University of Basrah – College of Engineering
Department of Civil Engineering

Numerical Analysis

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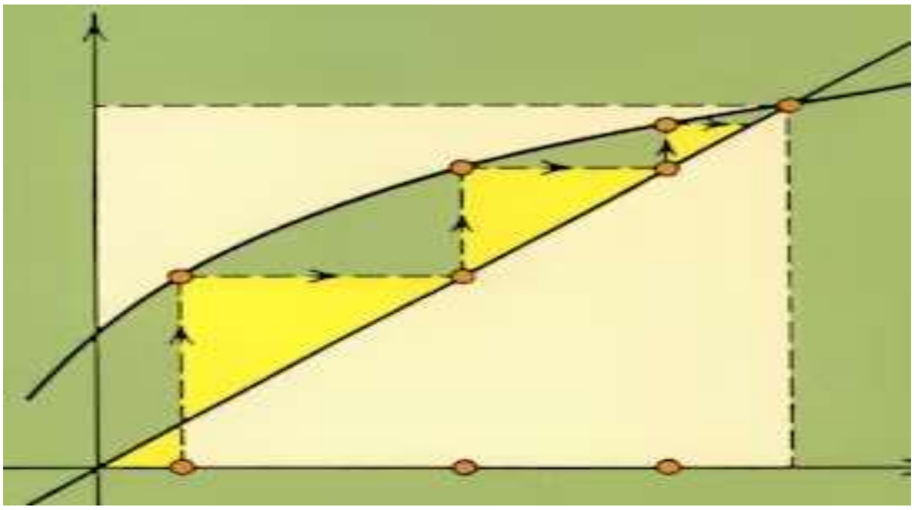


Syllabus

1- Introduction.
2- Numerical Solution of Algebraic Equations (Roots of equations).
3- Numerical Solution of Set of Algebraic Equations.
4- Taylor Series.
5- Numerical Differentiation (Finite Differences Calculus).
6- Numerical Integration.
7- Numerical Solution of Ordinary Differential Equations.
8- Curve Fitting.
9- Interpolation and Extrapolation.
10- Matrices and Determinants for Solving Simultaneous Algebraic Equations.

References

- Numerical Methods in Engineering Practice, by A. W. Al-Khafaji and J. R. Tooley.
- Numerical Methods, by R. W. Hornbeck.
- Numerical Methods for Engineers, by S. C. Chapra and R. P. Canale.
- Numerical Analysis, by R. L. Burden and J. D. Faires.

1-Introduction

Numerical methods

Numerical methods are a class of techniques used for solving a wide variety of mathematical problems in terms of numbers using only arithmetic and logic operations. The main advantage of numerical methods is their ability to solve problems that cannot be treated using classical analytical mathematics, such as non-linearity and complex geometries. The disadvantage is that the solutions using numerical methods are iterative, approximate, and not exact as those obtained by analytical methods.

Errors in numerical computations

1- Errors from the method of solution, since all numerical methods are only approximate.

2- Errors from solution truncation, since numerical methods are iterative and the iterations cannot continue infinite times.

3- Errors from numbers round off.

4- Errors from the mathematical model of the physical problems. For example in flexural formula the dx^2 term is neglected, also usually $\sin\theta$ is approximated to θ for small values of the later.

Error calculation

If x_{approx} is an approximate to x_{exact} then:

1- The absolute error is E or $\Delta = \left| x_{exact} - x_{approx} \right|$.

2- The relative error is $R = \left| \dfrac{x_{exact} - x_{approx}}{x_{exact}} \right|$.

3- The percent relative error is $P = \left| \dfrac{x_{exact} - x_{approx}}{x_{exact}} \right| \times 100$.

2- Numerical Solution of Algebraic Equations (Roots of Equations)

Introduction

A problem commonly encountered in engineering is that of determining the roots of an equation of the form $y = f(x)$. Finding the roots of an equation is equivalent to finding the values of x for which $f(x) = 0$. For this reason the roots of equation are often called the zeros of the equation. Different techniques of varying degrees of accuracy and rates of convergence were developed to determine these roots.

Root solving problem consists of finding the values of the independent variable which satisfy relationships, such as:

$$Ax^3 + Bx^2 = Cx + D.$$

The procedure for finding the roots will always be to collect all terms on one side of the equality sign, for example (for the above equation):

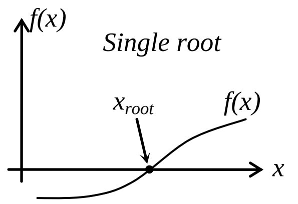
$$Ax^3 + Bx^2 - Cx - D = 0.$$

For any values of x other than the roots, this equation will not be satisfied. So in general:

$$f(x) = Ax^3 + Bx^2 - Cx - D.$$

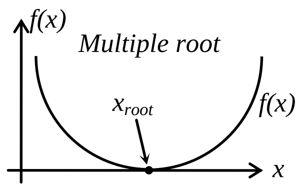
Now, finding the roots of the above equation is now equivalent to finding the values of x for which $f(x)$ is zero, i.e:

$$f(x) = 0.$$



Single and multiple roots

1- x_1 is a single (simple) root if $f(x_1) = 0$ and $f'(x_1) \neq 0$.



2- x_1 is a multiple root of :

multiplicity 2 if $f(x_1) = f'(x_1) = 0$ and $f''(x_1) \neq 0$,

multiplicity 3 if $f(x_1) = f'(x_1) = f''(x_1) = 0$ and $f'''(x_1) \neq 0$, and so on.

Accuracy in roots determination

All roots determination numerical methods are iterative, hence roots of different degrees of accuracy can be obtained depending on the method used and the number of iteration performed. The iteration should be continued until one (or more) of such following conditions are satisfied:

1- $\Delta = \left| x_i - x_{i-1} \right| \leq \varepsilon$, where ε is the allowed absolute difference between two successive trials (iterations).

2- $\left| f(x_i) \right| \leq E$, where E is the allowed absolute error in the value of the function.

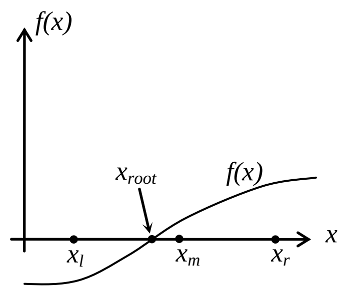
Solution of algebraic equations (determining roots of equations)

1- Bisection Method

This method, which is also known as interval halving method, is too inefficient for hand computation but is ideally suited to machine computation.

To find a real root of a given function *f(x)*, the following steps will be used:

1- Estimate two approximations of the root x_l and x_r such that $f(x_l) < 0$ ($f(x_l)$ is negative) and $f(x_r) > 0$ ($f(x_r)$ is positive).



2- Bisect the interval (x_l, x_r) to find its midpoint $x_m = \dfrac{x_r + x_l}{2}$ (which is considered as an improved approximation of root).

3- Check the sign of $f(x_m)$. If $f(x_m) < 0$, this mean that the root lies between x_m and x_r, then for the next iteration let $x_l = x_m$. If $f(x_m) > 0$, this mean that the root lies between x_l and x_m, then for the next iteration let $x_r = x_m$.

4- Repeat steps 2 and 3 until the required accuracy ε is achieved.

Notes:

1- For each iteration, the root is assumed to be the midpoint of the last interval found to contain it, i.e; the root is x_m.

2- For each iteration, the maximum absolute error Δ in the value of the root is no greater than one half the size of last interval found to contain the root, i.e;

$$\Delta = \frac{\left| x_r - x_l \right|}{2} \qquad \text{or} \qquad \Delta = \left| (x_m)_i - (x_m)_{i-1} \right|.$$

3- The maximum error Δ in the value of the root in a given iteration is one half its value in the previous iteration; $\Delta_i = \frac{1}{2}\Delta_{i-1}$. So this method has very slow convergence.

4- The bisection method cannot be used to find roots of functions that do not change their sign (from positive to negative or from negative to positive).

5- Since $\Delta_i = \frac{1}{2}\Delta_{i-1}$ and $\Delta = \frac{|x_r - x_l|}{2}$, so we can estimate the number of iterations *n* required to find a root to an accuracy of ε as follows:

$$\Delta \le \varepsilon \;\Rightarrow\; \frac{|x_r - x_l|}{2^n} \le \varepsilon \;\Rightarrow\; 2^n.\varepsilon \ge |x_r - x_l| \;\Rightarrow\; n\ln 2 + \ln\varepsilon \ge \ln|x_r - x_l|,$$

$$\therefore n \ge \frac{\ln|x_r - x_l| - \ln\varepsilon}{\ln 2} \quad \text{or} \quad n \ge \frac{\ln\left|\frac{x_r - x_l}{\varepsilon}\right|}{\ln 2}.$$

Example 1: Find the root(s) of the function $f(x) = x^3 - 5x^2 - 2x + 10$ using six iterations.

Solution:

Check the sign of $f(x)$ at different values of *x*:

x	- 2	- 1	0	1	2	3	4	5
$f(x)$	- 14	6	10	4	- 6	- 14	- 14	0

There are three roots: The first root lies between *x* = -2 and *x* = -1, the second root lies between *x* = 1 and *x* = 2, and the third root is *x* = 5 (exact value).

To find the first root by using the bisection method,

1st iteration: Let $x_l = -2$ and $x_r = -1$.

$$x_m = \frac{x_r + x_l}{2} \quad\Rightarrow\quad x_m = \frac{-1 + (-2)}{2} = -1.5$$

Check the sign of $f(x_m)$ $\Rightarrow$ $f(-1.5) = (-1.5)^3 - 5(-1.5)^2 - 2(-1.5) + 10 = -1.625$.

Since $f(x_m) < 0$, then for the next iteration $x_l = x_m = -1.5$ and $x_r = -1$ (unchanged)

2nd iteration: $x_l = -1.5$ and $x_r = -1$.

The calculations must be repeated as in the 1st iteration and continued until the required number of iterations is reached.

It is more preferred to put the calculations in a table as below:

No. of Iteration (i)	x_l	x_r	$x_m = \frac{x_r + x_l}{2}$	$f(x_m)$	$\Delta = \left\lvert \frac{x_r - x_l}{2} \right\rvert$
1	- 2	- 1	- 1.5	- 1.625	0.5
2	- 1.5	- 1	- 1.25	2.73….	0.25
3	- 1.5	- 1.25	- 1.375	0.69….	0.125
4	- 1.5	- 1.375	- 1.4375	- 0.42….	0.0625
5	- 1.4375	- 1.375	- 1.40625	0.14….	0.03125
6	- 1.4375	- 1.40625	- 1.421875	- 0.13….	0.015625

After six iterations the first approximate root is $x_{root} \approx -1.421875$.

To find the second root:

By using the bisection method,

<u>1st iteration:</u> Let $x_l = 2$ and $x_r = 1$.

$$x_m = \frac{x_r + x_l}{2} \quad \Rightarrow \quad x_m = \frac{1+2}{2} = 1.5$$

Check the sign of $f(x_m)$ $\Rightarrow$ $f(1.5) = (1.5)^3 - 5(1.5)^2 - 2(1.5) + 10 = -0.875$.

Since $f(x_m) < 0$, then for the next iteration $x_l = x_m = 1.5$ and $x_r = 1$ (unchanged).

<u>2nd iteration:</u> $x_l = 1.5$ and $x_r = 1$. And so on.

i	x_l	x_r	$x_m = \frac{x_r + x_l}{2}$	$f(x_m)$	$\Delta = \left\lvert \frac{x_r - x_l}{2} \right\rvert$
1	2	1	1.5	- 0.875	0.5
2	1.5	1	1.25	1.64….	0.25
3	1.5	1.25	1.375	0.39….	0.125
4	1.5	1.375	1.4375	- 0.23….	0.0625
5	1.4375	1.375	1.40625	0.08….	0.03125
6	1.4375	1.40625	1.421875	- 0.07….	0.015625

After six iterations the second approximate root is $x_{root} \approx 1.421875$.

Example 2: Find the point(s) of intersection of $y = \ln x$ and $y = 2x - 3$ accurately to three decimal places (i.e; $\varepsilon = 1 \times 10^{-3}$).

Solution:

To find the point(s) of intersection we put $y_1 = y_2 \quad \Rightarrow \quad \ln x = 2x - 3$,

$$\therefore \ln x - 2x + 3 = 0 \quad \Rightarrow \quad f(x) = 0 \text{ (Root finding problem)}$$

So we must find the root(s) of $f(x)$ where $f(x) = \ln x - 2x + 3$.

Check the sign of $f(x)$ at different values of *x*:

x	0.01	1	2	3	4	5
$f(x)$	- 1.625	1	- 0.306	- 1.9	- 3.6	- 5.39

There are two roots: The first root lies between *x* = 1 and *x* = 2 and the second root lies between *x* = 0.01 and *x* = 1. To find the first root by using the bisection method,

<u>1st iteration:</u> Let $x_l = 2$ and $x_r = 1 \Rightarrow x_m = \dfrac{x_r + x_l}{2} \Rightarrow x_m = \dfrac{1+2}{2} = 1.5$.

Check the sign of $f(x_m) \Rightarrow f(1.5) = \ln(1.5) - 2(1.5) + 3 = 0.40547$.

Since $f(x_m) > 0$, then for the next iteration $x_l = 2$ (unchanged) and $x_r = x_m = 1.5$.

<u>2nd iteration:</u> $x_l = 2$ and $x_r = 1.5$.

The calculations must be repeated as in the 1st iteration and continued until $\Delta \le \varepsilon$.

i	x_l	x_r	$x_m = \dfrac{x_r + x_l}{2}$	$f(x_m)$	$\Delta = \left\lvert \dfrac{x_r - x_l}{2} \right\rvert$
1	2	1	1.5	0.405…	0.5
2	2	1.5	1.75	0.059....	0.25
3	2	1.75	1.875	- 0.12….	0.125
4	1.875	1.75	1.8125	- 0.03….	0.0625
5	1.8125	1.75	1.78125	0.14….	0.03125
6	1.8125	1.78125	1.796875	- 0.007….	0.0156…
7	1.796875	1.78125	1.7890625	0.003…	0.007…
8	1.796875	1.7890625	1.79296875	- 0.002…	0.003…
9	1.79296875	1.7890625	1.791015625	- 0.0007…	0.001…
10	1.791015625	1.7890625	1.791992188	- 0.0006…	0.0009…$<\varepsilon$

After 10 iterations the first approximate root is $x_{root} \approx 1.791992$.

$y \approx \ln 1.791992 \approx 0.583327 \Rightarrow$ The first point of intersection is (1.791992,0.583327).

H.W:

The second point of intersection is (0.055439,-2.892471).

Note:

If we want to estimate the number of iterations required to find the above first root to the given accuracy, then:

$$n \geq \frac{\ln\left|\frac{x_r - x_l}{\varepsilon}\right|}{\ln 2} \quad \Rightarrow \quad n \geq \frac{\ln\left|\frac{1-2}{1\times 10^{-3}}\right|}{\ln 2} \quad \Rightarrow \quad n \geq 9.96 .$$

So we need 10 iterations.

2- Fixed point Method

A fixed point of a function $g(x)$ is a real number p such that $p = g(p)$. Graphically, fixed points of a function $y = g(x)$ are the points of intersection of $y = g(x)$ and $y = x$.

Fixed point method is used to determine roots of a function $f(x)$ as follows:

1- Rearrange the equation $f(x) = 0$ in the form $x = g(x)$ (so that x is on the left hand side of the equation).

2- Estimate an initial value to the root x_i and substitute it into $g(x)$ to get $g(x_i)$.

3- An improved estimation of the root is determined from $x_{i+1} = g(x_i)$ and so on.

Notes:

1- Fixed point method has very slow convergence.

2- For determining an expected root, lies in the interval (a, b), a certain expression of $x = g(x)$ seems to converge to this root if the absolute value of the slope of $g(x)$ is less than the slope of $y = x$, that is $|g'(x)| \leq 1$ for all $x \in (a,b)$.

3- A certain expression of $x = g(x)$ may converge to one root at more.

4- If we cannot get an expression of the form $x = g(x)$, then we could add x to both sides. For example, we can rewrite the equation $\sin x = 0$ in the form $x = \sin x + x$.

Example 1: Find numerically, to within 0.001, the value of *x* which makes the function $f(x) = (2-x)e^{-x/4}$ equal to 1.

Solution:

$f(x) = 1 \quad \Rightarrow \quad (2-x)e^{-x/4} = 1$

$\therefore (2-x)e^{-x/4} - 1 = 0 \quad \Rightarrow \quad h(x) = 0$. (Root finding problem)

So we must find a root of $h(x)$ where $h(x) = (2-x)e^{-x/4} - 1$

Check the sign of $h(x)$ at different values of *x*: (not necessary)

x	- 2	- 1	0	1	2	3
$h(x)$	1.4	1.3	1	- 0.22	- 1	- 1.47

Thus, there is a root lies between $x = 0$ and $x = 1$.

By using fixed point method, rearrange the equation $h(x) = 0$ in the form $x = g(x)$:

$$(2-x)e^{-x/4} - 1 = 0 \quad \Rightarrow \quad (2-x)e^{-x/4} = 1 \quad \Rightarrow \quad 2 - x = \frac{1}{e^{-x/4}}$$

$$2 - x = e^{x/4} \quad \Rightarrow \quad x = 2 - e^{x/4} \qquad \text{(In this expression } g(x) = 2 - e^{x/4}\text{)}$$

Let $x_o = 1$

<u>1st iteration:</u> $x_1 = g(x_o) \quad \Rightarrow \quad x_1 = g(1) = 2 - e^{(1)/4} = 0.715975$

<u>2nd iteration:</u> $x_1 = 0.715975 \quad \Rightarrow \quad x_2 = g(0.715975) = 2 - e^{(0.715975)/4} = 0.803987$

The calculations must be repeated and continued until $\Delta \le \varepsilon$.

i	x_i	$x_{i+1} = g(x_i)$	$\Delta_i = \lvert x_{i+1} - x_i \rvert$
0	1	0.715975	0.28….
1	0.715975	0.803987	0.08….
2	0.803987	0.777379	0.02….
3	0.777379	0.785485	8.1×10^{-3}
4	0.785485	0.783021	2.4×10^{-3}
5	0.783021	0.783771	$7.5 \times 10^{-4} < \varepsilon$

The required value is $x \approx 0.783771$.

