are trigonometric functions, use radian measure in calculator.

False Position Method

In Bisection method, the interval between $x_1 \& x_2$ is divided into two equal halves, irrespective of the location of the root. It may be possible that the root is closer to one as in figure 1.3, note that the root is closer to x_1.let us join the point $x_1 \& x_2$ by a straight line. The point of intersection of this line with x-axis gives and improved estimate root and is called false position of the root. Let this point is called x_3. This point then replaces one of initial guess. The process is then repeated with new values of $x_1 \& x_2$, since this method uses the false position of the root repeatedly it is called false position method. It is also called linear interpolation method.

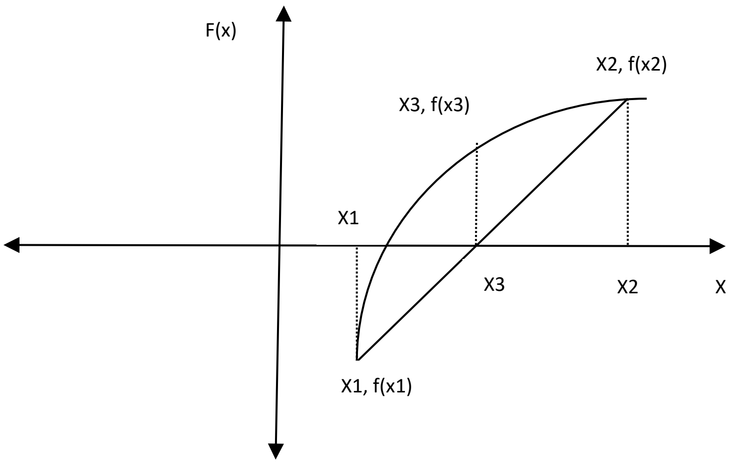


Figure1.3 : Illustration of False position method

The equation of the line joining $(x_1, f(x_1))$& $(x_2, f(x_2))$ is

$$y - y_1 = m(x - x_1)$$

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

$$y - f(x_1) = \frac{f(x_2) - f(x_1)}{x_2 - x_1}(x - x_1)$$

Let the line joining the points $(x_1, f(x_1))$& $(x_2, f(x_2))$ cuts x-axis at $(x_3, 0)$, then the point lies in the line, putting the value in the equation we get

$$0 - f(x_1) = \frac{f(x_2) - f(x_1)}{x_2 - x_1}(x_3 - x_1)$$

On solving the above equation, we get,

$$x_3 = x_1 - \frac{f(x_1)(x_2 - x_1)}{f(x_2) - f(x_1)}$$

This is the formula for calculating the new approximation in false position method.

Example 1: find the real root of the equation $x^3 - 2x - 5 = 0$ by the method of false position correct up to 4 decimal places.

Solution: Let $f(x) = x^3 - 2x - 5 = 0$, *Now we select the initial approximation, by selecting those values of x where their functional values have opposite sign.*

S.N	x	f(x)	
1	1	-6	
2	2	-1	
3	**3**	**16**	**Sign changed**
4	4	51	
5	5	110	
6	6	199	
7	7	324	
8	8	491	

From above table we can that the values of f(x) changes at x=2 & x=3, we can randomly test for the values without creating the table but it will be easy to find out if we use table.

now the initial approximation be $x_1 = 2,\ x_2 = 3$, then $f(2) = -1$ &$f(3) = 16$, where root lies in between 2 & 3, hence next approximation will be

$$x_3 = x_1 - \frac{f(x_1)(x_2 - x_1)}{f(x_2) - f(x_1)}$$

$$x_3 = 2 - \frac{(-1)(3-2)}{\big(16 - (-1)\big)}$$

$$x_3 = 2.0588$$

$f(2.0588) = -0.3908$. since $f(2.0588) * f(3) < 0$, a root lies in between 2.0588&3 now proceeding further in tabular form we get.

Itr	x1	f(x1)	x2	f(x2)	x3	f(x3)	error
1	2.0000	-1.0000	3.0000	16.0000	2.0588	-0.3908	1.0000
2	2.0588	-0.3908	3.0000	16.0000	2.0813	-0.1472	0.9412
3	2.0813	-0.1472	3.0000	16.0000	2.0896	-0.0547	0.9187

4	2.0896	-0.0547	3.0000	16.0000	2.0927	-0.0202	0.9104
5	2.0927	-0.0202	3.0000	16.0000	2.0939	-0.0075	0.9073
6	2.0939	-0.0075	3.0000	16.0000	2.0943	-0.0027	0.9061
7	2.0943	-0.0027	3.0000	16.0000	2.0945	-0.0010	0.9057
8	2.0945	-0.0010	3.0000	16.0000	2.0945	-0.0004	0.9055
9	2.0945	-0.0004	3.0000	16.0000	2.0945	-0.0001	0.9055
10	2.0945	-0.0001	3.0000	16.0000	2.0945	-0.0001	0.9055
11	2.0945	-0.0001	3.0000	16.0000	2.0945	0.0000	0.9055
12	2.0945	0.0000	3.0000	16.0000	2.0946	0.0000	0.9055

Therefore, the root of the equation is 2.0946, since the value of f(x3) = 0.0000.

Example 2: find the real root of the equation $x^2 - 4x - 10 = 0$ by the method of false position correct up to 6 decimal places.

Solution

Let $f(x) = x^2 - 4x - 10 = 0$, *Now we select the initial approximation, by selecting those values of x where their functional values have opposite sign.*

S.N	**x**	**f(x)**
1	-3	11
2	-2	2
3	-1	-5
4	0	-10
5	1	-13
6	2	-14
7	3	-13

From above table we can that the values of f(x) changes at x=-2 & x=-1, we can randomly test for the values without creating the table but it will be easy to find out if we use table.

now the initial approximation be $x_1 = -2, x_2 = -1$, then $f(-2) = 2$ &$f(-1) = -5$, where root lies in between -2 &-1, hence next approximation will be

$$x_3 = x_1 - \frac{f(x_1)(x_2 - x_1)}{f(x_2) - f(x_1)}$$

$$x_3 = -2 - \frac{(2)(-1-(-2))}{(-5-2)}$$

$$x_3 = -1.714286$$

$f(-1.714286) = -0.204082$. since $f(2) * f(-1.714286) < 0$, a root lies in between 2 &-1.714286 now proceeding further in tabular form we get.

Itr	x1	f(x1)	x2	f(x2)	x3	f(x3)	error
1	-2.000000	2.000000	-1.000000	-5.000000	-1.714286	-0.204082	1.000000
2	-2.000000	2.000000	-1.714286	-0.204082	-1.740741	-0.006859	0.285714
3	-2.000000	2.000000	-1.740741	-0.006859	-1.741627	-0.000229	0.259259
4	-2.000000	2.000000	-1.741627	-0.000229	-1.741656	-0.000008	0.258373
5	-2.000000	2.000000	-1.741656	-0.000008	-1.741657	0.000000	0.258344

Therefore, the root of the equation is -1.741657, since the value of f(x3) = 0.000000.

Practice: Find the real roots for the following equations , correct up to 5 decimal places.

1. $\mathbf{3x + \sin(x) - e^x = 0}$
2. $\mathbf{x - e^{-x} = 0}$
3. $\mathbf{x^3 - 4x^2 + x + 6 = 0}$
4. $\mathbf{3x^2 + 6x - 45 = 0}$
5. $\mathbf{4x^3 - 2x - 6 = 0}$

Open end methods:

This method uses single starting value or two values that do not necessarily bracket the root. The following methods fall under open end method:

1. Secant method
2. Newton method
3. Fixed point method

Secant Method

The secant method begins by finding two points on the curve of f(x), hopefully near to root. We draw a line through these two points and find the point where it intersects the x -axis. The two points may both be on one side of the root as seen in figure, but they can also be on opposite side.

If f(x) were truly linear, the straight line would intersect x-axis at the roots, but f(x) will never be linear because we would never use a root finding method on a linear function. That means the intersection of the line with x-axis in not at root, but that should be close to it. From the obvious similar triangles we can write

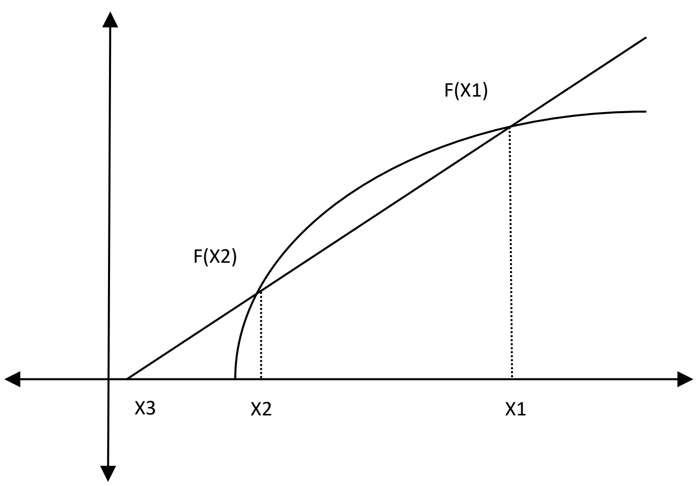


Figure 1.4: Illustration of Secant method

$$\frac{(x_2 - x_3)}{f(x_2)} = \frac{(x_1 - x_2)}{(f(x_1) - f(x_2))}$$

Now solving this for x_3 we get

$$x_3 = x_2 - \frac{f(x_2)(x_1 - x_2)}{f(x_1) - f(x_2)}$$

Because f(x) is not exactly linear, x_3 is not equal to root, but it should be closer than either of the two points.

Example 1: Find the real root of the equation $x^2 - 4x - 10 = 0$ by the method of secant method correct up to 6 decimal places.

Solution

Let $f(x) = x^2 - 4x - 10 = 0$, let the initial approximation be $x_1 = 4$, $x_2 = 6$, hence next approximation will be

$$x_3 = x_2 - \frac{f(x_2)(x_1 - x_2)}{f(x_1) - f(x_2)}$$

$$x_3 = 6 - \frac{(2)(4-6)}{(-10-2)}$$

$$x_3 = 5.666667$$

Proceeding further in tabular form we get.

Itr.	x1	f(x1)	x2	f(x2)	x3	f(x3)	error
1	4.000000	-10.000000	6.000000	2.000000	5.666667	-0.555556	2.000000
2	6.000000	2.000000	5.666667	-0.555556	5.739130	-0.018904	0.333333
3	5.666667	-0.555556	5.739130	-0.018904	5.741683	0.000191	0.072464
4	5.739130	-0.018904	5.741683	0.000191	5.741657	0.000000	0.002553
5	5.741683	0.000191	5.741657	0.000000	5.741657	0.000000	0.000026

Therefore, the root of the equation is 5.741657, since the value of f(x3) = 0.000000.

Practice: Find the real roots following equations, correct up to 5 decimal places.

1. $3x + \sin(x) - e^x = 0$

2. $4x^3 - 2x - 6 = 0$
3. $x^2 - 5x + 6 = 0$
4. $x \sin x - 1 = 0$
5. $e^x - 3x = 0$

Newton's method

One of the most widely used methods of solving non-linear equations is Newton's method (also called Newton Raphson Method). This method is also based on the linear approximation of the function, but does so using a tangent line to the curve. Figure gives the graphical description starting from a single initial estimate x_0, that is not too far from a root. We move along the tangent to its intersection with x-axis and take the next approximation. This is continued until either the successive x-value are sufficiently close or the value of the function is sufficiently near to zero.

The calculation scheme follows immediately from the right triangle shown in figure, which has the angle of inclination of the tangent line to the curve at $x = x_0$.

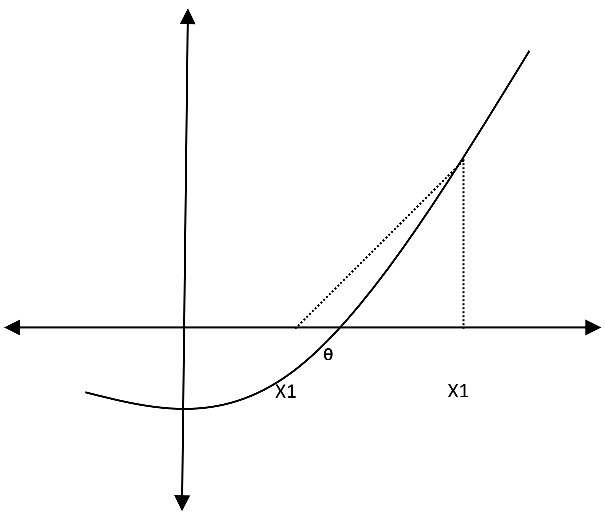


Figure 1.5: Illustration of Newton's Method

$$\tan\theta = f'(x_0) = \frac{f(x_0)}{x_0 - x_1}$$

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

In general,

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \; where \; n = 0,1,2,3 \ldots.$$

Newton's method is widely used because it is more rapidly convergent then any of the methods. Some important things that should be kept in mind while using Newton method:

1. When $f'(x_0)$ is very large, i.e. when the slope is large the root can be calculated in even less time.
2. If we choose the initial approximationx_0 close to the root then we get the root of the equation very quickly.
3. The process will evidently fail if $f'(x) = 0$, in that case use other methods
4. If the initial approximation to the root is not given choose two values of x such that its functional values are opposite, as this will ensure that the chosen point in near the root.

Example 1: Find the root of $x^3 - 3x^2 + 2x - 10 = 0$, using NR method

Solution: Let $x_0 = 2$ be an approximate of the root, then

$$f(x) = x^3 - 3x^2 + 2x - 10$$
$$f'(x) = 3x^2 - 6x + 2$$

At $x_0 = 2$

$$f(2) = 2^3 - 32^2 + 2 * 2 - 10 = -10$$
$$f'(2) = 32^2 - 6 * 2 + 2 = 2$$

Then the new approximate is :

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

$$x_1 = 2 - \frac{-10}{2}$$

$$= 7$$

Now

$$x_0 = x_1 = 7$$

Then doing further calculation, we get required root of the equation. In tabular form we get

Itr	x0	f(x0)	f'(x0)	x1	error
1	2.00000	-10.00000	2.00000	7.00000	5.00000
2	7.00000	200.00000	107.00000	7.00000	5.00000
3	5.13084	56.35721	50.19155	5.13084	1.86916
4	4.00800	14.20854	26.14417	4.00800	1.12284
5	3.46453	2.50479	17.22172	3.46453	0.54347
6	3.31909	0.15333	15.13448	3.31909	0.14544
7	3.30895	0.00071	14.99382	3.30895	0.01013
8	3.30891	0.00000	14.99316	3.30891	0.00005

Therefore, the root of the equation is 3.30891, since the value error=0.00005 correct up to 4 decimal place.

Practice :

1. $\sin(x) = 1 + x^3$
2. $f(x) = x^2 - 2x - 1$
3. $f(x) = x^3 - x - 3$
4. $f(x) = x^3 - 3x - 2$
5. $f(x) = \cos x$

Fixed point Iteration method

Any function in the form of $f(x) = 0$ can be manipulated such that x is on the left hand side of the equation as shown: $x = g(x)$. Both equations are equivalent. Observe that if $f(r) = 0$, where r is the root of f(x), it follows that r= $g(r)$, whenever we have r= $g(r)$r is said to be fixed point for the function g.

If x_i is an approximate solution then $x_{i+1} = g(x_i)$. The above transformation can be obtained either by algebraic manipulation of the given equation or by simply adding x to both sides of equation.

Example 1: locate the root of the equation $f(x) = x^2 - 2x - 3$.

Suppose we arrange to given the equivalent form $x = g_1(x) = \sqrt{2x+3}$, if we start with x=4 and iterate. Successive values of x are

$$x_0 = 4$$

$$x_1 = \sqrt{11} = 3.31662$$

$$x_2 = 3.10375$$

$$x_3 = 3.03439$$

$$x_4 = 3.01144$$

$$x_5 = 3.00381$$

$$x_6 = 3.00127$$

Therefore, it appears that the values are converging on the root at $x = 3$

Now if we re-arrange the terms then we get another equation

$$g_2(x) = \frac{3}{(x-2)} = x$$

Let us start the integration again with $x_0 = 4$, successive values then

$$x_0 = 4$$

$$x_1 = 1.5$$

$$x_2 = -6$$

$$x_3 = -0.375$$

$$x_4 = -1.26316$$

$$x_5 = -0.91935$$

$$x_6 = -1.02763$$

$$x_7 = -0.99087$$

$$x_8 = -1.00305$$

$$x_9 = -0.99898$$

$$x_{10} = -1.00034$$

$$x_{11} = -0.99989$$

$$x_{12} = -1.0004$$

$$x_{13} = -1.00000$$

It seems that we now converge to another root at $x = -1$, we also see that the converge is oscillatory rather than monotonic.

Consider another re-arrangement

$$x = g_2(x) = \frac{x^2 - 3}{2}$$

Starting with

$$x_0 = 4$$

$$x_1 = 6.5$$

$$x_2 = 19.625$$

$$x_3 = 191.070$$

From these results we see that the iterates are diverging.

NOTE: the g(x) formed must be such that $|g'(x)|$ around the real root should be less than 1, if this is not case change g(x).

Practice

Use the Fixed point iteration method to evaluate a root of the equation $x^2 - x - 1 = 0$, using the following forma of g(x)

a. $x = x^2 - 1$
b. $x = 1 + 2x - x^2$
c. $x = \frac{1+3x-x^2}{2}$

Starting with $x_0 = 1$ and $x_0 = 2$ and discuss the results

Convergence:

Convergence of Bisection method

In the bisection method, we choose a midpoint x_3 in the interval between $x_1 \& x_3$. Depending on the sign of the function $f(x_0), f(x_1) \& f(x_2)$. $x_1 \& x_2$ is set to equal to x_0, such that the new interval contains the root. In either case the interval containing the root is reduced by a factor 2. The same procedure is repeated n times, then the interval containing the root is reduced to the size $\frac{x_2-x_1}{2^n} = \frac{\Delta x}{2^n}$

After n iterations the root must lie within $\pm \frac{\Delta x}{2^n}$ of our estimate. This means that error bounds at n^{th} iteration is $E_n = \left|\frac{\Delta x}{2^n}\right|$

Similarly$E_{n+1} = \left|\frac{\Delta x}{2^{n+1}}\right| = \left|\frac{\Delta x}{2^n . 2}\right| = \frac{E_n}{2}$

that is the error decreases linearly with each step by a factor of 0.5. the bisection method is therefore linearly convergent. Since the convergence is slow to achieve a high degree of accuracy. Large number of iterations may be needed; however the bisection algorithm is guaranteed to converge.

Convergence of secant method and false position

Both of the secant method and false position uses iterations that can be written as

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

Which is similar to$x = g(x)$, except $x = g(x_n, x_{n-1})$ when we apply Taylor series the derivatives are pretty complicated, so we omit the details it turns out that the error relation is

$$e_{n+1} = \frac{g(\xi_1, \xi_2)}{2} * e_n e_{n+1}$$

Showing that the error is proportional to the product of the two pervious errors, we can conclude that the convergence is better than linear but poorer than quadratic

$$e_{n+1} \propto e_n * e_{n-1}$$

Convergence of Fixed point iteration:

The demonstration in example earlier shows that fixed point iterations seems to converge linearly. We now show when this is true.

We have $x_{n+1} = g(x_n)$ now writing above relation for the error after iteration n+1, where R is the true value of the root.

$$R - x_{n+1} = R - g(x_n) = g(R) - g(x_n)$$

Because where $x = R, R = g(R)$, multiplying and dividing by (R-x_n), we get

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

Now we can use the mean value theorem, if $g(x)$ and $g'(x)$ are continuous, to say that

$R - x_{n+1} = g'(\xi_n) * (R - x_n)$ where ξ_n lies between x_n *and* R, writing e_n for the error of the n^{th} iterate, we have $|e_{n+1}| = |g'(\xi_n) * e_n|$

Because e_n the error in x_n is $R - x_n$(we take absolute values because the successive iterates may oscillate around the root). Now from above equation we can say that the fixed point iteration will converge linearly, in the limit as x_n approaches R, provided that we start within the interval $|g'(\xi_n)| < K < 1$

Convergence of Newton's method

Newton's method uses iteration that resembles fixed point

$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = g(x_n)$, successively iterates will converge if $|g'(x)| < 1$ and doing the differentiation, we see that the method converge, if

$$|g'(x)| = \left|\frac{f(x) * f''(x)}{(f'(x))^2}\right| < 1 \ldots \ldots \ldots \ldots \ldots \ldots 1$$

Which requires that f(x) and its derivatives exits and be continuous. Newton method is shown to be quadratically convergent by the following as before

$$R - x_{n+1} = g(R) - g(x_n)$$

Now we expand $g(x_n)$ as Taylor series in terms of $(R - x_n)$ with the second derivative term as the remainder getting

$$g(x_n) = g(R) + g'(R) * (R - x_n) + \left(\frac{g''(\xi)}{2}\right) * (R - x_n)^2 \ldots \ldots \ldots \ldots 2$$

Where ξ lies within (x_n, R), however from equation 1

$$|g'(R)| = \left|\frac{f(R) * f''(R)}{(f'(R))^2}\right| = 0$$

Because $f(R) = 0$ at the root and equation 2 reduces to

$$g(x_n) = g(R) + \left(\frac{g'(\xi)}{2}\right) * (R - x_n)^2 \ldots\ldots\ldots\ldots .3$$

Using $e_n = R - x_n$ for the error on the n^{th} iterate equation 3 becomes

$$e_{n+1} = R - x_{n+1} = g(R) - g(x_n) = -(g''(\xi)/2)(e_n{}^2)$$

Providing that Newtons method is quadratically convergent

$$e_{n+1} \propto e_n{}^2$$

Chapter 2: Interpolation and approximation

The statement $y = f(x), x_0 \le x \le x_n$ means for every corresponding value of x in the range $x_0 \le x \le x_n$, there exists one or more values of y. assuming that $f(x)$ is single valued and continuous and that it is known explicitly then the values of $f(x)$ corresponding to certain given values of x, say $x_0, x_{1,}x_2 \ldots\ldots x_n$ can easily be computed and tabulated. The central problem of numerical analysis is the converse one,given the set of tabular values of $(x_0, y_0), (x_1, y_1), (x_2, y_2) \ldots\ldots (x_n, y_n)$ satisfying the relation $y = f(x)$ where the explicit nature of f(x) is not known, it is required to find a simpler function say $\phi(x)$ such that $f(x) and\ \phi(x)$agree at the set of tabulated points. Such a process is called interpolation. If $\phi(x)$ is polynomial then the process is called polynomial interpolation and $\phi(x)$ is called interpolating polynomial. Similarly different types of interpolation arise depending on $\phi(x)$.

An application of interpolation can be seen everyday in weather forcasting. The weather service people collect information on temperatures, wind speed and direction, humidity, pressure from hundreds of weather stations around the world. All these data items are entered into a massive computer program that models the weather.

Interpolation

$$e^x = a_0 + a_1x + a_2x^2 + a_3x^3 + \cdots \ldots\ldots . +a_nx^n$$

Taylor series expansion of e^x about x=0, a_0, a_1, a_2 … ..are coefficient to be determined

x	0	0.5	1	1.5	2	2.5	3
e^x	1	1.8487	2.7183	4.4817	7.3891	12.1825	20.085

If we have to find the value of $e^{2.2}$ or $e^{0.75}$ then interpolation inside the given range.

If we have to find the value of $e^{3.2}$ then extrapolation outside the given range.

Various method of interpolation

1. Lagrange interpolation
2. Newton's interpolation
3. Newton's Gregory forward interpolation
4. Spline interpolation

Polynomial form

The most common form of an n^{th} order polynomial is

$p(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots \ldots \ldots + a_n x^n$ known as power form.

Linear interpolation

The simplest form of interpolation is to approximate two data points by straight line, suppose we have two points $(x_1 f(x_1))$ &$(x_2 f(x_2))$. These two points can be connected linearly as shown in figure, using the concept of similar triangles we show that :

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

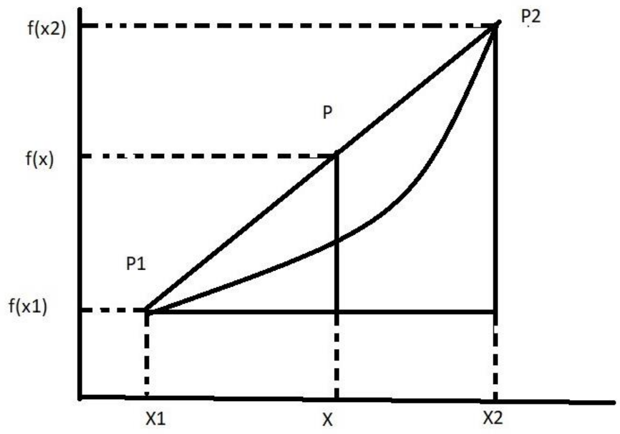


Figure: Graphical representation of Linear interpolation

On solving for f(x) we get

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

Above equation is known as linear interpolation formula, note that $\frac{f(x_2)-f(x_1)}{x_2-x_1}$ represents the slope of line.

Example : The table below shows square root for the integers, determine the square root of 2.5

x	1	2	3	4	5
F(x)	1	1.4142	1.7321	2	2.2361

The given value of 2.5 lies in between 2 and 3. Therefore $x_1 = 2, f(x_1) = 1.4142, x_2 = 3, f(x_2) = 1.7321,$

$$f(2.5) = f(x_1) + (x - x_1)\frac{f(x_2) - f(x_1)}{x_2 - x_1}$$

$$= f(2) + (2.5 - 2)\frac{f(3) - f(2)}{3 - 2}$$

$$= 1.4142 + (2.5 - 2)\frac{1.7321 - 1.4142}{3 - 2}$$

$$= 1.5732$$

Now if the two points taken are $x_1 = 2, x_2 = 4$

$$f(2.5) = f(1) + (2.5 - 2)\frac{f(4) - f(2)}{4 - 2}$$

$$f(2.5) = 1.4142 + 0.5\frac{(2 - 1.4142)}{2}$$

=1.5607

The correct answer is 1.5811, so from above values we can say that closer the points the more accurate results.

Lagrange Interpolation polynomial

Let $(x_0, y_0), (x_1, y_1), (x_2, y_2), (x_3, y_3)$ are given set of data points.Let $y = f(x)$ be a function which takes the (n+1) values $y_0, y_1, y_2, \dots \dots y_n$ corresponding to $x = x_0, x_1, x_2 \dots \dots x_n$. Now $f(x)$ can be represented as polynomial of n^{th} degree in x.

Let the polynomial be of the form

$$y = f(x) = a_0(x - x_1)(x - x_2) \dots \dots (x - x_n)$$

$$+a_1(x - x_0)(x - x_2) \dots \dots (x - x_n)$$

$$+a_2(x - x_0)(x - x_1) \dots \dots (x - x_n) \dots \dots$$

$$+a_n(x - x_0)(x - x_1) \dots \dots (x - x_{n-1}) \dots \dots . (1)$$

Putting $x = x_0, y = y_0$ in the equation 1 we get,

$$y_0 = a_0(x_0 - x_1)(x_0 - x_2) \dots \dots (x_0 - x_n)$$

$$a_0 = \frac{y_0}{(x_0 - x_1)(x_0 - x_2) \dots \dots (x_0 - x_n)}$$

Again putting $x = x_1, y = y_1$ in the equation 1 we get,

$$y_1 = a_1(x_1 - x_0)(x_1 - x_2) \dots \dots (x_1 - x_n)$$

$$a_1 = \frac{y_1}{(x_1 - x_0)(x_1 - x_2) \dots \dots (x_1 - x_n)}$$

On preceding

$$a_n = \frac{y_n}{(x_n - x_0)(x_n - x_1) \dots \dots (x_n - x_{n-1})}$$

Substituting the values of $a_0, a_{1,} a_2 \dots \dots a_n$ in equation 1 we get.

$$y = f(x) = \frac{(x - x_1)(x - x_2) \dots \dots (x - x_n)}{(x_0 - x_1)(x_0 - x_2) \dots \dots (x_0 - x_n)} y_0$$

$$+ \frac{(x - x_0)(x - x_2) \dots \dots (x - x_n)}{(x_1 - x_0)(x_1 - x_2) \dots \dots (x_1 - x_n)} y_1$$

$$+ \dots \dots$$

$$\frac{(x - x_0)(x - x_1) \dots \dots (x - x_{n-1})}{(x_n - x_0)(x_n - x_1) \dots \dots (x_n - x_{n-1})} y_n$$

this is known as Lagrange's interpolation formula

in general

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

This is Lagrange basic polynomial

Note:

1. *This formula can be used irrespective of whether the values* $x_{0,} x_{1,} x_{2,\dots.} x_{n,}$ *are equally spaced or not.*
2. *It is simple and easy to remember but its application is not speedy.*
3. *The main drawback of it is that if another interpolation value is inserted, then the interpolation coefficients are required to be recalculated.*

Example 1: Consider the problem to find the square root of 2.5 using the second order Lagrange interpolation polynomial.

Consider the following three points

$x_0 = 2$	$x_1 = 3$	$x_2 = 4$
$f_0 = 1.4142$	$f_1 = 1.7321$	$f_2 = 2$

We know that

$$f(x) = \sum_{i=0}^{2} y_i l_i$$

Where

$$l_i = \frac{\prod_{\substack{j=0 \\ j \neq i}}^{2} (x - x_j)}{\prod_{\substack{j=0 \\ j \neq i}}^{2} (x_i - x_j)}$$

so

$$l_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}$$

$$= \frac{(x-3)(x-4)}{(2-3)(2-4)}$$

$$= \frac{x^2 - 7x + 12}{2}$$

$$l_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}$$

$$= \frac{(x-2)(x-4)}{(3-2)(3-4)}$$

$$= \frac{x^2 - 6x + 8}{-1}$$

$$l_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

$$= \frac{(x-2)(x-3)}{(4-2)(4-3)}$$

$$= \frac{x^2 - 5x + 6}{2}$$

We know, $f(x) = y_0 l_0(x) + y_1 l_1(x) + y_2 l_2(x)$

$$= 1.4142 * \frac{x^2 - 7x + 12}{2} + 1.7321 * \frac{x^2 - 6x + 8}{-1} + 2 * \frac{x^2 - 5x + 6}{2}$$

$$= 0.7071 * (x^2 - 7x + 12) - 1.7321 * (x^2 - 6x + 8) + (x^2 - 5x + 6)$$

$$f(2.5) = 0.7071 * (2.5^2 - 7 * 2.5 + 12) - 1.7321 * (2.5^2 - 6 * 2.5 + 8) + (2.5^2 - 5 * 2.5 + 6)$$

$$= 0.5303 + 1.2991 - 0.25$$

$$= 1.5794$$

The square root of 2.5 is 1.5794 with some error.