<u>Notes:</u>

1- Another arrangement for the above table of calculations may be used as below:

i	x_i	$\Delta_i = \lvert x_{i+1} - x_i \rvert$
0	1	-
1	0.715975	0.28….
2	0.803987	0.08….
3	0.777379	0.02….
4	0.785485	8.1×10^{-3}
5	0.783021	2.4×10^{-3}
6	0.783771	$7.5\times10^{-4}<\varepsilon$

2- If we start with another possible expression of $x = g(x)$ like:

$$(2-x)e^{-x/4} - 1 = 0 \quad \Rightarrow \quad e^{-x/4} = \frac{1}{2-x} \quad \Rightarrow \quad e^{x/4} = 2-x$$

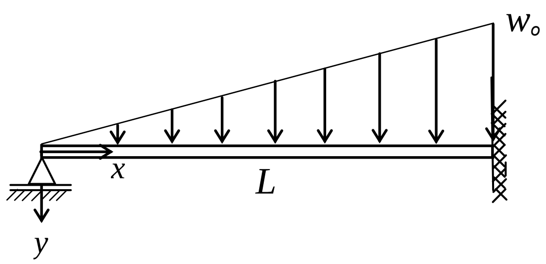
$$\frac{x}{4} = \ln(2-x) \quad \Rightarrow \quad x = 4\ln(2-x). \qquad \text{(In this expression } g(x) = 4\ln(2-x)\text{)}$$

Then, we get the following results:

i	x_i	$x_{i+1} = g(x_i)$	$\Delta_i = \lvert x_{i+1} - x_i \rvert$
0	1	0	1
1	0	2.772589	2.77….
2	2.772589	error	

Thus, this expression does not converge to the required root. Therefore we must search for another expression of $x = g(x)$.

<u>Example 2</u>: For the beam shown in the figure $L = 4\text{m}$, $w_o = 60\text{kN/m}$, and the deflection is given as $y = \dfrac{w_o}{120EIL}\left(x^5 - 2L^2x^3 + L^4x\right)$. Find numerically the value of the maximum deflection correct to three decimals.



Solution:

y_{max} occurs at $y' = 0$

$$y' = \frac{w_o}{120EIL}\left(5x^4 - 6L^2x^2 + L^4\right) = 0 \quad \Rightarrow \quad 5x^4 - 6L^2x^2 + L^4 = 0$$

$5x^4 - 6(4)^2 x^2 + 4^4 = 0 \quad \Rightarrow \quad 5x^4 - 96x^2 + 256 = 0$ [$f(x) = 0$ Finding roots problem]

where $f(x) = 5x^4 - 96x^2 + 256$

By using fixed point method, rearrange the equation $f(x) = 0$ in the form $x = g(x)$:

Try $5x^4 - 96x^2 + 256 = 0 \quad \Rightarrow \quad 96x^2 = 5x^4 + 256 \quad \Rightarrow \quad x = \sqrt{(5x^4 + 256)/96}$

[Here $g(x) = \sqrt{(5x^4 + 256)/96}$]

Let $x_o = 2$

1st iteration: $x_1 = g(2) = \sqrt{(5(2)^4 + 256)/96} = 1.870828693$

2nd iteration: $x_2 = \sqrt{(5(1.870828693)^4 + 256)/96} = 1.817879947$

The calculations must be repeated and continued until $\Delta \le \varepsilon$.

i	x_i	$x_{i+1} = g(x_i)$	$\Delta_i = \lvert x_{i+1} - x_i \rvert$
0	2	1.870828693	0.129….
1	1.870828693	1.817879947	0.052….
2	1.817879947	1.798740292	0.019….
3	1.798740292	1.792174023	6.5×10^{-3}
4	1.792174023	1.789963669	2.2×10^{-3}
5	1.789963669	1.78922445	$7.3 \times 10^{-4} < \varepsilon$

$\therefore \quad x \approx 1.788854$ m

$\therefore \quad y_{max} = y(1.788854)$

$$y_{max} = \frac{60}{120(1000)(4)}[(1.788854)^5 - 2(4)^2(1.788854)^3 + (4)^4(1.788854)]$$

$$\approx 0.036636 \text{ m} \approx 36.6 \text{ mm}$$

Note:

If we start with another possible expression of $x = g(x)$ like $x = \sqrt[4]{(96x^2 - 256)/5}$, then, thus, this expression will converge to another value (x = 4). Thus, we must try another expression of $x = g(x)$.

3- Newton-Raphson Method

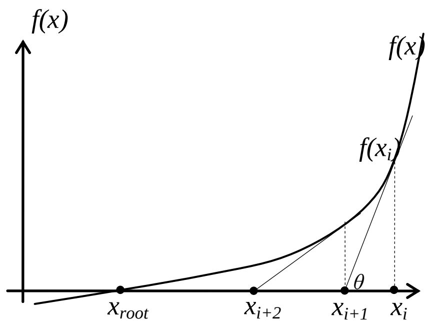
This is one of the more popular methods used for solving non-linear algebraic equations. It is also known as Newton's method or the tangent method. It is convergent faster than the previous methods. The formula of this method can be derived as follows.

Let x_i be an estimation to the required root of a given function $f(x)$. A better estimation x_{i+1} can be obtained by using the zero of the tangent to the function at x_i. The tangent line passes the x-axis at the improved root x_{i+1}. The value of x_{i+1} can be determined as follows:

$f'(x_i) = \tan\theta$, but from the shown figure:

$$\tan\theta = \frac{f(x_i)}{x_i - x_{i+1}} \quad \Rightarrow \quad \therefore f'(x_i) = \frac{f(x_i)}{x_i - x_{i+1}},$$

or $$x_i - x_{i+1} = \frac{f(x_i)}{f'(x_i)} \quad \Rightarrow \quad x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}.$$



Notes:

1. Newton-Raphson method has slow convergence in regions of multiple roots.
2. Near the maxima and minima points, Newton-Raphson method is either convergent to these points or convergent to a non-required root or divergent.

Example 1: Find the positive root of ($x^2 - 4\sin x$) to an accuracy of $\varepsilon = 1\times 10^{-6}$.

Solution:

Let $f(x) = x^2 - 4\sin x$, and check the sign of *f(x)*: (not necessary)

x	0	1	2	3
$f(x)$	0	- 2.366	0.363	8.4

There is a positive root lies between x = 1 and x = 2 and it is closer to x = 2.

To find this root by using Newton-Raphson method,

1st iteration: Let $x_o = 2$,

$$f(x) = x^2 - 4\sin x \quad \Rightarrow \quad f(x_o) = f(2) = (2)^2 - 4\sin 2 = 0.362810,$$

$$f'(x) = 2x - 4\cos x \quad \Rightarrow \quad f'(x_o) = f'(2) = 2(2) - 4\cos 2 = 5.664587,$$

$$x_1 = x_o - \frac{f(x_o)}{f'(x_o)} \quad \Rightarrow \quad x_1 = 2 - \frac{0.362810}{5.664587} = 1.935951.$$

2nd iteration: $x_1 = 1.935951.$

The calculations must be repeated as in the 1st iteration and continued until $\Delta \le \varepsilon$.

i	x_i	$f(x_i)$	$f'(x_i)$	$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$	$\Delta_i = \lvert x_{i+1} - x_i \rvert$
0	2	0.362810	5.664587	1.935951	0.064….
1	1.935951	0.011623	5.300277	1.933756	2.2×10^{-3}
2	1.933756	1.18×10^{-5}	5.287682	1.933754	2.2×10^{-6}
3	1.933754	1.25×10^{-6}	5.287671	1.933754	$\approx 2.3\times10^{-7} < \varepsilon$

After 4 iterations the positive root is $x_{root} \approx 1.933754$.

Note:

Another arrangement for the above table of calculations may be used as below:

i	x_i	$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} = x_i - \frac{x_i^2 - 4\sin x_i}{2x_i - 4\cos x_i}$	$\Delta_i = \lvert x_{i+1} - x_i \rvert$
0	2	1.935951	0.064….
1	1.935951	1.933756	2.2×10^{-3}
2	1.933756	1.933754	2.2×10^{-6}
3	1.933754	1.933754	$\approx 2.3\times10^{-7} < \varepsilon$

Example 2: Find the root of $f(x) = (2-x)e^{-x/4} - 1$ such that $\lvert f(x) \rvert < 1\times10^{-6}$.

Solution:

By using Newton-Raphson method,

$$f(x) = (2-x)e^{-x/4} - 1,$$

$$f'(x) = (2-x)e^{-x/4}(-1/4) + e^{-x/4}(-1) \quad \Rightarrow \quad f'(x) = (\frac{x}{4} - \frac{3}{2})e^{-x/4}.$$

1st iteration: Let $x_o = 3$ (chosen arbitrary)

$$f(x_o) = f(3) = (2-3)e^{-3/4} - 1 = -1.472366,$$

$$f'(x_o) = f'(3) = (\frac{3}{4} - \frac{3}{2})e^{-3/4} = -0.354275,$$

$$x_1 = x_o - \frac{f(x_o)}{f'(x_o)} \qquad \Rightarrow \qquad x_1 = 3 - \frac{-1.472366}{-0.354275} = -1.156000.$$

2nd iteration: $x_1 = -1.156000$.

The calculations must be repeated as above and continued until $|f(x)| < 1\times10^{-6}$.

i	x_i	$f(x_i)$	$f'(x_i)$	$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$
0	3	- 1.472366	- 0.354275	- 1.156000
1	- 1.156000	3.213550	- 2.388479	0.189438
2	0.189438	0.726814	- 1.385448	0.714043
3	0.714043	0.075722	- 1.105445	0.782542
4	0.782542	0.001130	- 1.072594	0.783596
5	0.783596	$3.4\times10^{-8} < 1\times10^{-6}$		

Hence the root is $x_{root} \approx 0.783596$.

Note:
If we choose $x_o = 8 \;\Rightarrow\; x_1 = 34.778112 \;\Rightarrow\; x_2 = 869.152844$. (Divergence)

Example 3: Solve, to three decimal-place accuracy, the following equation:

$$0.51e^{-0.1k} - 0.01e^{0.2k} = 0.25.$$

Solution:

$0.51e^{-0.1k} - 0.01e^{0.2k} = 0.25 \;\Rightarrow\; 0.51e^{-0.1k} - 0.01e^{0.2k} - 0.25 = 0$ [Root finding]

By using Newton-Raphson method,

$$k_1 = k_o - \frac{f(k_o)}{f'(k_o)}$$

where $f(k) = 0.51e^{-0.1k} - 0.01e^{0.2k} - 0.25$

and $f'(k) = -0.051e^{-0.1k} - 0.002e^{0.2k}$

Let $k_o = 0$

i	k_i	k_{i+1}	$\lvert\Delta_i\rvert$
0	0	4.716981132	4.716…
1	4.716981132	5.867556335	1.150…
2	5.867556335	5.904661726	0.037…
3	5.904661726	5.904692139	$3\times10^{-5} < \varepsilon$

$\therefore k = 5.90481551 \approx 5.905$.

4- Modified Newton Method

To find the roots of a function $f(x)$, define a new function $u(x)$ given by

$$u(x)=\frac{f(x)}{f'(x)} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ (1)$$

The function $u(x)$ has the same roots as does $f(x)$, since $u(x)$ becomes zero everywhere that $f(x)$ is zero. If $f(x)$ has a multiple root at $x=c$ of multiplicity r (this could occur, for example, if $f(x)$ contained a factor $(x-c)^r$). The $u(x)$ may be readily shown to have a single root at $x=c$.

$$f(x)=(x-c)^r \quad \Rightarrow \quad f'(x)=r(x-c)^{r-1},$$

$$u(x)=\frac{f(x)}{f'(x)} \quad \Rightarrow \quad u(x)=\frac{(x-c)^r}{r(x-c)^{r-1}} \quad \Rightarrow \quad u(x)=\frac{(x-c)}{r}.$$

Since Newton-Raphson method is effective for simple roots, we can apply this method to $u(x)$ instead of $f(x)$,

$$x_{i+1}=x_i-\frac{u(x_i)}{u'(x_i)}.$$

From Eq.(1), $$u'(x)=\frac{[f'(x)]^2-f(x).f''(x)}{[f'(x)]^2} \quad \Rightarrow \quad u'(x)=1-\frac{f(x).f''(x)}{[f'(x)]^2}.$$

The advantage of this method over the conventional Newton's method is in finding multiple roots with a faster convergence.

Example 1: Find numerically the positive root(s) for the function: $(\varepsilon=1\times10^{-5})$

$$f(x)=x^3-5.5x^2+4.0625x+10.5625.$$

Solution:

Sign test:

x	0	1	2	3	4	5
$f(x)$	10.5625	10.125	4.6875	0.25	2.8125	18.375

There is an expected root(s) lies in the interval (3,4).

To find this expected root, if any, by using the modified Newton method,

1st iteration: Let $x_o=3$

$$f(x)=x^3-5.5x^2+4.0625x+10.5625 \quad \Rightarrow \quad f(x_0)=f(3)=0.25$$

$$f'(x) = 3x^2 - 11x + 4.0625 \quad \Rightarrow \quad f'(x_0) = f'(3) = -1.9375$$

$$f''(x) = 6x - 11 \quad \Rightarrow \quad f''(x_0) = f''(3) = 7$$

$$u(x) = \frac{f(x)}{f'(x)} \quad \Rightarrow \quad u(x) = \frac{0.25}{-1.9375} = -0.129032\ldots$$

$$u'(x) = 1 - \frac{f(x).f''(x)}{[f'(x)]^2} \quad \Rightarrow \quad u'(x) = 1 - \frac{(0.25)(7)}{(-1.9375)^2} = 0.533818\ldots$$

$$x_1 = x_o - \frac{u(x_o)}{u'(x_o)} \quad \Rightarrow \quad x_1 = 3 - \frac{-0.129032\ldots}{0.533818\ldots} = 3.241715\ldots$$

<u>2nd iteration:</u> $x_1 = 3.241715\ldots$

The calculations must be repeated as in the 1st iteration and continued until $\Delta \le \varepsilon$

i	x_i	$u(x_i)$	$u'(x_i)$	$x_{i+1} = x_i - u(x_i)/u'(x_i)$	Δ_i
0	3	- 0.129032…	0.533818…	3.241715…	0.24….
1	3.241715…	$-4.146\ldots \times 10^{-3}$	0.500978…	3.249991…	8.2×10^{-3}
2	3.249991…	$-4.053\ldots \times 10^{-6}$	0.499998…	3.25	$8.1 \times 10^{-6} < \varepsilon$

After 3 iterations the root is $x_{root} = 3.25$

Check for multiple root, $f'(x_{root}) = f'(3.25) = 0 \Rightarrow x_{root} = 3.25$ is a multiple root

<u>Note:</u>
If we use Newton-Raphson method to find the above root, with the same initial value, then we will need more than 15 iterations to get the required accuracy. Thus, Newton-Raphson method has a very slow convergence in determining multiple roots.

<u>Example 2</u>: Find the smallest positive root of the function

$$f(x) = x^4 - 8.6x^3 - 35.51x^2 + 464.4x - 998.46. \qquad (\varepsilon = 1\times10^{-5})$$

Solution:

Check the sign of $f(x)$ at different values of x:

x	0	1	2	3	4	5	6	7	8
f(x)	- 998.46	- 577.17	- 264.5	- 76.05	- 3.42	- 14.21	- 52.02	- 36.45	136.9

There is a root lies between x = 7 and x = 8, but there is an expected root(s) lies between x = 4 and x = 5

To find this expected root, if any, by using the modified Newton method,

<u>1st iteration:</u>   Let $x_o = 4$

$$f(x) = x^4 - 8.6x^3 - 35.51x^2 + 464.4x - 998.46 \quad \Rightarrow \quad f(x_0) = f(4) = -3.42$$

$$f'(x) = 4x^3 - 25.8x^2 - 71.02x + 464.4 \quad \Rightarrow \quad f'(x_0) = f'(4) = 23.52$$

$$f''(x) = 12x^2 - 51.6x - 71.02 \quad \Rightarrow \quad f''(x_0) = f''(4) = -85.42$$

$$u(x) = \frac{f(x)}{f'(x)} \quad \Rightarrow \quad u(x) = \frac{-3.42}{23.52} = -0.145408$$

$$u'(x) = 1 - \frac{f(x).f''(x)}{[f'(x)]^2} \quad \Rightarrow \quad u'(x) = 1 - \frac{(-3.42)(-85.42)}{(23.52)^2} = 0.471906$$

$$x_1 = x_o - \frac{u(x_o)}{u'(x_o)} \quad \Rightarrow \quad x_1 = 4 - \frac{-0.145408}{0.471906} = 4.308129$$

<u>2nd iteration:</u> $x_1 = 4.308129$

The calculations must be repeated as in the 1st iteration and continued until $\Delta \le \varepsilon$

i	x_i	$u(x_i)$	$u'(x_i)$	$x_{i+1} = x_i - \frac{u(x_i)}{u'(x_i)}$	$\Delta_i = \lvert x_{i+1} - x_i \rvert$
0	4	- 0.145408	0.4719062	4.308129	0.308129
1	4.308129	4.0687×10^{-3}	0.5009915	4.300008	8.123×10^{-3}
2	4.300008	4.0315×10^{-6}	0.5000996	4.300000	$8\times10^{-6} < \varepsilon$

After 3 iterations the positive root is $x_{root} = 4.3$

Check for multiple root, $f'(x_{root}) = f'(4.3) = 0 \quad \Rightarrow \quad x_{root} = 4.3$ is a multiple root

3- Numerical Solution of Set of Algebraic Equations

Introduction

The solution of set of algebraic equations is an important step in wide variety of engineering problems, such as the numerical solution of differential equations, the structural analysis, network analysis, ….etc.

Iterative methods

In the these methods an initial set of values of the unknowns are assumed to determine improved approximate values of these unknowns which in turn are used to determine better approximations and so on. This iteration continues until sufficiently values are obtained.

Solution of Set of linear algebraic equations

1- Jacobi iteration

The system of equations:

$$\begin{aligned}
&a_{11}x_1 + a_{12}x_2 + \dots\dots + a_{1m}x_m = b_1\\
&a_{21}x_1 + a_{22}x_2 + \dots\dots + a_{2m}x_m = b_2\\
&\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \qquad \dots\dots\dots\dots\dots (1)\\
&a_{m1}x_1 + a_{m2}x_2 + \dots\dots + a_{mm}x_m = b_m
\end{aligned}$$

Can be written as:

$$\begin{aligned}
&x_1 = [b_1 - (a_{12}x_2 + \dots\dots + a_{1m}x_m)]/a_{11}\\
&x_2 = [b_2 - (a_{21}x_1 + \dots\dots + a_{2m}x_m)]/a_{22}\\
&\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \qquad \dots\dots\dots\dots\dots (2)\\
&x_m = [b_m - (a_{m1}x_1 + a_{m2}x_2 + \dots\dots)]/a_{mm}
\end{aligned}$$

In this method initial trial values are assumed which are substituted in the iterative equations (Eq.2) of the unknowns to obtain better approximations of the unknowns that are used to obtain new improved approximations. This method converges if :

$$\left|a_{ii}\right| > \sum_{j=1}^{n}\left|a_{ij}\right| \qquad j = 1,2,\dots\dots,n \text{ but } i \neq j \qquad \dots\dots\dots\dots\dots (3)$$

i.e. the absolute value of the element located on the main diagonal in each row is greater than the sum of the absolute values of the other elements in that row. So the procedure of solution in Jacobi method is as follows:

1- The equations are rearranged for condition of convergence in Eq.3.

2- The resulting equations are written in the iterative expressions of Eq.2.

3- A set of initial values of the unknowns are assumed.

4- These values are substituted in the iterative equations to obtain new values.

5- Step 3 is repeated until the required accuracy is achieved.

Example 1: Solve the following set of equations:

$$4x - 8y + z + 21 = 0,$$
$$-2x + y + 5z - 15 = 0,$$
$$4x - y + z - 7 = 0.$$

Solution:.

Use Jacobi iteration,

Step 1: Rearrange the equations for convergence:

$$4x - y + z = 7,$$
$$4x - 8y + z = -21,$$
$$-2x + y + 5z = 15.$$

Step 2: Find the iterative equations:

$$x_{i+1} = (7 + y_i - z_i)/4,$$
$$y_{i+1} = (21 + 4x_i + z_i)/8,$$
$$z_{i+1} = (15 + 2x_i - y_i)/5.$$

Step 3: Assume initial values:

$$x_o = y_o = z_o = 1.$$

Step 4: Substitute the initial values into the iterative equations to get new values:

1st iteration:

$$x_1 = (7 + 1 - 1)/4 = 1.75,$$
$$y_1 = (21 + 4(1) + 1)/8 = 3.25,$$
$$z_1 = (15 + 2(1) - 1)/5 = 3.2.$$

2nd iteration: $x_1 = 1.75$, $y_1 = 3.25$, and $z_1 = 3.2$.

The calculations must be repeated as in the 1st iteration and continued until the required accuracy (if any) is achieved.

No. of Iteration (i)	x_i	y_i	z_i
0	1	1	1
1	1.75	3.25	3.2
2	1.7625	3.9	3.05
3	1.9625	3.8875	2.925
4	1.990625	3.971875	3.0075
5	1.99109	3.99625	3.001875
…..	…..	…..	…..
…..	…..	…..	…..
	→2	→4	→3

2- Gauss-Seidel iteration

As $(x_1)_{i+1}$ is expected to be a better approximation than $(x_1)_i$,then it appears more advantageous to use the value of $(x_1)_{i+1}$ in determining $(x_2)_{i+1}$ rather than using $(x_1)_i$. Similarly, the value of $(x_1)_{i+1}$ and $(x_2)_{i+1}$ are used to determine the value of $(x_3)_{i+1}$, and so on. The using of this procedure will , in general, yield results that are more rapidly convergent than the conventional Jacobi iteration.

Example: Solve the following set of equations:

$$4x-8y+z+21=0,$$
$$-2x+y+5z-15=0,$$
$$4x-y+z-7=0.$$

Solution:.

Use Gauss-Seidel iteration,

Step 1: Rearrange the equations for convergence:

$$4x-y+z=7,$$
$$4x-8y+z=-21,$$
$$-2x+y+5z=15.$$

Step 2: Find the iterative equations:

$$x_{i+1} = (7 + y_i - z_i)/4,$$
$$y_{i+1} = (21 + 4x_{i+1} + z_i)/8,$$
$$z_{i+1} = (15 + 2x_{i+1} - y_{i+1})/5.$$

Step 3: Assume initial values:

$$x_o = y_o = z_o = 1.$$

Step 4: Substitute the initial values into the iterative equations to get new values:

1st iteration:

$$x_1 = (7 + 1 - 1)/4 = 1.75,$$
$$y_1 = (21 + 4(1.75) + 1)/8 = 3.625,$$
$$z_1 = (15 + 2(1.75) - 3.625)/5 = 2.975.$$

2nd iteration: $x_1 = 1.75$, $y_1 = 3.625$, and $z_1 = 2.975$.

The calculations must be repeated as in the 1st iteration and continued until the required accuracy (if any) is achieved.

i	x_i	y_i	z_i
0	1	1	1
1	1.75	3.625	2.975
2	1.9125	3.953125	2.974375
3	1.994688	3.994141	2.999047
…..	…..	…..	…..
…..	…..	…..	…..
	→2	→4	→3

Solution of Set of nonlinear algebraic equations

These equations can be solved by the Gauss- Seidel iteration.

Example 1: Solve the following system:

$$x + 4y + z^2 - 18 = 0,$$
$$x^2 + y + 4z - 15 = 0,$$
$$4x + y^2 + z - 11 = 0.$$

Solution:

Use Gauss-Seidel iteration,

Step 1: Rearrange the equations for convergence:

$$4x + y^2 + z = 11,$$

$$x + 4y + z^2 = 18,$$

$$x^2 + y + 4z = 15.$$

Step 2: Find the iterative equations:

$$x_{i+1} = (11 - y^2{}_i - z_i)/4,$$

$$y_{i+1} = (18 - x_{i+1} - z^2{}_i)/4,$$

$$z_{i+1} = (15 - x^2{}_{i+1} - y_{i+1})/4.$$

Step 3: Assume initial values:

$$x_o = y_o = z_o = 1.$$

Step 4: Substitute the initial values into the iterative equations to get new values:

1st iteration:

$$x_1 = (11 - 1^2 - 1)/4 = 2.25,$$

$$y_1 = (18 - 2.25 - 1^2)/4 = 3.6875,$$

$$z_1 = (15 - 2.25^2 - 3.6875)/4 = 1.5625.$$

2nd iteration: $x_1 = 2.25$, $y_1 = 3.6875$, and $z_1 = 1.562$.

The calculations must be repeated as in the 1st iteration and continued until the required accuracy (if any) is achieved.

No. of Iteration (i)	x_i	y_i	z_i
0	1	1	1
1	2.25	3.6875	1.5625
…..	…..	…..	…..
…..	…..	…..	…..
…..	…..	…..	…..
	→1	→2	→3

Example 2: Solve:

$$x^2 + xy = 10,$$

$$y + 3xy^2 = 57.$$

Solution:

Use the concept of Gauss-Seidel iteration,

Find the iterative equations:

$$x_{i+1} = \sqrt{10 - x_i y_i},$$

$$y_{i+1} = \sqrt{\frac{57 - y_i}{3x_{i+1}}}.$$

Assume initial values:

$$x_o = y_o = 1.$$

Step 4: Substitute the initial values into the iterative equations to get new values:

1st iteration:

$$x_1 = \sqrt{10 - (1)(1)} = 3,$$

$$y_1 = \sqrt{\frac{57 - 1}{3(3)}} = 2.494438.$$

2nd iteration: $x_1 = 3,\ y_1 = 2.494438.$

The calculations must be repeated as in the 1st iteration and continued until the required accuracy (if any) is achieved.

No. of Iteration (i)	x_i	y_i
0	1	1
1	3	2.494438
2	1.586407	3.384172
3	2.152052	2.881771
4	1.948917	3.042387
5	2.017583	2.985723
…..	…..	…..
…..	…..	…..
	→2	→3

Note: Other expressions for the iterative equations must be used if divergence is occurred.

4- Taylor Series

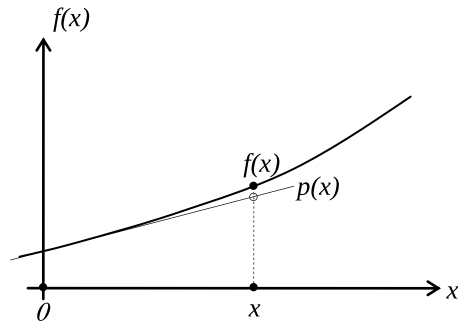
Introduction

Taylor series is the foundation of many numerical methods. Many of numerical techniques are derived directly from Taylor series, as are the estimates of the errors involved in employing these techniques.

Maclaurin series

Suppose that the value of the function $f(x)$, shown in the figure, and the values of all of its derivatives at $x=0$, i.e. $f(0), f'(0), f''(0), f'''(0),\ldots,$ are known and the value of this function at a point x is to be determined. One method is to approximate $f(x)$ by its tangent line at $x=0$, which has the equation:

$p(x)=c_0+c_1x.$ (polynomial of degree 1)



At $x=0$, $p(x)=p(0) \quad \Rightarrow \quad p(0)=c_0+c_1(0)$,

$\therefore \quad c_0=p(0)$, but $p(0)=f(0) \Rightarrow \quad c_0=f(0)$.

$p'(x)=c_1$.

At $x=0$, $p'(x)=p'(0) \quad \Rightarrow \quad p'(0)=c_1$,

but $p'(0)=f'(0) \quad \Rightarrow \quad c_1=f'(0)$.

$\therefore \; p(x)=f(0)+xf'(0) \quad \Rightarrow \quad f(x)\approx f(0)+xf'(0)$.

The accuracy of the approximation will be better improved as the degree of the approximation polynomial is increased. If a polynomial of infinite degree is used, then the following approximation is obtained:

$$f(x)=f(0)+xf'(0)+\frac{x^2}{2!}f''(0)+\frac{x^3}{3!}f'''(0)+\frac{x^4}{4!}f^{IV}(0)+\ldots\ldots\ldots,$$

or simply $\quad f(x)=\sum_{k=0}^{\infty}\frac{x^k}{k!}f^k(0)$.

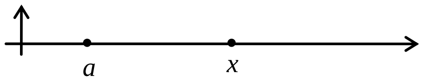
The above series (polynomial) is called the Maclaurin series (polynomial).

Taylor series

Maclaurin series gives an approximation of a function $f(x)$ in the vicinity of $x=0$. The more general case of approximating $f(x)$ in the vicinity of an arbitrary value $x=a$ is now considered. The basic idea is the same as before. Thus, if a polynomial of infinite degree is used to approximate a function $f(x)$ which its value and all its derivatives' values are known at $x=a$, then the following polynomial will obtained:

$$f(x)=f(a)+(x-a)f'(a)+\frac{(x-a)^2}{2!}f''(a)+\frac{(x-a)^3}{3!}f'''(a)+\frac{(x-a)^4}{4!}f^{IV}(0)+\ldots\ldots,$$

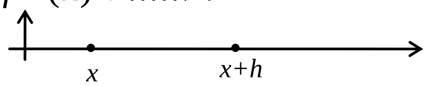
or simply $\quad f(x)=\sum_{k=0}^{\infty}\frac{(x-a)^k}{k!}f^k(a)$.



The above series (polynomial) is called the Taylor series expansion for the function f about $x=a$. It is obvious that Maclaurin series is a special case of Taylor series when the point of expansion is $x=0$ (i.e. $a=0$).

Another used formula of Taylor series expansion of a function f about x, where its value and all its derivatives' values are known at the point x, is

$$f(x+h)=f(x)+hf'(x)+\frac{h^2}{2!}f''(x)+\frac{h^3}{3!}f'''(x)+\frac{h^4}{4!}f^{IV}(x)+\ldots\ldots .$$



Order of error

The error in the value of $f(x)$ which refers to the error resulted from omitting terms beyond the term contains the nth derivative is denoted as $O(x-a)^{n+1}$.

If we take one term of Taylor series, then

$$f(x)=f(a)+O(x-a),$$

if we take two terms, then

$$f(x)=f(a)+(x-a)f'(a)+O(x-a)^2,$$

and if we take n terms, then

$$f(x)=f(a)+(x-a)f'(a)+\frac{(x-a)^2}{2!}f''(a)+\ldots.+\frac{(x-a)^{n-1}}{(n-1)!}f^{n-1}(a)+O(x-a)^n.$$

It is obvious that the error decreases as its order increases, i.e;

$$O(x-a)^{n+1}<O(x-a)^n.$$

Error in truncated Taylor series

The difference $R_n(x)$ (also called the error or remainder) between the exact value of the function $f(x)$ and the value obtained from the nth Taylor series $T_n(x)$ is

$R_n(x) = f(x) - T_n(x)$, which is known as the nth remainder, where

$$T_n(x) = \sum_{k=0}^{n} \frac{(x-a)^k}{k!} f^k(a) \quad \text{and} \quad R_n(x) = \sum_{k=n+1}^{\infty} \frac{(x-a)^k}{k!} f^k(a).$$

Thus the value of $f(x)$ can be written as:

$f(x) = T_n(x) + R_n(x)$, which is called Taylor formula with remainder.

The upper bound of the remainder in a truncated series can be estimated by:

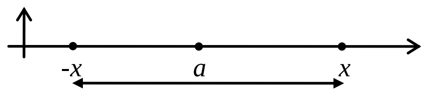
$$R(x) \le \left| \frac{(x-a)^r}{r!} f^r_{\max} \right| . \qquad \text{(Lagrange's form)}$$

where r is the power of $(x-a)$ in the first truncated term and the maximum value of the derivative f^r occurs at some point c lies in the interval $[x,a]$.

Notes:

1- Let the power series is $\sum_{k=0}^{\infty} U_k$. If the limit $f(x) = \lim_{k \to \infty} \left| \frac{U_{k+1}}{U_k} \right| = L$ exists, then

i- The series converges when $L < 1$.
ii- The series diverges when $L > 1$.
iii- The test fails when $L = 1$.



Interval of convergence

2- The number of terms of a given power series $\sum_{k=0}^{\infty} U_k$, that are required to compute x correct to a given accuracy ε, cab be estimated from $|U_k| < x.\varepsilon$.

Example 1: Find the Taylor series expansion for the function $f(x) = e^x$ about $x = 0$. Then use it to find $e^{0.5}$ to an error of order $O(x)^3$. Estimate the error and compare with the exact value.

Solution:

When the expansion is about $x = 0$, then Taylor series reduces to Maclaurin series.

$$f(x) = f(0) + xf'(0) + \frac{x^2}{2!} f''(0) + \frac{x^3}{3!} f'''(0) + \ldots\ldots\ldots$$

$$f(x) = e^x \;\Rightarrow\; f'(x) = f''(x) = f^n(x) = e^x \;\Rightarrow\; f(0) = f'(0) = f''(0) = f^n(0) = e^0 = 1$$

$\therefore\ f(x)=e^x=1+x.(1)+\dfrac{x^2}{2!}.(1)+\dfrac{x^3}{3!}.(1)+\ldots\ldots\ldots$ or $e^x=1+x+\dfrac{x^2}{2!}+\dfrac{x^3}{3!}+\ldots\ldots\ldots$

To compute $e^{0.5}\ \Rightarrow\ e^x=e^{0.5}\ \Rightarrow\ x=0.5$

$$\therefore\ e^{0.5}=1+0.5+\frac{(0.5)^2}{2!}+O(0.5)^3\ \Rightarrow\ e^{0.5}\approx 1+0.5+\frac{(0.5)^2}{2}\approx 1.625$$

The error can be estimated from $R(x)\le\left|\dfrac{(x-a)^r}{r!}f^{r}_{\max}\right|$.

Since the first truncated term in Taylor series contains the 3rd derivative (i.e. $r=3$),

$$\therefore\ R(x)\le\left|\frac{(0.5-0)^3}{3!}f'''_{\max}\right|$$

$f'''(x)=f'''(0.5)=e^{0.5}=1.648721$ & $f'''(a)=f'''(0)=e^0=1$

$$\therefore\ f'''_{\max}=1.648721\ \Rightarrow\ R(x)\le\left|\frac{(0.5-0)^3}{6}\times 1.648721\right|\ \Rightarrow\ R(x)\le 0.034348$$

The (exact) value is $e^{0.5}=1.648721$. (From the scientific calculator)

The absolute error $\Delta=|exact-approx|=|1.648721-1.625|=0.023721$ (<0.034348)

The percent relative error $P=\left|\dfrac{exact-approx}{exact}\right|\times 100=\left|\dfrac{1.648721-1.625}{1.648721}\right|\times 100=1.44\%$.

<u>Example 2</u>: Find the Taylor series expansion of $f(x)=e^{\sqrt{x}}$ about $x=0$.

Solution:

When the expansion is about $x=0$, then Taylor series reduces to Maclaurin series.

$$f(x)=f(0)+xf'(0)+\frac{x^2}{2!}f''(0)+\frac{x^3}{3!}f'''(0)+\ldots\ldots\ldots$$

$$f(x)=e^{\sqrt{x}}\ \Rightarrow\ f(0)=e^{\sqrt{0}}=1$$

$$f'(x)=e^{\sqrt{x}}.\frac{1}{2}x^{-1/2}\ \Rightarrow\ f'(x)=\frac{e^{\sqrt{x}}}{2\sqrt{x}}\ \Rightarrow\ f'(0)=\frac{e^{\sqrt{0}}}{2\sqrt{0}}=\frac{1}{0}\quad\text{(Undefined)}$$

Since $f'(0)$ does not exist (undefined) $\Rightarrow\ \therefore\ f(x)=e^{\sqrt{x}}$ cannot be expanded about $x=0$, or the Taylor series expansion of $f(x)=e^{\sqrt{x}}$ about $x=0$ does not exist.

Example 3: Find the interval of convergence of Maclaurin expansion for $\sin x$. How many terms are needed to compute $\sin(1/2)$ accurately to six decimals?