Practice :

1. Find the Lagrange interpolation polynomial to fit the following data.

i	0	1	2	3
x_i	0	1	2	3
$e^{x_i} - 1$	0	1.7183	6.3891	19.0855

Use the polynomial to estimate the value of $e^{1.5}$

2. Find the Lagrange interpolation polynomial to fit the following data.

x	1.0	1.1	1.2
$\cos x$	0.5403	0.4536	0.3624

Use the polynomial to estimate the value of cos 1.15

Newtons Interpolation formula

Given the set of data points $(x_0, y_0), (x_1, y_1), (x_2, y_2) \dots\dots (x_{n-1}, y_{n-1})$. Let us consider a polynomial function of the form known as newton form as

$$p_n(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + a_3(x - x_0)(x - x_1)(x - x_2) + \cdots + a_n(x - x_1) \dots (x - x_{n-1})$$

Of the order n which passes through all the given data points

At $x = x_0$, $p_n(x_0) = a_0 = y_0$

$$At, \quad x = x_1, p_n(x_1) = a_0 + a_1(x_1 - x_0) = y_1$$

$$a_1 = \frac{y_1 - a_0}{x_1 - x_0}$$

$$= \frac{y_1 - y_0}{x_1 - x_0}$$

$$At, \quad x = x_2, p_n(x_2) = a_0 + a_1(x_2 - x_0) + a_2(x_2 - x_0)(x_2 - x_1) = y_2$$

$$a_2 = \frac{y_2 - y_0 - a_1(x_2 - x_0)}{(x_2 - x_0)(x_2 - x_1)}$$

Substituting of the value of a_1

$$a_2 = \frac{y_2 - y_0 - \frac{y_1 - y_0}{x_1 - x_0}(x_2 - x_0)}{(x_2 - x_0)(x_2 - x_1)}$$

On further calculation we get the final result as

$$a_2 = \frac{\frac{y_2 - y_1}{x_2 - x_1} - \frac{y_1 - y_0}{x_1 - x_0}}{(x_2 - x_0)}$$

Now let us define new notation as

$$a_1 = \frac{y_1 - y_0}{x_1 - x_0} = f[x_0, x_1] \; divided \; difference$$

$$a_2 = \frac{\frac{y_2 - y_1}{x_2 - x_1} - \frac{y_1 - y_0}{x_1 - x_0}}{(x_2 - x_0)} = f[x_0, x_1, x_2]$$

$$a_2 = f[x_0, x_1, x_2, x_3] \dots \dots$$

$$a_n = f[x_0, x_1, x_2, x_3, \dots \dots x_n]$$

The polynomial $p_n(x)$ which passes through the given points is

$$p_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + f[x_0, x_1, x_2, x_3](x - x_0)(x - x_1)(x - x_2) \dots \dots . f[x_0, x_1, x_2, x_3 \dots \; x_n](x - x_0)(x - x_1)(x - x_2) \dots (x - x_{n-1})$$

This polynomial is called Newtons divided difference interpolation

Example : Given below is a table of data for $\log x$, estimate $\log 2.5$using second order newton

i	0	1	2	3
x_i	1	2	3	4
$\log x_i$	0	0.3010	0.4771	0.6021

Solution

$$a_0 = f[x_0] = y_0 = 0$$

$$a_1 = f[x_0, x_1] = \frac{y_1 - y_0}{x_1 - x_0} = \frac{0.3010 - 0}{2 - 1} = 0.3010$$

$$a_2 = f[x_0, x_1, x_2] = \frac{\frac{y_2 - y_1}{x_2 - x_1} - \frac{y_1 - y_0}{x_1 - x_0}}{(x_2 - x_0)} = \frac{\frac{0.4771 - 0.3010}{3-2} - \frac{0.3010 - 0}{2-1}}{(3-1)} = -0.0625\text{use}$$

Now,

$$p_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1)$$

$$= 0 + 0.3010 * (x - 1) + (-0.0625)(x - 1)(x - 2)$$

$$= 0.3010 * (x - 1) - 0.0625(x - 1)(x - 2)$$

$$p_n(2.5) = 0.3010 * (2.5 - 1) - 0.0625(2.5 - 1)(2.5 - 2)$$

$$= 0.3010 * 1.5 - 0.0469$$

$$= 0.4046$$

Newtons divided difference table:

The alternative way of finding the coefficients(a_0,a_1, a_2 *and so on*) values to use Newton divided difference table, for given (x_0,f_0),(x_1,f_1),(x_2,f_2),($x_3 f_3$) and (x_4,f_4) is called Newton's divided difference table.

Example : find the functional value for $x = 7$ using newton interpolation polynomial

x	5	6	9	11
f(x)	12	13	14	16

Since there are four data points the required polynomial will be of the order 3

$$p_3(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + a_3(x - x_0)(x - x_1)(x - x_2)$$

To get the value of a_0, a_1, a_2, a_3 we are going to use newton divided difference table

x	f		1st Order Difference	2nd Order Difference
5	12			
		$\frac{13-12}{6-5} = 1$		
6	13		$\frac{1/3 - 1}{9-5} = -1/6$	
		$\frac{14-13}{9-6} = 1/3$		$\frac{2/15-(-1/6)}{11-5} = 1/20$
9	14		$\frac{1-1/3}{11-6} = 2/5$	
		$\frac{16-14}{11-9} = 1$		
11	16			

From table $a_0 = 12, a_1 = 1, a_2 = -1/6, a_3 = 1/20$

Now $p_3(x) = 12 + 1(x - 5) - 1/6\,(x - 5)(x - 6) + 1/20\,(x - 5)(x - 6)(x - 9)$

Now substitute x=7 in above expression and we get

$$p_3(x) = 12 + 1(7 - 5) - 1/6\,(7 - 5)(7 - 6) + 1/20\,(7 - 5)(7 - 6)(7 - 9) = 13.47$$

Evenly spaced data

If x-value are evenly spaced getting an interpolating polynomial is considerably simplified. Most of the engineering and scientific table are available in this form.

Newton's forward difference interpolation/ Gregory Newton forward interpolation formula

let $y = f(x)$ be a function which takes the values $y_0, y_1 \ldots\ldots y_n$ for values (n+1), at $x_0, x_1, x_2 \ldots\ldots x_n$ of the independent variables x. let these values of x be equidistance i.e$x_i = x_0 + ih, i.e\ \ i = 0,1,2 \ldots n$. Let y(x) be the polynomial in x of the nth degree such that $y_i = f(x_i), i = 0,1,2 \ldots n$.

$$y(x) = A_0 + A_1(x - x_0) + A_2(x - x_0)(x - x_1) + A_3(x - x_0)(x - x_1)(x - x_2) \ldots\ldots\ldots (a)$$

Putting $x = x_0, x_1 \ldots\ldots x_n\ successively$

We get, putting $x = x_0$

$$y_0 = A_0$$

$$A_0 = y_0$$

putting $x = x_1$ and putting $A_0 = y_0$

$$y_1 = A_0 + A_1(x_1 - x_0)$$

$$A_1 = \frac{y_1 - A_0}{x_1 - x_0} = \frac{y_1 - y_0}{x_1 - x_0} = \frac{\Delta y_0}{h}$$

Where h =equidistant gap.

putting $x = x_2$ and putting values of A_0, A_1

$$y_2 = A_0 + A_1(x_1 - x_0) + A_2(x_2 - x_0)(x_2 - x_1)$$

$$A_2 = \frac{y_2 - A_0 - A_1(x_2 - x_0)}{(x_2 - x_0)(x_2 - x_1)}$$

$$= \frac{y_2 - y_0 - \frac{y_1 - y_0}{x_1 - x_0}(x_2 - x_0)}{(x_2 - x_0)(x_2 - x_1)}$$

$$x_2 - x_0 = (x_2 - x_1) + (x_1 - x_0) = h + h = 2h$$

$$= \frac{y_2 - y_0 - \frac{y_1 - y_0}{h} 2h}{(2h)(h)}$$

$$= \frac{y_2 - y_0 - 2y_1 + 2y_0}{2h^2}$$

$$= \frac{y_2 - 2y_1 + y_0}{2h^2}$$

$$= \frac{\Delta^2 y_0}{2!\, h^2}$$

Similarly

$$A_3 = \frac{\Delta^3 y_0}{3!\, h^3}$$

Similarly, and so on putting these values in equation (a), we get

$$y(x) = y_0 + \frac{\Delta y_0 (x - x_0)}{h} + \frac{\Delta^2 y_0 (x - x_0)(x - x_1)}{2!\, h^2} + \frac{\Delta^3 y_0 (x - x_0)(x - x_1)(x - x_2)}{3!\, h^3} \ldots\ldots..(b)$$

Putting $\frac{(x - x_0)}{h} = p, i.e\ x = x_0 + ph$ where p is a real number

Finally we get

$$y_p = y_0 + p\Delta y_0 + \frac{p(p-1)\Delta^2 y_0}{2!} + \frac{p(p-1)(p-2)\Delta^3 y_0}{3!} + \cdots + \frac{p(p-1)\ldots[p-(n-1)]\Delta^n y_0}{n!}$$

Where $y_p = y(x_0 + ph)$ is known as Gregory Newton forward interpolation formula.

Gregory Newton Backward Interpolation Formula

let $y = f(x)$ be a function which takes the values $y_0, y_1 \ldots\ldots y_n$ for values (n+1), at $x_0, x_1, x_2 \ldots\ldots x_n$ of the independent variables x. let these values of x be equidistance i.e$x_i = x_0 + ih, i.e\ \ i = 0,1,2 \ldots n$. Let y(x) be the polynomial in x of the nth degree such that $y_i = f(x_i), i = 0,1,2 \ldots n$. Suppose it is required to evaluate y(x) near the end of the table value, then we can assume that,

$$y(x) = A_0 + A_1(x - x_n) + A_2(x - x_n)(x - x_{n-1}) + A_3(x - x_n)(x - x_{n-1})(x - x_{n-2}) + \cdots + \cdots A_n(x - x_n)(x - x_{n-1}) \ldots (x - x_1) \ldots\ldots (a)$$

Putting $x = x_n, x_{n-1} \ldots\ldots x_0$ *successively in equation a*

We get, putting $x = x_n$

$$A_0 = y(x_n) = y_n$$

putting $x = x_{n-1}$ and putting $A_0 = y_n$

$$y(x_{n-1}) = y_{n-1} = A_0 + A_1(x_{n-1} - x_n)$$

putting $x = x_{n-2}$

$$y(x_{n-2}) = y_{n-2} = A_0 + A_1(x_{n-2} - x_n) + A_2(x_{n-2} - x_n)(x_{n-2} - x_{n-1})$$

Solving above equation for values of A, we get

$$A_1 = \frac{y_{n-1} - A_0}{x_{n-1} - x_n} = \frac{y_{n-1} - y_n}{x_{n-1} - x_n} = \frac{y_n - y_{n-1}}{x_n - x_{n-1}} = \frac{\nabla y_n}{h}$$

Where h =equidistant gap.

$$A_2 = \frac{y_{n-2} - A_0 - A_1(x_{n-2} - x_n)}{(x_{n-2} - x_n)(x_{n-2} - x_{n-1})}$$

$$= \frac{y_{n-2} - y_n - (y_n - y_{n-1})(-2)}{(-2h)(-h)} x \frac{1}{h}$$

$$= \frac{y_n - 2y_{n-1} + 2y_{n-2}}{2h^2}$$

$$= \frac{\nabla^2 y_n}{2!\, h^2}$$

Similarly

$$A_3 = \frac{\nabla^3 y_n}{3!\, h^3}$$

And so on

Putting these values in equation a we get

$$y(x) = y_n + \frac{\nabla y_n (x - x_n)}{h} + \frac{\nabla^2 y_n (x - x_n)(x - x_{n-1})}{2!\, h^2} + \frac{\nabla^3 y_n (x - x_n)(x - x_{n-1})(x - x_{n-2})}{3!\, h^3} \dots \dots . . (b)$$

Putting $\frac{(x - x_n)}{h} = p, i.e\ x = x_n + ph$ where p is a real number

Finally we get

$$y_p = y_n + p\Delta y_n + \frac{p(p+1)\nabla^2 y_n}{2!} + \frac{p(p+1)(p+2)\nabla^3 y_n}{3!} + \cdots + \frac{p(p+1)(p+2)\dots[p+(n-1)]\nabla^n y_n}{n!}$$

Where $y_p = y(x_n + ph)$ is known as Gregory Newton Backward interpolation formula.

Example 1: Estimate the value of $\sin\theta \; at \; \theta = 25^{\circ}$, using Newton Gregory Forward difference formula with the help of following table

θ	10	20	30	40	50
$\sin\theta$	0.1736	0.3420	0.5	0.6428	0.7660

Solution

In order to use newtons Gregory difference formula we need the values of Δ^n. These coefficients can be obtained from the difference table given below

θ	$\sin\theta$	Δy_n	$\Delta^2 y_n$	$\Delta^3 y_n$	$\Delta^4 y_n$
10	0.1736				
		0.1684			
20	0.3420		-0.0104		
		0.1580		-0.0048	
30	0.5		-0.0152		0.0004
		0.1428		-0.0041	
40	0.6428		-0.0196		
		0.1232			
50	0.7660				

The Newton's Forward Difference Interpolation Formula

$$y_p = y_0 + p\Delta y_0 + \frac{p(p-1)\Delta^2 y_0}{2!} + \frac{p(p-1)(p-2)\Delta^3 y_0}{3!} + \frac{p(p-1)(p-2)(p-3)\Delta^4 y_0}{4!}$$

Where $p = \frac{x - x_0}{h}$ for $\theta = 25, p = \frac{25-10}{10} = 1.5$

$$y_p = 0.1736 + 1.5 \times 0.1684 + \frac{1.6(1.5-1)(-0.0104)}{2!} + \frac{1.5(1.5-1)(1.5-2)(-0.0048)}{3!} + \frac{1.5(1.5-1)(1.5-2)(1.5-3)0.004}{4!}$$

$$= 0.1736 + 0.2526 - 0.0039 + 0.0003 + 0.0000$$

$$= 0.4226$$

Extra solving using backward formula

$$y_p = y_n + p\Delta y_n + \frac{p(p+1)\nabla^2 y_n}{2!} + \frac{p(p+1)(p+2)\nabla^3 y_n}{3!} + \frac{p(p+1)(p+2)(P+3)\nabla^4 y_n}{4!}$$

$$p = \frac{25-50}{10} = -2.5$$

$$y(25) = 0.7660 + (-2.5)(0.1232) + \frac{(-2.5)(-2.5+1)(-0.0196)}{2!} + \frac{(-2.5)(-2.5+1)(-2.5+2)(-0.0044)}{3!} + \frac{(-2.5)(-2.5+1)(-2.5+2)(-2.5+3)(0.0004)}{4!}$$

$$= 0.7660 - 0.3080 - 0.0368 + 0.0014 + 0$$

$$= 0.4226$$

Example 2 : Find the values of y for x=0.8 for the given set of values using Newton's Backward Difference Interpolation Formula

X	0.5	1	1.5	2	2.5	3
Y	2.1990	2.5	2.6761	2.8010	2.8979	2.9771

Now the difference table is

X	y	∇y_n	$\nabla^2 y_n$	$\nabla^3 y_n$	$\nabla^4 y_n$	$\nabla^5 y_n$
0.5	2.1990					
1	2.5	0.3010				
1.5	2.6761	0.1761	-0.1249			
2	2.8010	0.1249	-0.0512	0.0737		
2.5	2.8979	0.0969	-0.0280	0.0232	-0.0505	
3	2.9771	0.0792	-0.0177	0.0103	-0.0129	0.0376

Now, Newton's Backward Interpolation Formula

$$y_p = y_n + p\Delta y_n + \frac{p(p+1)\nabla^2 y_n}{2!} + \frac{p(p+1)(p+2)\nabla^3 y_n}{3!} + \frac{p(p+1)(p+2)(P+3)\nabla^4 y_n}{4!} + \frac{p(p+1)(p+2)(P+3)(P+4)\nabla^5 y_n}{5!}$$

Where

$$p = \frac{x - x_n}{h} = \frac{0.8 - 3}{0.5} = -4.4$$

Now

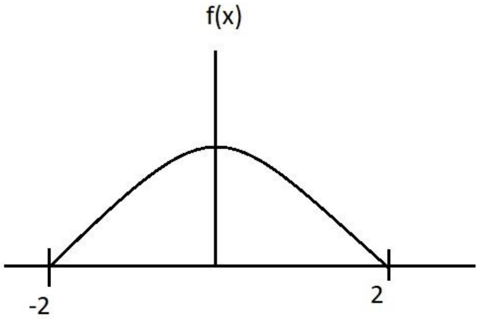
$$y_p = y(0.8) = 2.9771 + (-4.4)(0.0792) + \frac{(-4.4)(-4.4+1)(-0.0177)}{2!} + \frac{(-4.4)(-4.4+1)(-4.4+2)(0.0103)}{3!} + \frac{(-4.4)(-4.4+1)(-4.4+2)(-4.4+3)(-0.0129)}{4!} + \frac{(-4.4)(-4.4+1)(-4.4+2)(-4.4+3)(-4.4+4)(0.0376)}{5!}$$

$$= 2.9771 - 0.3485 - 0.1324 - 0.0616 - 0.0270 - 0.0063$$

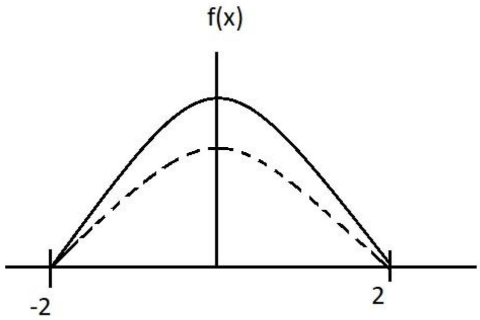
$$= 2.4013$$

Spline curves

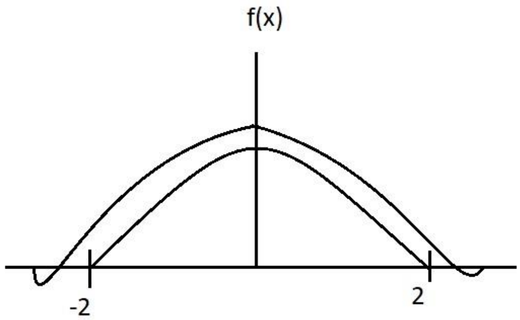
There are many times when fitting an interpolating polynomial to data points is very difficult. Here is an example where we try to fit to data pairs from known functions.



a) original function



b) fitted with quadratic function



c) fitted with p4(x)

None of the polynomial is a good representation of the function. In particular we observe that eight-degree polynomial derivatives widely near x=2.

One approach to overcome this problem is to divide the entire range of points into sub intervals and use local low order polynomials to interpolate each sub intervals, such polynomials are called piecewise polynomials.

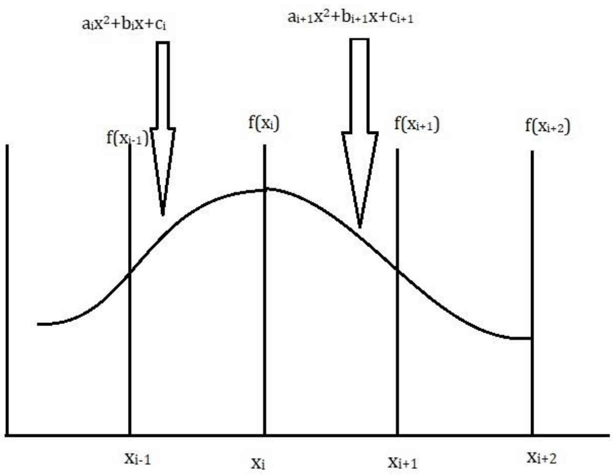
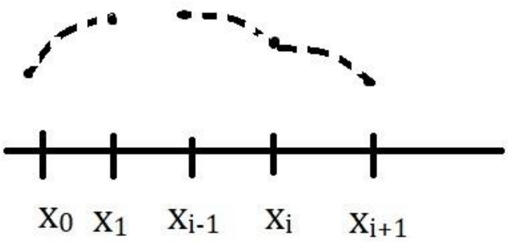


Figure piecewise polynomial interpolation

Such piecewise polynomials are called splines functions. So, the splines functions look smooth at the connecting points, the connecting points are called knots or nodes.



The formula for obtaining cubic spline function:

(1) We write the formula for a cubic polynomial $s_i(x)$ as,

$$s_i(x) = (a_{i-1}/6h_i)\,(h_i^2\, u_i - u_i^3) + (a_i/6h_i)\,(u_{i-1}^3 - h_i^2\, u_{i-1}) + 1/h_i\,(f_i\, u_{i-1} - f_{i-1}\, u_i)$$

where, $u_i = x - x_i$

(2) Formula for obtaining "a_i" values:

(I) For 3 data points:

$$h_i a_{i-1} + 2(h_i + h_{i+1})a_i + h_{i+1}a_{i+1} = 6\left(\frac{f_{i+1}-f_i}{h_{i+1}} - \frac{f_i - f_{i-1}}{h_i}\right)$$

(II) For 4 data points:

$$\begin{bmatrix} 2(h_1 + h_2) & h_2 \\ h_2 & 2(h_2 + h_3) \end{bmatrix}\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \end{bmatrix}$$

Where, $D_i = 6\left(\frac{f_{i+1}-f_i}{h_{i+1}} - \frac{f_i - f_{i-1}}{h_i}\right)$

Q.N. (1) Given the data points as below:

i	0	1	2
x_i	4 (x_0)	9 (x_1)	16 (x_2)
$f(x_i)$	2 (f_0)	3 (f_1)	4 (f_2)

Estimate the functional value at x=7 using cubic spline technique.

Solution : h_1 =5, h_2 =7 Now, using the formula,

$$h_i a_{i-1} + 2(h_i + h_{i+1})a_i + h_{i+1}a_{i+1} = 6\left(\frac{f_{i+1}-f_i}{h_{i+1}} - \frac{f_i - f_{i-1}}{h_i}\right) \text{...(A)}$$

Put i=1 since x=7 lies in the domain of $s_1(x)$. i.e.

$$h_1 a_0 + 2(h_1 + h_2)a_1 + h_2 a_2 = 6\left(\frac{f_2 - f_1}{h_2} - \frac{f_1 - f_0}{h_1}\right) \text{......(B)}$$

Now, we know from the cubic spline technique, $a_0 = a_n = 0$ i.e. $a_0 = a_2 = 0$

So, from (B) we get, 2(5+7) a_1=6[1/7-1/5].Therefore, a_1 = -0.0143

Now the cubic spline function,

$s_i(x) = (a_{i-1}/6h_i)(h_i^2 u_i - u_i^3) + (a_i/6h_i)(u_{i-1}^3 - h_i^2 u_{i-1}) + 1/h_i (f_i u_{i-1} - f_{i-1} u_i)$…(C)

where, $u_i = x - x_i$

put i=1 in (C) we get,

$s_1(x) = (a_0/6h_1)(h_1^2 u_1 - u_1^3) + (a_1/6h_1)(u_0^3 - h_1^2 u_0) + 1/h_1 (f_1 u_0 - f_0 u_1)$

where, $u_0 = x - x_0$ and $u_1 = x - x_1$

So, $s_1(7)$ = 2.6229 i.e. f(7) = 2.6229Ans.

Q.N. (2): Given the data points as below:

i	0	1	2	3
x_i	$1(x_0)$	$2(x_1)$	$3(x_2)$	$4(x_3)$
$f(x_i)$	$0.5(f_0)$	$0.3333(f_1)$	$0.25(f_2)$	$0.20(f_3)$

Estimate the functional value at x=2.5 using cubic spline technique.

Solution: $h_1 = 1$, $h_2 = 1$, $h_3 = 1$ and $a_0 = 0$, a_1, a_2, $a_3 = 0$ (from cubic spline technique)

$$\begin{bmatrix} 2(1+1) & 1 \\ 1 & 2(1+1) \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \end{bmatrix}$$

Now D_1 (i=1) = $6\left(\frac{f_2-f_1}{h_2} - \frac{f_1-f_0}{h_1}\right) = 0.5004$

and D_2(i=2) = $6\left(\frac{f_3-f_2}{h_3} - \frac{f_2-f_1}{h_2}\right) = 0.1995$

Now, $a_1 = 0.120$ and $a_2 = 0.0199$

Since x=2.5 lies on the domain of $s_2(x)$ i.e. i=2

Now, the cubic spline function,

$s_2(x) = (a_1/6h_2)(h_2^2 u_2 - u_2^3) + (a_2/6h_2)(u_1^3 - h_2^2 u_1) + 1/h_2 (f_2 u_1 - f_1 u_2)$

where, $u_2 = x - x_2$, $u_1 = x - x_1$

So, $s_2(2.5) = 0.2829$ i.e. $f(2.5) = 0.2829$

Practice questions:

1. Estimate the value of $\ln(3.5)$ using Newton-Gregory Forward Difference Formula using given data

x	1.0	2.0	3.0	4.0
$\ln x$	0.0	0.6931	1.0986	1.3863

2. Estimate the value of $\sin\theta$ at $\theta = 45^\circ \& 15^\circ$, using Newton Gregory Forward and Backward difference formula with the help of following table and compare the results

θ	10	20	30	40	50
$\sin\theta$	0.1736	0.3420	0.5	0.6428	0.7660

Curve Fitting:

In many applications it is often necessary to establish a mathematical relationship between experimental values, this relationship may be used for either testing existing mathematical model or establishing new ones. The mathematical equation can also be used to predict or forecast values of the dependent variables.

Suppose the value of y for the different values of x are given, if we want to know the effect of x and y then we may write a functional relationship $y = f(x)$

The variable y is called dependent variables and x is the independent variable. The relationship mat be either linear or non linear. We shall discuss the technique known as least squares regression to fit data under following situation.

Relationship is linear

Fitting a straight line is the simplest approach of regression analysis. Let us consider the mathematical equation of a straight line

$$y = a + bx = f(x)$$

We know that a is the intercept of the line and b is the slope. Consider the points(x_i, y_i), then the vertical distance of this point from the line $f(x) = a + bx$ is q_i , then

$$q_i = y_i - f(x_i)$$

$$= y_i - (a + bx_i)$$

There are various approaches that would be tries for fitting the best line through the data:

1. Minimize the sum of errors
2. Minimize the sum of absolute value of errors
3. Minimize the sum of squares of errors

Least Square regression:

Let the sum squares of individual errors be expressed as

$$Q = \sum_{i=1}^{n} {q_i}^2 = \sum_{i=1}^{n} [y_i - f(x_i)]^2$$

$$= \sum_{i=1}^{n} [y_i - a - bx_i]^2$$

In this method of least squares we choose a & b such that Q is minimum, since Q depends on a & b, a necessary condition for Q to be minimum is

$$\frac{\partial Q}{\partial a} = 0, \frac{\partial Q}{\partial b} = 0$$

Then

$$\frac{\partial Q}{\partial a} = -2\sum_{i=1}^{n} (y_i - a - bx_i) = 0$$

$$\frac{\partial Q}{\partial b} = -2\sum_{i=1}^{n} x_i(y_i - a - bx_i) = 0$$

Thus we can write as:

$$\sum_{i=1}^{n} (y_i - a - bx_i) = 0$$

$$\sum y_i = na + b\sum x_i \ldots\ldots\ldots\ldots\ldots \quad a$$

$$\sum x_i y_i = a\sum x_i + b\sum {x_i}^2 \ldots\ldots\ldots\ldots\ldots \quad b$$

These are called normal equations solving for a & b we get

$$b = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum {x_i}^2 - (\sum x_i)^2}$$

$$a = \frac{\sum y_i}{n} - b\frac{\sum x_i}{n} = \bar{y} - b\bar{x}$$

Where $\bar{x}$ *and* $\bar{y}$ are the average of x and y values.

Example: Fit a straight line to the following set of data

X	1	2	3	4	5
Y	3	4	5	6	8

Solution

The various summations are given below

	x_i	y_i	x_i^2	$x_i y_i$
	1	3	1	3
	2	4	4	8
	3	5	9	15
	4	6	16	24
	5	8	25	40
Σ	**15**	**26**	**55**	**90**

now

$$b = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - (\sum x_i)^2}$$

$$b = \frac{5 * 90 - 15 * 26}{5 * 55 - 15^2}$$

$$= 1.20$$

$$a = \frac{\sum y_i}{n} - b \frac{\sum x_i}{n}$$

$$= \frac{26}{5} - 1.2 \frac{15}{5}$$

$$= 1.6$$

Therefore, the linear equation is $y = 1.6 + 1.2x$

Practice :

1. Fit a linear curve through the following data points

X	1	2	3	4	5	6	7
Y	0.5	2.5	2.0	4.0	3.5	6.0	5.5

Answer :$y = 0.0714 + 0.839x$

2. In an organization , systematic efforts were introduces to reduce the employee absenteeism and result for the first 10 months are shown below, fit a linear least square lines to the data.

Months	1	2	3	4	5	6	7	8	9	10
Absentees(%)	10	9	9	8.5	9	8	8.5	7	8	7.5

3. The following table shows heights(h) and weights, find the regression line and estimate the weights of the person with the following heights.
   a) 140cm
   b) 163 cm
   c) 172.5 cm

h(cm)	175	165	160	180	150	170	155	185
w(kg)	68	58	59	71	51	62	53	68

Fitting Transcendental equations

In many cases of course data from experimental test are non linear, so we need to fit them some functions other than first degree polynomial some popular forms are

$$y = ax^b \; or \; y = ae^{bx}$$

Now for $y = ax^b$ if we take logarithms on both sides we get

$$\ln y = \ln a + \text{b}\ln x$$

now let is write as

$$z = A + bx$$

$$z = \ln y, A = \ln a\,, X = \ln x$$

This equation is similar in form to linear equation and therefore using the same procedure we can evaluate the parameters A & B.

$$b = \frac{n \sum \ln x_i \ln y_i - \sum \ln x_i \sum \ln y_i}{n \sum (\ln x_i)^2 - (\sum \ln x_i)^2}$$

$$\ln a = A = \frac{(\sum \ln y_i - b \sum \ln x_i)}{n}$$

$$a = e^A$$

Example : given the data table below , fit a power function model of the form $y = ax^b$

x	1	2	3	4	5
y	0.5	2	4.5	8	12.5

The various quantities requires are

x_i	y_i	$\ln x_i$	$\ln y_i$	$(\ln x_i)^2$	$(\ln x_i)(\ln y_i)$
1	0.5	0	-0.6931	0	0
2	2	0.6931	0.6931	0.4804	0.4804
3	4.5	1.0986	1.5041	1.2069	1.6524
4	8	1.3863	2.0794	1.9218	2.8827
5	12.5	1.6094	2.5257	2.5902	4.0649
$\sum$		4.7874	6.1092	6.1993	9.0804

$$b = \frac{n \sum \ln x_i \ln y_i - \sum \ln x_i \sum \ln y_i}{n \sum (\ln x_i)^2 - (\sum \ln x_i)^2}$$

$$= \frac{5 * 9.0804 - 4.7874 * 6.1092}{5 * 6.1993 - 4.7874^2}$$

$$= 2$$

$$A = \frac{(\sum \ln y_i - b \sum \ln x_i)}{n}$$

$$= \frac{6.1092 - 2 * 4.7874}{5}$$

$$= -0.6981$$

$$a = e^A = e^{-0.6931} = 0.5$$

$$y = ax^b = 0.5x^2$$

$$y = 0.5x^2$$

Practice:

1. The temperature of a metal strip was measured at various time intervals during heating and the values are given in the table

Time,t(min)	1	2	3	4
Temp,$T°(c)$	70	83	150	124

If the relationship between the temperature T and time t is of the form $T = be^{t/4} + a$, estimate temp at t=6min.