Solution:

Maclaurin series is $f(x) = f(0) + xf'(0) + \frac{x^2}{2!} f''(0) + \frac{x^3}{3!} f'''(0) + \ldots\ldots$

$$f(x) = \sin x \quad \Rightarrow \quad f(0) = \sin 0 = 0$$
$$f'(x) = \cos x \quad \Rightarrow \quad f'(0) = \cos 0 = 1$$
$$f''(x) = -\sin x \quad \Rightarrow \quad f''(0) = -\sin 0 = 0$$
$$f'''(x) = -\cos x \quad \Rightarrow \quad f'''(0) = -\cos 0 = -1$$

$$\therefore \ f(x) = \sin x = 0 + x(1) + \frac{x^2}{2!}.(0) + \frac{x^3}{3!}.(-1) + \ldots\ldots \Rightarrow \sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \ldots\ldots$$

Convergence test: Check $\lim_{k \to \infty} \left| \frac{U_{k+1}}{U_k} \right|$,

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \ldots\ldots \quad \Rightarrow \quad \sin x = \sum_{k=0}^{\infty} (-1)^k . \frac{x^{2k+1}}{(2k+1)!}$$

$$\therefore \lim_{k \to \infty} \left| \frac{U_{k+1}}{U_k} \right| = \lim_{k \to \infty} \left| \frac{\frac{x^{2(k+1)+1}}{(2(k+1)+1)!}}{\frac{x^{2k+1}}{(2k+1)!}} \right| = \lim_{k \to \infty} \left| \frac{\frac{x^{2k+3}}{(2k+3)!}}{\frac{x^{2k+1}}{(2k+1)!}} \right|$$

$$= \lim_{k \to \infty} \left| \frac{x^{2k+3}}{(2k+3)!} . \frac{(2k+1)!}{x^{2k+1}} \right| = \lim_{k \to \infty} \left| \frac{x^{2k+3}}{(2k+3)(2k+2)(2k+1)!} . \frac{(2k+1)!}{x^{2k+1}} \right|$$

$$= \lim_{k \to \infty} \left| \frac{x^2}{(2k+3)(2k+2)} \right| = \left| \frac{x^2}{(2\infty+3)(2\infty+2)} \right| = \left| \frac{x^2}{\infty} \right| = 0 < 1$$

$\therefore$ The series is convergent for all values of $x \in R$.

$\therefore$ The interval of convergence is $(-\infty, +\infty)$.

Estimation of terms No.: Use $\left| U_k \right| < x.\varepsilon$

$\frac{x^{2k+1}}{(2k+1)!} < x.\varepsilon$. Here $\varepsilon = 1 \times 10^{-6}$ & $\sin x = \sin(1/2) \Rightarrow x = 1/2$

$$\therefore \ \frac{(1/2)^{2k+1}}{(2k+1)!} < (1/2)(1 \times 10^{-6})$$

By trial and error $k = 4$. Thus, five terms are needed.

Example 4: Check whether the Maclaurin expansion for $\frac{1}{1-x}$ is valid to compute 4^{-1} or not.

Solution:

Maclaurin series is $f(x)=f(0)+xf'(0)+\frac{x^2}{2!}f''(0)+\frac{x^3}{3!}f'''(0)+\ldots\ldots$

$$f(x)=\frac{1}{1-x}=(1-x)^{-1} \quad\Rightarrow\quad f(0)=(1-0)^{-1}=1$$

$$f'(x)=-1(1-x)^{-2}.(-1)=(1-x)^{-2} \quad\Rightarrow\quad f'(0)=(1-0)^{-2}=1$$

$$f''(x)=-2(1-x)^{-3}.(-1)=2(1-x)^{-3} \quad\Rightarrow\quad f''(0)=2(1-0)^{-3}=2$$

$$f'''(x)=2.(-3)(1-x)^{-4}.(-1)=6(1-x)^{-4} \quad\Rightarrow\quad f'''(0)=6(1-0)^{-4}=6$$

$$\therefore\ f(x)=\frac{1}{1-x}=1+x(1)+\frac{x^2}{2!}.(2)+\frac{x^3}{3!}.(6)+\ldots\ldots\Rightarrow \frac{1}{1-x}=1+x+x^2+x^3+\ldots\ldots$$

<u>Convergence test</u>: Check $\lim_{k\to\infty}\left|\frac{U_{k+1}}{U_k}\right|$,

$$\frac{1}{1-x}=1+x+x^2+x^3+\ldots\ldots \quad\Rightarrow\quad \frac{1}{1-x}=\sum_{k=0}^{\infty}x^k$$

$$\therefore \lim_{k\to\infty}\left|\frac{U_{k+1}}{U_k}\right|=\lim_{k\to\infty}\left|\frac{x^{k+1}}{x^k}\right|=\lim_{k\to\infty}|x|=|x|$$

$\therefore$ The series converges when $|x|<1 \Rightarrow$ either $x<1$ or $-x<1 \Rightarrow x>-1$

$\therefore$ The interval of convergence is $(-1,1)$.

To compute $4^{-1} \;\Rightarrow\; 4^{-1}=\frac{1}{1-x} \;\Rightarrow\; \frac{1}{4}=\frac{1}{1-x} \;\Rightarrow\; 1-x=4 \;\Rightarrow\; x=-3\notin(-1,1)$

$\therefore$ Thus, the series is not valid to compute 4^{-1} (since it will diverge).

Example 5: Given the following DE: $y''=x-y'$, $y(0)=1$, $y'(0)=1$.

Using Taylor series, find the value of $y(0.5)$. $(\varepsilon=1\times10^{-3})$

Solution:

Taylor series is $f(x)=f(a)+(x-a)f'(a)+\frac{(x-a)^2}{2!}f''(a)+\ldots.$

Take $a=0$. Then, at $x=0.5 \Rightarrow y(0.5)=y(0)+0.5y'(0)+\frac{0.5^2}{2!}y''(0)+\frac{0.5^3}{3!}y'''(0)+..$

<u>1st iteration:</u> Use 4-terms of Taylor series

$y(0)=1$ & $y'(0)=1$ & $y''=x-y' \;\Rightarrow\; y''(0)=0-y'(0) \;\Rightarrow\; y''(0)=0-1=-1$

& $\quad y''' = 1 - y'' \quad \Rightarrow \quad y'''(0) = 1 - y''(0) \quad \Rightarrow \quad y'''(0) = 1 - (-1) = 2$

$\therefore \quad y(0.5) = 1 + 0.5(1) + \frac{0.5^2}{2!}(-1) + \frac{0.5^3}{3!}(2) = 1.416666$

<u>2nd iteration:</u> Use 5-terms of Taylor series

$y^{(4)} = 0 - y''' \quad \Rightarrow \quad y^{(4)} = -y''' \quad \Rightarrow \quad y^{(4)}(0) = -y'''(0) \quad \Rightarrow \quad y^{(4)}(0) = -(2) = -2$

$\therefore \quad y(0.5) = 1 + 0.5(1) + \frac{0.5^2}{2!}(-1) + \frac{0.5^3}{3!}(2) + \frac{0.5^4}{4!}(-2) = 1.411458$

The calculations must be repeated and continued until $\Delta \le \varepsilon$.

i	*No. of terms*	y_i	$\Delta_i = \left| y_{i+1} - y_i \right|$
1	4	1.416666	-
2	5	1.411458	5.2×10^{-3}
3	6	1.411979	$5.2 \times 10^{-4} < \varepsilon$

$\therefore \quad y(0.5) \approx 1.411$

<u>Note</u>: From the analytical solution $y = \frac{1}{2}x^2 - x - 2e^{-x} + 3$.

Thus, the exact value is $y(0.5) = \frac{1}{2}(0.5)^2 - 0.5 - 2e^{-0.5} + 3 = 1.411938$.

<u>Example 6</u>: After five seconds, the following information of a moving body is measured: position = 25 m, velocity = 10 m/s, and acceleration = 2 m/s^2. Using the principal of Taylor series, estimate the position after another five seconds.

Solution:

Taylor series is $f(t) = f(a) + (t-a)f'(a) + \frac{(t-a)^2}{2!}f''(a) + \ldots\ldots.$

If the position is $f(t)$, then the velocity is $f'(t)$ and the acceleration is $f''(t)$.

Expanding the function $f(t)$ about t = 5 s (i.e. $a = 5$) yields:

$$f(t) = f(5) + (t-5)f'(5) + \frac{(t-5)^2}{2!}f''(5) + \ldots. = 25 + (t-5)(10) + \frac{(t-5)^2}{2!}(2) + \ldots.$$

At t = 10 s $\quad \Rightarrow \quad f(10) = 25 + (10-5)(10) + \frac{(10-5)^2}{2!}(2) = 100$ m.

Example 7: Using Taylor series, compute the value of $\tan 47^\circ$ to an accuracy of three decimal places.

Solution:

Taylor series is $f(x) = f(a) + (x-a) f'(a) + \dfrac{(x-a)^2}{2!} f''(a) + \ldots\ldots$

Let $f(x) = \tan x$ and $a = 45^\circ = 45 \times \dfrac{\pi}{180} = \dfrac{\pi}{4}$ *radian*

$f(x) = \tan x \qquad \Rightarrow \qquad f(a) = f(45^\circ) = \tan(45^\circ) = 1$

$f'(x) = \sec^2 x = 1/\cos^2 x \qquad \Rightarrow \qquad f'(45^\circ) = 1/\cos^2(45^\circ) = 1/(1/\sqrt{2})^2 = 2$

$f''(x) = -2\cos^{-3} x.(-\sin x) = 2\sin x/\cos^3 x$

$\Rightarrow \quad f''(45^\circ) = 2\sin(45^\circ)/\cos^3(45^\circ) = 2.(1/\sqrt{2})/(1/\sqrt{2})^3 = 4$

$f'''(x) = 2(\sin x(-3\cos^{-4} x.(-\sin x)) + \cos x.\cos^{-3} x) = 6\sin^2 x/\cos^4 x + 2/\cos^2 x$

$f'''(45^\circ) = 6\sin^2(45^\circ)/\cos^4(45^\circ) + 2/\cos^2(45^\circ) = 6(1/\sqrt{2})^2/(1/\sqrt{2})^4 + 2(1/\sqrt{2})^2 = 16$

$$f(x) = 1 + (x - \frac{\pi}{4})(2) + \frac{(x-\frac{\pi}{4})^2}{2!}.(4) + \frac{(x-\frac{\pi}{4})^3}{3!}.(16) + \ldots\ldots$$

$$\therefore \quad \tan x = 1 + 2(x-\frac{\pi}{4}) + 2(x-\frac{\pi}{4})^2 + \frac{8}{3}(x-\frac{\pi}{4})^3 + \ldots\ldots$$

To compute $\tan 47^\circ \Rightarrow$ Use $x = 47^\circ = 47 \times \dfrac{\pi}{180} = \dfrac{47\pi}{180}$ *radian*

1st iteration: Use two terms of Taylor series

$$\tan 47^\circ = 1 + 2(\frac{47\pi}{180} - \frac{\pi}{4}) = 1.069813$$

2nd iteration: Use three terms of Taylor series

$$\tan 47^\circ = 1 + 2(\frac{47\pi}{180} - \frac{\pi}{4}) + 2(\frac{47\pi}{180} - \frac{\pi}{4})^2 = 1.072250$$

i	*No. of terms*	tan 46°	$\lvert\Delta\rvert$
1	2	1.069813	-
2	3	1.072250	2.4×10^{-3}
3	4	1.072364	$1.14 \times 10^{-4} < \varepsilon$

$\therefore \quad \tan 47^\circ \approx 1.072364$

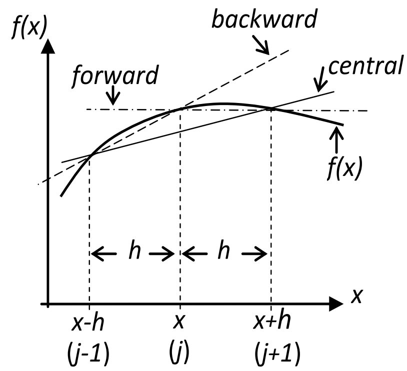
5- Numerical Differentiation
(Finite Difference Calculus)

Introduction

Numerical differentiation is the process of finding the numerical value of a derivative of a given function at a given point. In numerical analysis, numerical differentiation describes algorithms for estimating the derivative of a mathematical function using values of the function and perhaps other knowledge about the function.

Forward and backward differences

Consider a function $f(x)$ which is analytical (can be expanded by Taylor series) in the neighborhood of a point *x* as shown in the figure. We can find $f(x+h)$ by expanding $f(x)$ in a Taylor series about *x*:



$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \ldots ,$$

solving for $f'(x)$ yields:

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2!} f''(x) - \frac{h^2}{3!} f'''(x) - \ldots ,$$

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

This equation represents the first derivative of $f(x)$ with respect to *x* which is accurate to within an error of order *h*. employing the subscript notation:

$f(x) = f_j$ and $f(x+h) = f_{j+1}$, then

$$f'_j = \frac{f_{j+1} - f_j}{h} + O(h) \quad \text{or} \quad f'_j = \frac{\Delta f_j}{h} + O(h),$$

where Δf_j is the first forward difference of *f* at *j*, and $\frac{\Delta f_j}{h}$ is the first forward difference approximation to f' at *j* with an error order of *h*.

Similarly, we can find $f(x-h)$ by expanding $f(x)$ in a Taylor series about *x*:

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \ldots ,$$

solving for $f'(x)$ yields:

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \frac{h}{2!} f''(x) - \frac{h^2}{3!} f'''(x) - \ldots ,$$

or simply $f'_j = \dfrac{f_j - f_{j-1}}{h} + O(h)$ or $f'_j = \dfrac{\nabla f_j}{h} + O(h)$,

where ∇f_j is the first backward difference of *f* at *j*, and $\dfrac{\nabla f_j}{h}$ is the first backward difference approximation to f' at *j* with an error order of *h*.

How to find higher order derivatives

To find $f''(x)$, using Taylor series expansion of $f(x+h)$ and $f(x+2h)$ about *x* gives:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \ldots , \qquad \ldots\ldots\ldots\ldots (1)$$

$$f(x+2h) = f(x) + 2hf'(x) + \frac{4h^2}{2!} f''(x) + \frac{8h^3}{3!} f'''(x) + \ldots \qquad \ldots\ldots\ldots\ldots (2)$$

Multiplying Eq.1 by 2 and subtracting Eq.1 from Eq.2, then solving for $f''(x)$ yields:

$$f''(x) = \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} - hf'''(x) - \ldots ,$$

or simply, $f''_j = \dfrac{f_{j+2} - 2f_{j+1} + f_j}{h^2} + O(h)$ or $f''_j = \dfrac{\Delta^2 f_j}{h^2} + O(h)$,

where $\Delta^2 f_j$ is the second forward difference of *f* at *j*.

Similarly, by using the Taylor series expansion of $f(x-h)$ and $f(x-2h)$ about *x*, we can get:

$$f_j'' = \frac{f_j - 2f_{j-1} + f_{j-2}}{h^2} + O(h) \quad \text{or} \quad f_j'' = \frac{\nabla^2 f_j}{h^2} + O(h),$$

where $\nabla^2 f_j$ is the second backward difference of f at j.

Generally, any forward or backward difference may be obtained starting from the first forward or backward difference by using the following recurrence formulae:

$$\Delta^n f_j = \Delta(\Delta^{n-1} f_j) \quad \text{and} \quad \nabla^n f_j = \nabla(\nabla^{n-1} f_j).$$

For example,

$$\Delta^2 f_j = \Delta(\Delta f_j) = \Delta(f_{j+1} - f_j) = \Delta f_{j+1} - \Delta f_j = (f_{j+2} - f_{j+1}) - (f_{j+1} - f_j)$$
$$= f_{j+2} - 2f_{j+1} + f_j.$$

Thus, the derivatives of any order, with an error of order h, are given by:

$$\frac{d^n f_j}{dx^n} = \frac{\Delta^n f_j}{h^n} + O(h), \quad \text{or} \quad \frac{d^n f_j}{dx^n} = \frac{\nabla^n f_j}{h^n} + O(h).$$

Note: The 1st forward and backward difference approximations of $O(h)$ are exact for 1st polynomials (straight lines), and the 2nd forward and backward difference approximations of $O(h)$ are exact for 2nd degree polynomials. Generally, the nth difference approximations of $O(h)$ for $f^n(x)$ are exact for polynomials of n-degree.

How to find more accurate approximations

More accurate expressions for derivatives may be found by taking more terms in the Taylor series expansion. For example, to find $f'(x)$ with $O(h)^2$:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \ldots\ldots,$$

but $f''(x) = \dfrac{f(x+2h) - 2f(x+h) + f(x)}{h^2} + O(h)$, substituting above:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}\left[\frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} + O(h)\right] + \frac{h^3}{3!}f'''(x) + ..,$$

solving for $f'(x)$ yields:

$$f'(x) = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} + O(h)^2 \ ,$$

or simply, $$f'_j = \frac{-f_{j+2} + 4f_{j+1} - 3f_j}{2h} + O(h)^2 .$$

Note: This expression is exact for polynomials of degree 2 and lower (since the error involves only third and higher derivatives).

Central differences

Using Taylor series expansion of $f(x+h)$ and $f(x-h)$ about x gives:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + ... , \qquad .... (3)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + ... \qquad .... (4)$$

Subtracting Eq.4 from Eq.3 and solving for $f'(x)$ yields:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{3!}f'''(x) - ...... ,$$

or simply, $$f'_j = \frac{f_{j+1} - f_{j-1}}{2h} + O(h)^2 .$$

Note: This expression is exact for polynomials of degree 2 and lower.

To obtain $f''(x)$, one additional Taylor series expansion in each direction is required. In general:

$$\frac{d^n f_j}{dx^n} = \frac{\nabla^n f_{j+n/2} + \Delta^n f_{j-n/2}}{2h^n} + O(h)^2 \qquad n \text{ is even,}$$

$$\frac{d^n f_j}{dx^n} = \frac{\nabla^n f_{j+(n-1)/2} + \Delta^n f_{j-(n-1)/2}}{2h^n} + O(h)^2 \qquad n \text{ is odd.}$$

Note: The following table gives the most used finite difference approximations:

FORWARD DIFFERENCES	BACKWARD DIFFERENCES	Error
First Derivative	First Derivative	
$f'_j = \dfrac{-f_j + f_{j+1}}{h}$	$f'_j = \dfrac{f_j - f_{j-1}}{h}$	$O(h)$
$f'_j = \dfrac{-3f_j + 4f_{j+1} - f_{j+2}}{2h}$	$f'_j = \dfrac{3f_j - 4f_{j-1} + f_{j-2}}{2h}$	$O(h)^2$
Second Derivative	Second Derivative	
$f''_j = \dfrac{f_j - 2f_{j+1} + f_{j+2}}{h^2}$	$f''_j = \dfrac{f_j - 2f_{j-1} + f_{j-2}}{h^2}$	$O(h)$
$f''_j = \dfrac{2f_j - 5f_{j+1} + 4f_{j+2} - f_{j+3}}{h^2}$	$f''_j = \dfrac{2f_j - 5f_{j-1} + 4f_{j-2} - f_{j-3}}{h^2}$	$O(h)^2$
Third Derivative	Third Derivative	
$f'''_j = \dfrac{-f_j + 3f_{j+1} - 3f_{j+2} + f_{j+3}}{h^3}$	$f'''_j = \dfrac{f_j - 3f_{j-1} + 3f_{j-2} - f_{j-3}}{h^3}$	$O(h)$
$f'''_j = \dfrac{-5f_j + 18f_{j+1} - 24f_{j+2} + 14f_{j+3} - 3f_{j+4}}{2h^3}$	$f'''_j = \dfrac{5f_j - 18f_{j-1} + 24f_{j-2} - 14f_{j-3} + 3f_{j-4}}{2h^3}$	$O(h)^2$
Fourth Derivative	Fourth Derivative	
$f_j^{iv} = \dfrac{f_j - 4f_{j+1} + 6f_{j+2} - 4f_{j+3} + f_{j+4}}{h^4}$	$f_j^{iv} = \dfrac{f_j - 4f_{j-1} + 6f_{j-2} - 4f_{j-3} + f_{j-4}}{h^4}$	$O(h)$
$f_j^{iv} = \dfrac{3f_j - 14f_{j+1} + 26f_{j+2} - 24f_{j+3} + 11f_{j+4} - 2f_{j+5}}{h^4}$	$f_j^{iv} = \dfrac{3f_j - 14f_{j-1} + 26f_{j-2} - 24f_{j-3} + 11f_{j-4} - 2f_{j-5}}{h^4}$	$O(h)^2$

CENTRAL DIFFERENCES	Error
First Derivative	
$f'_j = \dfrac{-f_{j-1} + f_{j+1}}{2h}$	$O(h)^2$
$f'_j = \dfrac{f_{j-2} - 8f_{j-1} + 8f_{j+1} - f_{j+2}}{12h}$	$O(h)^4$
Second Derivative	
$f''_j = \dfrac{f_{j-1} - 2f_j + f_{j+1}}{h^2}$	$O(h)^2$
$f''_j = \dfrac{-f_{j-2} + 16f_{j-1} - 30f_j + 16f_{j+1} - f_{j+2}}{12h^2}$	$O(h)^4$
Third Derivative	
$f'''_j = \dfrac{-f_{j-2} + 2f_{j-1} - 2f_{j+1} + f_{j+2}}{2h^3}$	$O(h)^2$
$f'''_j = \dfrac{f_{j-3} - 8f_{j-2} + 13f_{j-1} - 13f_{j+1} + 8f_{j+2} - f_{j+3}}{8h^3}$	$O(h)^4$
Fourth Derivative	
$f_j^{iv} = \dfrac{f_{j-2} - 4f_{j-1} + 6f_j - 4f_{j+1} + f_{j+2}}{h^4}$	$O(h)^2$
$f_j^{iv} = \dfrac{-f_{j-3} + 12f_{j-2} - 39f_{j-1} + 56f_j - 39f_{j+1} + 12f_{j+2} - f_{j+3}}{6h^4}$	$O(h)^4$

Example 1: Find $f'(x)$ at $x=1$ for the function $f(x)=e^{x}$. Compare with the exact answer. (Use $h=0.1$)

Solution:

By central difference approximations with $O(h)^2$,

$$f_j' = \frac{-f_{j-1}+f_{j+1}}{2h} + O(h)^2,$$

0.9	1	1.1
j-1	*j*	*j+1*

At $x=1 \Rightarrow j=1, \quad j+1=x+h=1+0.1=1.1,$ and $j-1=x-h=1-0.1=0.9$.

$$f'(1) \approx \frac{-f(0.9)+f(1.1)}{2(0.1)} \quad \Rightarrow \quad f'(1) \approx \frac{-e^{0.9}+e^{1.1}}{0.2} \approx 2.722815.$$

The (exact) value is $e^{1}=2.718282$ (from the scientific calculator).

Percent relative error $P=\left|\frac{exact-approx.}{exact}\right| \times 100 = \left|\frac{2.718282-2.722815}{2.718282}\right| \times 100 = 0.17\%$

Notes:

* If we use forward difference approximations with $O(h)$,

$$f_j' = \frac{-f_{j}+f_{j+1}}{h} + O(h),$$

$$f'(1) \approx \frac{-f(1)+f(1.1)}{0.1} \quad \Rightarrow \quad f'(1) \approx \frac{-e^{1}+e^{1.1}}{0.1} \approx 2.858842.$$

The (exact) value is $e^{1}=2.718282$ (from the scientific calculator).

Percent relative error $P=\left|\frac{2.718282-2.858842}{2.718282}\right| \times 100 = 5.17\%$.

* If we use backward difference approximations with $O(h)$,

$$f_j' = \frac{f_{j}-f_{j-1}}{h} + O(h),$$

$$f'(1) \approx \frac{f(1)-f(0.9)}{0.1} \quad \Rightarrow \quad f'(1) \approx \frac{e^{1}-e^{0.9}}{0.1} \approx 2.586787.$$

Percent relative error $P=\left|\frac{2.718282-2.586787}{2.718282}\right| \times 100 = 4.8\%$.

Example 2: Given the function $f(x) = (x+1)^x$, find $f'(2)$ correct to three decimals.

Solution:

Use central difference approximations with $O(h)^2$,

$$f'_j = \frac{-f_{j-1} + f_{j+1}}{2h} + O(h)^2.$$

1.8 2 2.2
j-1 j j+1

1st iteration: Take $h_1 = 0.2$,

At $x = 2 \Rightarrow j = 2$, $j+1 = x + h_1 = 2 + 0.2 = 2.2$, and $j-1 = x - h_1 = 2 - 0.2 = 1.8$.

$$f'(2) \approx \frac{-f(1.8) + f(2.2)}{2(0.2)} \approx \frac{-(1.8+1)^{1.8} + (2.2+1)^{2.2}}{0.4} \approx 16.352674.$$

1.9 2 2.1
j-1 j j+1

2nd iteration: Take $h_2 = \frac{h_1}{2} = \frac{0.2}{2} = 0.1$,

$j+1 = x + h_2 = 2 + 0.1 = 2.1$, and $j-1 = x - h_2 = 2 - 0.1 = 1.9$.

$$f'(2) \approx \frac{-f(1.9) + f(2.1)}{2(0.1)} \approx \frac{-(1.9+1)^{1.9} + (2.1+1)^{2.1}}{0.2} \approx 16.002864.$$

The calculations must be continued until $\Delta \le \varepsilon$.

No. of Iteration (i)	h_i	f'_i	$\Delta_i = \left\| f'_i - f'_{i-1} \right\|$
1	0.2	16.352674	----
2	0.1	16.002864	0.34….
3	0.05	15.916291	0.08….
4	0.025	15.894702	0.02….
5	0.0125	15.889308	5.3×10^{-3}
6	0.00625	15.887960	1.3×10^{-3}
7	0.003125	15.887623	$3.3\times10^{-4} < \varepsilon$

$\therefore \quad f'(2) \approx 15.887623.$

Example 3: Find $f'(0)$ for the function $f(x) = \sqrt{x} + 7x$. $(\varepsilon = 1\times 10^{-3})$

Solution:

Use forward difference approximations with $O(h)$,

$$f'_j = \frac{-f_j + f_{j+1}}{h} + O(h).$$

1st iteration: Take $h_1 = 0.2$,

At $x = 0 \;\Rightarrow\; j = 0,\quad j+1 = x + h_1 = 0 + 0.2 = 0.2$.

$$f'(0) \approx \frac{-f(0) + f(0.2)}{0.2} \quad\Rightarrow\quad f'(0) \approx \frac{-(\sqrt{0} + 7(0)) + (\sqrt{0.2} + 7(0.2))}{0.2} \approx 9.236.$$

2nd iteration: Take $h_2 = \frac{h_1}{2} = \frac{0.2}{2} = 0.1$.

The calculations must be repeated as in the 1st iteration and continued until $\Delta \le \varepsilon$.

No. of Iteration (i)	h_i	f'_i	$\Delta_i = \left\| f'_i - f'_{i-1} \right\|$
1	0.2	9.236068	----
2	0.1	10.162278	0.92621
3	0.05	11.472136	1.309858
4	0.025	13.324555	1.852419 (divergence)

$\therefore\;\; f'(0)$ is undefined (does not exist).

Check: $f'(x) = \frac{1}{2\sqrt{x}} + 7 \;\Rightarrow\; f'(0) = \frac{1}{2\sqrt{0}} + 7 = \frac{1}{0} + 7$.   (undefined)

Example 4: Find $f'(0)$, $f'(2)$, $f'(4)$, and $f''(0)$ with error of $O(h)^2$ for the function of the following equally spaced data:

x	0	1	2	3	4
$f(x)$	30	33	28	12	- 22

Solution:

* At $x = 0$, forward differences must be used with $O(h)^2$,

$$f'_j = \frac{-3f_j + 4f_{j+1} - f_{j+2}}{2h} + O(h)^2,$$

$$\therefore f'(0)=\frac{-3f(0)+4f(1)-f(2)}{2(1)}=\frac{-3(30)+4(33)-(28)}{2}=7.$$

$$f_j''=\frac{2f_j-5f_{j+1}+4f_{j+2}-f_{j+3}}{h^2}+O(h)^2,$$

$$\therefore f''(0)=\frac{2f(0)-5f(1)+4f(2)-f(3)}{(1)^2}=\frac{2(30)-5(33)+4(28)-(12)}{1}=-5.$$

* At $x=2$, use central differences with $O(h)^2$,

$$f_j'=\frac{-f_{j-1}+f_{j+1}}{2h}+O(h)^2,$$

$$\therefore f'(2)=\frac{-f(1)+f(3)}{2(1)}=\frac{-(33)+(12)}{2}=-10.5.$$

* At $x=4$, backward differences must be used with $O(h)^2$,

$$f_j'=\frac{3f_j-4f_{j-1}+f_{j-2}}{2h}+O(h)^2,$$

$$\therefore f'(4)=\frac{3f(4)-4f(3)+f(2)}{2(1)}=\frac{3(-22)-4(12)+(28)}{2}=-43.$$

Example 5: The following data represent a polynomial. Find its equation.

x	0	1	2	3	4	5
$f(x)$	1.0	0.5	8.0	35.5	95.0	198.5

Solution:

The forward differences can be calculated as shown in the table below:

x	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
0	1.0	- 0.5	8	12	0
1	0.5	7.5	20	12	0
2	8.0	27.5	32	12	
3	35.5	59.5	44		
4	95.0	103.5			
5	198.5				

Since the 3rd difference (which is equivalent to the 3rd derivative) is constant, then the polynomial is of 3rd degree. The forward difference representation of the 3rd derivative is: $\dfrac{d^3 f}{dx^3} = \dfrac{\Delta^3 f}{h^3} + O(h)$.

However, for a 3rd degree polynomial, this expression is exact (i.e. $O(h) = 0$).

$$\frac{d^3 f}{dx^3} = \frac{\Delta^3 f}{h^3} = \frac{12}{1^3} = 12 \quad \Rightarrow \quad \frac{d^2 f}{dx^2} = 12x + A,$$

$$\frac{df}{dx} = 6x^2 + Ax + B \quad \Rightarrow \quad f(x) = 2x^3 + \frac{A}{2}x^2 + Bx + C.$$

We have 3 unknown constants, so we need 3 points. Substituting the three points $(0,1)$, $(1,0.5)$, and $(2,8)$ into the above equation gives respectively:

$$2(0)^3 + \frac{A}{2}(0)^2 + B(0) + C = 1 \quad \Rightarrow \quad C = 1$$

$$2(1)^3 + \frac{A}{2}(1)^2 + B(1) + 1 = 0.5 \quad \Rightarrow \quad A + 2B = -5 \qquad \text{……….. (I)}$$

$$2(2)^3 + \frac{A}{2}(2)^2 + B(2) + 1 = 8 \quad \Rightarrow \quad 2A + 2B = -9 \qquad \text{………. (II)}$$

Solving Eqs. I and II simultaneously gives:

$A = -4$ and $B = -1/2$

$$\therefore f(x) = 2x^3 + \frac{-4}{2}x^2 + \frac{-1}{2}x + 1 \quad \Rightarrow \quad f(x) = 2x^3 - 2x^2 - x/2 + 1.$$

Example 6: The deflections at selected locations in a beam, of $EI = 4 \times 10^6$ N.m^2 and $L = 4$ m, are:

Location (m)	0	0.5	1	1.5	2	2.5	3	3.5	4
Deflection (mm)	0	12.7	23.1	30.8	33.3	29.9	22.6	11.8	0

Determine, as accurate as possible, the slope and shear force at both ends and the bending moment at midspan.

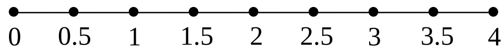
Solution:

Let x represents the location and y represents the deflection, then,

The slope $\theta = \dfrac{dy}{dx}$, shear force $V = -EI.\dfrac{d^3 y}{dx^3}$, and bending moment $M = -EI.\dfrac{d^2 y}{dx^2}$.

* At $x = 0$ m, forward differences must be used and we choose it with $O(h)^2$,

The slope $\theta_j = f'_j = \dfrac{-3f_j + 4f_{j+1} - f_{j+2}}{2h}$,



$$\therefore \theta_0 = \frac{-3y(0) + 4y(0.5) - y(1)}{2h} = \frac{-3(0) + 4(12.7) - (23.1)}{2(0.5)(1000)} = 27.7 \times 10^{-3}.$$

The shear force $V_j = -EI.f'''_j = -EI.\dfrac{-5f_j + 18f_{j+1} - 24f_{j+2} + 14f_{j+3} - 3f_{j+4}}{2h^3}$,

$$V_0 = -EI.\frac{-5y(0) + 18y(0.5) - 24y(1) + 14y(1.5) - 3y(2)}{2h^3},$$

$$V_0 = -4 \times 10^6.\frac{-5(0) + 18(12.7) - 24(23.1) + 14(30.8) - 3(33.3)}{2(0.5)^3(1000)} = -88000 \text{N}.$$

* At $x = 4$ m, backward difference must be used and we choose it with $O(h)^2$,

The slope $\theta_j = f'_j = \dfrac{3f_j - 4f_{j-1} + f_{j-2}}{2h}$,

$$\therefore \theta_4 = \frac{3y(4) - 4y(3.5) + y(3)}{2h} = \frac{3(0) - 4(11.8) + (22.6)}{2(0.5)(1000)} = -24.6 \times 10^{-3}.$$

The shear force $V_j = -EI.f'''_j = -EI.\dfrac{5f_j - 18f_{j-1} + 24f_{j-2} - 14f_{j-3} + 3f_{j-4}}{2h^3}$,

$$V_4 = -EI.\frac{5y(4) - 18y(3.5) + 24y(3) - 14y(2.5) + 3y(2)}{2h^3},$$

$$V_4 = -4 \times 10^6.\frac{5(0) - 18(11.8) + 24(22.6) - 14(29.9) + 3(33.3)}{2(0.5)^3(1000)} = -180800 \text{N}.$$

* At $x = 2$ m (midspan), using central difference and we choose it with $O(h)^4$,

The bending moment $M_j = -EI.f''_j = -EI.\dfrac{-f_{j-2} + 16f_{j-1} - 30f_j + 16f_{j+1} - f_{j+2}}{12h^2}$

$$M_2 = -EI.\frac{-y(1) + 16y(1.5) - 30y(2) + 16y(2.5) - y(3)}{12h^2},$$

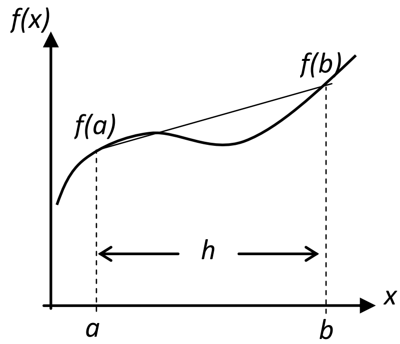
$$M_2 = -4 \times 10^6.\frac{-(23.1) + 16(30.8) - 30(33.3) + 16(29.9) - (22.6)}{12(0.5)^2(1000)} = 98000 \text{N.m}.$$

6- Numerical Integration

Introduction

The primary purpose of numerical integration (also called quadrature) is the evaluation of integrals which are either impossible or else very difficult to evaluate analytically. Numerical integration is also essential in the evaluation of integrals of functions available only at discrete points. Such functions often result from the numerical solution of differential equations or from experimental data taken at discrete intervals.

An integral of a given function represents the area enclosed by this function and the x-axis. So, evaluating this area is equivalent to evaluate the integral of this function. In the following, some of numerical techniques, which are used to evaluate an integral, are presented.



1- Trapezoidal rule

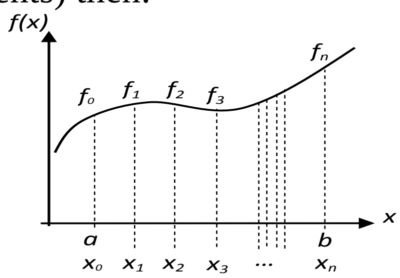
Consider the integral:

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

If $f(x)$ is replaced by a straight line (1st order polynomial) connecting two points, then the area under this function can be computed from:

$$I = \frac{h}{2}.(f_a + f_b) . \qquad \text{[Trapezoidal rule for one segment (panel)]}$$

If we divide the interval [a,b] into n equal subintervals (segments) then:



$$h = \Delta x = \frac{b-a}{n} ,$$

$$I = \frac{h}{2}.(f_0 + f_1) + \frac{h}{2}.(f_1 + f_2) + ...+ \frac{h}{2}.(f_{n-1} + f_n) ,$$

or $\quad I = \frac{h}{2}.(f_0 + 2\sum_{i=1}^{n-1} f_i + f_n) , \qquad$ (trapezoidal rule for n segments)

where, $f_0 = f_a = f(a)$ and $f_n = f_b = f(b)$.

Notes:

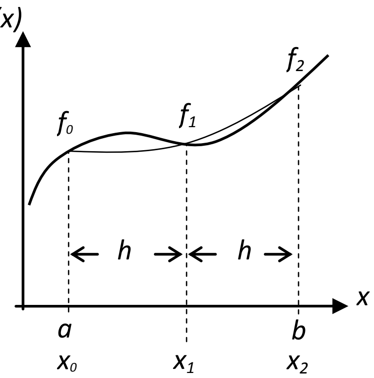
1- The trapezoidal rule gives an answer with an error of order $O(h)^2$.