2. Use the exponential model $y = ae^{bx}$ to fit the data

X	0.4	0.8	1.2	1.6	2.0	2.4
Y	75	100	140	200	270	375

Fitting a polynomial function

When a given set of data does not appear to satisfy a linear equation, we can try a suitable polynomial as regression curve to fit the data. The least squares technique can be readily used to fit the data to a polynomial

Consider a polynomial of degree m-1.

$$f(x) = y = a_1 + a_1 x + a_3 x^2 + a_4 x^3 + \cdots \ldots + a_m x^{m-1}$$

If the data contains n set of x any y values, then the sum squares of the errors is given by

$$Q = \sum_{i=1}^{n} [y_i - f(x_i)]^2$$

Since f(x) is a polynomial and contains coefficient $a_1, a_2, a_{3\dots}$ we have to estimate all m coefficients as before we have the following m equations that can be solved for these coefficients i.e

$$\frac{\partial Q}{\partial a_1} = 0, \frac{\partial Q}{\partial a_2} = 0 \dots . \frac{\partial Q}{\partial a_m} = 0$$

Consider a general term

$$\frac{\partial Q}{\partial a_j} = -2\sum_{i=1}^{n}[y_i - f(x_i)]\frac{\partial f(x_i)}{\partial a_j} = 0$$

$$\frac{\partial f(x_i)}{\partial a_j} = {x_i}^{j-1}$$

Thus, we have

$$\sum_{i=1}^{n}[y_i - f(x_i)]{x_i}^{j-1} = 0 \;\; j = 1,2,3 \dots \dots m$$

$$\sum_{i=1}^{n}\left[y_i{x_i}^{j-1} - {x_i}^{j-1}f(x_i)\right] = 0$$

Substituting for $f(x_i)$

$$\sum_{i=1}^{n}{x_i}^{j-1}\,(a_1 + a_1x_i + a_3{x_i}^2 + a_4{x_i}^3 + \cdots \dots + \; a_m{x_i}^{m-1}) = \sum_{i=1}^{n}y_i{x_i}^{j-1}$$

These are m equations and each summation is for i=1 to n

$$a_1n + a_2\sum x_i + a_3\sum {x_i}^2 + a_4\sum {x_i}^3 + \cdots \dots + \; a_m\sum {x_i}^{m-1} = \sum y_i$$

$$a_1\sum x_i + a_2\sum {x_i}^2 + a_3\sum {x_i}^3 + a_4\sum {x_i}^4 + \cdots \dots + \; a_m\sum {x_i}^m = \sum y_ix_i \dots$$

$$a_1\sum {x_i}^{m-1} + a_2\sum {x_i}^m + a_3\sum {x_i}^{m+1} + a_4\sum {x_i}^{m+2} + \cdots \dots + \; a_m\sum {x_i}^{2m-2} = \sum y_i{x_i}^{m-1}$$

The set of m equation can be represented in matrix as CA=B

$$C = \begin{bmatrix} n & \sum x_i & \sum x_i{}^2 & \cdots & \sum x_i{}^{m-1} \\ \sum x_i & \sum x_i{}^2 & \sum x_i{}^3 & \cdots & \sum x_i{}^m \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \sum x_i{}^{m-1} & \sum x_i{}^m & \sum x_i{}^{m+1} & \cdots & \sum x_i{}^{2m-2} \end{bmatrix}$$

$$A = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_m \end{bmatrix} B = \begin{bmatrix} \sum y_i \\ \sum y_i x_i \\ \sum y_i x_i{}^2 \\ \vdots \\ \sum y_i x_i{}^{m-1} \end{bmatrix}$$

Example : Fit a second order polynomial to the data in the table

x	1.0	2	3	4
y	6	11	18	27

The order of the polynomial is 2 and therefore we will have 3 simultaneous equations as shown below:

$$a_1 n + a_2 \sum x_i + a_3 \sum x_i{}^2 = \sum y_i$$

$$a_1 \sum x_i + a_2 \sum x_i{}^2 + a_3 \sum x_i{}^3 = \sum y_i x_i$$

$$a_1 \sum x_i{}^2 + a_2 \sum x_i{}^3 + a_3 \sum x_i{}^4 = \sum y_i x_i{}^2$$

	x	y	x^2	x^3	x^4	yx	yx^2
	1	6	1	1	1	6	6
	2	11	4	8	16	22	44
	3	18	9	27	81	54	162
	4	27	16	64	256	108	432
$\sum$	**10**	**62**	**30**	**100**	**354**	**190**	**644**

Substituting these values, we get,

$$4a_1 + 10a_2 + 30a_3 = 62$$

$$10a_1 + 30a_2 + 100a_3 = 190$$

$$30a_1 + 100a_2 + 354a_3 = 644$$

On solving these equations gives,

$$a_1 = 3, a_2 = 2, a_3 = 1$$

Therefore, the least square quadratic polynomial is $y = 3 + 2x + x^2$

Chapter 3: Numerical Differentiation and Integration

Let us consider a set of values (x_i, y_i) of a function. The process of computing the derivative or derivatives of that function at some values of x from the given set of values is called Numerical Differentiation. This may be done by first approximating the function by suitable interpolation formula and then differentiating.

Derivatives using Newton's Forward Difference formula

Newton's forward interpolation formula

$$y_p = y_0 + p\Delta y_0 + \frac{p(p-1)\Delta^2 y_0}{2!} + \frac{p(p-1)(p-2)\Delta^3 y_0}{3!} + \frac{p(p-1)(p-2)(p-3)\Delta^4 y_0}{4!} \ldots (1)$$

$$p = \frac{x - x_0}{h}$$

Differentiating both sides of above equation with respect to p, we have

$$\frac{dy}{dp} = \Delta y_0 + \frac{(2p-1)\Delta^2 y_0}{2!} + \frac{(3p^2 - 6p + 2)\Delta^3 y_0}{3!} + \cdots \quad (2)$$

Now

$$\frac{dy}{dx} = \frac{dy}{dp}\frac{dp}{dx} = \frac{dy}{dp}\frac{1}{h}$$

$$\because \frac{dp}{dx} = \frac{1}{h}$$

$$\frac{dy}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{(2p-1)\Delta^2 y_0}{2!} + \frac{(3p^2 - 6p + 2)\Delta^3 y_0}{3!} + \frac{(4p^3 - 18p^2 + 22p - 6)\Delta^4 y_0}{4!}\right] \ldots (3)$$

At $x = x_0, p = 0$, hence putting p=0 in equation 3 we get

$$\left.\frac{dy}{dx}\right|_{x=x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{\Delta^2 y_0}{2} + \frac{\Delta^3 y_0}{3} - \frac{\Delta^4 y_0}{4}\right] \ldots (4)$$

Differentiating equation 3 again with respect to x we get

$$\frac{d^2y}{dx^2} = \frac{d}{dp}\left(\frac{dy}{dx}\right)\frac{dp}{dx} = \frac{1}{h}\frac{d}{dp}\left(\frac{dy}{dx}\right)$$

$$= \frac{1}{h^2}\left[\Delta^2 y_0 + \frac{(p-1)\Delta^3 y_0}{1!} + \frac{(6p^2 - 18p + 11)\Delta^4 y_0}{12} + \cdots\right] \quad (5)$$

Putting $p = 0$ in equation 5

$$\left.\frac{d^2y}{dx^2}\right|_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0\right]$$

Similarly

$$\left.\frac{d^3y}{dx^3}\right|_{x=x_0} = \frac{1}{h^3}\left[\Delta^3 y_0 - \frac{3}{2}\Delta^4 y_0 \ldots\right]$$

Derivates using Newton's Backward Difference Formula

Newton's backward interpolation formula is

$$y = y_n + p\nabla y_n + \frac{p(p+1)\nabla^2 y_n}{2!} + \frac{p(p+1)(p+2)\nabla^3 y_n}{3!} + \frac{p(p+1)(p+2)(P+3)\nabla^4 y_n}{4!} \ldots (8)$$

$$p = \frac{x - x_n}{h} \ldots\ldots (9)$$

$$\frac{dy}{dx} = \frac{dy}{dp}\frac{dp}{dx} = \frac{dy}{dp}\frac{1}{h}$$

$$\frac{dy}{dp} = \frac{1}{h}\left[\nabla y_n + \frac{2p+1}{2!}\nabla^2 y_n + \frac{3p^2 + 6p + 2}{3!}\nabla^3 y_0 + \cdots\right] \ldots (10)$$

At $x = x_n, p = 0$, hence putting p=0 in equation 10 we get

$$\left.\frac{dy}{dx}\right|_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{\nabla^2 y_n}{2} + \frac{\nabla^3 y_n}{3} + \frac{\nabla^4 y_n}{4}\right] \dots (11)$$

Again, differentiating equation 10 with respect to x

$$\frac{d^2y}{dx^2} = \frac{d}{dp}\left(\frac{dy}{dx}\right)\frac{dp}{dx} = \frac{1}{h}\frac{d}{dp}\left(\frac{dy}{dx}\right)$$

$$= \frac{1}{h^2}\left[\nabla^2 y_n + \frac{6p+6}{3!}\nabla^3 y_n + \frac{6p^2+18p+11}{4!}\nabla^4 y_n + \cdots\right] \dots (12)$$

Putting $p = 0$

$$\left.\frac{d^2y}{dx^2}\right|_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \cdots\right] \dots (13)$$

Similarly

$$\left.\frac{d^3y}{dx^3}\right|_{x=x_n} = \frac{1}{h^3}\left[\nabla^3 y_n + \frac{3}{2}\nabla^4 y_n + \cdots\right] \dots (14)$$

Note: first derivative is also as rate of change, so it can also be asked to find the velocity, second derivative to find acceleration etc.

Example: Find the first, second and third derivate of $f(x) at\ x = 1.5$ if

x	1.5	2.0	2.5	3.0	3.5	4.0
$f(x)$	3.375	7.0	13.625	24	38.875	59.0

Solution

We have to find the derivate at the points $x = 1.5$, which is at the beginning of the given data. Therefore, we use the derivate of Newton's Forward Interpolation formula.

Forward difference table is

x	$y = f(x)$	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
1.5	3.375					
		3.625				
2.0	7.0		3			
		6.6250		0.75		
2.5	13.625		3.750		0	
		10.3750		0.75		0
3.0	24.0		4.5		0	
		14.8750		0.75		
3.5	38.875		5.25			
		20.1250				
4.0	59.0					

Here $x_0 = 1.5, y_0 = 3.375, \Delta y_0 = 3.625, \Delta^2 y_0 = 3, \Delta^3 y_0 = 0.75, \Delta^4 y_0 = 0, h = 0.5$

Now using equation for finding the derivate

$$\left.\frac{dy}{dx}\right|_{x=x_0} = f'(x_0) = \frac{1}{h}\left[\Delta y_0 - \frac{\Delta^2 y_0}{2} + \frac{\Delta^3 y_0}{3} - \frac{\Delta^4 y_0}{4} + \cdots\right]$$

$$f'(1.5) = \frac{1}{0.5}\left[3.625 - \frac{3}{2} + \frac{0.75}{3} - \frac{0}{4} + \cdots\right]$$

$$= 4.75$$

Now

$$\left.\frac{d^2 y}{dx^2}\right|_{x=x_0} = f''(1.5) = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12} * 0\right]$$

$$= \frac{1}{1.5^2}\left[3 - 0.75 + \frac{11}{12} * 0\right]$$

$$= 9$$

Again

$$\left.\frac{d^3y}{dx^3}\right|_{x=x_0} = \frac{1}{h^3}\left[\Delta^3 y_0 - \frac{3}{2}\Delta^4 y_0 \ldots\right]$$

$$= \frac{1}{1.5^3}[0.75]$$

$$= 6$$

Example:

The population of a certain town (as obtained from central data) is shown in the following table

Year	1951	1961	1971	1981	1991
population (thousand)	19.36	36.65	58.81	77.21	94.61

Find the rate of growth of the population in the year 1981

Solution

Here we have to find the derivate at 1981 which is near the end of the table, hence we use the derivative of Newtons Backward difference formula. The table if difference is as follows:

x(year)	$y = f(x)$(population)	∇y	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$
1951	19.96				
		16.69			
1961	36.65		5.47		
		22.16		-9.23	
1971	58.81		-3.76		11.99
		18.40		2.76	
1981	77.21		-1		
		17.40			
1991	94.61				

Here $h = 10, x_n = 1991, \nabla y_n = 17.4, \nabla^2 y_n = -1, \nabla^3 y_n = 2.76, \nabla^4 y_n = 11.99$

We know derivative for backward difference is:

$$\frac{dy}{dp} = \frac{1}{h}\left[\nabla y_n + \frac{2p+1}{2!}\nabla^2 y_n + \frac{3p^2+6p+2}{3!}\nabla^3 y_0 + \frac{2p^3+9p^2+11p+3}{4!}\nabla^4 y_0\right]$$

Now we have to find out the rate of growth of the population in year 1981, so

$$p = \frac{x - x_n}{h} = \frac{1981 - 1991}{10} = -1$$

$$\therefore p = -1, h = 10$$

$$y'(1981) = \frac{1}{10}\left[17.4 + \frac{2(-1)+1}{2} * (-1) + \frac{3(-1)^2 + 6(-1) + 2}{6} 2.76 + \frac{2(-1)^3 + 9(-1)^2 + 11(-1) + 3}{12} 11.99\right]$$

$$= \frac{1}{10}[17.4 + 0.5 - 0.46 - 0.992]$$

$$= 1.6441$$

Therefore, the rate of growth of the population in the year is 1981 is 1.6441

Maxima and minima of tabulated function

We know Newton's forward interpolation formula as :

$$\frac{dy}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{(2p-1)\Delta^2 y_0}{2!} + \frac{(3p^2 - 6p + 2)\Delta^3 y_0}{3!} + \frac{(4p^3 - 18p^2 + 22p - 6)\Delta^4 y_0}{4!} \dots\right]$$

We know that maximum and minimum values of a function $y = f(x)$ can be found by equating dy/dx to zero and solution for x

$$\left[\Delta y_0 + \frac{(2p-1)\Delta^2 y_0}{2!} + \frac{(3p^2-6p+2)\Delta^3 y_0}{3!} + \frac{(4p^3-18p^2+22p-6)\Delta^4 y_0}{4!} + \cdots\right]$$

Now for keeping only up to third difference we have

$$\Delta y_0 + \frac{(2p-1)\Delta^2 y_0}{2!} + \frac{(3p^2-6p+2)\Delta^3 y_0}{3!} = 0$$

Solving this for p, by substituting $\Delta y_0, \Delta^2 y_0, \Delta^3 y_0$, we get x as $x_0 + ph$ at which y is a maximum or minimum

Example: Given the following data, find the maximum value of y

x	-1	1	2	3
y	-21	15	12	3

Since the arguments (x -points) aren't equally spaced we use Newton's Divided Difference formula

$$y(x) = a_0 + a_1(x-x_0) + a_2(x-x_0)(x-x_1) + a_3(x-x_0)(x-x_1)(x-x_2) \ldots$$

x	$f(x)$			
-1	-21			
		18^*		
1	15		-7^{**}	
		-3		1
2	12		-3	
		-9		
3	3			

Note :

$$* \; 18 = \frac{15-(-21)}{1-(-1)}$$

$$** -7 = \frac{-3-18}{2-(-1)}$$

From above table,

$a_0 = -21, a_1 = 18, a_2 = -7, a_3 = 1,$

$$f(x) = -21 + 18(x+1) + (x+1)(x-1)(-7) + (x+1)(x-1)(x-2)(1)$$

$$f(x) = x^3 - 9x^2 + 17x + 6$$

For maxima and minima $\frac{dy}{dx} = 0$

$$3x^2 - 18x + 17 = 0$$

On solving, we get,

$$x = 4..8257 \; or \; 1.1743$$

Since x=4.8257 is out of range [-1 to 3] , we take x=1.1743

$$\therefore y_{max} = x^3 - 9x^2 + 17x + 6$$

$$= 1.1743^3 - 9 * 1.1734^2 + 17 * 1.1743 + 6$$

$$= 15.171612$$

Differentiating continuous functions:

If the process of approximating the derivative $f'(x)$ of the function f(x), when the function itself is available

Forward Difference Quotient

consider a small increment $\Delta x = h$ in x, according to Taylor's theorem, we have

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(\theta) \ldots (1) \quad for\; x + \theta \leq x + h$$

by re-arranging the terms, we get

$f'(x) = \frac{f(x+h)-f(x)}{h} - \frac{h^2}{2} f''(\theta) \dots . (2)$

Thus if h is chosen to be sufficiently small , $f'(x)$ can be approximated by

$f'(x) = \frac{f(x+h)-f(x)}{h} \dots .(3)$

With a truncation error of

$$E_t(h) = -\frac{h^2}{2} f''(\theta) \dots . (4)$$

Equation 3 is called first order forward difference quotient. This is also known as two-point formula. The truncation error is in the order of h and can be decreased by decreasing h.

Similarly, we can show that the first order backward difference quotient is

$$f'(x) = \frac{f(x) - f(x-h)}{h} \dots (5)$$

Central Difference Quotient

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

This equation is called second order difference quotient. Note that this is the average of the forward difference quotient and backward difference equation. This is also called as three-point formula.

Example: Estimate approximate derivative of $f(x) = x^2 \; at \; x = 1$, for h=0.2,0.1,0.05 and 0.01, using first order forward difference formula

We know that

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

$$f'(x) = \frac{f(1+h) - f(x)}{h}$$

Derivative approximation is tabulated below as:

h	$f'(1)$
0.2	2.2
0.1	2.1
0.05	2.05
0.01	2.01

Note that the correct answer is 2. The derivative approximation approaches the exact value as h decreases.

Now for central difference quotient

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

$$f'(x) = \frac{f(1+h) - f(1-h)}{2h}$$

h	$f'(1)$
0.2	2
0.1	2
0.05	2

Example Practice:

1. Find the first and second derivates of the function tabulated below at point x=19

x	1.0	1.2	1.4	1.6	1.8	2.0
f(x)	0	0.128	0.544	1.296	2.432	4.00

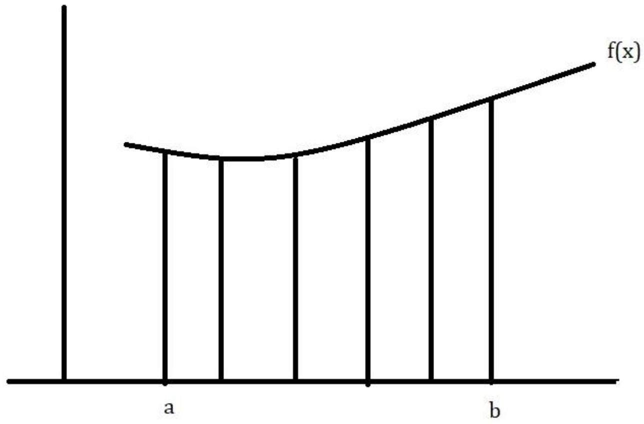
Result :0.63,6.6

2. The following data gives corresponding values of pressure and specific volume of super-heated steam.

v	2	4	6	8	10
P	105	42.07	25.3	16.7	13

a. Find the rate of change of pressure with respect to volume when v=2

b. Find the rate of change of volume with respect to pressure when p=105



Numerical Integration:

The process of computing $\int_a^b y\,dx, where\ y = f(x)$ is given by a set of tabulated values $[x_i, y_i]$, i=0,1,2 ….n ,$a = x_0$, $b = x_n$ is called numerical integration since $y = f(x)$ is a single variable function, the process in general is known as quadrature, like that of numerical differentiation here also we replace f(X) by an interpolation formula and integrate it in between given limits.

Newtons Cotes Formula:

This is the most popular and widely used in numerical integration. Numerical integration method uses an interpolating polynomial $p_n(x)$ in place of f(x)

Thus $I = \int_a^b f(x)dx = \int_a^b p_n(x)dx \dots\dots (1)$

We know, Newton's interpolation formula as:

$$f(x) = f_0 + p\Delta f_0 + \frac{p(p-1)}{2!}\Delta^2 f_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 f_0 + \cdots$$

Integrating term by term, since $x = x_0 + ph$

$$dx = hdp$$

$$I = \int_0^n \left[f_0 + p\Delta f_0 + \frac{p(p-1)}{2!}\Delta^2 f_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 f_0 + \cdots\right] hdp$$

$$I = h\left[nf_0 + \frac{n^2}{2}\Delta f_0 + \frac{1}{2!}\left(\frac{n^3}{3} - \frac{n^2}{2}\right)\Delta^2 f_0 + \frac{1}{3!}\left(\frac{n^4}{4} - n^3 + n^2\right)\Delta^3 f_0 + \cdots\right] \ldots .(1)$$

Above equation is known as **Newton's Cote's quadrature formula**, used for numerical integration.

If the limits of integration a and b are in the set of interpolating points xi=0,1,2,3…..n, then the formula is referred as closed form. If the points a and b lie beyond the set of interpolating points, then the formula is termed as open form. Since the open form formula is not used for definite integration, we consider here only the closed form methods. They include:

1. Trapezoidal rule
2. Simpson's 1/3 rule
3. Simpson's 3/8 rule

Trapezoidal rule (2 Point Formula)

Putting n=1 in equation 1 and neglecting second and higher order differences we get

$$\int_{x_0}^{x_n} f(x)dx = h\left[f_0 + \frac{\Delta f_0}{2}\right]$$

$$I = h\left[f_0 + \frac{1}{2}(f_1 - f_0)\right]$$

$$I = \frac{h}{2}[f_0 + f_1]$$

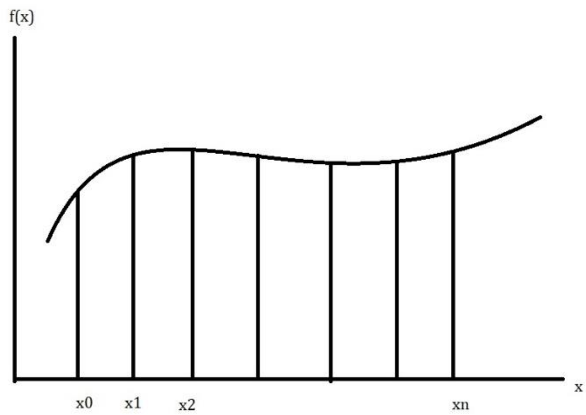
Composite Trapezoidal Rule:

If the range to be integrated is large, the trapezoidal rule can be improved by dividing the interval (a,b) into a number of small intervals. The sum of areas of all the sub-intervals is the integral of the intervals (a,b) or (x_0,x_n). this is known as composite trapezoidal rule.

As seen in the figure, there are n+1 equally spaced sampling point that create n segments of equal width h given by

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

$$x_i = a + ih \qquad i = 0,1,2, \dots n$$



From the equation of trapezoidal rule,

$$I_i = \int_{x_{i-1}}^{x_i} p_1(x)dx$$

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

The total area of all the n segments is

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

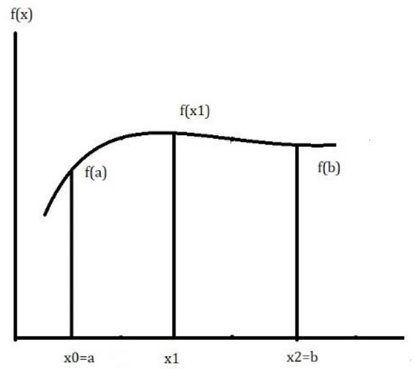
$$I = \frac{h}{2}[f(x_0) + f(x_1)] + \frac{h}{2}[f(x_1) + f(x_2)] + \cdots + \frac{h}{2}[f(x_{n-1}) + f(x_n)]$$

Now let us denote $f_i = f(x_i)$ then

$$I = \frac{h}{2}\left[f_0 + 2\sum_{i=1}^{n-1} f_i + f_n\right]$$

Above equation is known as composite trapezoidal rule

Simpson's $^1/_3$ rule (3 Point Formula)



Another popular method is Simpson's 1/3 rule. Here the function f(x) is approximated by second order polynomial $p_2(x)$ which passes through three sampling points as shown in figure. The three points include the end point a & b and midpoint between $x_1 = (a+b)/2$. The width of the segment h is given by $h = {}^{(b-a)}/_{n}$. Take n=2 and neglecting the third and higher order differences we get (in newton's cote formula)

$$I = h\left[2f_0 + \frac{2^2}{2}\Delta f_0 + \frac{1}{2!}\left(\frac{2^3}{3} - \frac{2^2}{2}\right)\Delta^2 f_0\right]$$

$$\int_a^b f(x)dx = h\left[2f_0 + 2(f_1 - f_0) + \frac{1}{2}(\frac{8}{3} - 2)(f_1 - f_0)^2\right]$$

$$= h\left[2f_0 + 2f_1 - 2f_0 + \frac{1}{3}(\Delta f_2 - \Delta f_1)\right]$$

$$= \frac{h}{3}\left[2f_0 + 2f_1 - 2f_0 + \frac{1}{3}(f_2 - f_1 - (f_1 - f_0))\right]$$

$$= \frac{h}{3}[f_0 + 4f_1 + f_2]$$

Composite Simpson's 1/3 rule:

$$\int_a^b f(x)dx = \frac{h}{3}[(f_0 + f_n) + 4(f_1 + f_3 + f_5 + \cdots) + 2(f_2 + f_4 + f_6 + \cdots)]$$

Simpson's 3/8 rule (4 Point Rule)

We have Newton's cotes formula

$$I = h\left[nf_0 + \frac{n^2}{2}\Delta f_0 + \frac{1}{2!}\left(\frac{n^3}{3} - \frac{n^2}{2}\right)\Delta^2 f_0 + \frac{1}{3!}\left(\frac{n^4}{4} - n^3 + n^2\right)\Delta^3 f_0 + \cdots\right]$$

Putting n=3 and neglecting 4th terms in above formula

$$I = h\left[3f_0 + \frac{3^2}{2}\Delta f_0 + \frac{1}{2}\left(\frac{3^3}{3} - \frac{3^2}{2}\right)\Delta^2 f_0 + \frac{1}{6}\left(\frac{3^4}{4} - 3^3 + 3^2\right)\Delta^3 f_0 + \cdots\right]$$

On solving we get

$$I = \frac{3h}{8}[(f_0 + f_3) + 3f_1 + 3f_2]$$

Adding all these integrals where n is a multiple of 3 we get

$$\int f(x)dx = \frac{3h}{8}[(f_0 + f_n) + 3(f_1 + f_2 + f_4 + f_5 + f_7 + \cdots) + 2(f_3 + f_6 + f_9 + \cdots)]$$

This is composite Simpson's 3/8 rule.

Example:

1. Evaluate $\int_0^{10} \frac{dx}{1+x^2}$ using
   a. Trapezoidal rule
   b. Simpson's 1/3 rule
   c. Simpson's 3/8 rule

Solution:

Taking h=1, divide the whole range of the integration [0,10] into ten equal parts. The value of the integrand for each point of sub division.

$x_i = x$	$x_0 = 0$	1	2	3	4	5	6	7	8	9	10
$f_i = y$	1	0.5	0.2	0.1	0.0588	0.0385	0.0270	0.020	0.0154	0.0122	0.0099

a. By Trapezoidal rule

$$\int_0^{10} \frac{dx}{1+x^2} = \frac{h}{2}[f_0 + f_1]$$

$$= \frac{1}{2}[1 + 0.5]$$

$$= 0.75$$

b. By Simpson's 1/3 rule

$$\int_0^{10} \frac{dx}{1+x^2} = \frac{h}{3}[f_0 + 4f_1 + f_2]$$

$$= \frac{1}{3}[1 + 4 \times 0.5 + 0.2]$$

$$= 1.0667$$

c. By Simpson's 3/8 rule

$$\int_0^{10} \frac{dx}{1+x^2} = \frac{3h}{8}[(f_0 + f_3) + 3f_1 + 3f_2]$$

$$= \frac{3 \times 1}{8}[(1 + 0.1) + 3 \times 0.5 + 3 \times 0.2]$$

$$= 1.2$$

Composite methods:

a. Trapezoidal rule

$$\int_0^{10} \frac{dx}{1+x^2} = \frac{h}{2}\left[f_0 + 2\sum_{i=1}^{n-1} f_i + f_n\right]$$

$$= \frac{h}{2}\left[f_0 + 2\sum_{i=1}^{9} f_i + f_{10}\right]$$

$$= \frac{1}{2}[1 + 2(0.5 + 0.2 + 0.1 + 0.0588 + 0.0385 + 0.0270 + 0.020 + 0.0154 + 0.0122) + 0.0099]$$

$$= 1.4769$$

b. By Simpson's 1/3 rule

$$\int_0^{10} \frac{dx}{1 + x^2} = \frac{h}{3}[(f_0 + f_{10}) + 4(f_1 + f_3 + f_5 + f_7 + f_9) + 2(f_2 + f_4 + f_6 + f_8)]$$

$$= \frac{1}{3}[(1 + 0.0099) + 4(0.5 + 0.1 + 0.0385 + 0.020 + 0.0122) + 2(0.2 + 0.0588 + 0.0270 + 0.0154)]$$

$$= \frac{1}{3}[1.0099 + 2.6828 + 0.6024]$$

$$= 1.4317$$

c. Simpson's 3/8 rule

$$\int_0^{10} \frac{dx}{1 + x^2} = \frac{3h}{8}[(f_0 + f_{10}) + 3(f_1 + f_2 + f_4 + f_5 + f_7 + f_8) + 2(f_3 + f_6 + f_9)]$$

$$= \frac{3}{8}[(1 + 0.0099) + 3(0.5 + 0.2 + 0.0588 + 0.0385 + 0.020 + 0.0154) + 2(0.1 + 0.0270 + 0.0270 + 0.0122)]$$

$$= 1.4199$$

Romberg integration formula/ Richardson's deferred approach to the limit or Romberg method

Take an arbitrary value of h and calculate

$$I_1 = \int_a^b f(x)dx = \frac{h}{2}[(f_0 + f_n) + 2(f_1 + f_2 + f_3 + f_{n-1})]$$

$$I_2 = \int_a^b f(x)dx = \frac{h}{4}[(f_0 + f_n) + 2(f_1 + f_2 + f_3 + f_{n-1})]$$

$$I_3 = \int_a^b f(x)dx = \frac{h}{8}[(f_0 + f_n) + 2(f_1 + f_2 + f_3 + f_{n-1})]$$

Now better estimate of I_1 & I_2 can be found as

$$I_1{}^* = I_2 + \frac{1}{3}(I_2 - I_1)$$

$$I_2{}^* = I_3 + \frac{1}{3}(I_3 - I_2)$$

If $I_1{}^* = I_2{}^*$ then stop else continue as $I_1{}^{**} = I_2{}^* + \frac{1}{3}(I_2{}^* - I_1{}^*)$ and so on

Example: Evaluate $\int_0^1 \frac{dx}{1+x^2}$ using Romberg's method correct up to four decimal places. Hence find approximate value of π.

Solution

By taking n=2, $h = \frac{b-a}{n} = \frac{1-0}{2} = 0.5$

a. When h=0.5

x	0	0.5	1
f_i	1	0.8	0.5

$$I_1 = \frac{h}{2}[(f_0 + f_2) + 2(f_1)] = \frac{0.5}{2}[(1 + 0.5) + 2(0.8)] = 0.7750$$

b. When h=0.5/2=0.25

x	0	0.25	0.5	0.75	1
f_i	1	0.9412	0.8	0.64	0.5

$$I_2 = \frac{h}{2}[(f_0 + f_4) + 2(f_1 + f_2 + f_3)]$$

$$= \frac{0.25}{2}[(1 + 0.5) + 2(0.941 + 0.8 + 0.64)] = 0.7828$$

c. When h=0.25/2=0.125

x	0	0.125	0.25	0.375	0.5	0.625	0.75	0.875	1
f_i	1	0.9846	0.9412	0.8767	0.8	0.7191	0.64	0.5664	0.5

$$I_3 = \frac{h}{2}[(f_0 + f_8) + 2(f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + f_7)]$$

$$= \frac{0.125}{2}[(1 + 0.5) + 2(0.9846 + 0.9412 + 0.8767 + 0.8 + 0.7191 + 0.64 + 0.5664)] = 0.78475$$

$$I_1{}^* = I_2 + \frac{1}{3}(I_2 - I_1) = 0.7828 + \frac{1}{3}(0.7828 - 0.7750) = 0.7854$$

$$I_2{}^* = I_3 + \frac{1}{3}(I_3 - I_2) = 0.7848 + \frac{1}{3}(0.7848 - 0.7828) = 0.7854$$

Since these two are the same value, we conclude that the value of the integral =0.7854

i.e $\int_0^1 \frac{dx}{1+x^2} = 0.7854$

$$\int_0^1 \frac{dx}{1 + x^2} = [\tan^{-1} x]_0^1 = \tan^{-1} 1 - \tan^{-1} 0 = \frac{\pi}{4} = 0.7854$$

$$\therefore \pi \approx 3.1416$$

Gaussian integration:

Gaussian integration is based on the concept that the accuracy of numerical integration can be improved by choosing sampling points wisely rather than on the basis of equal sampling. The problem is to compute the values of x_1& x_2 given the value of a and b and to choose approximate weights w_1 & w_2 . The method of implementing the strategy of finding approximate values of x_i & w_i and obtaining the integral of f(x) is called Gaussian integration or quadrature.

Gaussian integration assumes an approximation of the form

$$I_g = \int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} w_i f(x_i) \ldots.(1)$$

The above equation 1 contains 2n unknowns to be determined. For example for n=2, we need to find the values of w_1,w_2,x_1,x_2. We assume that the integral will be exact up to cubic polynomial. This implies the function $1,x,x^2$&x^3 can be numerically integrated to obtain exact results.

Assume f(x)=1 (assume the integral is exact up to cubic polynomial)

1. f(x)=1

$$w_1 + w_2 = \int_{-1}^{1} dx = 2$$

2. f(x)=x

$$\mathrm{w_1x_1 + w_2x_2} = \int_{-1}^{1} \mathrm{f(x)dx} = 0$$

3. f(x)=x^2

$$\mathrm{w}_1 x_1{}^2 + \mathrm{w}_2 x_2{}^2 = \int_{-1}^{1} \mathrm{f(x)dx} = \int_{-1}^{1} x^2 \mathrm{dx} = \frac{2}{3}$$

4. f(x)=x3

$$\mathrm{w}_1 x_1{}^3 + \mathrm{w}_2 x_2{}^3 = \int_{-1}^{1} \mathrm{f(x)dx} = \int_{-1}^{1} x^3 \mathrm{dx} = 0$$

Solving above equation we get

$$w_1 = 1, w_2 = 1$$

$$x_1 = {}^{-1}/_{\sqrt{3}} = -0.5773502$$
$$x_2 = {}^{1}/_{\sqrt{3}} = 0.5773502$$

Thus, we have the Gaussian Quadrature formula, for n=2

$$\int_{-1}^{1} f(x)dx = f(-{}^{1}/_{\sqrt{3}}) + f({}^{1}/_{\sqrt{3}})$$

This formula will give correct value for the integral of f(x) in the range (-1,1) for any function up to third order. The above equation is also called Gauss Legendre formula.

Example : Compute $\int_{-1}^{1} e^x$ using two point Gaussian integration formula

$$I = \int_{-1}^{1} e^x dx = w_1 f(x_1) + w_2 f(x_2)$$

Where x_1 and x_2 are Gaussian quadrature points and are given by

$$x_1 = {}^{-1}/_{\sqrt{3}} = -0.5773502, w_1 = 1$$
$$x_2 = {}^{1}/_{\sqrt{3}} = 0.5773502, w_2 = 1$$

$$f(x) = e^x$$

we know that,

$$I = w_1 f\left(-{}^{1}/_{\sqrt{3}}\right) + w_2 f\left({}^{1}/_{\sqrt{3}}\right)$$

$$= e^{-1/\sqrt{3}} + e^{1/\sqrt{3}}$$

$$= 0.5614 + 1.7813$$

$$= 2.3427$$

Changing limits of Integration

Note that the Gaussian formula imposed a restriction on the limits of integration to be from -1 to 1. The restriction can be overcome by using the techniques of the “interval transformation” used in calculus, let

$$\int_a^b f(x)dx = c\int_{-1}^{1} g(z)\,dz$$

Assume the following transformation between x and new variable z. by following relation.

i.e x=Az+B

this must satisfy the following conditions at x=a, z=-1 & x=b, z=1

i.e B-A=a, A+B=b

$$A = \frac{b-a}{2}, B = \frac{a+b}{2}$$

$\therefore\ \mathrm{x} = (\frac{b-a}{2})\mathrm{z} + (\frac{a+b}{2})$

$$dx = (\frac{b-a}{2})dz$$

here $C = \frac{b-a}{2}$

∴ the integral becomes

$$\frac{b-a}{2}\int_{-1}^{1} g(z)dz$$

The Gaussian formula for this integration is

$$\frac{b-a}{2}\int_{-1}^{1} g(z)dz = (\frac{b-a}{2})\sum_{i=1}^{n} w_i g(z_i)$$

Where w_i and z_i are the weights and quadrature points for the integration domain (-1,1)

Example: Compute the integral

$I = \int_{-2}^{2} e^{-x/2}$ by using Gaussian two points formula

Here n=2

$I = \frac{b-a}{2}\int_{-1}^{1} g(z)dz = \frac{b-a}{2}\sum_{i=1}^{n} w_i g(z_i) = \left(\frac{b-a}{2}\right)[w_1 g(z_1) + w_2 g(z_2)]$

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

$$= \frac{2-(-2)}{2}z + \frac{2+(-2)}{2}$$

$$= 2z$$

$$\therefore g(z) = e^{-x/2} = e^{-2z/2} = e^{-z}$$

For two point formula :

$$w_1 = w_2 = 1$$

$$z_1 = -1/\sqrt{3}, z_2 = 1/\sqrt{3}$$

$$I = \frac{b-a}{2}[w_1 g(z_1) + w_2 g(z_2)]$$

$$= \frac{2-(-2)}{2}[e^{-(-1/\sqrt{3})} + e^{-(1/\sqrt{3})}]$$

$$= 2(0.5614 + 1.7813)$$

$$= 4.8654$$

Values for gaussian quadrature

Number of terms	Values of x	Weighting factor	Valid to degree
2	-0.5773502	1	3
	0.5773502	1	
3	-0.77459667	0.55555555	
	0	0.88888889	5
	0.77459667	0.55555555	
4	-0.86113631	0.34785485	
	-0.33998104	0.65214515	7
	0.33998104	0.65214515	
	0.86113631	0.34785485	

Example: Use Gaussian integration 3 point formula to evaluate $\int_2^4 (x^4 + 1)dx$

Given n=3, a=2, b=4

$$I = \frac{b-a}{2}\sum_{i=1}^{3} w_i g(z_i)$$

$$I = \frac{b-a}{2}[w_1 g(z_1) + w_2 g(z_2) + w_3 g(z_3)]$$

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

$$= (\frac{4-2}{2})z + (\frac{4+2}{2})$$

$$= z + 3$$

$$\therefore g(z) = (z+3)^4 + 1$$

For n=3

$w_1 = 0.55556$ $z_1 = -0.77460$

$w_2 = 0.88889$ $z_2 = 0$

$w_3 = 0.55556$ $z_3 = 0.77460$

$$I = 0.55556[(-0.77460 + 3)^4 + 1] + 0.88889[(0 + 3)^4 + 1] + 0.55556[(0.77460 + 3)^4 + 1]$$

$$= 14.1814 + 72.8890 + 113.3310$$

$$= 200.4014$$

Chapter 4: solution of Linear Algebraic Equations

Linear equations:

First mathematical models of many of the real world problems are either linear or can be approximated reasonably well using linear relationships. Analysis of linear relationship of variables is generally easier than that of non-linear relationships.

A linear equation involving two variables x and y has the standard form $ax + by = c$, where a, b& c are real numbers and a and b both cannot be equal to zero.

The equation becomes non-linear if any of the variables has the exponent other than one, example

$$4x + 5y = 15 \; linear$$

$$4x - xy + 5y = 15 \;\; non - linear$$

$$x^2 + 5y^2 = 15 \;\; non - linear$$

Linear equation occurs in more than two variables as$a_1x_1 + a_2x_2 + a_3x_3 + \cdots a_nx_n = b$. The set of equations is known as system of simultaneous equations, in matrix form it can be represented as $Ax = B$

$$3x_1 + 2x_2 + 4x_3 = 14$$

$$x_1 - 2x_2 = -7$$

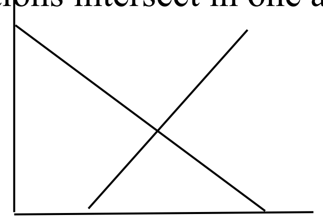
$$-x_1 + 3x_2 + 2x_3 = 2$$

$$\begin{bmatrix} 3 & 2 & 4 \\ 1 & -2 & 0 \\ -1 & 3 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 14 \\ -7 \\ 2 \end{bmatrix}$$

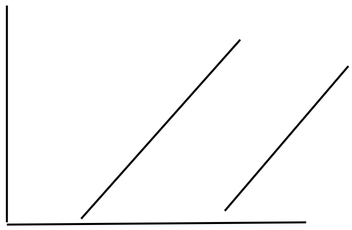
Existence of solution

In solving system of equations, we find values of variables that satisfy all equations in the system simultaneously. There may be 4 possibilities in solving the equations.

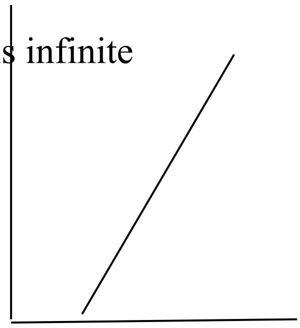
1. System with unique solution
   here the lines or equations intersect in one and only one point.



2. System with no solution
   Here the lines or equation never intersect or parallel lines.



3. System with infinite solution
   Here two equation or lines overlap, so that there is infinite Solutions



4. ILL conditioned system:
   There may be situation where the system has a solution but it is very close to being singular, i.e, any equation have solution but is very difficult to

identify the exact point at which the lines intersect. If there is any slight changes in the value in the equation then we will see huge change in the solution, this type of equation is called ILL condition system, we should be careful in solving these kind of solutions. Example

$$\begin{bmatrix} 1.01 & 0.99 \\ 0.99 & 1.01 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 2.00 \\ 2.00 \end{bmatrix}$$

$$1.01x + 0.99y = 2$$

$$0.99x + 1.01y = 2$$

On solving these equations, we get the solution at x=1 & y=1, however if we make small changes in b i.e.

$$\begin{bmatrix} 1.01 & 0.99 \\ 0.99 & 1.01 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 2.02 \\ 1.98 \end{bmatrix}$$

$$1.01x + 0.99y = 2.02$$

$$0.99x + 1.01y = 1.98$$

On solving these equations, we get x=2 & y=0

So slight changes results in huge change in solution.

Methods of solutions (Direct Methods)

Elimination method

Elimination method is a method of solving simultaneous linear. This method involves elimination of a term containing one of the unknowns in all but one equation, one such step reduces the order of equations by one, repeated elimination leads finally to one equation with one unknown.

Example: solve the following equation using elimination method

$$4x_1 - 2x_2 + x_3 = 15 \dots \dots (1)$$

$$-3x_1 - x_2 + 4x_3 = 8 \dots \dots (2)$$

$$x_1 - x_2 + 3x_3 = 13 \dots \dots (3)$$

Here multiply $R_1\ by\ 3\ \&R_2\ by\ 4$ and add to eliminate $x_1$from 2. Multiply $R_1\ by - 1\&R_3\ by\ 4$ and add to eliminate $x_1$from 3

$$4x_1 - 2x_2 + x_3 = 15$$

$$-10x_2 + 19x_3 = 77$$

$$-2x_2 + 11x_3 = 37$$

Now to eliminate x_2 from third equation multiply second row by 2 and third row by -10 and adding

$$4x_1 - 2x_2 + x_3 = 15$$

$$-10x_2 + 19x_3 = 77$$

$$-72x_3 = -216$$

Now we have a triangular system and solution is readily obtained from back-substitution

$$x_3 = 3$$

$$x_2 = \frac{77 - 19 * 3}{-10} = -2$$

$$x_1 = \frac{15 + 2 * (-2) - 3}{4} = 2$$

Gauss Elimination Method

The procedure in above example may not be satisfactory for large systems because the transformed coefficients can become very large as we convert to a triangular system. So, we use another method called Gaussian Elimination method that avoid this by subtracting $^{a_{i1}}/_{a_{11}}$ times the first equation from i^{th} equation to make the transformed numbers in the first column equal to zero and proceed on.

However, we must always be cautious against divide by zero, a useful strategy to avoid divide by zero is to re-arrange the equations so as to put the coefficient of large magnitude on the diagonal at each step, this is called pivoting. Complete pivoting method require both row and column interchange but this is much difficult and not frequently done. Changing only row called partial pivoting which places a coefficient of larger magnitude on the diagonal by row interchange only. This will be guaranteeing a non-zero divisors if there is a solution to set of equations and will have the added advantage of giving improved arithmetic precision. The diagonal elements that result are called pivot elements.

Example (without pivoting element)

$$0.143x_1 + 0.357x_2 + 2.01x_3 = -5.173$$

$$-1.31x_1 + 0.911x_2 + 1.99x_3 = -5.458$$

$$11.2x_1 - 4.30x_2 - 0.605x_3 = 4.415$$

Augmented matrix is

$$\begin{bmatrix} 0.143 & 0.357 & 2.01 & -5.173 \\ -1.31 & 0.911 & 1.99 & -5.458 \\ 11.2 & -4.30 & -0.605 & 4.415 \end{bmatrix}$$

$$R_2 \to \left({R_1}/{0.143}\right) 1.31 + R_2\,, R_3 \to \left({R_1}/{0.143}\right) * (-11.2) + R_3$$

$$\begin{bmatrix} 0.143 & 0.357 & 2.01 & -5.173 \\ 0 & 4.181 & 20.403 & -52.847 \\ 0 & -32.261 & -158.032 & 409.573 \end{bmatrix}$$

$$R_3 \to \left({R_2}/{4.181}\right) 32.261 + R_2$$

$$\begin{bmatrix} 0.143 & 0.357 & 2.01 & -5.173 \\ 0 & 4.181 & 20.403 & -52.847 \\ 0 & 0 & -0.6 & 1.8 \end{bmatrix}$$

$$x_3 = {1.8}/{-0.6} = -3.001$$

$$4.181x_2 + 20.403x_3 = -52.847$$

$$x_2 = \frac{-52.847 - 20.403 * -3.001}{4.181} = 2.005$$

$$0.143x_1 + 0.357x_2 + 2.01x_3 = -5.173$$

$$x_1 = \frac{-5.173 - 0.357x_2 - 2.01x_3}{0.143}$$

$$x_1 = \frac{-5.173 - 0.35 * 2.005 - 2.01 - 3.001}{0.143}$$

$$x_1 = 0.749$$

Example (with pivoting element)

$$0.143x_1 + 0.357x_2 + 2.01x_3 = -5.173$$

$$-1.31x_1 + 0.911x_2 + 1.99x_3 = -5.458$$

$$11.2x_1 - 4.30x_2 - 0.605x_3 = 4.415$$

Augmented matrix is

$$\begin{bmatrix} 0.143 & 0.357 & 2.01 & -5.173 \\ -1.31 & 0.911 & 1.99 & -5.458 \\ 11.2 & -4.30 & -0.605 & 4.415 \end{bmatrix}$$

$$R_1 \leftrightarrow R_3 (Pivoting)$$

$$\begin{bmatrix} 11.2 & -4.30 & -0.605 & 4.415 \\ -1.31 & 0.911 & 1.99 & -5.458 \\ 0.143 & 0.357 & 2.01 & -5.173 \end{bmatrix}$$

$$R_2 \to \left({R_1}/{11.2}\right) 1.31 + R_2 \, , R_3 \to \left({R_1}/{11.2}\right) * (-0.143) + R_3$$

$$\begin{bmatrix} 11.2 & -4.30 & -0.605 & 4.415 \\ 0 & 0.408 & 1.919 & -4.942 \\ 0 & 0.412 & 2.018 & -5.229 \end{bmatrix}$$

$$R_2 \leftrightarrow R_3$$

$$\begin{bmatrix} 11.2 & -4.30 & -0.605 & 4.415 \\ 0 & 0.412 & 2.018 & -5.229 \\ 0 & 0.408 & 1.919 & -4.942 \end{bmatrix}$$

$$R_3 \to \left({R_2}/{0.412}\right) * (-0.408) + R_3$$

$$\begin{matrix} 11.2 & -4.30 & -0.605 & 4.415 \\ 0 & 0.412 & 2.018 & -5.229 \\ 0 & 0 & -0.079 & 0.236 \end{matrix}$$

$$x_3 = {0.236}/{-0.079} = -2.990$$

$$0.412x_2 + 2.018x_3 = -5.229$$

$$x_2 = \frac{-5.229 - 2.018 * -2.990}{0.412} = 1.953$$

$$11.2x_1 - 4.30x_2 - 0.605x_3 = 4.415$$

$$x_1 = \frac{4.415 + 4.30 * 1.953 + 0.605 * -2.990}{11.2}$$

$$x_1 = 0.982$$

Hence $x_1 = 2, x_2 = 1.953, x_3 = -2.990$

Practice: Solve the following system of equations(without pivoting)

1. $3x_1 + 6x_2 + x_3 = 16,\quad 2x_1 + 4x_2 + 3x_3 = 13,\quad x_1 + 3x_2 + 2x_3 = 9$
2. $2x_1 + 3x_2 + 4x_3 = 5,\quad 3x_1 + 4x_2 + 5x_3 = 6,\quad 4\,x_1 + 5x_2 + 6x_3 = 7$
3. **Solve above equations again using pivoting techniques.**

Gauss Jordan Method

Gauss Jordan method is another popular method used for solving a system of linear equations. In this method the elements above the diagonal are made zero at the same time that zero are created below the diagonal, usually the diagonal elements are made ones at the same time the reduction is performed, this transforms the coefficient matrix into identity matrix. When this has been accomplished the column of right-hand side has been transformed into the solution vector. Pivoting is normally employed to preserve arithmetic accuracy.

Example solution using Gauss-Jordan method

$$2x_1 + 4x_2 - 6x_3 = -8$$

$$x_1 + 3x_2 + x_3 = 10$$

$$2x_1 - 4x_2 - 2x_3 = -12$$

Augmented matrix is

$$\begin{bmatrix} 2 & 4 & -6 & -8 \\ 1 & 3 & 1 & 10 \\ 2 & -4 & -2 & -12 \end{bmatrix}$$

$$R_1 \to \left({}^{R_1}/_{2}\right)$$

$$\begin{bmatrix} 1 & 2 & -3 & -4 \\ 1 & 3 & 1 & 10 \\ 2 & -4 & -2 & -12 \end{bmatrix}$$

$$R_2 \to R_1 - R_2\,, R_3 \to -2R_1 + R_3$$

$$\begin{bmatrix} 1 & 2 & -3 & -4 \\ 0 & -1 & -4 & -14 \\ 0 & -8 & 4 & -4 \end{bmatrix}$$

$$R_2 \to \left({R_2}/{-1}\right)$$

$$\begin{matrix} 1 & 2 & -3 & -4 \\ 0 & 1 & 4 & 14 \\ 0 & -8 & 4 & -4 \end{matrix}$$

$$R_1 \to -2R_2 + R_1\,, R_3 \to 8R_2 + R_3$$

$$\begin{matrix} 1 & 0 & -11 & -32 \\ 0 & 1 & 4 & 14 \\ 0 & 0 & 36 & 108 \end{matrix}$$

$$R_3 \to \left({R_3}/{36}\right)$$

$$\begin{matrix} 1 & 0 & -11 & -32 \\ 0 & 1 & 4 & 14 \\ 0 & 0 & 1 & 3 \end{matrix}$$

$$R_1 \to 11R_3 + R_1\,, R_2 \to -4R_3 + R_2$$

$$\begin{matrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 2 \\ 0 & 0 & 1 & 3 \end{matrix}$$

Hence $x_1 = 1, x_2 = 2, x_3 = 3$

Example Solution using Gauss-Jordan method (with pivoting)

$$2x_1 + 4x_2 - 6x_3 = -8$$

$$x_1 + 3x_2 + x_3 = 10$$

$$2x_1 - 4x_2 - 2x_3 = -12$$

Augmented matrix is:

$$\begin{bmatrix} 2 & 4 & -6 & -8 \\ 1 & 3 & 1 & 10 \\ 2 & -4 & -2 & -12 \end{bmatrix}$$

$$R_1 \to \left({R_1}/{2}\right)$$

$$\begin{bmatrix} 1 & 2 & -3 & -4 \\ 1 & 3 & 1 & 10 \\ 2 & -4 & -2 & -12 \end{bmatrix}$$

$$R_2 \to R_1 - R_2 \,, R_3 \to -2R_1 + R_3$$

$$\begin{bmatrix} 1 & 2 & -3 & -4 \\ 0 & -1 & -4 & -14 \\ 0 & -8 & 4 & -4 \end{bmatrix}$$

$$R_2 \leftrightarrow R_3$$

$$\begin{matrix} 1 & 2 & -3 & -4 \\ 0 & -8 & 4 & -4 \\ 0 & 1 & 4 & -14 \end{matrix}$$

$$R_2 \to \left({R_2}/{-8}\right)$$

$$\begin{matrix} 1 & 2 & -3 & -4 \\ 0 & 1 & -0.5 & 0.5 \\ 0 & 1 & 4 & 14 \end{matrix}$$

$$R_1 \to -2R_2 + R_1 \,, R_3 \to -R_2 + R_3$$

$$\begin{matrix} 1 & 0 & -2 & -5 \\ 0 & 1 & -0.5 & 0.5 \\ 0 & 0 & 4.5 & 13.5 \end{matrix}$$

$$R_3 \to \left({R_3}/{4.5}\right)$$

$$\begin{matrix} 1 & 0 & -2 & -5 \\ 0 & 1 & -0.5 & 0.5 \\ 0 & 0 & 1 & 3 \end{matrix}$$

$$R_1 \to 2R_3 + R_1\ , R_2 \to 0.5R_3 + R_2$$

$$\begin{matrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 2 \\ 0 & 0 & 1 & 3 \end{matrix}$$

Hence $x_1 = 1, x_2 = 2, x_3 = 3$

Practice: Solve the following system of equations using GJ elimination method.

1. $x_1 + 2x_2 - 3x_3 = 4, \quad 2x_1 + 4x_2 - 6x_3 = 8, \quad x_1 - 2x_2 + 5x_3 = 4$
2. $2x_1 + x_2 + x_3 = 7, \quad 4x_1 + 2x_2 + 3x_3 = 4, \quad x_1 - x_2 + x_3 = 0$

The inverse of a matrix

The division a matrix is not defined but the equivalent is obtained from the inverse of the matrix. If the product of two square matrices A*B equals identity matrix I, B is said to be inverse of A (also A is inverse of B). the usual notation of the matrix is A^{-1} . we can say as $AB = I, A = B^{-1}, B = A^{-1}$.

Example: Given matrix A, find the inverse of A using Gauss Jordan method.

$$A = \begin{bmatrix} 1 & -1 & 2 \\ 3 & 0 & 1 \\ 1 & 0 & 2 \end{bmatrix}$$

The augmented matrix with identity matrix is $\begin{bmatrix} 1 & -1 & 2 & 1 & 0 & 0 \\ 3 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 2 & 0 & 0 & 1 \end{bmatrix}$

$$R_2 \to -3R_1 + R_2\ , R_3 \to -R_1 + R_3$$

$$\begin{bmatrix} 1 & -1 & 2 & 1 & 0 & 0 \\ 0 & 3 & -5 & -3 & 1 & 0 \\ 0 & 1 & 0 & -1 & 0 & 1 \end{bmatrix}$$

$$R_2 \to \left({}^{R_2}/_3\right)$$

$$\begin{bmatrix} 1 & -1 & 2 & 1 & 0 & 0 \\ 0 & 1 & -1.6667 & -1 & 0.333 & 0 \\ 0 & 1 & 0 & -1 & 0 & 1 \end{bmatrix}$$

$$R_1 \to R_1 + R_2\ , R_3 \to R_2 - R_3$$

$$\begin{bmatrix} 1 & 0 & 0.3333 & 0 & 0.3333 & 0 \\ 0 & 1 & -1.6667 & -1 & 0.3333 & 0 \\ 0 & 0 & -1.6667 & 0 & 0.3333 & -1 \end{bmatrix}$$

$$R_3 \rightarrow \left({}^{R_3}/_{-1.6667} \right)$$

$$\begin{bmatrix} 1 & 0 & 0.3333 & 0 & 0.3333 & 0 \\ 0 & 1 & -1.6667 & -1 & 0.333 & 0 \\ 0 & 0 & 1 & 0 & -0.2 & 0.6 \end{bmatrix}$$

$$R_1 \rightarrow -0.3333R_3 + R_1 \, , R_2 \rightarrow 1.6667R_3 + R_2$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0.4 & -0.2 \\ 0 & 1 & 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & 0 & -0.2 & 0.6 \end{bmatrix}$$

$$A^{-1} = \begin{bmatrix} 0 & 0.4 & -0.2 \\ -1 & 0 & 1 \\ 0 & -0.2 & 0.6 \end{bmatrix}$$

Practice: Find the inverse of the following matrix using Gauss Jordan elimination method.

$$A = \begin{bmatrix} 2 & 3 & 4 \\ 4 & 2 & 3 \\ 3 & 4 & 2 \end{bmatrix}$$

Method of factorization

Consider the following system of equations

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$

$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

These equations can be written in matrix form as:

$$AX = B$$

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} B = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

In this method, we use the fact that the square matrix A can be factorized into the form LU, where L is lower triangular matrix and U can be upper triangular matrix such that $A = LU$

$$L = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \quad U = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

$$LUX = B$$

Let us assume $UX = Z$, then $LZ = B$

Now we can solve the system A$X = B$ in two stages

1. Solve the equation, $LZ = B$ for Z by forward substitution
2. Solve the equation, $UX = Z$ for X using Z by backward substitution.

The elements of L and U can be determined by comparing the elements of the product of L and U with those of A. The decomposition with L having unit diagonal values is called the ***Dolittle LU*** decomposition while the other one with U having unit diagonal elements is called ***Crout's LU*** decomposition.

Dolittle LU decomposition:

$$\begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} \\ l_{21}u_{11} & l_{21}u_{12} + u_{22} & l_{21}u_{13} + u_{23} \\ l_{31}u_{11} & l_{31}u_{12} + l_{32}u_{22} & l_{31}u_{13} + l_{32}u_{23} + u_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

Equating the corresponding coefficients, we get the values of L and U

Example: Find L & U by using Doolittle algorithm.

$$2x - 3y + 10z = 3$$

$$-x + 4y + 2z = 20$$

$$5x + 2y + z = -12$$

The given system is $Ax = B$,

Where,

$$A = \begin{bmatrix} 2 & -3 & 10 \\ -1 & 4 & 2 \\ 5 & 2 & 1 \end{bmatrix} X = \begin{bmatrix} x \\ y \\ z \end{bmatrix} B = \begin{bmatrix} 3 \\ 20 \\ -12 \end{bmatrix}$$ here, A=LU

$$\begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix} = \begin{bmatrix} 2 & -3 & 10 \\ -1 & 4 & 2 \\ 5 & 2 & 1 \end{bmatrix}$$

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} \\ l_{21}u_{11} & l_{21}u_{12} + u_{22} & l_{21}u_{13} + u_{23} \\ l_{31}u_{11} & l_{31}u_{12} + l_{32}u_{22} & l_{31}u_{13} + l_{32}u_{23} + u_{33} \end{bmatrix} = \begin{bmatrix} 2 & -3 & 10 \\ -1 & 4 & 2 \\ 5 & 2 & 1 \end{bmatrix}$$

Now comparing both sides we get,

$$u_{11} = 2\,, u_{12} = -3, u_{13} = 10$$

$$l_{21}u_{11} = -1$$

$$l_{21} = -{}^{1}\!/_{2}$$

$$l_{21}u_{12} + u_{22} = 4$$

$$u_{22} = {}^{5}\!/_{2}$$

$$l_{21}u_{13} + u_{23} = 2$$

$$u_{23} = 7$$

$$l_{31}u_{11} = 5$$

$$l_{31} = {}^{5}\!/_{2}$$

$$l_{31}u_{12} + l_{32}u_{22} = 2$$

$$l_{32} = {}^{19}\!/_{5}$$

$$l_{31}u_{13} + l_{32}u_{23} + u_{33} = 1$$

$$u_{33} = -{}^{253}\!/_{5}$$

So, we have,

$$L = \begin{bmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 \\ \frac{5}{2} & \frac{19}{5} & 1 \end{bmatrix} \quad U = \begin{bmatrix} 2 & -3 & 10 \\ 0 & \frac{5}{2} & 7 \\ 0 & 0 & -\frac{253}{5} \end{bmatrix}$$

Now $LZ = B$ where Z is the matrix of order 3×3.

$$\begin{bmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 \\ \frac{5}{2} & \frac{19}{5} & 1 \end{bmatrix} \begin{bmatrix} Z_1 \\ Z2 \\ Z_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 20 \\ -12 \end{bmatrix}$$

$$Z_1 = 3$$

$$-\frac{1}{2} Z_1 + Z_2 = 20$$

$$Z_2 = \frac{43}{2}$$

$$\frac{5}{2} Z_1 + \frac{19}{5} Z_2 + Z_3 = -12$$

$$Z_3 = -\frac{506}{5}$$

Now UX= Z

$$\begin{bmatrix} 2 & -3 & 10 \\ 0 & \frac{5}{2} & 7 \\ 0 & 0 & -\frac{254}{5} \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 3 \\ \frac{43}{2} \\ -\frac{506}{5} \end{bmatrix}$$

$$z = 2$$

$$\frac{5}{2} y + 7z = \frac{43}{2}$$

$$y = 3$$

$$2x - 3y + 10z = 3$$

$$x = -4$$

Practice: Solve the following system of equations by factorization using Doolittle method.

$$x + 3y + 8z = 4$$

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

$$x + 3y + 4z = 1$$

Note: the process of solution by using method of factorization can be repeatedly applied to solve the equation multiple times for different B. in this case it is faster to do an LU decomposition of the matrix A once and then solve the triangular matrices for different B, rather than using Gaussian elimination each time.