2- The trapezoidal rule gives an answer which is exact for 1st degree polynomial and approximate for other polynomials of higher degree.

3- Reducing h will, in general, provide more accurate answers.

2- Simpson's rule

2.1- Simpson's 1/3 rule



If $f(x)$ is replaced by a 2nd order polynomial (parabola) connecting three points, then the area under this function can be computed from:

$$I=\frac{h}{3}.(f_0+4f_1+f_2)$$.(Simpson's 1/3 rule for two segments)

If we divide the interval [a,b] into n equal subintervals (n is even) then:

$$I=\frac{h}{3}.(f_0+4f_1+f_2)+\frac{h}{3}.(f_2+4f_3+f_4)+.......+\frac{h}{3}.(f_{n-2}+4f_{n-1}+f_n),$$

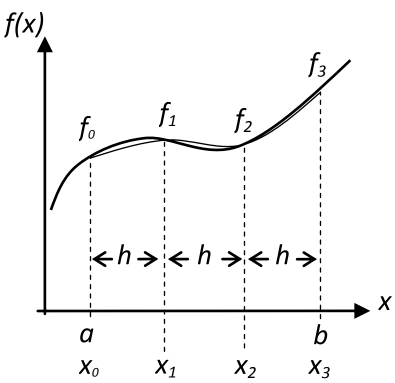
or $$I=\frac{h}{3}.(f_0+4\sum_{i=1,3,5,..}^{n-1}f_i+2\sum_{i=2,4,6,..}^{n-2}f_i+f_n).$$ [Simpson's 1/3 rule for n (even) segments]

Notes:

1- Simpson's 1/3 rule gives answers with an error of order $O(h)^4$.

2- Simpson's 1/3 gives answers which are exact for polynomials of 2nd degree or lower and approximate for other polynomials of higher degree.

2.2- Simpson's 3/8 rule



If $f(x)$ is replaced by a 3rd order polynomial (cubic equation) connecting four points, then the area under this function can be computed from:

$$I=\frac{3h}{8}.(f_0+3f_1+3f_2+f_3).$$ (Simpson's 3/8 rule for three segments)

If we divide the interval [a,b] into n equal subintervals (segments) then:

$$I=\frac{3h}{8}.(f_0+3f_1+3f_2+f_3)+\frac{3h}{8}.(f_3+3f_4+3f_5+f_6)+..+\frac{3h}{8}.(f_{n-3}+3f_{n-2}+3f_{n-1}+f_n)$$

or $\quad I=\dfrac{3h}{8}.[f_0+3(f_1+f_2+f_4+f_5+\ldots)+2\sum\limits_{i=3,6,9,..}^{n-4}f_i+f_n].$ (3/8 rule for n segments)

Notes:

1- Simpson's 3/8 rule gives answers with an error of order $O(h)^4$.

2- Simpson's 3/8 rule gives answers which are exact for polynomials of 3rd degree or lower and approximate for other polynomials of higher degree.

Example 1: Evaluate $I=\int_0^{\pi}\sin x dx$ using six segments. Compare with the exact answer.

f_0	f_1	f_2	f_3	f_4	f_5	f_6
0	π/6	2π/6	3π/6	4π/6	5π/6	π

Solution:

Since $n=6 \quad \Rightarrow \quad h=\Delta x=\dfrac{b-a}{n}=\dfrac{\pi-0}{6}=\dfrac{\pi}{6}$.

By using the trapezoidal rule (which is of error of $O(h)^2$) $\Rightarrow I=\dfrac{h}{2}.(f_0+2\sum\limits_{i=1}^{n-1}f_i+f_n)$,

$$I=\frac{\pi/6}{2}.\{f_0+2(f_1+f_2+f_3+f_4+f_5)+f_6\},$$

$$=\frac{\pi}{12}[\sin 0+2\{\sin(\pi/6)+\sin(2\pi/6)+\sin(3\pi/6)+\sin(4\pi/6)+\sin(5\pi/6)\}+\sin(\pi)]$$

$$\approx 1.954097.$$

The exact value is $I=\left[-\cos x\right]_0^{\pi}=(-\cos\pi)-(-\cos 0)=\{-(-1)\}-\{-(1)\}=2$.

Percent relative error $P=\left|\dfrac{exact-approx.}{exact}\right|\times 100=\left|\dfrac{2-1.954097}{2}\right|\times 100=2.3\%$.

Notes:

* If we use the Simpson's 1/3 rule (which is of error of $O(h)^4$) then,

$$I=\frac{h}{3}.(f_0+4\sum_{i=1,3,5,..}^{n-1}f_i+2\sum_{i=2,4,..}^{n-2}f_i+f_n),$$

$$I=\frac{\pi/6}{3}.\{f_0+4(f_1+f_3+f_5)+2(f_2+f_4)+f_6\},$$

$$= \frac{\pi}{18}[\sin 0 + 4\{\sin(\pi/6) + \sin(3\pi/6) + \sin(5\pi/6)\} + 2\{\sin(2\pi/6) + \sin(4\pi/6)\} + \sin(\pi)]$$

$$\approx 2.000863.$$

Percent relative error $P = \left|\frac{exact - approx.}{exact}\right| \times 100 = \left|\frac{2 - 2.000863}{2}\right| \times 100 = 0.04\%.$

* If we use the Simpson's 3/8 rule (which is of error of $O(h)^4$) then,

$$I = \frac{3h}{8}.[f_0 + 3(f_1 + f_2 + f_4 + f_5 + \ldots) + 2\sum_{i=3,6,9,..}^{n-4} f_i + f_n],$$

$$I = \frac{3(\pi/6)}{8}.\{f_0 + 3(f_1 + f_2 + f_4 + f_5) + 2(f_3) + f_6\},$$

$$= \frac{\pi}{16}[\sin 0 + 3\{\sin(\pi/6) + \sin(2\pi/6) + \sin(4\pi/6) + \sin(5\pi/6)\} + 2\sin(3\pi/6) + \sin(\pi)]$$

$$\approx 2.000005.$$

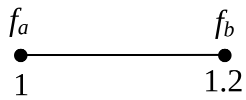
Percent relative error $P = \left|\frac{exact - approx.}{exact}\right| \times 100 = \left|\frac{2 - 2.000005}{2}\right| \times 100 = 0.0003\%.$

Example 2: Given the function $f(x) = (x+1)^x$, find $\int_1^{1.2} f(x)dx$ correct to three decimal places.

Solution:

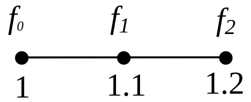
By using the trapezoidal rule,

1st iteration: Take $n = 1$ $\Rightarrow$ $h = \frac{b-a}{n} = \frac{1.2-1}{1} = 0.2,$



$$I = \frac{h}{2}.(f_a + f_b) = \frac{h}{2}.[f(1) + f(1.2)] = \frac{0.2}{2}.[(1+1)^1 + (1.2+1)^{1.2}] = 0.457577.$$

2nd iteration: Take $n = 2$ $\Rightarrow$ $h = \frac{b-a}{n} = \frac{1.2-1}{2} = 0.1,$



$$I = \frac{h}{2}.(f_0 + 2f_1 + f_2) = \frac{h}{2}.[f(1) + 2f(1.1) + f(1.2)] = \frac{0.1}{2}.[(1+1)^1 + 2(1.1+1)^{1.1} + (1.2+1)^{1.2}] = 0.454962$$

The calculations must be continued until $\Delta \le \varepsilon$.

No. of Iteration (i)	h_i	I_i	$\Delta_i = \lvert I_i - I_{i-1} \rvert$
1	0.2	0.457577	----
2	0.1	0.454962	2.6×10^{-3}
3	0.05	0.454306	$6.5 \times 10^{-4} < \varepsilon$

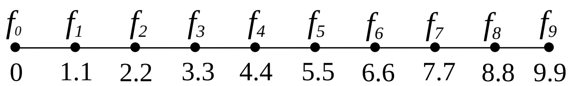
$$\therefore \int_{1}^{1.2} f(x)dx \approx 0.454306.$$

<u>Example 3</u>: Evaluate $\int_{0}^{9.9} f(x)dx$ using the following data:

x	0	1.1	2.2	3.3	4.4	5.5	6.6	7.7	8.8	9.9
$f(x)$	0	0.6	0.8	0.6	0.1	- 0.2	- 0.1	0.1	0.3	0.4

Solution:

Here we have $n = 9$ and $h = 1.1$.



<u>Solution I</u>: By using the trapezoidal rule $\Rightarrow$ $I = \frac{h}{2}.(f_0 + 2\sum_{i=1}^{n-1} f_i + f_n)$,

$$I = \frac{h}{2}.\{f_0 + 2(f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + f_7 + f_8) + f_9\},$$

$$= \frac{1.1}{2}[0 + 2\{0.6 + 0.8 + 0.6 + 0.1 + (-0.2) + (-0.1) + 0.1 + 0.3\} + 0.4] = 2.64.$$

<u>Solution II</u>: Since n = 9 (odd), so we cannot use the Simpson's 1/3 rule directly. Instead, we can apply it for the first 8 segments and the trapezoidal rule for the last segment:

$$I = \frac{h}{3}.\{f_0 + 4(f_1 + f_3 + f_5 + f_7) + 2(f_2 + f_4 + f_6) + f_8\} + \frac{h}{2}.(f_8 + f_9),$$

$$= \frac{1.1}{3}[0 + 4\{0.6 + 0.6 + (-0.2) + 0.1\} + 2\{0.8 + 0.1 + (-0.1)\} + 0.3] + \frac{1.1}{2}[0.3 + 0.4] = 2.695 \cdot$$

<u>Solution III</u>: We can apply the Simpson's 1/3 rule for the first 6 segments and the 3/8 rule for the last 3 segments, then:

$$I = \frac{h}{3}.\{f_0 + 4(f_1 + f_3 + f_5) + 2(f_2 + f_4) + f_6\} + \frac{3h}{8}.\{f_6 + 3(f_7 + f_8) + f_9\},$$

$$= \frac{1.1}{3}[0 + 4\{0.6 + 0.6 + (-0.2)\} + 2(0.8 + 0.1) + (-0.1)] + \frac{3(1.1)}{8}[-0.1 + 3(0.1 + 0.3) + 0.4] = 2.70875 \cdot$$

Solution IV: Since $n = 9 = (3\times3)$, so we can use the Simpson's 3/8 rule directly:

$$I = \frac{3h}{8}.\{f_0 + 3(f_1 + f_2) + f_3\} + \frac{3h}{8}.\{f_3 + 3(f_4 + f_5) + f_6\} + \frac{3h}{8}.\{f_6 + 3(f_7 + f_8) + f_9\},$$

or $$I = \frac{3h}{8}.\{f_0 + 3(f_1 + f_2 + f_4 + f_5 + f_7 + f_8) + 2(f_3 + f_6) + f_9\},$$

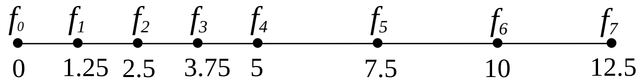
$$= \frac{3(1.1)}{8}[0 + 3\{0.6 + 0.8 + 0.1 + (-0.2) + 0.1 + 0.3\} + 2\{0.6 + (-0.1)\} + 0.4] = 2.68125.$$

Example 4: A rectangular swimming pool is (7.5 m) wide and (12.5 m) long. The depth of water (h) of distance (x) from one end of the pool is measured and found to be as follows:

Distance, x, (m)	0	1.25	2.5	3.75	5	7.5	10	12.5
Depth, h, (m)	1.5	2.05	2.275	2.475	2.625	2.875	3.075	3.25

Determine, as accurate as possible, the volume of water in the pool.

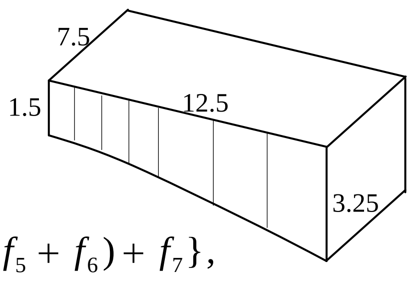
Solution:



Volume of water = Lateral area of water $\times$ wide = $\left(\int_0^{12.5} h.dx\right) \times 7.5$.

Here we have 4 segments of $h_1 = 1.25$ m and 3 segments of $h_2 = 2.5$ m.

By using the Simpson's 1/3 rule for the first 4 segments and the 3/8 rule for the last 3 segments we get:



$$I = \frac{h_1}{3}.(f_0 + 4f_1 + f_2) + \frac{h_1}{3}.(f_2 + 4f_3 + f_4) + \frac{3h_2}{8}.\{f_4 + 3(f_5 + f_6) + f_7\},$$

$$= \frac{1.25}{3}.\{1.5 + 4(2.05) + 2.275\} + \frac{1.25}{3}.\{2.275 + 4(2.475) + 2.625) + \frac{3(2.5)}{8}.\{2.625 + 3(2.875 + 3.075) + 3.25\}$$

$\approx 35.63\ \text{m}^2$.

$\therefore$ Volume of water $\approx 35.63 \times 7.5 \approx 267.225\ \text{m}^3$.

Example 5: Evaluate $I = \int_{2}^{3} \int_{x}^{2x^3} (x^2 + y)dydx$. (Use 4 segments in each direction)

Solution:

Let $f(x,y) = x^2 + y \quad \Rightarrow \qquad g(x) = \int_{x}^{2x^3} f(x,y)dy$ (the inner integral)

$\therefore I = \int_{2}^{3} g(x)dx$. $\qquad h_x = \dfrac{3-2}{4} = 0.25$

g_0	g_1	g_2	g_3	g_4
2	2.25	2.5	2.75	3

By using the Simpson's 1/3 rule, $\quad I = \dfrac{h}{3}.(f_0 + 4\sum_{i=1,3,5,..}^{n-1} f_i + 2\sum_{i=2,4,6,..}^{n-2} f_i + f_n)$,

$$I = \frac{h_x}{3}.\{g_0 + 4(g_1 + g_3) + 2g_2 + g_4\},$$

$$= \frac{0.25}{3}.[g(2) + 4\{g(2.25) + g(2.75)\} + 2g(2.5) + g(3)].$$

To find $g(2)$: $\quad g(2) = \int_{2}^{2(2)^3} f(2,y)dy = \int_{2}^{16} f(2,y)dy$.

f_0	f_1	f_2	f_3	f_4
2	5.5	9	12.5	16

$$h_y = \frac{16-2}{4} = 3.5$$

$$\therefore g(2) = \frac{h_y}{3}.[f_0 + 4(f_1 + f_3) + 2f_2 + f_4]$$

$$= \frac{3.5}{3}.[f(2,2) + 4\{f(2,5.5) + f(2,12.5)\} + 2f(2,9) + f(2,16)]$$

$f(2,2) = 2^2 + 2 = 6$, $\qquad f(2,5.5) = 2^2 + 5.5 = 9.5$, $\qquad f(2,9) = 2^2 + 9 = 13$,
$f(2,12.5) = 2^2 + 12.5 = 16.5$, $\qquad$ and $\qquad f(2,16) = 2^2 + 16 = 20$,

$$\therefore g(2) = \frac{3.5}{3}.[6 + 4(9.5 + 16.5) + 2(13) + 20] = 182.$$

Similarly,
$g(2.25) = 360.9009$, $\quad g(2.5) = 664.8438$, $\quad g(2.75) = 1154.995$, and $\quad g(3) = 1912.5$,

(Note: h_y is different for each of these inner integrals)

$$\therefore I \approx \frac{0.25}{3}.[182 + 4(360.9009 + 1154.995) + 2(664.8438) + 1912.5] \approx 790.6478.$$

The exact answer is: $I = \int_{2}^{3} \int_{x}^{2x^3} (x^2 + y)dydx = \int_{2}^{3} \left[x^2 y + \dfrac{y^2}{2} \right]_{x}^{2x^3} dx$,

$$= \int_{2}^{3} \left(2x^5 + 2x^6 - x^3 - \frac{x^2}{2} \right) dx = \left[\frac{2x^6}{6} + \frac{2x^7}{7} - \frac{x^4}{4} - \frac{x^3}{2(3)} \right]_{2}^{3} = 790.5357.$$

Romberg integration

This powerful and efficient numerical integration technique is based on the use of the trapezoidal rule combined with Richardson extrapolation. Richardson extrapolation is carried out according to:

$$I_k = \frac{1}{4^{k-1} - 1}.\left(4^{k-1} I_m - I_l\right),$$

where I_m and I_l are the more and less accurate integrals, respectively.

If $k = 2$, then $I_2 = \frac{1}{3}.\left(4I_m - I_l\right)$ which gives approximations with $O(h)^4$.

If $k = 3$, then $I_3 = \frac{1}{15}.\left(16I_m - I_l\right)$ which gives approximations with $O(h)^6$.

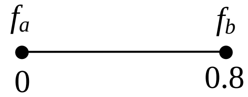
If $k = 4$, then $I_4 = \frac{1}{63}.\left(64I_m - I_l\right)$ which gives approximations with $O(h)^8$.

If $k = 5$, then $I_5 = \frac{1}{255}.\left(256I_m - I_l\right)$ which gives approximations with $O(h)^{10}$.

Example 1: Evaluate $\int_0^{0.8} e^{-x^2}\,dx$ using Romberg integration with an absolute convergence criterion of $\varepsilon = 10^{-6}$.