Crout's method

$$\begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\begin{bmatrix} l_{11} & l_{11}u_{12} & l_{11}u_{13} \\ l_{21} & l_{21}u_{12} + l_{22} & l_{21}u_{13} + l_{22}u_{23} \\ l_{31} & l_{31}u_{12} + l_{32} & l_{31}u_{13} + l_{32}u_{23} + l_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

Equating the corresponding coefficients, we get the values of l and u

Example Solve the following system by the method of Crout's factorization method.

$$2x - 3y + 10z = 3$$

$$-x + 4y + 2z = 20$$

$$5x + 2y + z = -12$$

The given system is $Ax = B$, where

$$A = \begin{bmatrix} 2 & -3 & 10 \\ -1 & 4 & 2 \\ 5 & 2 & 1 \end{bmatrix} X = \begin{bmatrix} x \\ y \\ z \end{bmatrix} B = \begin{bmatrix} 3 \\ 20 \\ -12 \end{bmatrix} \text{ here A=LU}$$

$$\begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 2 & -3 & 10 \\ -1 & 4 & 2 \\ 5 & 2 & 1 \end{bmatrix}$$

Now comparing, we get,

$$l_{11} = 2\,, l_{21} = -1, l_{13} = 5$$

$$l_{11}u_{12} = -3$$

$$u_{12} = -{}^{3}/_{2}$$

$$l_{11}u_{13} = 10$$

$$u_{13} = {}^{10}/_{2} = 5$$

$$l_{21}u_{12} + l_{22} = 4$$

$$l_{22} = {}^{5}/_{2}$$

$$l_{21}u_{13} + l_{22}u_{23} = 2$$

$$u_{23} = {}^{14}/_{5}$$

$$l_{31}u_{12} + l_{32} = 2$$

$$l_{32} = {}^{19}/_{2}$$

$$l_{31}u_{13} + l_{32}u_{23} + l_{33} = 1$$

$$l_{33} = -{}^{253}/_{5}$$

So, we have,

$$L = \begin{bmatrix} 2 & 0 & 0 \\ -1 & {}^{5}/_{2} & 0 \\ 5 & {}^{19}/_{5} & -{}^{253}/_{5} \end{bmatrix} \quad U = \begin{bmatrix} 1 & -{}^{3}/_{2} & 5 \\ 0 & 1 & {}^{14}/_{5} \\ 0 & 0 & 1 \end{bmatrix}$$

Now $Lz = B$

$$\begin{bmatrix} 2 & 0 & 0 \\ -1 & {}^{5}/_{2} & 0 \\ 5 & {}^{19}/_{5} & -{}^{253}/_{5} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 20 \\ -12 \end{bmatrix}$$

$$Z_1 = {}^{3}/_{2}$$

$$-Z_1 + \frac{5}{2}Z_2 = 20$$

$$Z_2 = {}^{43}/_{2}$$

$$5Z_1 + {}^{19}/_{2}\,Z_2 - \frac{253}{5}Z_3 = -12$$

$$Z_3 = 2$$

Now UX= Z

$$\begin{bmatrix} 1 & -{}^{3}/_{2} & 5 \\ 0 & 1 & {}^{14}/_{5} \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} {}^{3}/_{2} \\ {}^{43}/_{5} \\ 2 \end{bmatrix}$$

$$z = 2$$

$$y + \frac{14}{5}z = {}^{43}/_{5}$$

$$y = 3$$

$$x - \frac{3}{2}y + 5z = \frac{3}{2}$$

$$x = -4$$

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

Practice: Solve the following system using Doolittle and Crout's decomposition methods.

1. $x_1 + 2x_2 - 3x_3 = 4, \quad 2x_1 + 4x_2 - 6x_3 = 8, \quad x_1 - 2x_2 + 5x_3 = 4$
2. $2x_1 + x_2 + x_3 = 7, \quad 4x_1 + 2x_2 + 3x_3 = 4, \quad x_1 - x_2 + x_3 = 0$

Choleskys method:

In case of A is symmetric, the LU decomposition can be modified so that upper factor in matrix is the transpose of the lower one (vice versa)

i.e.

$$A = LL^T = U^T U$$

$$\begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

Just as other method, perform as before.

Symmetric matrix

A square matrix A = $[\boldsymbol{a_{ij}}]$ is called symmetric if $\boldsymbol{a_{ij} = a_{ji}}$ for all i and j

Example: Factorize the matrix, using Cholesky algorithm

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 8 & 22 \\ 3 & 22 & 82 \end{bmatrix}$$

Now decomposition becomes,

$$\begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 8 & 22 \\ 3 & 22 & 82 \end{bmatrix}$$

Equating, we get:

$$l_{11}{}^2 = 1, l_{11} = 1$$

$$l_{11} l_{21} = 2, l_{21} = 2$$

$$l_{11} l_{31} = 3, l_{31} = 3$$

$l_{21} l_{21} + l_{22} l_{22} = 8 , l_{22} = 2$

$l_{31}{}^2 + l_{32}{}^2 + l_{33}{}^2 = 82 , l_{33} = 3$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 2 & 0 \\ 3 & 8 & 3 \end{bmatrix}$$

Practice: Find the Cholesky decomposition of the matrix

$$A = \begin{bmatrix} 4 & 1 & 1 \\ 1 & 5 & 2 \\ 1 & 2 & 3 \end{bmatrix}$$

Iterative methods (Indirect Methods)

Gauss elimination and its derivatives are called direct method, an entirely different way to solve many systems is through iteration. In this we start with an initial estimate of the solution vector and proceed to refine this estimate.

When the system of equation can be ordered so that each diagonal entry of the coefficient matrix is larger in magnitude that the sum of the magnitude of the other coefficients in that row, then such system is called diagonally dominant and the iteration will converge for any stating values. Formally we say that an nxn matrix A is diagonally dominant if and only if for each i=1, 2, 3….n

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}| \; for\ all\ i$$

The iterative method depends on the arrangement of the equations in this manner

Let us consider a system of n equations in n unknowns

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2$$

$$a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n$$

We write the original system as

$$x_1 = \frac{b_1 - (a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n)}{a_{11}}$$

$$x_2 = \frac{b_2 - (a_{21}x_1 + a_{23}x_3 + \cdots + a_{2n}x_n)}{a_{22}}$$

$$x_n = \frac{b_n - (a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn-1}x_n)}{a_{nn}}$$

Now we can computer $x_1, x_2 \dots x_n$ by using initial guess for these values. The new values area gain used to compute the next set of x values. The process can continue till we obtain a desired level of accuracy in x values.

1.Gauss Jacobi Iteration method:

Example:

Solve the equation using Gauss Jacobi iteration method

$$6x_1 - 2x_2 + x_3 = 11$$

$$x_1 + 2x_2 - 5x_3 = -1$$

$$-2x_1 + 7x_2 + 2x_3 = 5$$

Now, first we recorder the equation so that coefficient matrix is diagonally dominant

$$6x_1 - 2x_2 + x_3 = 11$$

$$-2x_1 + 7x_2 + 2x_3 = 5$$

$$x_1 + 2x_2 - 5x_3 = -1$$

Now,

$$x_1 = \frac{11 - (-2x_2 + x_3)}{6}$$

$$x_2 = \frac{5 - (-2x_1 + 2x_3)}{7}$$

$$x_3 = -(\frac{-1 - (x_1 + 2x_2)}{5})$$

We can simplify as:

$$x_1 = \frac{11}{6} + \frac{2}{6}x_2 - \frac{1}{6}x_3$$

$$x_2 = \frac{5}{7} + \frac{2}{7}x_1 - \frac{2}{7}x_3$$

$$x_3 = \frac{1}{5} + \frac{1}{5}x_2 + \frac{2}{5}x_3$$

We begin with some initial approximation to the value of the variables, let's take as:

$$x_1 = 0, x_2 = 0, x_3 = 0,$$

Then new approximation using above formula will be as follows

x_1=1.833333
x_2=0.714286
x_3=0.200000
2 Iteration
x_1=2.038095
x_2 =1.180952
x_3=0.852381
3 Iteration
x_1=2.084921
x_2=1.053061
x_3=1.080000
4 Iteration
x_1=2.004354
x_2=1.001406
x_3=1.038209
5 Iteration
x_1=1.994100
x_2=0.990327
x_3=1.001433
6 Iteration
x_1=1.996537
x_2=0.997905
x_3=0.994951
7 Iteration
x_1=2.000143
x_2=1.000453

x_3=0.998469
8Iteration
x_1=2.000406
x_2=1.000478
x_3=1.000210
9 Iteration
x_1=2.000124
x_2=1.000056
x_3=1.000273
10 Iteration
x_1=1.999973
x_2=0.999958
x_3=1.000047
11 Iteration
x_1=1.999978
x_2=0.999979
x_3=0.999978
12 Iteration
x_1=1.999997
x_2=1.000000
x_3=0.999987
12 Iteration
the final result is :
x_1=1.999997
x_2=1.000000
x_3=0.999987

Practice: Solve the equation using Gauss Jacobi Iteration method.

$$10x_1 - 2x_2 - x_3 - x_4 = 11$$

$$-2x_1 + 10x_2 - x_3 - x_4 = 15$$

$$-x_1 - x_2 + 10x_3 - 2x_4 = 27$$

$$-x_1 - x_2 - 2x_3 + 10x_4 = -9$$

result

$$x_1 = 1, x_2 = 2, x_3 = 3, x_4 = 0,$$

2.Gauss Seidel Iteration method

This is simple modification of Gauss Jacobi method, as before

Let us consider a system of n equations in n unknowns

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2$$

$$a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n$$

We write the original system as:

$$x_1 = \frac{b_1 - (a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n)}{a_{11}}$$

$$x_2 = \frac{b_2 - (a_{21}x_1 + a_{23}x_3 + \cdots + a_{2n}x_n)}{a_{22}}$$

$$x_n = \frac{b_n - (a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn-1}x_n)}{a_{nn}}$$

Now, we can compute: $x_1, x_2 \dots x_n$ by using initial guess for these values. Here we use the updated values of $x_1, x_2 \dots x_n$ in calculating new values of x in each iteration till we obtain a desired level of accuracy in x values. This method is more rapid in convergence than gauss Jacobi method. The rate of convergence of gauss seidel method is roughly twice that of gauss Jacobi.

Example

Solve the equation using Gauss Seidel iteration method .

$$8x_1 - 3x_2 + 2x_3 = 20$$

$$6x_1 + 3x_2 + 12x_3 = 35$$

$$4x_1 + 11x_2 - x_3 = 33$$

Now, first we know the equation so that coefficient matrix is diagonally dominant

$$8x_1 - 3x_2 + 2x_3 = 20$$

$$4x_1 + 11x_2 - x_3 = 33$$

$$6x_1 + 3x_2 + 12x_3 = 35$$

Now

$$x_1 = \frac{20 + 3x_2 - 2x_3}{8}$$

$$x_2 = \frac{33 - 4x_1 + x_3}{11}$$

$$x_3 = \frac{35 - 6x_1 - 3x_2}{12}$$

We begin with some initial approximation to the value of the variables, let's take as:

$$x_2 = 0, x_3 = 0,$$

Then new approximation using above formula will be as follows

$$x_1 = \frac{20 + 3 * 0 - 2 * 0}{8} = 2.5$$

$$x_2 = \frac{33 - 4 * 2.5 + 0}{11} = 2.0909$$

$$x_3 = \frac{35 - 6 * 2.5 - 3 * 2.0909}{12} = 1.1439$$

2 iteration

$$x_1 = \frac{20 + 3 * 2.0909 - 2 * 1.1439}{8} = 2.9981$$

$$x_2 = \frac{33 - 4 * 2.9981 + 1.1439}{11} = 2.0138$$

$$x_3 = \frac{35 - 6 * 2.9981 - 3 * 1.7018}{12} = 0.9142$$

3 iteration

$$x_1 = \frac{20 + 3 * 2.0138 - 2 * 0.9142}{8} = 3.0266$$

$$x_2 = \frac{33 - 4 * 3.0266 + 0.9142}{11} = 1.9825$$

$$x_3 = \frac{35 - 6 * 3.0266 - 3 * 1.9825}{12} = 0.9077$$

4 iteration

$$x_1 = \frac{20 + 3 * 1.9825 - 2 * 0.9077}{8} = 3.0165$$

$$x_2 = \frac{33 - 4 * 3.0165 + 0.9077}{11} = 1.9856$$

$$x_3 = \frac{35 - 6 * 3.0165 - 3 * 1.9856}{12} = 0.9120$$

5 iteration

$$x_1 = \frac{20 + 3 * 1.9856 - 2 * 0.9120}{8} = 3.0166$$

$$x_2 = \frac{33 - 4 * 3.0166 + 0.9120}{11} = 1.9860$$

$$x_3 = \frac{35 - 6 * 3.0166 - 3 * 1.9860}{12} = 0.9119$$

6 iteration

$$x_1 = \frac{20 + 3 * 1.9860 - 2 * 0.9119}{8} = 3.0168$$

$$x_2 = \frac{33 - 4 * 3.0168 + 0.9119}{11} = 1.9859$$

$$x_3 = \frac{35 - 6 * 3.0168 - 3 * 1.9859}{12} = 0.9118$$

7 iteration

$$x_1 = \frac{20 + 3 * 1.9859 - 2 * 0.9118}{8} = 3.0168$$

$$x_2 = \frac{33 - 4 * 3.0168 + 0.9118}{11} = 1.9859$$

$$x_3 = \frac{35 - 6 * 3.0168 - 3 * 1.9859}{12} = 0.9118$$

Since the 6^{th} and 7^{th} approximate are almost same up to 4 decimal places, we can say the solution vector is :

$$x_1 = 3.0168, x_2 = 1.9859, x_3 = 0.9118$$

Practice:

Solve the equation using Gauss Seidel iteration method

$$2x_1 + x_2 + x_3 = 5$$

$$3x_1 + 5x_2 + 2x_3 = 15$$

$$2x_1 + x_2 + 4x_3 = 8$$

Practice: Solve the following systems using Jacobi and Gauss Seidel method

1. $3x_1 - 2x_2 = 5, \quad -x_1 + 2x_2 - x_3 = 0, -2x_2 + x_3 = -1$
2. $2x_1 - 7x_2 - 10x_3 = -17, \quad 5x_1 + x_2 + 3x_3 = 14, \quad x_1 + 10x_2 + 9x_3 = 7$

3.Relaxation Iterative method:

Solve the following system of equations by relaxation method:

$$10x - 2y + z = 12$$

$$x + 9y - z = 10$$

$$2x - y + 11z = 20$$

Now obtaining residues:

$12 - 10x + 2y - z = R_1$

$10 - x - 9y + z = R_2$

$20 - 2x + y - 11z = R_3$

Now, the increments in x, y, z are dx, dy, dz so, dx= $-R_1/-10$, dy = $-R_2/-9$ and dz = $-R_3/-11$

Iterative Table:

i	x	y	z	R_1	R_2	R_3	Incrmnts.
1	0	0	0	12	10	20	dz=-20/-11=1.8182
2	0	0	1.8182	10.1818	11.8182	-0.0002	dy=-11.8182/-9=1.3131
3	0	1.3131	1.8182	12.8080	0.0003	0.0003	dx=-12.8080/-10=1.2808
4	1.2808	1.3131	1.8182	0	-1.2805	-1.2487	dy=-(-1.2805)/-9=-0.142
5	1.2808	1.1708	1.8182	-0.2846	0.002	-1.3910	dz=-(-1.3910)/-11=-0.126
6	1.2808	1.1708	1.6917	-0.1581	-0.1263	0.0005	dx=-(-0.1581)/-10= -0.158
7	1.2650	1.1708	1.6917	-0.0001	-0.1105	0.0321	dy=-(-0.1105)/-9= -0.0123

Therefore, the solution vector, X = $\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1.2650 \\ 1.1708 \\ 1.6917 \end{bmatrix}$ Ans.

Power method:

Power method is a single value method used for determining the dominant eigen value of a matrix. It as an iterative method implemented using an initial starting vector x. the starting vector can be arbitrary if no suitable approximation is available. Power method is implemented as follows

$$Y = AX - - - - - - (a)$$

$$X = \frac{Y}{k} - - - - - - (b)$$

The new value of X is obtained in b is the used in equation a to compute new value of Y and the process is repeated until the desired level of accuracy is obtained. The parameter k is called scaling factor is the element of Y with largest magnitude.

Example: find the largest Eigen value λ and the corresponding vector v, of the matrix using power method

$$A = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Solution assume X be column vector to be eigen vector of given matrix, now let $X = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$ be the eigen vector

Now iteration 1

$$Y = AX = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} \qquad X = \frac{Y}{k} = \frac{1}{2} \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0.5 \\ 0 \end{bmatrix}$$

iteration 2

$$Y = AX = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0.5 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 2.5 \\ 0 \end{bmatrix} \qquad X = \frac{Y}{k} = \frac{1}{2.5} \begin{bmatrix} 2 \\ 2.5 \\ 0 \end{bmatrix} = \begin{bmatrix} 0.8 \\ 1 \\ 0 \end{bmatrix}$$

iteration 3

$$Y = AX = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0.8 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2.8 \\ 2.6 \\ 0 \end{bmatrix} \qquad X = \frac{Y}{k} = \frac{1}{2.8} \begin{bmatrix} 2.8 \\ 2.6 \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ 0.929 \\ 0 \end{bmatrix}$$

iteration 4

$$Y = AX = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0.929 \\ 0 \end{bmatrix} = \begin{bmatrix} 2.858 \\ 2.928 \\ 0 \end{bmatrix} \qquad X = \frac{Y}{k}$$

$$= \frac{1}{2.928} \begin{bmatrix} 2.858 \\ 2.928 \\ 0 \end{bmatrix} = \begin{bmatrix} 0.976 \\ 1 \\ 0 \end{bmatrix}$$

iteration 5

$$Y = AX = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0.976 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2.976 \\ 2.952 \\ 0 \end{bmatrix} \qquad X = \frac{Y}{k}$$

$$= \frac{1}{2.976} \begin{bmatrix} 2.976 \\ 2.952 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0.992 \\ 0 \end{bmatrix}$$

iteration 6

$$Y = AX = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0.992 \\ 0 \end{bmatrix} = \begin{bmatrix} 2.984 \\ 2.992 \\ 0 \end{bmatrix} \qquad X = \frac{Y}{k}$$

$$= \frac{1}{2.992} \begin{bmatrix} 2.984 \\ 2.992 \\ 0 \end{bmatrix} = \begin{bmatrix} 0.997 \\ 1 \\ 0 \end{bmatrix}$$

iteration 7

$$Y = AX = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0.997 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2.997 \\ 2.994 \\ 0 \end{bmatrix} \qquad X = \frac{Y}{k}$$

$$= \frac{1}{2.997} \begin{bmatrix} 2.997 \\ 2.994 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0.999 \\ 0 \end{bmatrix}$$

iteration 8

$$Y = AX = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0.999 \\ 0 \end{bmatrix} = \begin{bmatrix} 2.998 \\ 2.999 \\ 0 \end{bmatrix} \qquad X = \frac{Y}{k}$$

$$= \frac{1}{2.999} \begin{bmatrix} 2.998 \\ 2.999 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

iteration 9

$$Y = AX = \begin{bmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ 0 \end{bmatrix} \qquad X = \frac{Y}{k} = \frac{1}{3} \begin{bmatrix} 3 \\ 3 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

Since the value of X is same for 8th and 9th iteration so eigen value is $\lambda = 3$ and eigen vector is $X = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$

Practice: Determine the Numerically largest eigen value and the corresponding eigen vector of the following matrix, using power method

$$\begin{bmatrix} \mathbf{25} & \mathbf{1} & \mathbf{2} \\ \mathbf{1} & \mathbf{3} & \mathbf{0} \\ \mathbf{2} & \mathbf{0} & \mathbf{-4} \end{bmatrix}$$

Eigen value is 25.18, eigen vector = $\begin{bmatrix} \mathbf{1} \\ \mathbf{0.04508} \\ \mathbf{0.06854} \end{bmatrix}$

Chapter 5 Solution of ordinary differential Equations

Many of the laws in physics, chemistry, engineering, economics are based on empirical observations that describe changes in the state of the system. Mathematical models that describe the state of such system are often expressed in terms of not only certain system parameters but also their derivatives, such mathematical model which uses differential calculus to express relationship between variables are known as differential equations.

Examples:

1. Kirchhoff's law $L\frac{di}{dt} + iR = v$
2. $m\frac{dv}{dt} = F$
3. $m\frac{d^2y}{dt^2} + a\frac{dy}{dt} + ky = 0$

Here

- The quantity y that is being differentiated is called dependent variable.
- The quantity with respect to which the dependent variable is differentiated is called independent variable.
- If there is only one independent variable then the equation is called an ordinary differential equation.

- If the equation contains more than one independent variable then it is called partial differential equation

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

Order of equation:

The highest derivative that appears in the equation is called order. If there is only first derivative then it called first order differential equation.

Degree of equation:

The degree of differential equation is the power of the highest order derivative

$$xy'' + x^2 y' = 2y + 3 \quad order = 2, degree = 1$$

$$(y''')^2 + 5y' = 2y + 3 \quad order = 3, degree = 2$$

Initial value problem (IVP)

In order to obtain the values of the integration constant, we need additional information for example consider the solution $y = ae^x$ to the equation $y' = y$. if we are giving a value of y for some x, the constant a can be dertermined, suppose y=1 when x=0, then $y(0) = ae^0 = 1$,

$\therefore a = 1$ and particular solution is $y = e^x$

It is also possible to specify the condition at different values of the independent variables such problems are called boundary value problem (BVP).

Example

$y'' = f(x, y, y')\ y(a) = A, y(b) =$
$B\ \ where\ a\ \&\ b\ are\ two\ different\ points.$

Solution of ordinary differential equations

1. Taylor's series method
2. Euler's method
3. Heun's method
4. Runge's method
5. Runge's Kutta 4th order method
6. Shooting method
7. Picard's method
8. R.K method for simultaneous equations
9. Solution of higher order differential equation

1. Taylor's series

Taylor series is often used in determining the order of errors for methods and the series itself is the basic for some numerical procedures.

Let $y' = f(x,y), \qquad y(x_0) = y_0$
(7)

Be the differential equation to which the numerical solution is required. Expanding $y(x)$ about $x = x_0$ by Taylor Series we get

$$y(x) = y(x_0) + \frac{(x-x_0)y'(x_0)}{1!} + \frac{(x-x_0)^2 y''(x_0)}{2!} + \cdots \qquad (8)$$

$$= y_0 + \frac{(x-x_0)y_0'}{1!} + \frac{(x-x_0)^2 y_0''}{2!} + \cdots \qquad (9)$$

Putting $x = x_0 + h = x_1$, h=difference we have

$$y_1 = y(x_1) = y_0 + \frac{hy_0'}{1!} + \frac{h^2 y_0''}{2!} + \frac{h^3 y_0'''}{3!} \ldots \qquad (10)$$

Here y_0', y_0'', y_0''' ... can be found using equation (1) and its successive differentiation at $x = x_0$. The series in (4) can be truncated at any stage if 'h' is small. Now having obtained $y_1$we can calculate y_1', y_1'', y_1''' from equation (1) at $x = x_0 +$ h

Now expanding $y(x)$ by Taylor series about $x = x_1$, we get

$$y_2 = y_1 + \frac{hy_1'}{1!} + \frac{h^2 y_1''}{2!} + \frac{h^3 y_1'''}{3!} \ldots \qquad (11)$$

Proceeding further we get

$$y_n = y_{n-1} + \frac{hy_{n-1}'}{1!} + \frac{h^2 y_{n-2}''}{2!} + \frac{h^3 y_{n-3}'''}{3!} \ldots \qquad (12)$$

By taking sufficient number of terms in above series the value of y_n can be obtained without much error

If a Taylor series is truncated while there are still non-zero derivatives of higher order the truncated power series will not be exact. The error term for a truncated Taylor Series can be written in several ways but the most useful form when the series is truncated after n^{th} term is

Example:

Using Taylor series method, solve $\frac{dy}{dx} = x^2 - y, y(0) = 1$ at $x =$ 0.1,0.2,0.3 &0.4.

Solution

Given $y' = x^2 - y$,$y(0) = 1$,

$x_0 = 0, y_0 = 1, \mathrm{h} = 0.1, x = 0.1, x = 0.2, x = 0.3, x = 0.4$

Now

$y' = x^2 - y \qquad y_0' = x_0^2 - y_0 = 0 - 1 = -1$

$y'' = 2x - y' \qquad y_0'' = 2x_0 - y_0' = 2 * 0 - (-1) = 1$

$y''' = 2 - y'' \qquad y_0''' = 2 - y_0'' = 1$

$y^{iv} = -y''' \qquad y_0^{iv} = -y_0''' = -1$

By Taylor Series

$$y_1 = y_0 + \frac{hy_0'}{1!} + \frac{h^2 y_0''}{2!} + \frac{h^3 y_0'''}{3!} + \frac{h^4 y_0^{iv}}{4!} \ldots$$

$y_1 = y(0.1)$

$= 1 + \frac{0.1(-1)}{1!} + \frac{(0.1)^2 * 1}{2!} + \frac{0.1^3 * 1}{3!} + \frac{0.1^4 * (-1)}{4!} \ldots$

$= 1 - 0.1 + 0.005 + 0.0001667 - 0.00000417$

$= 0.90516$

Now

$y_1' = x_1^2 - y_1 = (0.1)^2 - 0.90516$=-0.89516

$y_1'' = 2x_1 - y_1' = 2 * (0.1) - (-0.89516) = 1.09516$

$y_1''' = 2 - y_1'' = 2 - 1.0951 = 0.90484$

$y_1^{iv} = -y_1''' = -0.90484$

By Taylor Series

$$y_2 = y_1 + \frac{hy_1'}{1!} + \frac{h^2y_1''}{2!} + \frac{h^3y_1'''}{3!} + \frac{h^4y_1^{iv}}{4!} \dots$$

$y_2 = y(0.2)$

$= 0.90516 + \frac{0.1*(-0.89516)}{1!} + \frac{(0.1)^2*1.09516}{2!} + \frac{0.1^3*0.90484}{3!} + \frac{0.1^4*(-)}{4!} \dots$

$= 0.90516 - 0.089516 + 0.0054758 + 0.000150 - 0.00000377$

=0.821266

Now

$y_2' = x_2^2 - y_2 = (0.2)^2 - 0.8212352 = -0.7812352$

$y_2'' = 2x_2 - y_2' = 2*(0.2) - (-0.7812352) = 1.1812352$

$y_2''' = 2 - y_2'' = 2 - 1.1812352 = 0.8187648$

$y_2^{iv} = -y_2''' = -0.8187648$

By Taylor Series

$$y_3 = y_2 + \frac{hy_2'}{1!} + \frac{h^2y_2''}{2!} + \frac{h^3y_2'''}{3!} + \frac{h^4y_2^{iv}}{4!} \dots$$

$y_3 = y(0.3)$

$$= 0.8212352 + \frac{0.1*(-0.7812352)}{1!} + \frac{(0.1)^2*1.1812352}{2!} + \frac{0.1^3*0.8187648}{3!} + \frac{0.1^4*(-0.8187648)}{4!} \dots$$

$= 0.7491509$

Now

$y_3' = x_3^2 - y_3 = (0.3)^2 - 0.7491509 = -0.6591509$

$y_3'' = 2x_3 - y_3' = 2*(0.3) - (-0.6591509) = 1.2591509$

$y_3''' = 2 - y_3'' = 2 - 1.2591509 = 0.740849$

$y_3^{iv} = -y_3''' = -0.740849$

By Taylor Series

$$y_4 = y_3 + \frac{hy_3'}{1!} + \frac{h^2 y_3''}{2!} + \frac{h^3 y_3'''}{3!} + \frac{h^4 y_3^{iv}}{4!} \ldots$$

$y_4 = y(0.4)$

$$= 0.7491509 + \frac{0.1 * (-0.6591509)}{1!} + \frac{(0.1)^2 * 1.2591509}{2!} + \frac{0.1^3 * 0.740849}{3!} + \cdots$$

$$= 0.6896519$$

Similarly we can find the values of y_n for n=5, 6, 7…..

2. Euler's method:

Euler's method is the simplest one step method. It has limited application because of its low accuracy. From Taylor's theorem we have

$$\mathrm{y(x)} = y(x_0) + \frac{(x - x_0)y'(x_0)}{1!} + \frac{(x - x_0)^2 y''(x_0)}{2!} + \cdots$$

Taking only first two terms only

$$y(x) = y(x_0) + y'(x_0)(x - x_0)$$

Now, we get,

$$y(x_1) = y_1 = y(x_0) + (x_1 - x_0)f(x_0, y_0)$$

where $x = x_1, f(x_0, y_0) = y'(x_0)$

Now let $h = x_1 - x_0$

$$y_1 = y_0 + hf(x_0, y_0)$$

Similarly

$$y_2 = y_1 + hf(x_1, y_1)$$

In general

$$y_{i+1} = y_i + hf(x_i, y_i)$$

This formula is known as Euler's method and can be used recursively to evaluate y_1, y_2 … starting from the initial condition $y_0 = y(x_0)$

- A new value of y is estimated using the previous value of y as initial condition.
- The term $hf(x_i,y_i)$ represents the incremental value of y and $f(x_i,y_i)$ is the slope of y(x) at (x_i,y_i), the new value is obtained by extrapolating linearly over the step size h using the slope at its previous value.
  i.e. new value =old value + slope x step size

Example : Given the equation $y'(x) = 3x^2 + 1$, with y(1)=2, estimate y(2), using Euler's method using h=0.5 & h=0.25,
Solution

$$y'(x) = f(x, y) = 3x^2 + 1$$
$$y(1) = 2, y(x_0) = y_0, x_0 = 1, y_0 = 2$$

We know that

$$y_{i+1} = y_i + hf(x_i, y_i)$$

a. h=0.5

$$y_1 = y(1 + 0.5) = y(1.5) = y_0 + hf(x_0, y_0)$$
$$= y(1) + 0.5 \times (3 \times 1^2 + 1)$$
$$= 2 + 0.5 \times 4$$
$$= 4$$
$$y_1 = y(2.0) + y(1.5 + 0.5) = y_1 + hf(x_1, y_1) = y(1.5) + 0.5 \times f(x_{1.5}, y_{1.5})$$
$$= 4 + 0.5 \times (3 \times 1.5^2 + 1)$$
$$= 7.8750$$
$$\therefore y(2) = 7.8750$$

b. h=0.25

$y(1) = 2$

$y_1 = y(1 + 0.25) = y(1.25) = y_0 + hf(x_0, y_0) = 2 + 0.25 \times f(1,2)$

$= 2 + 0.25(3 \times 1^2 + 1) = 3$

$y_2 = y(1.25 + 0.25) = y(1.5) = y_1 + hf(x_1, y_1) = 3 + 0.25 \times f(1.25,3)$

$$= 3 + 0.25(3 \times 1.25^2 + 1) = 4.4218$$

$$y_3 = y(1.5 + 0.25) = y(1.75) = y_2 + hf(x_2, y_2)$$
$$= 4.4218 + 0.25 \times f(1.5, 4.4218)$$
$$= 4.4218 + 0.25(3 \times 1.5^2 + 1) = 6.3593$$

$$y_4 = y(1.75 + 0.25) = y(2.0) = y_3 + hf(x_3, y_3)$$
$$= 6.3593 + 0.25 \times f(1.75, 6.3593)$$
$$= 6.3593 + 0.25(3 \times 1.75^2 + 1) = 8.9061$$
$$\therefore y(2.0) = 8.9061$$

3. Heun's method:

Euler's method is the simplest of all one step methods. It is easy to implement on computers. One of the major weakness is large truncation error in Euler's method. This is due to the fact that Euler's method uses only the first two terms of Taylor's series. Now heun's method also called improved Euler's method.

In Euler's method the slope at the beginning of the interval is used to extrapolate y_i to y_{i+1} over the entire interval, thus $y_{i+1} = y_i + m_1 h \ldots\ldots\ldots a$ where m_1 is the slope at(x_i, y_i).

Alternative is to use the line which is parallel to the tangent at the point $[x_{i+1}, y(x_{i+1})]$ to extrapolate from $y_i \; to \; y_{i+1}$

$$y_{i+1} = y_i + m_2 h \ldots\ldots\ldots b$$

Where, m_2 is the slope at $[x_{i+1}, y(x_{i+1})]$. Note that the estimate appears to be overestimated.

Now a third approach is to use a line whose slope is the average of the slopes at the end points of the interval, i.e

$$y_{i+1} = y_i + (\frac{m_1 + m_2}{2})h \ldots\ldots\ldots c$$

This gives the better approximation to y_{i+1}, this approach is known as Heun's method.