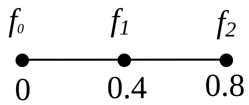
Solution:

1st iteration: Take $n = 1$ $\Rightarrow$ $h = \frac{b-a}{n} = \frac{0.8-0}{1} = 0.8,$



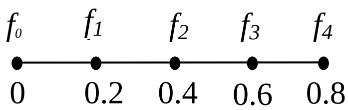
$$I = \frac{h}{2}.(f_a + f_b) = \frac{h}{2}.[f(0) + f(0.8)] = \frac{0.8}{2}.[e^{-(0)^2} + e^{-(0.8)^2}] = 0.610917.$$

2nd iteration: Take $n = 2$ $\Rightarrow$ $h = \frac{b-a}{n} = \frac{0.8-0}{2} = 0.4,$



$$I = \frac{h}{2}(f_0 + 2f_1 + f_2) = \frac{h}{2}[f(0) + 2f(0.4) + f(0.8)] = \frac{0.4}{2}[e^{-(0)^2} + 2e^{-(0.4)^2} + e^{-(0.8)^2}] = 0.646316$$

3rd iteration: Take $n = 4$ $\Rightarrow$ $h = \frac{b-a}{n} = \frac{0.8-0}{4} = 0.2,$



$$I = \frac{h}{2}.(f_0 + 2\sum f_i + f_n) = \frac{h}{2}.[f(0) + 2\{f(0.2) + f(0.4) + f(0.6)\} + f(0.8)]$$

$$= \frac{0.2}{2}.[e^{-(0)^2} + 2\{e^{-(0.2)^2} + e^{-(0.4)^2} + e^{-(0.6)^2}\} + e^{-(0.8)^2}] = 0.654851.$$

The calculations must be continued until $\Delta \le \varepsilon$.

i	n	I_1	$I_2 = \frac{1}{3}.\left(4I_m - I_l\right)$	$I_3 = \frac{1}{15}.\left(16I_m - I_l\right)$	$I_4 = \frac{1}{63}.\left(64I_m - I_l\right)$
1	1	0.610917			
2	2	0.646316	0.658116		
3	4	0.654851	0.657696	0.657668	
4	8	0.656966	0.657671	0.657669	0.657669
$\lvert\Delta\rvert$			0.04….	4.4×10^{-4}	$1 \times 10^{-6} \le \varepsilon$

$$\therefore \int_0^{0.8} e^{-x^2}\,dx \approx 0.657669.$$

Example 2: (Final 2014) A rod is subjected to an axial tensile load and the stress-strain data, up to the point of rupture, is tabulated below. The area under the stress-strain curve, up to the point of rupture, is called the modulus of toughness. Compute this modulus to $O(h)^8$.

Strain, ε $(\times 10^{-3})$	0	5	10	15	20	25	30	35	40
Stress, σ, (N/mm^2)	0	5	10	16	21	25	28	30	31

Solution:

Since the modulus of toughness represents the area under the stress-strain curve,

$$\therefore \text{ the modulus of toughness } = \int_0^{40\times10^{-3}} \sigma.d\varepsilon$$

Since the answer is required to $O(h)^8$, then we must use Romberg integration .

1st iteration: For $n = 1$ $\Rightarrow$ $h = \dfrac{b-a}{n} = \dfrac{40\times10^{-3} - 0}{1} = 40\times10^{-3}$,

σ_a σ_b

0 40×10^{-3}

$$I = \frac{h}{2}.(\sigma_a + \sigma_b) = \frac{40\times10^{-3}}{2}.[0+31] = 0.62.$$

2nd iteration: Take $n = 2$ $\Rightarrow$ $h = \dfrac{b-a}{n} = \dfrac{40\times10^{-3} - 0}{2} = 20\times10^{-3}$,

σ_0 σ_1 σ_2

0 20×10^{-3} 40×10^{-3}

$$I = \frac{h}{2}.(\sigma_0 + 2\sigma_1 + \sigma_2) = \frac{20\times10^{-3}}{2}.[0 + 2(21) + 31] = 0.73.$$

The calculations must be continued until the required order of error is achieved.

i	n	I_1	$I_2 = \frac{1}{3}.\left(4I_m - I_l\right)$	$I_3 = \frac{1}{15}.\left(16I_m - I_l\right)$	$I_4 = \frac{1}{63}.\left(64I_m - I_l\right)$
1	1	0.62			
2	2	0.73	0.766667		
3	4	0.745	0.75	0.748889	
4	8	0.7525	0.755	0.755333	0.755435
Order of error			$O(h)^4$	$O(h)^6$	$O(h)^8$

$\therefore$ The modulus of toughness ≈ 0.755435 N/mm^2.

7- Numerical Solution of Ordinary Differential Equations

Introduction

An n^{th} order differential equation requires n conditions to obtain a unique solution. If all conditions are specified at the same value of the independent variable, then the problem is called an *initial value problem*, such as

$$y'' + 2y = \ln x, \qquad y(0) = 1 \text{ and } y'(0) = 0.$$

If the conditions are specified at different values of the independent variable, then it is a *boundary value problem*, such as

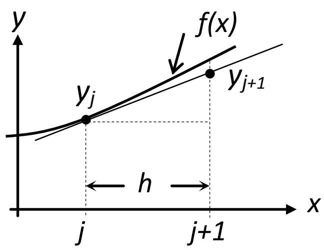
$$EIy'' = -M, \qquad y(0) = 0 \text{ and } y(L) = 0.$$

I- Solution of initial value problems

I-a- Solution of 1st order ODEs

Different numerical methods are used to solve 1st ordinary differential equations. Consider the following 1st order ordinary differential equation $y' = f(x, y)$:

1- Euler's method



From the figure $y'_j = \dfrac{y_{j+1} - y_j}{h}$,

$$\therefore \frac{y_{j+1} - y_j}{h} = f(x_j, y_j),$$

or $\quad y_{j+1} = y_j + h.f(x_j, y_j)$. (New value = old value + step size × slope)

Note: Euler's method gives approximations with an error of 1st order $O(h)$.

2- Second order Runge-Kutta method

$$y_{j+1} = y_j + h.k_2,$$

where $\quad k_1 = f(x_j, y_j) \quad$ and $\quad k_2 = f(x_j + \frac{h}{2}, y_j + \frac{h}{2}k_1)$.

Note: The 2nd order Runge-Kutta method gives approximations with an error of 2nd order $O(h)^2$.

3- Fourth order Runge-Kutta method

$$y_{j+1} = y_j + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4),$$

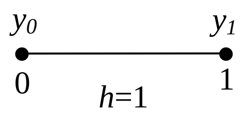
where $k_1 = f(x_j, y_j)$, $\quad k_2 = f(x_j + \frac{h}{2}, y_j + \frac{h}{2}k_1)$,

$k_3 = f(x_j + \frac{h}{2}, y_j + \frac{h}{2}k_2)$, and $\quad k_4 = f(x_j + h, y_j + hk_3)$.

Note: The 4th order Runge-Kutta method gives approximations with an error of 4th order $O(h)^4$.

Example 1: Find $y(1)$ if $\frac{dy}{dx} = \frac{1}{2}(x - y)$, $\quad y(0) = 1$. (Use h = 1)

Solution:



The slope $f(x, y) = y' = \frac{1}{2}(x - y)$

With the given step size $h = 1$, we need one step to move from the start point $x = 0$ (where condition is given) to the end point $x = 1$ (where y is required).

Solution I: By Euler's method $\Rightarrow$ $y_{j+1} = y_j + h.f(x_j, y_j)$.

$x_j = 0$ and $y_j = y(x_j) = y(0) = 1$,

$$\therefore \quad y_1 = 1 + h.f(0,1) = 1 + (1)[\frac{1}{2}(0 - 1)] = 0.5.$$

* From the analytical solution:

$$y = x - 2 + 3e^{-x/2} \Rightarrow y(1) = 1 - 2 + 3e^{-1/2} = 0.819592. \quad \text{(Exact answer)}$$

* Percent relative error $P = \left|\frac{exact - approx.}{exact}\right| \times 100 = \left|\frac{0.819592 - 0.5}{0.819592}\right| \times 100 \approx 39\%$.

Solution II: By the 2nd order Runge-Kutta method $\Rightarrow$ $y_{j+1} = y_j + h.k_2$,

where $k_1 = f(x_j, y_j)$ and $k_2 = f(x_j + \frac{h}{2}, y_j + \frac{h}{2}k_1)$.

$x_j = 0$ and $y_j = y(x_j) = y(0) = 1$,

$k_1 = f(0,1) = \frac{1}{2}(0 - 1) = -0.5$,

$$k_2 = f((0+\frac{1}{2}),(1+\frac{1}{2}\times(-0.5))) = f(0.5,0.75) = \frac{1}{2}(0.5-0.75) = -0.125,$$

$$\therefore y_1 = 1 + (1)(-0.125) = 0.875.$$

* Percent relative error $P = \left|\dfrac{0.819592 - 0.875}{0.819592}\right| \times 100 \approx 6.8\%$.

<u>Solution III</u>: By the 4th order Runge-Kutta method,

$$y_{j+1} = y_j + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4),$$

where $k_1 = f(x_j, y_j)$, $\qquad k_2 = f(x_j + \frac{h}{2}, y_j + \frac{h}{2}k_1)$,

$$k_3 = f(x_j + \frac{h}{2}, y_j + \frac{h}{2}k_2), \text{ and } \quad k_4 = f(x_j + h, y_j + hk_3).$$

$x_j = 0$ and $\quad y_j = y(x_j) = y(0) = 1$,

$$k_1 = f(0,1) = \frac{1}{2}(0-1) = -0.5,$$

$$k_2 = f((0+\frac{1}{2}),(1+\frac{1}{2}\times(-0.5))) = f(0.5,0.75) = \frac{1}{2}(0.5-0.75) = -0.125,$$

$$k_3 = f((0+\frac{1}{2}),(1+\frac{1}{2}\times(-0.125))) = f(0.5,0.9375) = \frac{1}{2}(0.5-0.9375) = -0.21875,$$

$$k_4 = f((0+1),(1+1\times(-0.21875))) = f(1,0.78125) = \frac{1}{2}(1-0.78125) = 0.109375,$$

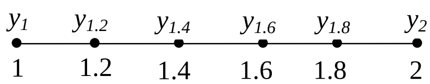
$$\therefore y_1 = 1 + \frac{1}{6}(-0.5 + 2(-0.125) + 2(-0.21875) + 0.109375) = 0.820313.$$

* Percent relative error $P = \left|\dfrac{0.819592 - 0.820313}{0.819592}\right| \times 100 \approx 0.09\%$.

<u>Example 2</u>: Use Euler's method to find y at $x = 2$, given that

$$dy - e^{x+0.1y}dx = 0, \qquad y(1) = 0. \qquad \text{(Use } h = 0.2\text{)}$$

Solution:



$$\frac{dy}{dx} = e^{x+0.1y} \qquad \Rightarrow \qquad \text{The slope is } f(x,y) = e^{x+0.1y}.$$

With the given step size $h = 0.2$, we need 5 steps to move from the start point $x = 1$ (where condition is given) to the end point $x = 2$ (where y is required).

Using Euler's method $\Rightarrow$ $y_{j+1} = y_j + h.f(x_j, y_j)$.

Step 1: $x_j = 1$ and $y_j = y(x_j) = y(1) = 0$,

$$y_{1.2} = y_1 + h.f(1,0) = 0 + 0.2 \times e^{1+0.1(0)} = 0.543656.$$

Step 2: $x_j = 1.2$ and $y_j = y_{1.2} = 0.543656$,

$$y_{1.4} = y_{1.2} + h.f(1.2, 0.543656) = 0.543656 + 0.2 \times e^{1.2+0.1(0.543656)} = 1.244779.$$

The calculations must be continued for 5 steps.

No. of Step (j)	x_j	y_j	$f(x_j, y_j) = e^{x_j+0.1y_j}$	$y_{j+1} = y_j + h.f(x_j, y_j)$
1	1	0	2.718282	0.543656
2	1.2	0.543656	3.505614	1.244779
3	1.4	1.244779	4.592745	2.163328
4	1.6	2.163328	6.149266	3.393181
5	1.8	3.393181	8.493644	5.091910

$\therefore$ $y(2) \approx 5.091910$.

I-b- Solution of a set of 1st order ODEs

To solve a set of ordinary differential equations we can use the previous methods (either Euler's or Runge-Kutta method).

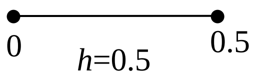
Example: For the following set of ordinary differential equations, if at $x = 0$, $y = 4$ and $z = 6$, then by one step of the 2nd order Runge-Kutta method, find y and z at $x = 0.5$.

$$\frac{dy}{dx} = x - 0.5y + z, \qquad \frac{dz}{dx} = x - y + 2z.$$

Solution:

Let $f_1(x, y, z) = y' = x - 0.5y + z$ (which is used to find y),

and $f_2(x, y, z) = z' = x - y + 2z$ (which is used to find z).



From the start point $x = 0$ to the end point $x = 0.5$, by one step, we need a step size of $h = 0.5$.

By using the 2nd order Runge-Kutta method,

$$y_{j+1} = y_j + h.(k_2)_1 \qquad \text{and} \qquad z_{j+1} = z_j + h.(k_2)_2 \qquad \text{where,}$$

$$(k_1)_1 = f_1(x_j, y_j, z_j) \qquad \text{and} \qquad (k_2)_1 = f_1(x_j + \frac{h}{2}, y_j + \frac{h}{2}(k_1)_1, z_j + \frac{h}{2}(k_1)_2).$$

$$(k_1)_2 = f_2(x_j, y_j, z_j) \qquad \text{and} \qquad (k_2)_2 = f_2(x_j + \frac{h}{2}, y_j + \frac{h}{2}(k_1)_1, z_j + \frac{h}{2}(k_1)_2).$$

$$x_j = 0, \qquad y_j = y(x_j) = y(0) = 4, \quad \text{and} \qquad z_j = z(x_j) = z(0) = 6.$$

$$(k_1)_1 = f_1(0,4,6) = 0 - 0.5(4) + 6 = 4,$$

$$(k_1)_2 = f_2(0,4,6) = 0 - 4 + 2(6) = 8,$$

$$(k_2)_1 = f_1((0 + \frac{0.5}{2}),(4 + \frac{0.5}{2} \times 4),(6 + \frac{0.5}{2} \times 8)) = f_1(0.25,5,8) = 0.25 - 0.5(5) + 8 = 5.75,$$

$$(k_2)_2 = f_2((0 + \frac{0.5}{2}),(4 + \frac{0.5}{2} \times 4),(6 + \frac{0.5}{2} \times 8)) = f_2(0.25,5,8) = 0.25 - 5 + 2(8) = 11.25,$$

$$\therefore y_{0.5} = 4 + (0.5)(5.75) = 6.875, \text{ and}$$

$$z_{0.5} = 6 + (0.5)(11.25) = 11.625.$$

I-c- Solution of second order ODEs

To solve a 2nd order ordinary differential equations we can use ***either*** the previous methods (but first we must transform the problem into a set of two 1st order ODEs.) ***or*** we use suitable finite differences approximations.

Example 1: Using $h = 0.1$, find $y(0.1)$ to $O(h)^2$ if

$$\frac{d^2y}{dt^2} = y + e^t, \qquad\qquad y(0) = 1, \ \frac{dy}{dt}(0) = 0.$$

By using the 2nd order Runge-Kutta method which is of $O(h)^2$.

We must first transform the problem into a set of two 1st order ODEs.

Let $\quad \dfrac{dy}{dt} = z \qquad \Rightarrow \qquad \dfrac{dz}{dt} = \dfrac{d^2y}{dt^2} = y + e^t$.

Put $f_1(z) = y' = z$ (which is used to find *y*),

and $f_2(t, y) = z' = y + e^t$ (which is used to find *z*).

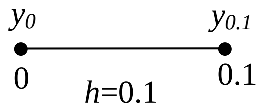
$y_{j+1} = y_j + h.(k_2)_1$ and $z_{j+1} = z_j + h.(k_2)_2$ where,

$(k_1)_1 = f_1(t_j, y_j, z_j)$ and $(k_2)_1 = f_1(t_j + \frac{h}{2}, y_j + \frac{h}{2}(k_1)_1, z_j + \frac{h}{2}(k_1)_2)$.

$(k_1)_2 = f_2(t_j, y_j, z_j)$ and $(k_2)_2 = f_2(t_j + \frac{h}{2}, y_j + \frac{h}{2}(k_1)_1, z_j + \frac{h}{2}(k_1)_2)$.

Since $h = 0.1$, then we need one step to move from the start point $t = 0$ to the end point $t = 0.1$.

$$t_j = 0, \quad y_j = y(t_j) = y(0) = 1, \text{ and } \quad z_j = \frac{dy}{dt}(t_j) = 0.$$



$(k_1)_1 = f_1(0,1,0) = 0$,

$(k_1)_2 = f_2(0,1,0) = 1 + e^0 = 2$,

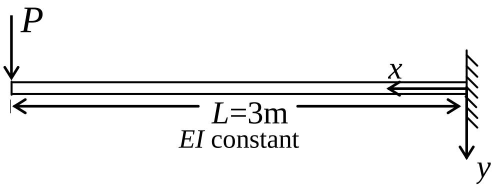
$(k_2)_1 = f_1((0 + \frac{0.1}{2}), (1 + \frac{0.1}{2} \times 0), (0 + \frac{0.1}{2} \times 2)) = f_1(0.05, 1, 0.1) = 0.1$,

$(k_2)_2 = f_2((0 + \frac{0.1}{2}), (1 + \frac{0.1}{2} \times 0), (0 + \frac{0.1}{2} \times 2)) = f_2(0.05, 1, 0.1) = 1 + e^{0.05} = 2.051271$,

$\therefore y_{0.1} = 1 + (0.1)(0.1) = 1.01$, and

$z_{0.1} = 0 + (0.1)(2.051271) = 0.205127$. (Not required, representing the slope)

Example 2: For the shown cantilever, find numerically the deflection at the free end. (Use $h = 1$ m)

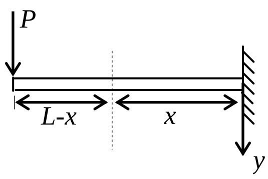


Solution:

$EIy'' = -M$.

From left, $M = -P(L - x) \Rightarrow EIy'' = P(L - x)$,

Or $y'' = \frac{P}{EI}(3 - x)$, $\quad y(0) = 0$, $y'(0) = 0$.



By using the 2nd order Runge-Kutta method which is of $O(h)^2$.

We must first transform the problem into a set of two 1st order ODEs.

Let $y' = z \Rightarrow z' = y'' = \frac{P}{EI}(3 - x)$.

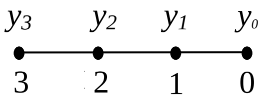
Put $f_1(z) = y' = z$ (which is used to find y), and $f_2(x) = z' = \dfrac{P}{EI}(3-x)$ (which is used to find z).

$$y_{j+1} = y_j + h.(k_2)_1 \qquad \text{and} \qquad z_{j+1} = z_j + h.(k_2)_2 \qquad \text{where,}$$

$$(k_1)_1 = f_1(x_j, y_j, z_j) \qquad \text{and} \qquad (k_2)_1 = f_1(x_j + \frac{h}{2}, y_j + \frac{h}{2}(k_1)_1, z_j + \frac{h}{2}(k_1)_2).$$

$$(k_1)_2 = f_2(x_j, y_j, z_j) \qquad \text{and} \qquad (k_2)_2 = f_2(x_j + \frac{h}{2}, y_j + \frac{h}{2}(k_1)_1, z_j + \frac{h}{2}(k_1)_2).$$

Since $h = 1$ m, then we need three steps to move from the start point $x = 0$ to the end point $x = 3$ m.