The formula for implementing Heun's method can be constructed easily as

$$y'(x) = f(x, y)$$

We can obtain:

$$m_1 = y'(x_i) = f(x_i, y_i)$$

$$m_2 = y'(x_{i+1}) = f(x_{i+1}, y_{i+1})$$

$$\therefore m = \frac{m_1 + m_2}{2} = \frac{f(x_i, y_i) + f(x_{i+1}, y_{i+1})}{2}$$

Now, the equation (c) becomes:

$$y_{i+1} = y_i + \frac{h}{2}[f(x_i, y_i) + f(x_{i+1}, y_{i+1})] \ldots\ldots d$$

Note that the term y_{i+1} appears on both sides. The value y_{i+1} cannot be calculated until the value of y_{i+1} inside the function $f(x_{i+1}, y_{i+1})$ is available. This value can be predicted using Euler's formula as

$$y_{i+1} = y_i + hf(x_i, y_i)$$

Then, the Heun's formula can be written as:

$$y_{i+1} = y_i + \frac{h}{2}\left[f(x_i, y_i) + f(x_{i+1}, y_{e^{i+1}})\right]$$

Putting the value of Euler's formula in above equation we get

$$y_{i+1} = y_i + \frac{h}{2}[f(x_i, y_i) + y_i + hf(x_i, y_i)]$$

Example : Given the equation $y'(x) = \frac{2y}{x}$ with y(1)=2, estimate y(2) using 1) Euler's method 2) Heun's method and compare the result. Take h=0.25

I. Euler's method
   h=0.25, y(1)=2

$$y(1.25) = y_1 = y_0 + hf(x_0, y_0) = 2 + 0.25f(1,2) = 2 + 0.25 \times \frac{2 \times 2}{1} = 3$$

$$y(1.5) = y_2 = y_1 + hf(x_1, y_1) = 3 + 0.25f(1.25,3) = 3 + 0.25 \times \frac{2 \times 3}{1.25}$$
$$= 4.2$$

$$y(1.75) = y_3 = y_2 + hf(x_2, y_2) = 4.2 + 0.25f(1.5,4.2)$$
$$= 4.2 + 0.25 \times \frac{2 \times 4.2}{1.5} = 5.6$$
$$y(2) = y_4 = y_3 + hf(x_3, y_3) = 5.6 + 0.25f(1.75,5.6)$$
$$= 5.6 + 0.25 \times \frac{2 \times 5.6}{1.75} = 7.2$$

II. Heun's method:

Iteration 1:

we know

$$y_{i+1} = y_i + (\frac{m_1 + m_2}{2})h$$

$$y_i = y_0 + (\frac{m_1 + m_2}{2})h$$

Given the initial condition $y(x_0) = y_0 = y(1) = 2$

$$y(1 + 0.25) = y(1.25) = y_1 = y_0 + (\frac{m_1 + m_2}{2})h$$

$$m_1 = f(x_{0,}y_0) = f(1,2) = \frac{2 \times 2}{1} = 4$$

$$m_2 = f(x_0 + h, y_0 + m_1 h)$$

$$= f(1 + 0.25,2 + 4 \times 0.25)$$

$$= f(1.25,3)$$

$$= \frac{2 \times 3}{1.25}$$

$$= 4.8$$

$$y(1.25) = y_0 + \left(\frac{m_1 + m_2}{2}\right)h = 2 + \left(\frac{4 + 4.8}{2}\right)0.25 = 3.1$$

Iteration 2:

$$y(1.25 + 0.25) = y(1.5) = y_2 = y_1 + (\frac{m_1 + m_2}{2})h$$

$$m_1 = f(x_1 y_1) = f(1.25,3.1) = \frac{2 \times 3.1}{1.25} = 4.96$$

$$m_2 = f(x_1 + h, y_1 + m_1 h)$$

$$= f(1.25 + 0.25, 3.1 + 4.96 \times 0.25)$$

$$= f(1.5, 4.34)$$

$$= \frac{2 \times 4.34}{1.5}$$

$$= 5.7867$$

$$y(1.5) = y_1 + \left(\frac{m_1 + m_2}{2}\right)h = 3.1 + \left(\frac{4.96 + 5.7867}{2}\right)0.25 = 4.44$$

Iteration 3:

$$y(1.5 + 0.25) = y(1.75) = y_3 = y_2 + (\frac{m_1 + m_2}{2})h$$

$$m_1 = f(x_2 y_2) = f(1.5, 4.44) = \frac{2 \times 4.44}{1.5} = 5.92$$

$$m_2 = f(x_2 + h, y_2 + m_1 h)$$

$$= f(1.5 + 0.25, 4.44 + 5.92 \times 0.25)$$

$$= f(1.75, 5.92)$$

$$= \frac{2 \times 5.92}{1.75}$$

$$= 6.77$$

$$y(1.75) = y_3 = y_2 + \left(\frac{m_1 + m_2}{2}\right)h = 4.44 + \left(\frac{5.92 + 6.77}{2}\right)0.25 = 6.03$$

Iteration 4:

$$y(1.75 + 0.25) = y(1.5) = y_4 = y_3 + (\frac{m_1 + m_2}{2})h$$

$$m_1 = f(x_3 y_3) = f(1.75, 6.03) = \frac{2 \times 6.03}{1.75} = 6.89$$

$$m_2 = f(x_3 + h, y_3 + m_1 h)$$

$$= f(1.75 + 0.25, 6.03 + 6.89 \times 0.25)$$

$$= f(2,7.75)$$

$$= \frac{2 \times 7.75}{2}$$

$$= 7.75$$

$$y(2) = y_4 = y_3 + \left(\frac{m_1 + m_2}{2}\right) h = 6.03 + \left(\frac{6.89 + 7.75}{2}\right) 0.25 = 7.86$$

The above equation can be done using the following formula, note this is same problem but done using later formula, you can use any method which ever you feel easy to use.

Iteration 1:

We know that

$$y_{i+1} = y_i + \frac{h}{2}\left[f(x_i, y_i) + f(x_{i+1}, y_{e^{i+1}})\right]$$

We know

$$f(x_0, y_0) = f(1,2) = \frac{2y}{x} = \frac{2 \times 2}{1} = 4$$

$$y_e(1.25) = y(1) + h \times f\big(x_1, y(1)\big)$$

$$= 2 + 0.25 f(1,2)$$

$$= 2 + 0.25 \times \frac{2 \times 2}{1}$$

$$= 3$$

$$y(1.25) = y(1) + \frac{h}{2}\left[f(x_1, y_1) + f\big(x_{i+1}, y_{e^{i+1}}\big)\right]$$

$$= 2 + \frac{0.25}{2}[f(1,2) + f(1.25,3)]$$

$$2 + \frac{0.25}{2}\left[\frac{2 \times 2}{1} + \frac{2 \times 3}{1.25}\right]$$
$$= 3.1$$

Iteration 2:

$$y(1.5) = y(1.25) + \frac{h}{2}[f(x_{1.25}, y_{1.25}) + f(x_{1.5}, y_{e^{1.5}})]$$

$$y(1.5) = y(1.25) + \frac{h}{2}[f(1.25,3.1) + f(x_{1.5}, y_{e^{1.5}})]$$

$$y_e(1.25) = y(1.25) + h \times f(x_{1.25}, y_{1.25})$$
$$= 3.1 + 0.25f(1.25,3.1)$$
$$= 3.1 + 0.25 \times \frac{2 \times 3.1}{1.25}$$
$$= 4.34$$
$$y(1.5) = y(1.25) + \frac{h}{2}[f(1.25,3.1) + f(x_{1.5}, y_{e^{1.5}})]$$
$$y(1.5) = 3.1 + \frac{0.25}{2}[f(1.25,3.1) + f(1.5,4.34)]$$
$$= 3.1 + \frac{0.25}{2}\left[2 \times \frac{3.1}{1.25} + 2 \times \frac{4.34}{1.5}\right]$$
$$= 4.4433$$

Iteration 3:

$$y(1.75) = y(1.5) + \frac{h}{2}[f(x_{1.5}, y_{1.5}) + f(x_{1.75}, y_{e^{1.75}})]$$

$$y_e(1.75) = y(1.5) + h \times f(x_{1.5}, y_{1.5})$$
$$= 4.4433 + 0.25f(1.5,4.4433)$$
$$= 4.4433 + 0.25 \times \frac{2 \times 4.4433}{1.5}$$
$$= 5.9244$$
$$y(1.75) = y(1.5) + \frac{h}{2}[f(1.5,4.4433) + f(x_{1.5}, 5.9244)]$$
$$= 4.4433 + \frac{0.25}{2}\left[2 \times \frac{4.4433}{1.5} + 2 \times \frac{5.9244}{1.75}\right]$$
$$= 6.0302$$

Iteration 4:

$$y(2) = y(1.75) + \frac{h}{2}[f(x_{1.75}, y_{1.75}) + f(x_2, y_{e^2})]$$

$$y_e(2) = y(1.75) + h \times f(x_{1.75}, y_{1.75})$$
$$= 6.0302 + 0.25f(1.75, 6.0302)$$
$$= 6.0302 + 0.25 \times \frac{2 \times 6.0302}{1.75}$$
$$= 7.7531$$
$$y(2) = y(1.75) + \frac{h}{2}[f(1.75, 6.0302) + f(2, 7.7531)]$$
$$= 6.0302 + \frac{0.25}{2}\left[2 \times \frac{6.0302}{1.75} + 2 \times \frac{7.7531}{2}\right]$$
$$= 7.8608$$

The exact solution of the equation $y'(x) = 2\frac{y}{x}$ with $y(1) = 2$ is obtained as

$$y(x) = 2x^2$$
$$y(2) = 2 \times 2^2 = 8$$

error =8-7.8608=0.1392

Runge Kutta method:

Runge Kutta method refers to a family of one step methods used for numerical solution of initial value problems. They are all based on the general form of the extrapolation equation:

$$y_{i+1} = y_i + slope \times interval\ size$$
$$= y_i + mh$$

Where m represents the slope that is weighted averages of the slope at various points in the interval h. Runge Kutta (RK) methods are known by their order. For instance an RK method is called r-order Runge Kutta method when slope at r points are used to construct the weighted average slope m.

Euler's method is the first order RK method because it uses only one slope at (x_i, y_i) to estimate y_{i+1}.

Huen's method is a second order RK method because it employs slope at two ends points of the interval. It demonstrated that higher order would be better the accuracy of estimates.

Fourth order Runge Kutta method (Classical fourth order Runge Kutta method)

The classical fourth order Runge Kutta method is given as:

$$y_{i+1} = y_i + (\frac{m_1 + 2m_2 + 2m_3 + m_4}{6})h$$

Where

$$m_1 = f(x_i, y_i)$$

$$m_2 = f(x_i + \frac{h}{2}, y_i + \frac{m_1 h}{2})$$

$$m_3 = f(x_i + \frac{h}{2}, y_i + \frac{m_2 h}{2})$$

$$m_4 = f(x_i + h, y_i + m_3 h)$$

Runge Kutta (3^{rd} order RK method)

$$y_{i+1} = y_i + (\frac{m_1 + 4m_4 + m_3}{6})h$$

Where,

$$m_1 = f(x_i, y_i)$$

$$m_2 = f(x_i + h, y_i + m_1 h)$$

$$m_3 = f(x_i + h, y_i + m_2 h)$$

$$m_4 = f(x_i + \frac{h}{2}, y_i + m_1 \frac{h}{2})$$

Example : Use the classical RK method to estimate y(0.4) when $y'(x) = x^2 + y^2$with $y(0) = 0$, assume h=0.2.

Solution

Given condition

$$y(0) = 0, f(x, y) = x^2 + y^2$$

We know that,

$$y_{i+1} = y_i + (\frac{m_1 + 2m_2 + 2m_3 + m_4}{6})h$$

Where,

$$m_1 = f(x_i, y_i)$$

$$m_2 = f(x_i + \frac{h}{2}, y_i + \frac{m_1 h}{2})$$

$$m_3 = f(x_i + \frac{h}{2}, y_i + \frac{m_2 h}{2})$$

$$m_4 = f(x_i + h, y_i + m_3 h)$$

iteration 1:

$$y(0.2) = y_0 + (\frac{m_1 + 2m_1 + 2m_3 + m_4}{6})h$$

$$m_1 = f(x_0, y_0) = f(0,0) = 0$$

$$m_2 = f(x_0 + \frac{h}{2}, y_0 + \frac{m_1 h}{2}) = f(0 + \frac{0.2}{2}, 0 + \frac{0 \times 0.2}{2}) = f(0.1,0)$$
$$= 0.1^2 + 0.0^2 = 0.01$$

$$m_3 = f(x_0 + \frac{h}{2}, y_0 + \frac{m_2 h}{2}) = f(0 + \frac{0.2}{2}, 0 + \frac{0.01 \times 0.2}{2}) = f(0.1,0.001)$$
$$= 0.1^2 + 0.001^2 = 0.01$$

$$m_4 = f(x_0 + h, y_0 + m_3 h) = f(0 + 0.2, 0 + 0.01 \times 0.2) = f(0.2,0.002)$$
$$= 0.1^2 + 0.002^2 = 0.04$$

$$y(0.2) = y_0 + \left(\frac{m_1 + 2m_1 + 2m_3 + m_4}{6}\right)h$$

$$y(0.2) = 0 + \left(\frac{0 + 2 \times 0.01 + 2 \times 0.01 + 0.04}{6}\right)0.2 = 0.00267$$

Iteration 2

$$y(0.4) = y_1 + (\frac{m_1 + 2m_1 + 2m_3 + m_4}{6})h$$

$$y_1 = y(0.2)$$

$$m_1 = f(x_{0.2}, y_{0.2}) = f(0.2,0.00267) = 0.04$$

$$m_2 = f(0.2 + \frac{0.2}{2}, 0.00267 + \frac{0.04 \times 0.2}{2}) = f(0.3,0.0067)$$
$$= 0.3^2 + 0.0067^2 = 0.09004$$

$$m_3 = f(0.2 + \frac{0.2}{2}, 0.00267 + \frac{0.09004 \times 0.2}{2}) = f(0.3,0.01167)$$
$$= 0.3^2 + 0.01167^2 = 0.09014$$

$$m_4 = f(0.2 + 0.2, 0.00267 + 0.9014 \times 0.2) = f(0.4,0.02070)$$
$$= 0.4^2 + 0.02070^2 = 0.16043$$

$$y(0.4) = y_0 + \left(\frac{m_1 + 2m_1 + 2m_3 + m_4}{6}\right) h$$

$$y(0.4) = 0.00267 + \left(\frac{0.04 + 2 \times 0.09004 + 2 \times 0.09014 + 0.16043}{6}\right) 0.2$$
$$= 0.02136$$

Runge Kutta method for simultaneous first order equations:

Consider the simultaneous equation

$$\frac{dy}{dx} = f_1(x, y, z) \quad \& \quad \frac{dx}{dz} = f_2(x, y, z)$$

With the initial conditions $y(x_0) = y_0, z(x_0) = z_0$ now starting from (x_0, y_0, z_0) the increment k and l in y and z are given by the following formula

$$k_1 = hf_1(x_0, y_0, z_0)\ ;\ \ l_1 = hf_2(x_0, y_0, z_0)$$

$$k_2 = hf_1(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}, z_0 + \frac{l_1}{2})\ ;\ \ l_2 = hf_2(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}, z_0 + \frac{l_1}{2})$$

$$k_3 = hf_1(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}, z_0 + \frac{l_2}{2})\ ;\ \ l_3 = hf_2(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}, z_0 + \frac{l_2}{2})$$

$$k_4 = hf_1(x_0 + h, y_0 + k_3, z_0 + l_3)\ ;\ \ l_4 = hf_2(x_0 + h, y_0 + k_3, z_0 + l_3)$$

$$k = \frac{(k_1 + 2k_2 + 2k_3 + k_4)}{6}$$

$$l = \frac{(l_1 + 2l_2 + 2l_3 + l_4)}{6}$$

$$y_1 = y_0 + k, \; z_1 = z_0 + l$$

To compute y_2, z_2 we simply replace x_0, y_0, z_0 by x_1, y_1, z_1 in the above formulae

If we consider the second order R.K method

$$k_1 = hf_1(x_0, y_0, z_0) \; ; \; \; l_1 = hf_2(x_0, y_0, z_0)$$

$$k_2 = hf_1(x_0 + h, y_0 + k_1, z_0 + l_1) \; ; \; \; l_2 = hf_2(x_0 + h, y_0 + k_1, z_0 + l_1)$$

$$k = \frac{k_1 + k_2}{2} \; ; \quad l = \frac{l_1 + l_2}{2}$$

$$y_1 = y_0 + k \; ; \; z_1 = z_0 + k$$

Example: Solve $\frac{dy}{dx} = yz + x; \frac{dz}{dx} = xz + y$ given that y(0)=1,z(0)=-1 for y(0.1),z(0.1)

Solution:

Here,

$$f_1(x, y, z) = yz + x \; ; \; f_2(x, y, z) = xz + y$$

let h=0.1 x_0=0, y_0=1, z_0=-1

$$k_1 = hf_1(x_0, y_0, z_0) = 0.1f_1(0,1,-1) = 0.1(1 \times -1 + 0) = -0.1$$

$$l_1 = hf_2(x_0, y_0, z_0) = 0.1f_2(0,1,-1) = 0.1(0 \times -1 + 1) = 0.1$$

$$k_2 = hf_1\left(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}, z_0 + \frac{l_1}{2}\right)$$

$$= 0.1f_1\left(0 + \frac{0.1}{2}, 1 + \frac{-0.1}{2}, -1 + \frac{0.1}{2}\right)$$

$$= 0.1f_1(0.05, 0.95, -0.95)$$

$$= 0.1(0.95 \times -0.95 + 0.05)$$

$$= -0.08525$$

$$l_2 = hf_2\left(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}, z_0 + \frac{l_1}{2}\right)$$

$$= 0.1f_2\left(0 + \frac{0.1}{2}, 1 + \frac{-0.1}{2}, -1 + \frac{0.1}{2}\right)$$

$$= 0.1(0.05 \times -0.95 + 0.95)$$

$$= 0.09025$$

$$k_3 = hf_1\left(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}, z_0 + \frac{l_2}{2}\right)$$

$$= 0.1f_1\left(0 + \frac{0.1}{2}, 1 + \frac{-0.08525}{2}, -1 + \frac{0.09025}{2}\right)$$

$$= 0.1f_1(0.05, 0.95738, -0.95738)$$

$$= 0.1(0.95738 \times -0.95738 + 0.05) = -0.08666$$

$$l_3 = hf_2(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}, z_0 + \frac{l_2}{2})$$

$$= 0.1f_2\left(0 + \frac{0.1}{2}, 1 + \frac{-0.0891}{2}, -1 + \frac{0.0903}{2}\right)$$

$$= 0.1f_2(0.05, 0.95738, -0.95738)$$

$$= 0.1(0.05 \times -0.95738, +0.95738)$$

$$= 0.09095$$

$$k_4 = hf_1(x_0 + h, y_0 + k_3, z_0 + l_3)$$

$$= 0.1f_1(0 + 0.1, 1 + (-0.08666), -1 + 0.09095)$$

$$= 0.1f_1(0.1, 0.91334, -0.90905)$$

$$= 0.1(0.91334 \times -0.90905 + 0.1)$$

$$= -0.07303$$

$$l_4 = hf_2(x_0 + h, y_0 + k_3, z_0 + l_3)$$

$$= 0.1f_2(0 + 0.1, 1 + (-0.0862), -1 + 0.0907)$$

$$= 0.1f_2(0.1, 0.91334, -0.90905)$$

$$= 0.1(0.1 \times -0.90905 + 0.91334)$$

$$= 0.08224$$

$$k = \frac{(k_1 + 2k_2 + 2k_3 + k_4)}{6}$$

$$= \frac{(-0.1 + 2 \times -0.8525 + 2 \times -0.08666 - 0.07303)}{6}$$

$$= -0.08614$$

$$l = \frac{(l_1 + 2l_2 + 2l_3 + l_4)}{6}$$

$$= \frac{(0.1 + 2 \times 0.09025 + 2 \times 0.09095 + 0.082224)}{6}$$

$$= 0.09077$$

$$y_1 = y(0.1) = y_0 + k = 1 + (-0.08614) = 0.91386$$

$$z_1 = z(0.1) = z_0 + l = -1 + 0.09077 = -0.90923$$

Practice: Compute y(0.2) & z(0.2) in the above solution.

Higher order equations:

A higher order differential equation is in the form

$$\frac{d^m y}{dx^m} = f(x, y, \frac{dy}{dx}, \frac{d^2 y}{dx^2} \ldots.) \ldots\ldots a$$

With m initial conditions given as

$$y(x_0) = a_1, y'(x_0) = a_2 \ldots.. y^{m-1}(x_0) = a_m$$

we can replace equation a by a system of first order equation as follows. Let us denote

$$y = y_1, \frac{dy}{dx} = y_2, \frac{d^2y}{dx^2} = y_3 \ldots .$$

then

$$\frac{dy_1}{dx} = y_2 \qquad y_1(x_0) = y_{1,0} = a_1$$

$$\frac{dy_2}{dx} = y_3 \qquad y_2(x_0) = y_{2,0} = a_2$$

$$\ldots .$$

$$\frac{dy_{m-1}}{dx} = y_m \qquad y_{m-1}(x_0) = y_{m-1,0} = a_{m-1}$$

$$\frac{dy_m}{dx} = f(x_1, y_2, y_2 \ldots y_m) \qquad y_m(x_0) = y_{m,0} = a_m$$

This system is similar to the system of first order with the condition,

$$f_i = y_{i+1}, i = 1,2, \ldots . m - 1$$

$$f_m = f(x, y_1, y_2 \ldots y_m)$$

RK method for second order differential equations:

Consider the second order differential equation

$$\frac{d^2y}{dx^2} = \phi\left[x, y, \frac{dy}{dx}\right] \qquad y(x_0) = y_0, y'(x_0) = y'_0, z(x_0) = z_0 \ldots \ldots . (a)$$

Let $\frac{dy}{dx} = z, then, \frac{d^2y}{dx^2} = \frac{dz}{dx}$

Substituting equation (a) we get

$\frac{dz}{dx} = z = \emptyset(x, y, z), y(x_0) = y_0, z(x_0) = z_0$

The problem reduces to

$\frac{dy}{dx} = z = f_1(x, y, z)$ & $\frac{dz}{dx} = z' = f_2(x, y, z)$ subjected to $y(x_0) = y_0, z(x_0) = z_0$ and this can be solved as before.

Example : Solve $y'' = xy' - y, y(0) = 3, y'(0) = 0$ to approximate y(0.1).

Given:

$$y'' = xy' - y, y(0) = 3, y'(0) = 0, h = 0.1$$

Let $\frac{dy}{dx} = y' = z$, then $y'' = z'$, above equation reduces to

$$y' = z = f_1(x, y, z)$$

$$y'' = z' = xy' - y = xz - y = f_2(x, y, z)$$

Subjected to y(0)=3 & z(0) =0 .i.e $x_0 = 0,\ y_0 = 3,\ z_0 = 0$

Now,

$$k_1 = hf_1(x_0, y_0, z_0) = h(z_0) = 0.1 \times 0 = 0$$

$$l_1 = hf_2(x_0, y_0, z_0) = hf_2(0,3,0) = 0.1 \times (0 \times 0 - 3) = -0.3$$

$$k_2 = hf_1\left(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}, z_0 + \frac{l_1}{2}\right)$$

$$= hf_1\left(0 + \frac{0.1}{2}, 3 + \frac{0}{2}, 0 + \left(-\frac{0.3}{2}\right)\right)$$

$$= hf_1(0.05,3,-0.15)$$

$$= 0.1(-0.15)$$

$$= -0.015$$

$$l_2 = 0.1f_2\left(0 + \frac{0.1}{2}, 3 + \frac{0}{2}, 0 - \frac{0.3}{2}\right)$$

$$= 0.1f_2(0.05,3,-0.15)$$

$$= 0.1(0.05 \times -0.0015 - 3) = -0.3001$$

$$k_3 = hf_1\left(0 + \frac{0.1}{2}, 3 + \frac{-0.15}{2}, 0 + \frac{-0.3001}{2}\right)$$

$$= 0.1f_1(0.05, 2.925, -0.1501)$$

$$= 0.1 \times -0.1501$$

$$= -0.0150$$

$$l_3 = hf_2(0 + \frac{0.1}{2}, 3 + \frac{-0.15}{2}, 0 + \frac{-0.3001}{2})$$

$$= 0.1f_2(0.05, 2.925, -0.1501)$$

$$= 0.1(0.05 \times -0.1501 - 2.925)$$

$$= -0.2933$$

$$k_4 = hf_1(0 + 0.1, 3 + (-0.0150), 0 + (-0.2933))$$

$$= 0.1f_1(0.1, 2.9850, -2.933)$$

$$= 0.1 \times -0.2933$$

$$= -0.0293$$

$$l_4 = hf_2(0 + 0.1, 3 + (-0.0150), 0 + (-0.2933))$$

$$= 0.1f_2\big((0.1, 2.9850, -2.933)\big)$$

$$= 0.1(0.1 \times -0.293 - 2.9850)$$

$$= -0.3014$$

$$k = \frac{(k_1 + 2k_2 + 2k_3 + k_4)}{6}$$

$$= \frac{(0 + 2 \times -0.015 + 2 \times -0.0150 - 0.0293)}{6}$$

$$= -0.0149$$

$$l = \frac{(l_1 + 2l_2 + 2l_3 + l_4)}{6}$$

$$= \frac{(-0.3 + 2 \times -0.3001 + 2 \times -0.2933 - 0.3014)}{6}$$

$$= -0.2980$$

$$y_1 = y(0.1) = y_0 + k = 3 + (-0.3014) = 2.6986$$

$$z_1 = z(0.1) = z_0 + l = 0 - 0.2980 = -0.2980$$

Picard method of successive approximation

Consider the first order differential equation $\frac{dy}{dx} = f(x, y)$ subjected to $y(x_0) = y_0$. We can integrate this to obtain the solution in the interval(x_0,x).

The above equation can be written as $\mathrm{dy} = \mathrm{f(x, y)dx}$

Integrating between the limits , we get

$$\int_{y_0}^{y} dy = \int_{x_0}^{x} f(x, y)dx$$

$$y - y_0 = \int_{x_0}^{x} f(x, y)dx$$

$$y = y_0 + \int_{x_0}^{x} f(x, y)dx$$

$$y(x) = y(x_0) + \int_{x_0}^{x} f(x, y)dx$$

Since y appears under the integral sign on the right, the integration cannot be formed. The dependent variable should be replaced by either a constant or a function of x, since we know the initial value of y at x=x_0 we may use this as a first approximation to the solution and the result can be used on the right hand side to obtain the next approximation.

Now by Picard's methods first approximation we replace y by y_0 in f(x,y) i.e

$$y_1 = y_0 + \int_{x_0}^{x} f(x, y_0)dx$$

For second approximation y_2 replace y by y_1

$$y_2 = y_0 + \int_{x_0}^{x} f(x, y_1)dx \; \ldots..$$

$$y_n = y_0 + \int_{x_0}^{x} f(x, y_{n-1})dx$$

The process is to be stopped when two values of y, are same to desired degree of accuracy

Note:

1. *This method is applicable only to a limited class of equations in which the successive integration can be perform easily.*
2. *Sometimes it may not be possible to carry out the integration.*
3. *It is not convenient method for computer-based solution.*

Example : Use Picard's method to approximate the value of y when x=0.1,0.2,0.3,0.4 & 0.5. given that y=1 at x=0, y'=1+xy, correct up to three decimal places

Given

$$\frac{dy}{dx} = 1 + xy\,;\; y(0) = 1$$

$$f(x, y) = 1 + xy, y_0 = 1, x_0 = 0$$

first approximation

$$y_1 = y_0 + \int_{x_0}^{x} f(x, y_0)dx = 1 + \int_{0}^{x} (1 + xy_0)dx$$

$$= 1 + \int_{0}^{x} (1 + x)dx$$

$$= 1 + x + \frac{x^2}{2}$$

Second approximation

$$y_2 = y_0 + \int_{x_0}^{x} f(x, y_1)dx$$

$$= 1 + \int_0^x (1 + xy_1)dx$$

$$= 1 + \int_0^x \left(1 + x\left(1 + x + \frac{x^2}{2}\right)\right)dx$$

$$= 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{8}$$

Third approximation

$$y_3 = y_0 + \int_{x_0}^{x} f(x, y_2)dx$$

$$= 1 + \int_0^x (1 + xy_2)dx$$

$$= 1 + \int_0^x \left(1 + x\left(1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{8}\right)\right)dx$$

$$= 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{8} + \frac{x^5}{15} + \frac{x^6}{48}$$

Fourth approximation

$$y_4 = y_0 + \int_{x_0}^{x} f(x, y_3)dx$$

$$= 1 + \int_0^x (1 + xy_3)dx$$

$$= 1 + \int_0^x \left(1 + x\left(1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{8} + \frac{x^5}{15} + \frac{x^6}{48}\right)\right)dx$$

$$= 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{8} + \frac{x^5}{15} + \frac{x^6}{48} + \frac{x^7}{105} + \frac{x^8}{348}$$

Now at x=0.1

Y_1=1.1050

Y_2=1.1053

Y_3=1.1053

Since the value is correct up to three decimal places y(0.1)=1.105

Shooting method

This method is called shooting method because it resembles an artillery problem. In this method the given boundary value problem is first converted into an equivalent initial value problem an then solved using any of the method discussed in previous section.

Consider the equation

$y'' = f(x, y, y')\ y(a) = A, y(b) = B$

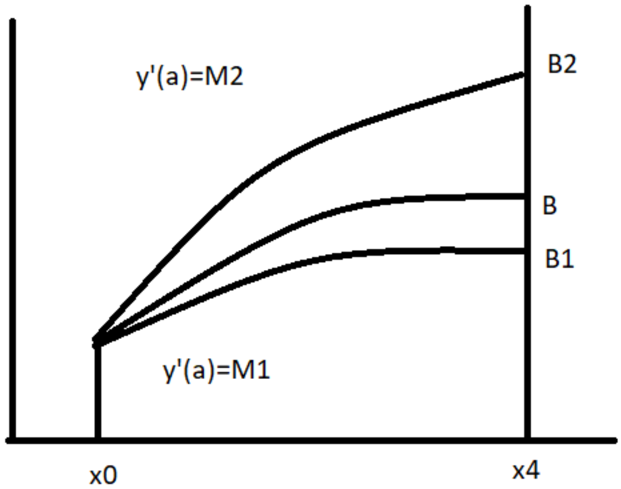
Letting $y' = z$, we obtain the following set of two equations $y' = z\,, z' = f(x, y, z)$. In order to solve this set as initial value problem we need two conditions at x=a, we have one condition y(a)=A and therefore require another condition for z at x=a. let us assume that $z(a) = M_1$, where M_1 is a guess. Note M_1 represents the slope $y'(x)\ at\ x = a$ thus the problem is reduced to as system two first order equation with initial conditions

$$y' = z \qquad y(a) = A$$

$$z' = f(x, y, z) \qquad z(a) = M_1 \dots\dots (a)$$

Equation a can be solved for y and z, using any one step method, using steps of h, until the solution at x=b is reached. Let the estimated value of y(x) at x=b be B_1, if B_1=B then we have obtained the required solution. In practice it is very unlikely that our initial guess z(a)=M_1 is correct.

If $B_1 \neq B$ then we obtain the solution with another guess say z(a) =M_2. Let new estimate of y(x) be at x=b be B_2. If B_2 is not equal to B then process is continued till we obtain the correct estimate of y(b). However the procedure can be accelerated by suing an improves guess for z(a) after estimates of B_1 & B_2 are obtained.



Let us assume that z(a)=M_3 lead to the value of y(b)=B, if we assume that values of M and B are linearly related then

$$\frac{M_3 - M_2}{B - B_2} = \frac{M_2 - M_1}{B_2 - B_1}$$

$$M_3 = M_2 + \frac{B - B_2}{B_2 - B_1}(M_2 - M_1)$$

$$M_3 = M_2 - \frac{B_2 - B}{B_2 - B_1}(M_2 - M_1)$$

Now with z(a)=M_3, we can again obtain the solution of y(x).

Example : using shooting method solve the equation $\frac{d^2y}{dx^2} = 6x,\ y(1) = 2, y(2) = 9$ in the interval (1,2)

Solution

By transformation

$$\frac{dy}{dx} = z = f_1(x,y,z), y(1) = 2\,, \frac{dz}{dx} = 6x = f_2(x,y,z)$$

Let us assume that $z(1) = y'(1) = 2(M_1\ say)$, applying Heun's method we obtain the solution as follows

Iteration 1:

h=0.5, x_0=1, y(1)=y_0=2, z(1)=z_0=2

$$y_{i+1} = y_i + (\frac{m_1 + m_2}{2})h$$

$$m_1(1) = f_1(x_0, y_0, z_0) = f_1(1,2,2) = z_0 = 2$$

$$m_1(2) = f_2(x_0, y_0, z_0) = f_2(1,2,2) = 6x_0 = 6 \times 1 = 6$$

$$m_2(1) = f_1\big(x_0 + h, y_0 + m_1(1)h, z_0 + \mathrm{hm}_1(2)\big)$$

$$= f_1(1 + 0.5, 2 + 2 \times 0.5, 2 + 6 \times 0.5)$$

$$= f_1(1.5,3,5)$$

$$= 5$$

$$m_2(2) = f_2\big(x_0 + h, y_0 + m_1(1)h, z_0 + \mathrm{hm}_1(2)\big)$$

$$= f_2(1 + 0.5, 2 + 2 \times 0.5, 2 + 6 \times 0.5)$$

$$= f_1(1.5,3,5)$$

$$= 6 \times x$$

$$= 6 \times 1.5$$

$$= 9$$

$$m(1) = \frac{m_1(1) + m_2(1)}{2} = \frac{2 + 5}{2} = 3.5$$

$$m(2) = \frac{m_1(2) + m_2(2)}{2} = \frac{6 + 9}{2} = 7.5$$

$$y(x_1) = y(1.5) = y(1) + m(1)h = 2 + 3.5 \times 0.5 = 3.75$$

$$z(x_1) = z(1.5) = z(1) + m(2)h = 2 + 7.5 \times 0.5 = 5.75$$

iteration 2 :

h=0.5, x_1=1.5, y_1=3.75, z1=5.75

$$m_1(1) = f_1(x_1, y_1, z_1) = z_1 = 5.75$$

$$m_1(2) = f_2(x_1, y_1, z_1) = 6x_1 = 6 \times 1.5 = 9$$

$$m_2(1) = f_1\left(x_1 + h, y_1 + m_1(1)h, z_1 + \mathrm{hm}_1(2)\right)$$

$$= f_1(1.5 + 0.5, 3.75 + 5.75 \times 0.5, 5.75 + 9 \times 0.5)$$

$$= f_1(2, 6.625, 10.25)$$

$$= 10.25$$

$$m_2(2) = f_2\left(x_1 + h, y_1 + m_1(1)h, z_1 + \mathrm{hm}_1(2)\right)$$

$$= f_2(1.5 + 0.5, 3.75 + 5.75 \times 0.5, 5.75 + 9 \times 0.5)$$

$$= f_1(2, 6.625, 10.25)$$

$$= 6 \times x$$

$$= 6 \times 2$$

$$= 12$$

$$m(1) = \frac{m_1(1) + m_2(1)}{2} = \frac{5.75 + 10.25}{2} = 8$$

$$m(2) = \frac{m_1(2) + m_2(2)}{2} = \frac{9 + 12}{2} = 10.5$$

$$y(x_2) = y(2) = y(1) + m(1)h = 3.75 + 8 \times 0.5 = 7.75$$

This gives B_1=7.75 which is less than B=9

Now let us assume z (1) =y' (1) =4(M_2) and again estimate y (2)

Iteration 1:

h=0.5, x_0=1, y(1)=y_0=2, z(1)=z_0=4

$$y_{i+1} = y_i + (\frac{m_1 + m_2}{2})h$$

$$m_1(1) = f_1(x_0, y_0, z_0) = f_1(1,2,4) = z_0 = 4$$

$$m_1(2) = f_2(x_0, y_0, z_0) = f_2(1,2,4) = 6x_0 = 6 \times 1 = 6$$

$$m_2(1) = f_1\big(x_0 + h, y_0 + m_1(1)h, z_0 + \mathrm{hm}_1(2)\big)$$

$$= f_1(1 + 0.5, 2 + 4 \times 0.5, 4 + 6 \times 0.5)$$

$$= f_1(1.5,4,7)$$

$$= 7$$

$$m_2(2) = f_2\big(x_0 + h, y_0 + m_1(1)h, z_0 + \mathrm{hm}_1(2)\big)$$

$$= f_2(1 + 0.5, 2 + 4 \times 0.5, 4 + 6 \times 0.5)$$

$$= f_1(1.5,4,7)$$

$$= 6 \times x$$

$$= 6 \times 1.5$$

$$= 9$$

$$m(1) = \frac{m_1(1) + m_2(1)}{2} = \frac{4 + 7}{2} = 5.5$$

$$m(2) = \frac{m_1(2) + m_2(2)}{2} = \frac{6 + 9}{2} = 7.5$$

$$y(x_1) = y(1.5) = y(1) + m(1)h = 2 + 5.5 \times 0.5 = 4.75$$

$$z(x_1) = z(1.5) = z(1) + m(2)h = 4 + 7.5 \times 0.5 = 7.75$$

iteration 2 :

h=0.5, x_1=1.5, y_1=4.75, z1=7.75

$$m_1(1) = f_1(x_1, y_1, z_1) = z_1 = 7.75$$

$$m_1(2) = f_2(x_1, y_1, z_1) = 6x_1 = 6 \times 1.5 = 9$$

$$m_2(1) = f_1\big(x_1 + h, y_1 + m_1(1)h, z_1 + \mathrm{hm}_1(2)\big)$$

$$= f_1(1.5 + 0.5, 4.75 + 7.75 \times 0.5, 7.75 + 9 \times 0.5)$$

$$= f_1(2, 8.625, 12.25)$$

$$= 12.25$$

$$m_2(2) = f_2\big(x_1 + h, y_1 + m_1(1)h, z_1 + \mathrm{hm}_1(2)\big)$$

$$= f_2(1.5 + 0.5, 4.75 + 7.75 \times 0.5, 7.75 + 9 \times 0.5)$$

$$= f_1(2, 8.625, 12.25)$$

$$= 6 \times x$$

$$= 6 \times 2$$

$$= 12$$

$$m(1) = \frac{m_1(1) + m_2(1)}{2} = \frac{7.75 + 12.25}{2} = 10$$

$$m(2) = \frac{m_1(2) + m_2(2)}{2} = \frac{9 + 12}{2} = 10.5$$

$$y(x_2) = y(2) = y(1) + m(1)h = 4.75 + 10 \times 0.5 = 9.75$$

Which is greater than B=9, now let us have the third estimate of z(1)=M_3 using the relationship

$$M_3 = M_2 - \frac{B_2 - B}{B_2 - B_1}(M_2 - M_1)$$

$$M_3 = 4 - \frac{9.75 - 9}{9.75 - 7.75}(4 - 2)$$

$$= 3.25$$

The new estimate for z(1)=y'(1)=3.25

Iteration 1:

h=0.5, x_0=1, y(1)=y_0=2, z(1)=z_0=3.25

$$y_{i+1} = y_i + (\frac{m_1 + m_2}{2})h$$

$$m_1(1) = f_1(x_0, y_0, z_0) = f_1(1,2,3.25) = z_0 = 3.25$$

$$m_1(2) = f_2(x_0, y_0, z_0) = f_2(1,2,3.25) = 6x_0 = 6 \times 1 = 6$$

$$m_2(1) = f_1\left(x_0 + h, y_0 + m_1(1)h, z_0 + \mathrm{hm}_1(2)\right)$$

$$= f_1(1 + 0.5, 2 + 3.25 \times 0.5, 3.25 + 6 \times 0.5)$$

$$= f_1(1.5, 3.625, 6.25)$$

$$= 6.25$$

$$m_2(2) = f_2\left(x_0 + h, y_0 + m_1(1)h, z_0 + \mathrm{hm}_1(2)\right)$$

$$= f_2(1 + 0.5, 2 + 3.25 \times 0.5, 3.25 + 6 \times 0.5)$$

$$= f_1(1.5, 3.625, 6.25)$$

$$= 6 \times x$$

$$= 6 \times 1.5$$

$$= 9$$

$$m(1) = \frac{m_1(1) + m_2(1)}{2} = \frac{3.25 + 6.25}{2} = 4.75$$

$$m(2) = \frac{m_1(2) + m_2(2)}{2} = \frac{6 + 9}{2} = 7.5$$

$$y(x_1) = y(1.5) = y(1) + m(1)h = 2 + 4.75 \times 0.5 = 4.375$$

$$z(x_1) = z(1.5) = z(1) + m(2)h = 3.25 + 7.5 \times 0.5 = 7.$$

iteration 2 :

h=0.5, x_1=1.5, y_1=4.375, z1=7

$$m_1(1) = f_1(x_1, y_1, z_1) = z_1 = 7$$

$$m_1(2) = f_2(x_1, y_1, z_1) = 6x_1 = 6 \times 1.5 = 9$$

$$m_2(1) = f_1\big(x_1 + h, y_1 + m_1(1)h, z_1 + \mathrm{hm}_1(2)\big)$$

$$= f_1(1.5 + 0.5, 4.375 + 7 \times 0.5, 7 + 9 \times 0.5)$$

$$= f_1(2, 7.875, 11.5)$$

$$= 11.5$$

$$m_2(2) = f_2\big(x_1 + h, y_1 + m_1(1)h, z_1 + \mathrm{hm}_1(2)\big)$$

$$= f_2(1.5 + 0.5, 4.375 + 7 \times 0.5, 7 + 9 \times 0.5)$$

$$= f_1(2, 7.875, 11.5)$$

$$= 6 \times x$$

$$= 6 \times 2$$

$$= 12$$

$$m(1) = \frac{m_1(1) + m_2(1)}{2} = \frac{7 + 11.5}{2} = 9.25$$

$$m(2) = \frac{m_1(2) + m_2(2)}{2} = \frac{9 + 12}{2} = 10.5$$

$$y(x_2) = y(2) = y(1) + m(1)h = 4.375 + 9.25 \times 0.5 = 9$$

The solution is y(1)=2, y(1.5)=4.375, y(2)=9 the exact solution is $y(x) = x^3 + 1$ and therefore y(1.5)=4.375

Practice :

1. Solve $\frac{dy}{dx} = 1 - y, y(0) = 0\ in\ the\ range\ 0 \le x \le 0.3$, using
   a. Euler's method b. Heun's method
2. Solve $\frac{dy}{dx} = y - \frac{2x}{y}, y(0) = 0\ in\ the\ range\ 0 \le x \le 0.2$, using
   b. Euler's method b. Heun's method
3. Using Runge Kutta method of fourth order solve for y(0.1), y(0.2) & y(0.3) given that $y' = xy + y^2$,y(0)=1
4. Solve the following equation by Picard's method $y'(x) = x^2 + y^2, y(0) = 0$ estimate y(0.1),y(0.2)
5. Applying shooting method to solve the boundary value problem, solve $y'' = y(x), y(0) = 0\ and\ y(1) = 1$, i.e find $y'(0)$

Chapter 6: Solution of partial differential equations

Many physical phenomena in applied science and engineering when formulated into mathematical models fall into a category of system known as partial differential equations. A partial differential equation is a differential equation involving more than one in independent variables.

We can write a second order equation involving two independent variables in general form as :

$$\frac{a\partial^2 f}{\partial x^2} + \frac{b\partial^2 f}{\partial x \partial y} + \frac{c\partial^2 f}{\partial y^2} = F(x, y, \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}) \ldots\ldots\ldots 1$$

Where a,b,c may be constant or function of x & y

The equation 1 is classified as

i. Elliptical if $b^2 - 4ac < 0$
ii. Parabolic if $b^2 - 4ac = 0$
iii. Hyperbolic if $b^2 - 4ac > 0$

Two approaches of solving PDEs are:

1. Finite difference method (where regions are regular).
2. Finite element method (where regions are irregular).

Finite difference method:

The finite difference method is based on the formula for approximating first and second order derivatives of a function. In this method derivatives that occurs in partial differential equation are replaced by their finite difference equivalents. The difference equation is then written for each grid points using function values at the surrounding grid points. Solving these equations simultaneously give the values of the function of each grid points.

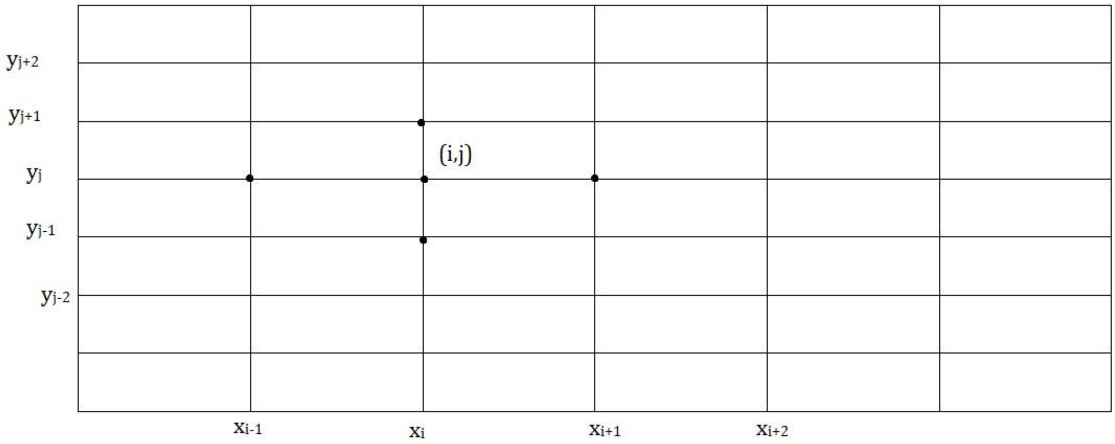


Figure: two-dimensional finite difference grid

$$x_{i+1} = x_i + h$$

$$y_{i+1} = y_i + h$$

We have already discussed that if the function f(x) has a continuous fourth derivative, then it's first and second derivatives are given by the following central difference approximation.

$$f'(x_i) = \frac{f(x_i + h) - f(x_i - h)}{2h}$$

$$f'_i = \frac{f_{i+1} - f_{i-1}}{2h} \quad ....2$$

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

$$f''_i = \frac{f_{i+1} - 2f_i - f_{i-1}}{h^2} \quad ....3$$

The subscripts on f indicate the x value at which the function is evaluated. When f is a function of two variables x and y, the partial derivatives of f with respect x or y are the ordinary derivatives of f with respect to x or y when y or x does not change. We can use the equations 2 and 3 in the x direction to determine derivatives with respect to x and in the y direction to determine derivatives with respect to y. thus we have

$$\frac{\partial f(x_i, y_j)}{\partial x} = f_x(x_i, y_j) = \frac{f(x_{i+1}, y_j) - f(x_{i-1}, y_j)}{h}$$

$$\frac{\partial f(x_i, y_j)}{\partial y} = f_y(x_i, y_j) = \frac{f(x_i, y_{j+1}) - f(x_i, y_{j-1})}{k}$$

$$\frac{\partial^2 f(x_i, y_j)}{\partial x^2} = f_{xx}(x_i, y_j) = \frac{f(x_{i+1}, y_j) - 2f(x_i, y_j) + f(x_{i-1}, y_j)}{h^2}$$

$$\frac{\partial^2 f(x_i, y_j)}{\partial y^2} = f_{yy}(x_i, y_j) = \frac{f(x_i, y_{j+1}) - 2f(x_i, y_j) + f(x_i, y_{j-1})}{k^2}$$

$$\frac{\partial^2 f(x_i, y_j)}{\partial x \partial y} = \frac{f(x_{i+1}, y_{j+1}) - f(x_{i+1}, y_{j-1}) - f(x_{i-1}, y_{j+1}) + f(x_{i-1}, y_{j-1})}{4hk}$$

It would be convenient to use double subscripts i,j on f to indicate x and y values. Then above equation become

$$f_{x,i,j} = \frac{f_{i+1,j} - f_{i-1,j}}{h}$$

$$f_{y,i,j} = \frac{f_{i,j+1} - f_{i,j-1}}{k}$$

$$f_{xx,i,j} = \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{h^2}$$

$$f_{yy,i,j} = \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{k^2}$$

$$f_{xy,i,j} = \frac{f_{i+1,j+1} - f_{i+1,j-1} - f_{i-1,j+1} + f_{i-1,j-1}}{2hk}$$

We will use these finite difference equivalents of the partial derivatives to construct various types of differential equations.

Elliptical equations

Elliptical equations are governed by condition on the boundary of closed domain. We consider here the two most commonly encountered elliptical equations.

a. Laplace’s equation

b. Poisson's equation

Laplace's equation

Any equation of the form $\nabla^2 f = 0$ is called laplace's equation, where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \ldots\ldots 4$$

$$\therefore \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = \nabla^2 f = 0 \ldots\ldots 5$$

Where a=1,b=0,c=1 and F(x,y,$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}$)=0

Where ∇^2 is called Laplacian operator, above equation can be written as

$$U_{xx} + U_{yy} = 0$$

Replacing the second order derivatives by their finite difference equivalents, at points (x_i, y_i) we get

$$\nabla^2 f_{ij} = \frac{f_{i+1,j} - 2f_{ij} + f_{i-1,j}}{h^2} + \frac{f_{i,j+1} - 2f_{ij} + f_{i,j-1}}{k^2} = 0 \ldots\ldots 6$$

If we assume for simplicity, h=k, then we get

$$\nabla^2 f_{ij} = \frac{f_{i+1,j} - 2f_{ij} + f_{i-1,j}}{h^2} + \frac{f_{i,j+1} - 2f_{ij} + f_{i,j-1}}{h^2}$$

$$\nabla^2 f_{ij} = \frac{f_{i+1,j} + f_{i-1,j} - 4f_{ij} + f_{i,j+1} + f_{i,j-1}}{h^2} \ldots\ldots 7$$

$$f_{i+1,j} + f_{i-1,j} - 4f_{ij} + f_{i,j+1} + f_{i,j-1} = 0$$

This is called Laplace's equation

Above equation contains four neighboring points around central points (x_i, y_i) as shown in figure, the above equation is known as five point difference formula for Laplace's equation.

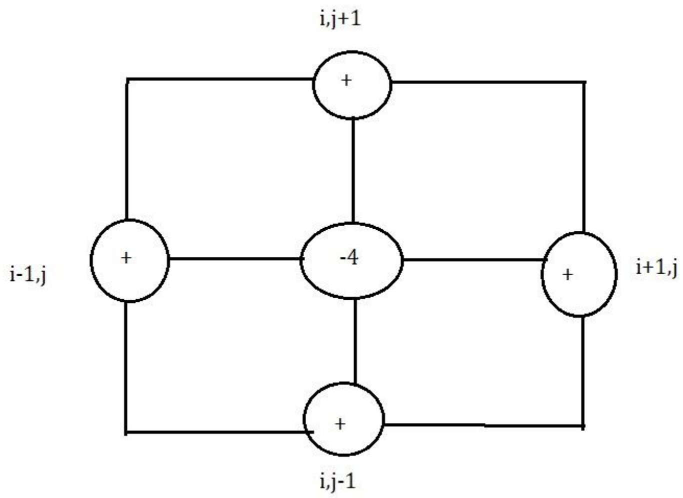


figure: Grid for Laplace equation

we can also represent the relationship of pivotal values pictorially as below.

$$\nabla^2 f_{ij} = \frac{1}{h^2}\begin{Bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{Bmatrix} f_{ij} = 0 \ldots\ldots .8$$

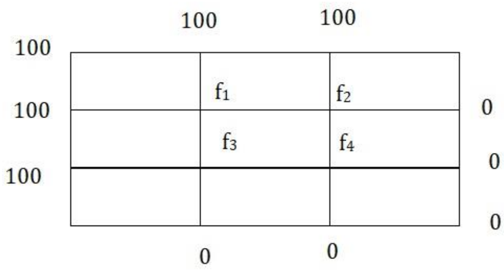
From above equation we can show that the function value at grid point(x_i, y_i) is the average of the values at the four adjoining points. i.e

$f_{ij} = \frac{1}{4}(f_{i+1,j} + f_{i-1,j} + f_{i,j+1} + f_{i,j-1}) \ldots\ldots .9$

To evaluate numerically the solution of Laplace equation at the grid points we can apply equation 9 at the grid points where f_{ij} is required thus obtaining a system of linear equations in the pivotal values of f_{ij}. The system of linear equations may be solved using either direct or iterative methods.

Example: Consider a steel plate of size 15cm x 15cm, if two of the sides are held at 100°c and other two sides are held at 0°c, what are the steady state temperatures at interior points assuming a grid of size 5cm x 5cm.

Note: A problem with values known on each boundary is said to have Dirichlet boundary condition. This problem is illustrated below.



The system of equation is as follows:

Point 1:

$$100 + 100 + f_3 + f_2 - 4f_1 = 0 \ldots\ldots..1$$

Point 2:

$$f_1 + 100 + f_4 + 0 - 4f_2 = 0 \ldots\ldots.2$$

Point 3:

$$100 + f_1 + 0 + f_4 - 4f_3 = 0 \ldots\ldots.3$$

Point 4:

$$f_3 + f_2 + 0 + 0 - 4f_4 = 0 \ldots\ldots.4$$

On solving above four equations we get the values as:

$$f_1 = 75, f_2 = 50, f_3 = 50, f_4 = 25$$

So we can see the interior temperature points as above.

Note: for solving use any iterative methods that you have learned in chapter 4.

Poisson's equation

If we put a=1, b=0, c=1 in the equation and F(x,y,f,f_x, f_y)=g(x,y) then

$$\frac{a\partial^2 f}{\partial x^2} + \frac{b\partial^2 f}{\partial x\partial y} + \frac{c\partial^2 f}{\partial y^2} = F\left(x, y, \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right)$$

We get

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

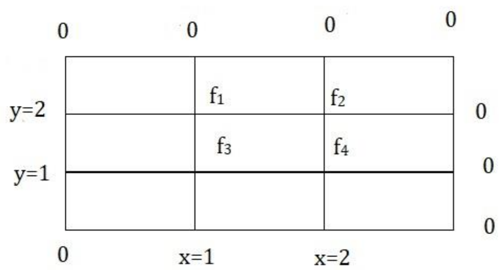
$$\nabla^2 f = g(x, y) \ldots \ldots . . a$$

The above equation a is called poisson's equation using the notation $g_{ij} = g(x_i, y_i)$ and laplace equation may be modified to solve the equation a. the finite difference formula for solving poisson's equation then takes of the form

$$f_{i+1,j} + f_{i-1,j} + f_{i,j+1} + f_{i,j-1} - 4f_{ij} = h^2 g_{ij} \ \ldots \ldots . . b$$

Example: Solve the poisson's equation $\nabla^2 f = 2x^2y^2$ over the square domain $0 \leq x \leq 3$ & $0 \leq y \leq 3$ with f=0 on the boundary and h=1.

The domain is divided into squares of one unit size as in figure.



By applying equations b at each grid points

Point 1:

$$0 + 0 + f_3 + f_2 - 4f_1 = 1^2 g(1,2)$$

$$f_2 + f_3 - 4f_1 = 2x1^2x2^2$$

$$f_2 + f_3 - 4f_1 = 8 \ldots\ldots\ldots 1$$

Point 2:

$$f_1 + 0 + 0 + f_4 - 4f_2 = 1^2 g(2,2)$$

$$f_1 + f_4 - 4f_2 = 2x2^2x2^2$$

$$f_1 - 4f_2 + f_4 = 32 \ldots\ldots\ldots 2$$

Point 3:

$$0 + f_1 + 0 + f_4 - 4f_3 = 1^2 g(1,1)$$

$$f_1 + f_4 - 4f_3 = 2x1^2x1^2$$

$$f_1 - 4f_3 + f_4 = 2 \ldots\ldots\ldots 3$$

Point 4:

$$f_3 + f_2 + 0 + 0 - 4f_4 = 1^2 g(2,1)$$

$$f_2 + f_3 - 4f_4 = 2x2^2$$

$$f_2 + f_3 - 4f_4 = 8 \ldots\ldots\ldots 4$$

On solving we get

$$f_1 = -\frac{22}{4}, f_2 = -\frac{43}{4}, f_3 = -\frac{13}{4}, f_4 = -\frac{22}{4}$$

Therefore the interior points are as above.

Note: we can use any problem-solving methods already discussed for solving the values of fi

Parabolic equations

Elliptical equations studies previously described problems that are time independent, such problems are known as steady state problems, but we come across problems that are not steady state. This means that the function is dependent on both space and time. Parabolic equations for which $b^2 - 4ac = 0$, describes the problem that depend on space and time variables.

A popular case for parabolic type of equation is the study of heat flow in one-dimensional direction in an insulated rod, such problems are governed by both boundary and initial conditions.

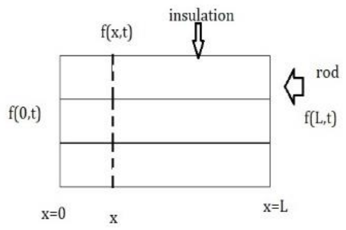


Figure : heat flow in a rod

Let f represent the temperature at any points in rod, whose distance from left end is x. Heat is flowing from left to right under the influence of temperature gradient. The temperature f(x,t) in the at position x and time t governed by the heat equation.

$$k_1 \frac{\partial f}{\partial x^2} = k_2 k_3 \frac{\partial f}{\partial t} \dots \dots . . a$$

Where $k_1$is coefficient of thermal conductivity, k_2 is the specific heat and k_3 is density of the material.

Equation a can be simplified as

$$k f_{xx}(x,t) = f_t(x,t) \dots \dots . b$$

Where $k = \frac{k_1}{k_2 k_3}$

The initial condition will be the initial temperatures at all points along the rod .

$$f(x,0) = f(x)\ 0 \le x \le L$$

The boundary conditions f(0,t) and f(L,t) describes the temperature at each end of the rod as function of time, if they are held at constant then

$$f(0,t) = c_1 0 \le t \le \infty$$

$$f(L,t) = c_2\ 0 \le t \le \infty$$

solution of heat equation

we can solve the heat equation in equation using the finite difference formula given below.

$$f_t(x,t) = \frac{f(x,t+\tau) - f(x,t)}{\tau}$$

$$= \frac{1}{\tau}\left(f_{i,j+1} - f_{i,j}\right) \dots \dots . c$$

$$f_{xx}(x,t) = \frac{f(x-h,t) - 2f(x,t) + f(x+h,t)}{h^2}$$

$$= \frac{1}{h^2}\left(f_{i-1,j} - 2f_{i,j} + f_{i+1,j}\right) \dots \dots d$$

Substituting c and d in equation b we can obtain

$$\frac{1}{\tau}\left(f_{i,j+1} - f_{i,j}\right) = \frac{k}{h^2}\left(f_{i-1,j} - 2f_{ij} + 2f_{i+1,j}\right) \dots \dots e$$

Solving for $f_{i,j+1}$

$$f_{i,j+1} = \left(1 - \frac{2\tau k}{h^2}\right) f_{ij} + \frac{\tau k}{h^2}\left(f_{i-1,j} + f_{i+1,j}\right)$$
$$= (1 - 2\gamma) f_{ij} + \gamma\left(f_{i-1,j} + f_{i+1,j}\right) \dots . . f$$

Where $\gamma = \frac{\tau k}{h^2}$

Bender Schmidt method

The recurrence of equation allows us to evaluate f at each point x and at any point t. if we choose step size Δt & Δx, such that

$$1 - 2\gamma = 1 - \frac{2\tau k}{h^2} = 0 \ \ldots\ldots g$$

Equation f simplifies to

$$f_{i,j+1} = \frac{1}{2}\left(f_{i+1,j} + f_{i-1,j}\right) \ldots\ldots h$$

Equation h is known as Bender Schmidt recurrence equation. This equation determines the value of f at $x = x_i$, at time $t = t_i + \tau$ as the average of the values right and left of x_i at time t_j.

Note that the step size in Δt obtained from equation g.

$$\tau = \frac{h^2}{2k}$$

Gives the equation h , equation f is stable if and only if the we step size τ satisfies the condition

$$\tau \leq \frac{h^2}{2k}$$

Example : Solve the parabolic equation $2f_{xx}(x,t) = f_t(x,t)$, given the initial condition

$$f(x,0) = 50(4 - x) \ \ 0 \leq x \leq 4$$

And boundary conditions

$$f(0,t) = 0$$

$$f(4,t) = 0, \quad 0 \leq t \leq 1.5$$

Solution

If we assume $\Delta x = h = 1, \Delta t = \tau$ (using Bender Schmidt method)

$$\tau \leq \frac{h^2}{2k} = \frac{1^2}{2x2} = 0.25$$

Taking $\tau = 0.25$, we have

$$f_{i,j+1} = \frac{1}{2}\left(f_{i-1,j} + f_{i+1,j}\right)$$

From the initial boundary condition : $f(0,t) = 0$ or, f(0,j) =0 for all values of j.
i.e. $f(0,0) = 0$

$f(0,1) = 0$

$f(0,2) = 0$

$f(0,3) = 0$

$f(0,4) = 0$

$f(0,5) = 0$

$f(0,6) = 0$

From the final boundary condition: $f(4,t) = 0$ or $f(4,j) = 0$ for all values of j.

$$f(4,0) = 0$$

$$f(4,1) = 0$$

$$f(4,2) = 0$$

$$f(4,3) = 0$$

$$f(4,4) = 0$$

Now, again from the given initial condition:

$$f(x,0) = 50(4 - x)$$

Or, $f(i,0) = 50(4 - i)$ for all values of i.

$$f(1,0) = 50(4 - 1) = 150$$

$$f(2,0) = 50(4 - 2) = 100$$

$$f(3,0) = 50(4 - 3) = 50$$

Now, again from Bender Schmidt recursive formula,

$f_{i,j+1} = \frac{1}{2}\left(f_{i-1,j} + f_{i+1,j}\right)$ ………(A)

Put j=0 in (A) we get,

$f_{i,1} = \frac{1}{2}\left(f_{i-1,0} + f_{i+1,0}\right)$……….(B)

Put i=1, 2, 3 respectively in (B) we get,

$f_{1,1} = \frac{1}{2}\left(f_{0,0} + f_{2,0}\right)=\frac{1}{2}(0 + 100)=50$

$f_{2,1} = \frac{1}{2}\left(f_{1,0} + f_{3,0}\right)=\frac{1}{2}(150 + 50)=100$

$f_{3,1} = \frac{1}{2}\left(f_{2,0} + f_{4,0}\right)=\frac{1}{2}(100 + 0)=50$

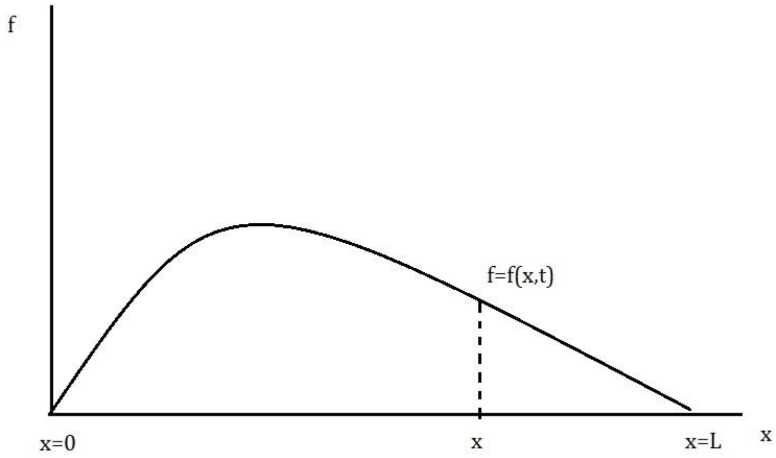
Again take j=1 and i= 1.2, 3 respectively to find $f_{1,2}$ $f_{2,2}f_{3,2}$ and take j=2, j=3, j=4 and j=6 and find the corresponding values for i=1, i=2 and i=3 for each 'j' .

Using the formula we can generate successfully f(x,t). the estimated are recorded in the following table at each interior point, the temperature at any single point is just average of the values at the adjacent points of the previous points.

x / t	0 (i=0)	1(i=1)	2 (i=2)	3(i=3)	4(i=4)
0.00(j=0)	0	150	100	50	0
0.25 (j=1)	0	50($f_{1,1}$)	100($f_{2.1}$)	50($f_{3,1}$)	0
0.50(j=2)	0	50	50	50	0
0.75 (j=3)	0	25	50	25	0
1.00(j=4)	0	25	25	25	0

Hyperbolic equation

Hyperbolic equation models the vibration of structure such as building beams and machines we here consider the case of a vibrating string that is fixed at both the ends as figure.



The lateral displacement of string f varies with time t and distance x along the string. The displacement f(x,t) is governed by the wave equation

$$T\frac{\partial^2 f}{\partial x^2} = \rho\frac{\partial^2 f}{\partial t^2}$$

Where T is the tension in the string and ρ is the mass per unit length.

Hyperbolic problems are governed by both boundary and initial conditions, if time is one of the independent variables. Two boundary conditions are the vibrating string problems under consideration are

$$f(0,t) = 0, \quad 0 \le t \le b$$

$$f(L,t) = 0, \quad 0 \le t \le b$$

Two initial conditions are:

$$f(x,0) = f(x), 0 \le t \le \alpha$$

$$f_t(x,0) = g(x), 0 \le t \le a$$

Solution hyperbolic equations

The domain of interest $0 \le t \le a \; and \; 0 \le t \le b$ is partitioned as shown in figure, the rectangle size is $\Delta x = h, \Delta t = \tau$

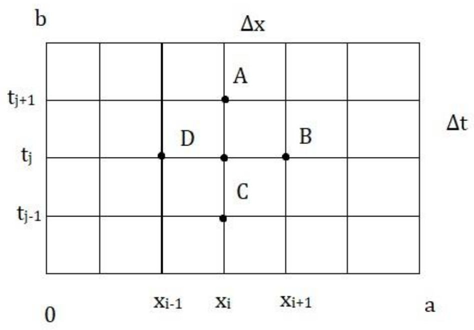


Figure : Grid for solving hyperbolic equation

The difference equation for $f_{xx}(x,t)$ *and* $f_{tt}(x,t)$ are

$$f_{xx}(x,t) = \frac{f(x-h,t) - 2f(x,t) + f(x+h,t)}{h^2}$$

$$f_{tt}(x,t) = \frac{f(x,t-\tau) - 2f(x,t) + f(x,t+\tau)}{\tau^2}$$

This implies that

$$T\frac{f_{i-1,j} - 2f_{ij} + f_{i+1,j}}{h^2} = \rho\frac{f_{i,j-1} - 2f_{ij} + f_{i,j+1}}{\tau^2}$$

Solving this for $f_{i,j+1}$, we obtain

$$f_{i,j+1} = -f_{i,j-1} + 2\left(1 - \frac{T\tau^2}{\rho h^2}\right)f_{ij} + \frac{T\tau^2}{\rho h^2}\left(f_{i+1,j} + f_{i-1,j}\right)$$

If we make $1 - \frac{T\tau^2}{\rho h^2} = 0$

Then we have

$$f_{i,j+1} = -f_{i,j-1} + f_{i+1,j} + f_{i-1,j} \;\;\dots\dots\dots d$$

The values of f at $x = x_i$ and $t = t_j + \tau$ is equal to the um of the values of f, at the point $x = x_i - h$ and $x = x_i + h$ at the time $t = t_j(previous\ time)$ minus the value of f at $x = x_i$ at time $t = t_j - \tau$. From figure we can say $f_A = f_B + f_D - f_C$

Starting values

We need two rows of starting values, corresponding to j=1 and j=2, in order to computer the values of the third row. First row is obtained using the condition.

$$f(x,0) = f(x)$$

The 2nd row can be obtained using the 2nd initial condition as $f_t(x,0) = g(x)$

We know that

$$f_t(x,0) = \frac{f_{i,0+1} - f_{i,0-1}}{2\tau} = g_i$$

$$f_{i,-1} = f_{i,1} - 2\tau g_i\ for\ t = 0\ only$$

Substituting this in equation d, we get for $t = t_1$

$$f_{i,1} = \frac{1}{2}\left(f_{i+1,0} + f_{i-1,0}\right) + \tau g_i\ \dots\dots.e$$

In many cases $g(x_i) = 0$ then we have

$$f_{i,1} = \frac{1}{2}\left(f_{i+1,0} + f_{i-1,0}\right)$$

Example: Solve numerically the wave equation

$$f_{tt}(x,t) = 4f_{xx}(x,t) 0 \le x \le 5\ \&\ 0 \le t \le 2.5$$

With boundary condition

$$f(0,t) = 0\ \ and f(5,t) = 0$$

And initial values

$$f(x,0) = f(x) = x(5-x)$$

$$f_t(x,0) = g(x) = 0$$

Solution

Let h=1

Given $\frac{T}{\rho} = 4$

Assuming $1 - 4\frac{\tau^2}{1^2} = 0$

We get

$$\tau = \frac{1}{2}$$

The values estimated using equations d and e

x \ t	0	1	2	3	4	5
0.0	0	4	6	6	4	0
0.5	0	3 *	5 **	5	3	0
1.0	0	1	2	2	1	0
1.5	0	-1***	-2	-2	-1	0
2.0	0	-3	-5	-5	-3	0
2.5	0	-4	-6	-6	-4	0

$* = \frac{0+6}{2}$ $** = \frac{4+6}{2}$ $*** = 2+0-3$

Chapter 6: Solution of partial differential equations

Many physical phenomena in applied science and engineering when formulated into mathematical models fall into a category of system known as partial differential equations. A partial differential equation is a differential equation involving more than one in independent variables.

We can write a second order equation involving two independent variables in general form as :

$$\frac{a\partial^2 f}{\partial x^2} + \frac{b\partial^2 f}{\partial x \partial y} + \frac{c\partial^2 f}{\partial y^2} = F(x, y, \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}) \ldots\ldots\ldots 1$$

Where a,b,c may be constant or function of x & y

The equation 1 is classified as

iv. Elliptical if $b^2 - 4ac < 0$
v. Parabolic if $b^2 - 4ac = 0$
vi. Hyperbolic if $b^2 - 4ac > 0$

Two approaches of solving are

3. Finite difference method (where regions are regular)
4. Finite element method (where regions are irregular)

Finite difference method

The finite difference method is based on the formula for approximating first and second order derivatives of a function. In this method derivatives that occurs in partial differential equation are replaced by their finite difference equivalents. The difference equation is then written for each grid points using function values at the surrounding grid points. Solving these equations simultaneously give the values of the function of each grid points.

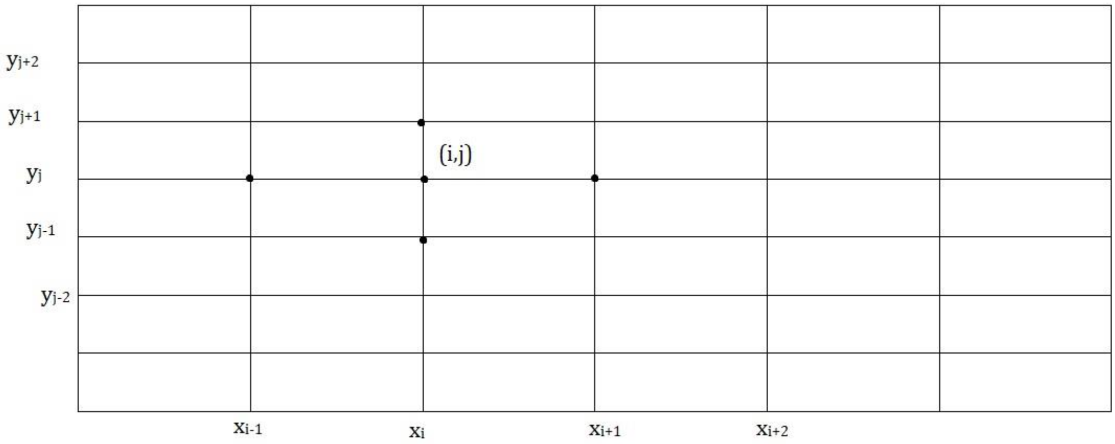


Figure: two-dimensional finite difference grid

$$x_{i+1} = x_i + h$$

$$y_{i+1} = y_i + h$$

We have already discussed that if the function f(x) has a continuous fourth derivative, then it's first and second derivatives are given by the following central difference approximation.

$$f'(x_i) = \frac{f(x_i + h) - f(x_i - h)}{2h}$$

$$f'_i = \frac{f_{i+1} - f_{i-1}}{2h} \quad \ldots\ldots\ldots 2$$

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

$$f''_i = \frac{f_{i+1} - 2f_i - f_{i-1}}{h^2} \quad \ldots\ldots\ldots 3$$

The subscripts on f indicate the x value at which the function is evaluated. When f is a function of two variables x and y, the partial derivatives of f with respect x or y are the ordinary derivatives of f with respect to x or y when y or x does not change. We can use the equations 2 and 3 in the x direction to determine derivatives with respect to x and in the y direction to determine derivatives with respect to y. thus we have

$$\frac{\partial f(x_i, y_j)}{\partial x} = f_x(x_i, y_j) = \frac{f(x_{i+1}, y_j) - f(x_{i-1}, y_j)}{2h}$$

$$\frac{\partial f(x_i, y_j)}{\partial y} = f_y(x_i, y_j) = \frac{f(x_i, y_{j+1}) - f(x_i, y_{j-1})}{2k}$$

$$\frac{\partial^2 f(x_i, y_j)}{\partial x^2} = f_{xx}(x_i, y_j) = \frac{f(x_{i+1}, y_j) - 2f(x_i, y_j) + f(x_{i-1}, y_j)}{h^2}$$

$$\frac{\partial^2 f(x_i, y_j)}{\partial y^2} = f_{yy}(x_i, y_j) = \frac{f(x_i, y_{j+1}) - 2f(x_i, y_j) + f(x_i, y_{j-1})}{k^2}$$

$$\frac{\partial^2 f(x_i, y_j)}{\partial x \partial y} = \frac{f(x_{i+1}, y_{j+1}) - f(x_{i+1}, y_{j-1}) - f(x_{i-1}, y_{j+1}) + f(x_{i-1}, y_{j-1})}{4hk}$$

It would be convenient to use double subscripts i,j on f to indicate x and y values. Then above equation become

$$f_{x,i,j} = \frac{f_{i+1,j} - f_{i-1,j}}{h}$$

$$f_{y,i,j} = \frac{f_{i,j+1} - f_{i,j-1}}{k}$$

$$f_{xx,i,j} = \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{h^2}$$

$$f_{yy,i,j} = \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{k^2}$$

$$f_{xy,i,j} = \frac{f_{i+1,j+1} - f_{i+1,j-1} - f_{i-1,j+1} + f_{i-1,j-1}}{2hk}$$

We will use these finite difference equivalents of the partial derivatives to construct various types of differential equations.

Elliptical equations

Elliptical equations are governed by condition on the boundary of closed domain. We consider here the two most commonly encountered elliptical equations.

c. Laplace's equation

d. Poisson's equation

Laplace's equation

Any equation of the form $\nabla^2 f = 0$ is called laplace's equation, where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \ldots\ldots 4$$

$$\therefore \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = \nabla^2 f = 0 \ldots\ldots 5$$

Where a=1,b=0,c=1 and F(x,y,$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}$)=0

Where ∇^2 is called Laplacian operator, above equation can be written as

$$U_{xx} + U_{yy} = 0$$

Replacing the second order derivatives by their finite difference equivalents, at points (x_i, y_i) we get

$$\nabla^2 f_{ij} = \frac{f_{i+1,j} - 2f_{ij} + f_{i-1,j}}{h^2} + \frac{f_{i,j+1} - 2f_{ij} + f_{i,j-1}}{k^2} = 0 \ldots\ldots 6$$

If we assume for simplicity, h=k, then we get

$$\nabla^2 f_{ij} = \frac{f_{i+1,j} - 2f_{ij} + f_{i-1,j}}{h^2} + \frac{f_{i,j+1} - 2f_{ij} + f_{i,j-1}}{h^2}$$

$$\nabla^2 f_{ij} = \frac{f_{i+1,j} + f_{i-1,j} - 4f_{ij} + f_{i,j+1} + f_{i,j-1}}{h^2} \ldots\ldots 7$$

$$f_{i+1,j} + f_{i-1,j} - 4f_{ij} + f_{i,j+1} + f_{i,j-1} = 0$$

This is called Laplace's equation

Above equation contains four neighboring points around central points (x_i, y_i) as shown in figure, the above equation is known as five point difference formula for Laplace's equation.

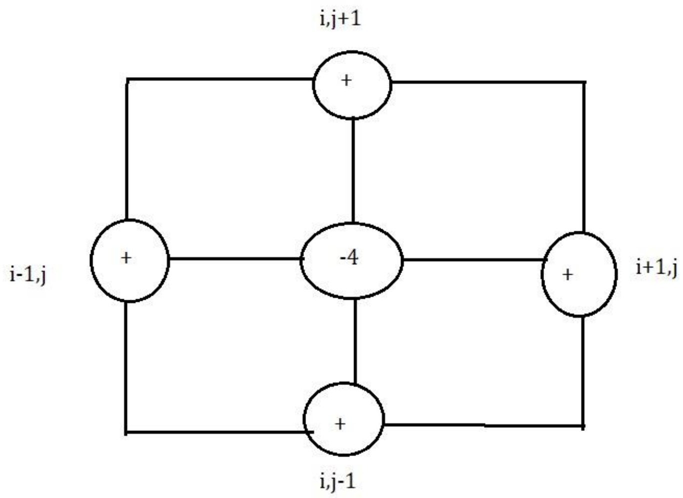


figure: Grid for Laplace equation

we can also represent the relationship of pivotal values as,

$$\nabla^2 f_{ij} = \frac{1}{h^2}\begin{Bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{Bmatrix} f_{ij} = 0 \ldots\ldots. 8$$

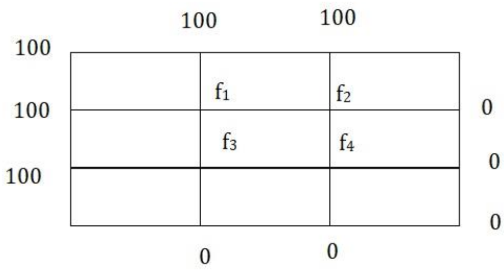
From above equation we can show that the function value at grid point(x_i, y_i) is the average of the values at the four adjoining points. i.e

$f_{ij} = \frac{1}{4}(f_{i+1,j} + f_{i-1,j} + f_{i,j+1} + f_{i,j-1}) \ldots\ldots. 9$

To evaluate numerically the solution of Laplace equation at the grid points we can apply equation 9 at the grid points where f_{ij} is required thus obtaining a system of linear equations in the pivotal values of f_{ij}. The system of linear equations may be solved using either direct or iterative methods.

Example: Consider a steel plate of size 15cm x 15cm, if two of the sides are held at 100°c and the other two sides are held at 0°c. What are the steady state temperatures at interior points(nodes) assuming a grid of 5cm x 5cm.

Note: a problem with values known on each boundary is said to have Dirichlet boundary condition. This problem is illustrated below.



The system of equation is as follows

Point 1:

$$100 + 100 + f_3 + f_2 - 4f_1 = 0 \ldots \ldots ..1$$

Point 2:

$$f_1 + 100 + f_4 + 0 - 4f_2 = 0 \ldots \ldots ..2$$

Point 3:

$$100 + f_1 + 0 + f_4 - 4f_3 = 0 \ldots \ldots ..3$$

Point 4:

$$f_3 + f_2 + 0 + 0 - 4f_4 = 0 \ldots \ldots ..4$$

On solving above four equations we get the values as:

$$f_1 = 75, f_2 = 50, f_3 = 50, f_4 = 25$$

So we can see the interior temperature points as above.

Note: for solving use any methods that have learned in before chapters.

Poisson's equation

If we put a=1, b=0, c=1 in the equation and F(x,y,f,f_x, f_y)=g(x,y) then

$$\frac{a\partial^2 f}{\partial x^2} + \frac{b\partial^2 f}{\partial x\partial y} + \frac{c\partial^2 f}{\partial y^2} = F\left(x, y, \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right)$$

We get

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

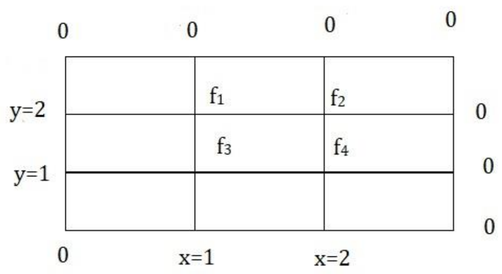
$$\nabla^2 f = g(x, y) \dots \dots . . a$$

The above equation a is called poisson's equation using the notation $g_{ij} = g(x_i, y_i)$ and laplace equation may be modified to solve the equation a. the finite difference formula for solving poisson's equation then takes of the form

$$f_{i+1,j} + f_{i-1,j} + f_{i,j+1} + f_{i,j-1} - 4f_{ij} = h^2 g_{ij} \dots \dots . . b$$

Example: Solve the poisson's equation $\nabla^2 f = 2x^2y^2$ over the square domain $0 \leq x \leq 3$ & $0 \leq y \leq 3$ with f=0 on the boundary and h=1.

The domain is divided into squares of one unit size as in figure.



By applying equations b at each grid points

Point 1:

$$0 + 0 + f_3 + f_2 - 4f_1 = 1^2 g(1,2)$$

$$f_2 + f_3 - 4f_1 = 2x1^2x2^2$$

$$f_2 + f_3 - 4f_1 = 8 \ldots\ldots\ldots 1$$

Point 2:

$$f_1 + 0 + 0 + f_4 - 4f_2 = 1^2 g(2,2)$$

$$f_1 + f_4 - 4f_2 = 2x2^2x2^2$$

$$f_1 - 4f_2 + f_4 = 32 \ldots\ldots\ldots 2$$

Point 3:

$$0 + f_1 + 0 + f_4 - 4f_3 = 1^2 g(1,1)$$

$$f_1 + f_4 - 4f_3 = 2x1^2x1^2$$

$$f_1 - 4f_3 + f_4 = 2 \ldots\ldots\ldots 3$$

Point 4:

$$f_3 + f_2 + 0 + 0 - 4f_4 = 1^2 g(2,1)$$

$$f_2 + f_3 - 4f_4 = 2x2^2$$

$$f_2 + f_3 - 4f_4 = 8 \ldots\ldots\ldots 4$$

On solving we get

$$f_1 = -\frac{22}{4}, f_2 = -\frac{43}{4}, f_3 = -\frac{13}{4}, f_4 = -\frac{22}{4}$$

Therefore the interior points are as above.

Note: we can use any problem-solving methods already discussed for solving the values of fi

Parabolic equations

Elliptical equations studies previously described problems that are time independent, such problems are known as steady state problems, but we come across problems that are not steady state. This means that the function is dependent on both space and time. Parabolic equations for which $b^2 - 4ac = 0$, describes the problem that depend on space and time variables.

A popular case for parabolic type of equation is the study of heat flow in one-dimensional direction in an insulated rod, such problems are governed by both boundary and initial conditions.

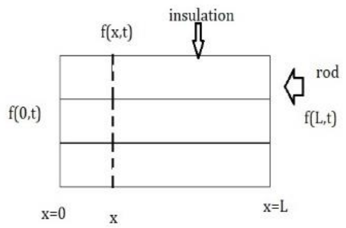


Figure : heat flow in a rod

Let f represent the temperature at any points in rod, whose distance from left end is x. Heat is flowing from left to right under the influence of temperature gradient. The temperature f(x,t) in the at position x and time t governed by the heat equation.

$$k_1 \frac{\partial f}{\partial x^2} = k_2 k_3 \frac{\partial f}{\partial t} \dots \dots . . a$$

Where $k_1$is coefficient of thermal conductivity, k_2 is the specific heat and k_3 is density of the material.

Equation a can be simplified as

$$k f_{xx}(x,t) = f_t(x,t) \dots \dots . b$$

Where $k = \frac{k_1}{k_2 k_3}$

The initial condition will be the initial temperatures at all points along the rod .

$$f(x,0) = f(x)\ 0 \le x \le L$$

The boundary conditions f(0,t) and f(L,t) describes the temperature at each end of the rod as function of time, if they are held at constant then

$$f(0,t) = c_1 0 \le t \le \infty$$

$$f(L,t) = c_2\ 0 \le t \le \infty$$

solution of heat equation

we can solve the heat equation in equation using the finite difference formula given below.

$$f_t(x,t) = \frac{f(x,t+\tau) - f(x,t)}{\tau}$$

$$= \frac{1}{\tau}\left(f_{i,j+1} - f_{i,j}\right) \dots \dots .c$$

$$f_{xx}(x,t) = \frac{f(x-h,t) - 2f(x,t) + f(x+h,t)}{h^2}$$

$$= \frac{1}{h^2}\left(f_{i-1,j} - 2f_{i,j} + f_{i+1,j}\right) \dots \dots d$$

Substituting c and d in equation b we can obtain

$$\frac{1}{\tau}\left(f_{i,j+1} - f_{i,j}\right) = \frac{k}{h^2}\left(f_{i-1,j} - 2f_{ij} + 2f_{i+1,j}\right) \dots \dots e$$

Solving for $f_{i,j+1}$

$$f_{i,j+1} = \left(1 - \frac{2\tau k}{h^2}\right) f_{ij} + \frac{\tau k}{h^2}\left(f_{i-1,j} + f_{i+1,j}\right)$$
$$= (1-2\gamma) f_{ij} + \gamma\left(f_{i-1,j} + f_{i+1,j}\right) \dots \dots f$$

Where $\gamma = \frac{\tau k}{h^2}$

Bender Schmidt method

The recurrence of equation allows us to evaluate f at each point x and at any point t. if we choose step size Δt & Δx, such that

$$1 - 2\gamma = 1 - \frac{2\tau k}{h^2} = 0 \quad \dots \dots g$$

Equation f simplifies to

$$f_{i,j+1} = \frac{1}{2}\left(f_{i+1,j} + f_{i-1,j}\right) \dots \dots . h$$

Equation h is known as Bender Schmidt recurrence equation. This equation determines the value of f at $x = x_i$, at time $t = t_i + \tau$ as the average of the values right and left of x_i at time t_j.

Note that the step size in Δt obtained from equation g.

$$\tau = \frac{h^2}{2k}$$

Gives the equation h , equation f is stable if and only if the we step size τ satisfies the condition

$$\tau \leq \frac{h^2}{2k}$$

Example: Solve the equation $2f_{xx}(x,t) = f_t(x,t)$ *and* given the initial condition:

$$f(x,0) = 50(4 - x) \quad 0 \leq x \leq 4$$

And boundary conditions:

$$f(0,t) = 0,$$

$$f(4,t) = t + 1, \quad 0 \leq t \leq 1.5$$

Solution

If we assume $\Delta x = h = 1, \Delta t = \tau$ (using Bender Schmidt method)

$$\tau \leq \frac{h^2}{2k} = \frac{1^2}{2x2} = 0.25$$

Taking $\tau = 0.25$, we have

$$f_{i,j+1} = \frac{1}{2}\left(f_{i-1,j} + f_{i+1,j}\right)$$

Using the formula we can generate successfully f(x,t). the estimated are recorded in the following table at each interior point, the temperature at any single point is just average of the values at the adjacent points of the previous points.

X(i) / t (j)	0	1	2	3	4
0.00(0)	0	150	100	50	0
0.25(1)	0	50($f_{1,1}$)	100	50	0
0.50(2)	0	50	50	50	0
0.75	0	25	25	25	0
1.00	0	12.5	25	12.5	0
1.25	0	12.5	12.5	12.5	0
1.50	0	6.25	12.5	6.25	0

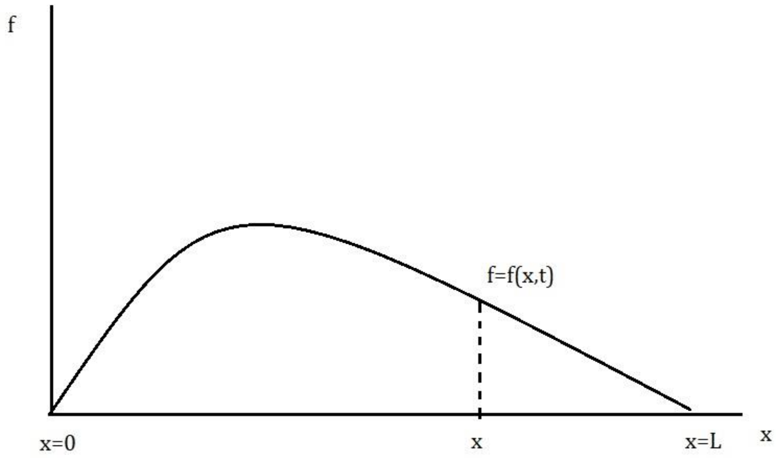
f(0,t) =0 , f(0,j)=0 for all values of j.

Again from the given final boundary condition: f(4,t) =0 , f(4,j)=0 for all values of j.

Also from the given initial condition: $f(i,0) = 50(4-i)$ for all values of i.

Hyperbolic equation

Hyperbolic equation models the vibration of structure such as building beams and machines we here consider the case of a vibrating string that is fixed at both the ends as figure.



The lateral displacement of string f varies with time t and distance x along the string. The displacement f(x,t) is governed by the wave equation

$$T\frac{\partial^2 f}{\partial x^2} = \rho\frac{\partial^2 f}{\partial t^2}$$

Where T is the tension in the string and ρ is the mass per unit length.

Hyperbolic problems are governed by both boundary and initial conditions, if time is one of the independent variables. Two boundary conditions are the vibrating string problems under consideration are

$$f(0,t) = 0, \quad 0 \le t \le b$$

$$f(L,t) = 0, \quad 0 \le t \le b$$

Two initial condition are

$$f(x,0) = f(x), 0 \le t \le \alpha$$

$$f_t(x,0) = g(x), 0 \le t \le a$$

Solution hyperbolic equations

The domain of interest $0 \le t \le a \; and \; 0 \le t \le b$ is partitioned as shown in figure, the rectangle size is $\Delta x = h, \Delta t = \tau$

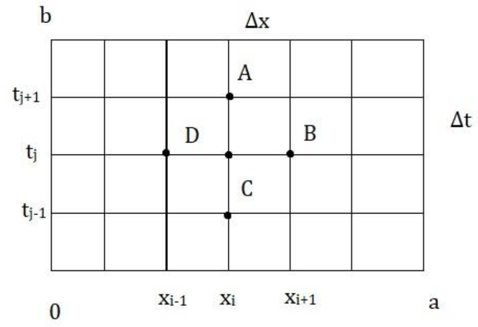


Figure : Grid for solving hyperbolic equation

The difference equation for $f_{xx}(x,t)$ and $f_{tt}(x,t)$ are

$$f_{xx}(x,t) = \frac{f(x-h,t) - 2f(x,t) + f(x+h,t)}{h^2}$$

$$f_{tt}(x,t) = \frac{f(x,t-\tau) - 2f(x,t) + f(x,t+\tau)}{\tau^2}$$

This implies that

$$T\frac{f_{i-1,j} - 2f_{ij} + f_{i+1,j}}{h^2} = \rho\frac{f_{i,j-1} - 2f_{ij} + f_{i,j+1}}{\tau^2}$$

Solving this for $f_{i,j+1}$, we obtain

$$f_{i,j+1} = -f_{i,j-1} + 2\left(1 - \frac{T\tau^2}{\rho h^2}\right)f_{ij} + \frac{T\tau^2}{\rho h^2}\left(f_{i+1,j} + f_{i-1,j}\right)$$

If we make $1 - \frac{T\tau^2}{\rho h^2} = 0$

Then we have

$$f_{i,j+1} = -f_{i,j-1} + f_{i+1,j} + f_{i-1,j} \quad \dots\dots\dots d$$

The values of f at $x = x_i$ and $t = t_j + \tau$ is equal to the um of the values of f, at the point $x = x_i - h$ and $x = x_i + h$ at the time $t = t_j(previous\ time)$ minus the value of f at $x = x_i$ at time $t = t_j - \tau$. From figure we can say $f_A = f_B + f_D - f_C$

Starting values

We need two rows of starting values, corresponding to j=1 and j=2, in order to computer the values of the third row. First row is obtained using the condition.

$$f(x,0) = f(x)$$

The 2nd row can be obtained using the 2nd initial condition as $f_t(x,0) = g(x)$

We know that

$$f_t(x,0) = \frac{f_{i,0+1} - f_{i,0-1}}{2\tau} = g_i$$

$$f_{i,-1} = f_{i,1} - 2\tau g_i\ for\ t = 0\ only$$

Substituting this in equation d, we get for $t = t_1$

$$f_{i,1} = \frac{1}{2}\left(f_{i+1,0} + f_{i-1,0}\right) + \tau g_i \ldots \ldots e$$

In many cases $g(x_i) = 0$ then we have

$$f_{i,1} = \frac{1}{2}\left(f_{i+1,0} + f_{i-1,0}\right)$$

Example: solve numerically the wave equation

$$f_{tt}(x,t) = 4f_{xx}(x,t) 0 \le x \le 5\ \&\ 0 \le t \le 2.5$$

With boundary condition

$$f(0,t) = 0\ \ and f(5,t) = 0$$

And initial values

$$f(x,0) = f(x) = x(5-x)$$

$$f_t(x,0) = g(x) = 0$$

Solution

Let h=1

Given $\frac{T}{\rho} = 4$

Assuming $1 - 4\frac{\tau^2}{1^2} = 0$

We get

$$\tau = \frac{1}{2}$$

The values estimated using equations d and e

x / t	0	1	2	3	4	5
0.0	0	4	6	6	4	0
0.5	0	3 *	5 **	5	3	0
1.0	0	1	2	2	1	0
1.5	0	-1***	-2	-2	-1	0
2.0	0	-3	-5	-5	-3	0
2.5	0	-4	-6	-6	-4	0

$* = \frac{0+6}{2}$ $** = \frac{4+6}{2}$ $*** = 2+0-3$