Step 1: $x_j = 0$, $y_j = 0$, and $z_j = y'(x_j) = 0$.

$$(k_1)_1 = f_1(0,0,0) = 0,$$

$$(k_1)_2 = f_2(0,0,0) = \frac{P}{EI}(3-0) = \frac{3P}{EI},$$

$$(k_2)_1 = f_1((0+\frac{1}{2}),(0+\frac{1}{2}\times 0),(0+\frac{1}{2}\times\frac{3P}{EI})) = f_1(\frac{1}{2},0,\frac{3P}{2EI}) = \frac{3P}{2EI},$$

$$(k_2)_2 = f_2(\frac{1}{2},0,\frac{3P}{2EI}) = \frac{P}{EI}(3-\frac{1}{2}) = \frac{5P}{2EI},$$

$$\therefore y_1 = 0 + (1)(\frac{3P}{2EI}) = \frac{3P}{2EI}, \qquad \text{(deflection at } x = 1 \text{ m)}$$

$$\therefore z_1 = 0 + (1)(\frac{5P}{2EI}) = \frac{5P}{2EI}. \qquad \text{(slope at } x = 1 \text{ m)}$$

Step 2: $x_j = 1$, $y_j = \dfrac{3P}{2EI}$, and $z_j = \dfrac{5P}{2EI}$.

$$(k_1)_1 = f_1(1,\frac{3P}{2EI},\frac{5P}{2EI}) = \frac{5P}{2EI},$$

$$(k_1)_2 = f_2(1,\frac{3P}{2EI},\frac{5P}{2EI}) = \frac{P}{EI}(3-1) = \frac{2P}{EI},$$

$$(k_2)_1 = f_1((1+\frac{1}{2}),\ldots,(\frac{5P}{2EI}+\frac{1}{2}\times\frac{2P}{EI})) = f_1(\frac{3}{2},\ldots,\frac{7P}{2EI}) = \frac{7P}{2EI},$$

$$(k_2)_2 = f_2(\frac{3}{2},\ldots,\frac{7P}{2EI}) = \frac{P}{EI}(3-\frac{3}{2}) = \frac{3P}{2EI},$$

$$\therefore y_2 = \frac{3P}{2EI} + (1)(\frac{7P}{2EI}) = \frac{5P}{EI}, \qquad \text{(deflection at } x = 2 \text{ m)}$$

$$\therefore z_2 = \frac{5P}{2EI} + (1)(\frac{3P}{2EI}) = \frac{4P}{EI}. \qquad \text{(slope at } x = 2 \text{ m)}$$

<u>Step 3</u>: $x_j = 2$, $y_j = \dfrac{5P}{EI}$, and $z_j = \dfrac{4P}{EI}$.

$$(k_1)_1 = f_1(2, \frac{5P}{EI}, \frac{4P}{EI}) = \frac{4P}{EI},$$

$$(k_1)_2 = f_2(2, \frac{5P}{EI}, \frac{4P}{EI}) = \frac{P}{EI}(3-2) = \frac{P}{EI},$$

$$(k_2)_1 = f_1((2+\frac{1}{2}), \ldots, (\frac{4P}{EI} + \frac{1}{2} \times \frac{P}{EI})) = f_1(\frac{5}{2}, \ldots, \frac{9P}{2EI}) = \frac{9P}{2EI},$$

$$(k_2)_2 = f_2(\frac{5}{2}, \ldots, \frac{9P}{2EI}) = \frac{P}{EI}(3-\frac{5}{2}) = \frac{P}{2EI},$$

$$\therefore y_3 = \frac{5P}{EI} + (1)(\frac{9P}{2EI}) = \frac{19P}{2EI}, \qquad \text{(deflection at } x = 3 \text{ m)}$$

$$\therefore z_3 = \frac{4P}{EI} + (1)(\frac{P}{2EI}) = \frac{9P}{2EI}. \qquad \text{(slope at } x = 3 \text{ m)}$$

$\therefore$ The deflection at the free end is $y_3 \approx \dfrac{19P}{2EI}$.

II- Solution of boundary value problems

To solve this type of ordinary differential equations, finite differences approximations are used.

<u>Example 1</u>: Find $y(2)$ and $y(3)$: (Use $h = 1$)

$$x^2 \frac{d^2y}{dx^2} + x\frac{dy}{dx} - y = 0, \qquad y(1) = 6, \quad y(4) = 9.$$

Solution:

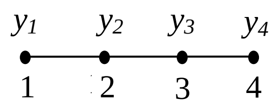
By using central finite differences approximations:

For the given ODE, using central finite differences approximations of $O(h)^2$ we get,

$$x_j^2 \left(\frac{y_{j-1} - 2y_j + y_{j+1}}{h^2} \right) + x_j \left(\frac{-y_{j-1} + y_{j+1}}{2h} \right) - y_j = 0,$$

$$x_j^2 (y_{j-1} - 2y_j + y_{j+1}) + \frac{hx_j}{2}(-y_{j-1} + y_{j+1}) - h^2 y_j = 0,$$

$$(x_j^2 - \frac{hx_j}{2}) y_{j-1} - (2x_j^2 + h^2) y_j + (x_j^2 + \frac{hx_j}{2}) y_{j+1} = 0.$$



(*Two unknowns*)

At $x_j = 2$,   (*Note*: from the given conditions $y_1 = 6$ and $y_4 = 9$)

$$(2^2 - \frac{1\times 2}{2})y_1 - (2\times 2^2 + 1^2)y_2 + (2^2 + \frac{1\times 2}{2})y_3 = 0,$$

$$3(6) - 9y_2 + 5y_3 = 0 \quad \Rightarrow \quad -9y_2 + 5y_3 = -18. \qquad \ldots\ldots(1)$$

At $x_j = 3$,

$$(3^2 - \frac{1\times 3}{2})y_2 - (2\times 3^2 + 1^2)y_3 + (3^2 + \frac{1\times 3}{2})y_4 = 0,$$

$$7.5y_2 - 19y_3 + 10.5(9) = 0 \quad \Rightarrow \quad 7.5y_2 - 19y_3 = -94.5. \qquad \ldots\ldots(2)$$

In matrix form: $\begin{bmatrix} -9 & 5 \\ 7.5 & -19 \end{bmatrix}\begin{Bmatrix} y_2 \\ y_3 \end{Bmatrix} = \begin{bmatrix} -18 \\ -94.5 \end{bmatrix}$.

Use Cramer's rule:

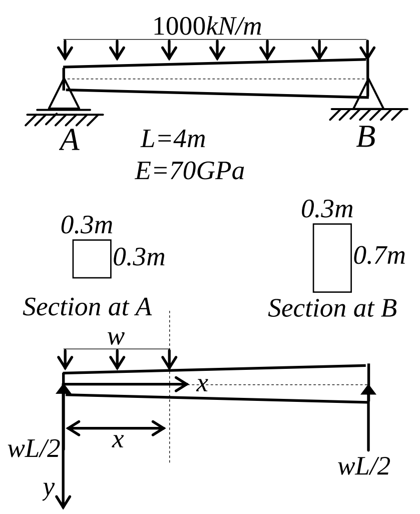
$$y_2 = \frac{\begin{vmatrix} -18 & 5 \\ -94.5 & -19 \end{vmatrix}}{\begin{vmatrix} -9 & 5 \\ 7.5 & -19 \end{vmatrix}} = \frac{-18(-19) - 5(-94.5)}{-9(-19) - 5(7.5)} = \frac{814.5}{133.5} = 6.101124.$$

$$y_3 = \frac{\begin{vmatrix} -9 & -18 \\ 7.5 & -94.5 \end{vmatrix}}{\begin{vmatrix} -9 & 5 \\ 7.5 & -19 \end{vmatrix}} = \frac{-9(-94.5) - (-18)(7.5)}{133.5} = \frac{985.5}{133.5} = 7.382023.$$

<u>*Note*</u>: The analytical solution is $y = \frac{4}{x} + 2x \Rightarrow y(2) = 6$ and $y(3) = 7.333333$.

<u>Example 2</u>: Find, numerically to $O(h)^2$, the deflection at midspan. (Use $h = 1m$)

Solution:



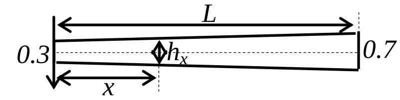
$$EI_x \frac{d^2y}{dx^2} = -M_x \quad \Rightarrow \quad \frac{d^2y}{dx^2} = -\frac{M_x}{EI_x}$$

$$M_x = \frac{wL}{2}.x - w.x.\frac{x}{2},$$

$$M_x = \frac{1000\times 10^3 \times 4}{2}.x - 1000\times 10^3 x.\frac{x}{2}$$

$$= 2\times 10^6 x - 5\times 10^5 x^2$$

$$I_x = \frac{b.(h_x)^3}{12} = \frac{b.(0.3+\frac{0.4x}{L})^3}{12} = \frac{0.3(0.3+\frac{0.4x}{4})^3}{12}$$



$$\frac{h_x - 0.3}{x} = \frac{0.7-0.3}{L} \Rightarrow h_x = 0.3 + \frac{0.4x}{L}$$

$$= 0.025(0.3+0.1x)^3$$

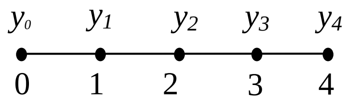
$$\therefore \frac{d^2y}{dx^2} = -\frac{2\times10^6 x - 5\times10^5 x^2}{70\times10^9 \times 0.025(0.3+0.1x)^3} \quad \Rightarrow \quad \frac{d^2y}{dx^2} = 2.857\times10^{-4}\frac{x^2-4x}{(0.3+0.1x)^3}$$

Boundary conditions: $y(0)=0$ and $y(L)=0$.

For the obtained ODE, using central finite differences of $O(h)^2$ we get,

$f_j'' = \dfrac{f_{j-1} - 2f_j + f_{j+1}}{h^2}$, substituting into the ODE yields:

$$\frac{y_{j-1} - 2y_j + y_{j+1}}{h^2} = 2.857\times10^{-4}\frac{x_j^{\,2} - 4x_j}{(0.3+0.1x_j)^3},$$



or $$y_{j-1} - 2y_j + y_{j+1} = 2.857\times10^{-4}h^2\frac{x_j^{\,2} - 4x_j}{(0.3+0.1x_j)^3}.$$

At $x_j = 1$, (*Note*: from the boundary conditions $y_0 = 0$ and $y_4 = 0$)

$$y_0 - 2y_1 + y_2 = 2.857\times10^{-4}(1)^2\frac{1^2 - 4(1)}{(0.3+0.1(1))^3} \quad \Rightarrow \quad -2y_1 + y_2 = -0.0134 \quad \ldots.(1)$$

At $x_j = 2$,

$$y_1 - 2y_2 + y_3 = 2.857\times10^{-4}(1)^2\frac{2^2 - 4(2)}{(0.3+0.1(2))^3} \Rightarrow y_1 - 2y_2 + y_3 = -0.00914 \ \ldots (2)$$

At $x_j = 3$,

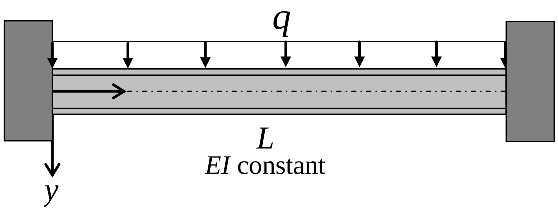
$$y_2 - 2y_3 + y_4 = 2.857\times10^{-4}(1)^2\frac{3^2 - 4(3)}{(0.3+0.1(3))^3} \quad \Rightarrow \quad y_2 - 2y_3 = -0.004 \quad \ldots.(3)$$

In matrix form: $$\begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix}\begin{Bmatrix} y_1 \\ y_2 \\ y_3 \end{Bmatrix} = \begin{bmatrix} -0.0134 \\ -0.00914 \\ -0.004 \end{bmatrix}.$$

$$y_2 = \frac{\begin{vmatrix} -2 & -0.0134 & 0 \\ 1 & -0.00914 & 1 \\ 0 & -0.004 & -2 \end{vmatrix}}{\begin{vmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{vmatrix}} = \frac{-2\begin{vmatrix} -0.00914 & 1 \\ -0.004 & -2 \end{vmatrix} - \begin{vmatrix} -0.0134 & 0 \\ -0.004 & -2 \end{vmatrix} + 0}{-2\begin{vmatrix} -2 & 1 \\ 1 & -2 \end{vmatrix} + (-1)\begin{vmatrix} 1 & 0 \\ 1 & -2 \end{vmatrix} + 0} = \frac{-0.07136}{-4} = 0.01784m$$

$\therefore$ The deflection at midspan is $y_2 \approx 17.8mm$.

<u>Example 3</u>: Estimate, numerically, the deflection at midspan. (Use $h = L/4$)



Solution:

$$EI\frac{d^4y}{dx^4} = w \quad \Rightarrow \quad EI\frac{d^4y}{dx^4} = q$$

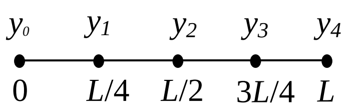
or $\quad \dfrac{d^4y}{dx^4} = \dfrac{q}{EI}$, $\qquad y(0) = 0$, $y'(0) = 0$, $y(L) = 0$, and $y'(L) = 0$.

***Method I*:** (By using mixed finite difference approximations)

For the obtained ODE, using central finite differences of $O(h)^2$ we get,

$$f_j^{iv} = \frac{f_{j-2} - 4f_{j-1} + 6f_j - 4f_{j+1} + f_{j+2}}{h^4}$$, substituting into the ODE yields:

$$\frac{y_{j-2} - 4y_{j-1} + 6y_j - 4y_{j+1} + y_{j+2}}{h^4} = \frac{q_j}{EI},$$



or $\quad y_{j-2} - 4y_{j-1} + 6y_j - 4y_{j+1} + y_{j+2} = \dfrac{q_j h^4}{EI}$.

At $x_j = L/2$, $\qquad$ (*Note*: from the conditions $y_0 = 0$ and $y_4 = 0$)

$$y_0 - 4y_1 + 6y_2 - 4y_3 + y_4 = \frac{q(L/4)^4}{EI},$$

$$\therefore \; -4y_1 + 6y_2 - 4y_3 = \frac{qL^4}{256EI}. \qquad \text{.........(1)}$$

For the condition $y'(0)=0$, using forward differences of $O(h)^2$, we get,

$$f'_j=\frac{-3f_j+4f_{j+1}-f_{j+2}}{2h}\text{, substituting into this condition yields:}$$

$$\therefore \frac{-3y_0+4y_1-y_2}{2h}=0 \qquad \Rightarrow \qquad 4y_1-y_2=0 \qquad \ldots\ldots(2)$$

For the condition $y'(L)=0$, using backward differences of $O(h)^2$, we get,

$$f'_j=\frac{3f_j-4f_{j-1}+f_{j-2}}{2h}\text{, substituting into this condition yields:}$$

$$\therefore \frac{3y_4-4y_3+y_2}{2h}=0 \qquad \Rightarrow \qquad y_2-4y_3=0 \qquad \ldots\ldots(3)$$

In matrix form: $\begin{bmatrix}-4 & 6 & -4\\ 4 & -1 & 0\\ 0 & 1 & -4\end{bmatrix}\begin{Bmatrix}y_1\\ y_2\\ y_3\end{Bmatrix}=\begin{bmatrix}qL^4/256EI\\ 0\\ 0\end{bmatrix}.$

$$y_2=\frac{\begin{vmatrix}-4 & \dfrac{qL^4}{256EI} & -4\\ 4 & 0 & 0\\ 0 & 0 & -4\end{vmatrix}}{\begin{vmatrix}-4 & 6 & -4\\ 4 & -1 & 0\\ 0 & 1 & -4\end{vmatrix}}=\frac{(-1)\dfrac{qL^4}{256EI}\begin{vmatrix}4 & 0\\ 0 & -4\end{vmatrix}+0}{-4\begin{vmatrix}-1 & 0\\ 1 & -4\end{vmatrix}+(-1)(4)\begin{vmatrix}6 & -4\\ 1 & -4\end{vmatrix}+0}=\frac{\dfrac{qL^4}{16EI}}{64}=\frac{qL^4}{1024EI}.$$

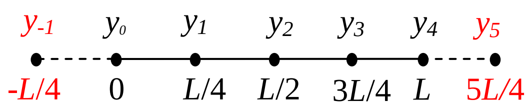
$\therefore$ The deflection at midspan is $y_2\approx\dfrac{qL^4}{1024EI}$.

Method II**:** (To get more accurate result by using central finite differences)

For the obtained ODE, using central finite differences of $O(h)^2$ we get,

$$f_j^{iv}=\frac{f_{j-2}-4f_{j-1}+6f_j-4f_{j+1}+f_{j+2}}{h^4}\text{, substituting into the ODE yields:}$$

$$\frac{y_{j-2}-4y_{j-1}+6y_j-4y_{j+1}+y_{j+2}}{h^4}=\frac{q_j}{EI},$$



or $\quad y_{j-2}-4y_{j-1}+6y_j-4y_{j+1}+y_{j+2}=\dfrac{q_j h^4}{EI}.$

For the condition $y'(0)=0$, using central differences of $O(h)^2$, we get,

$$f'_j=\frac{-f_{j-1}+f_{j+1}}{2h} \quad \Rightarrow \quad \frac{-y_{-1}+y_1}{2h}=0 \quad \Rightarrow \quad -y_{-1}+y_1=0 \quad \Rightarrow \quad y_{-1}=y_1.$$

Similarly, for $y'(L)=0$ we get $\dfrac{-y_3+y_5}{2h}=0 \quad \Rightarrow \quad -y_3+y_5=0 \quad \Rightarrow \quad y_5=y_3.$

$x_j=L/4,$ (*Note*: from the boundary conditions $y_0=0$ and $y_4=0$)

$$y_{-1}-4y_0+6y_1-4y_2+y_3=\frac{q(L/4)^4}{EI} \quad \Rightarrow \quad 7y_1-4y_2+y_3=\frac{qL^4}{256EI} \qquad \text{.... (1)}$$

At $x_j=L/2,$ $\quad y_0-4y_1+6y_2-4y_3+y_4=\dfrac{q(L/4)^4}{EI},$

$$\therefore\ -4y_1+6y_2-4y_3=\frac{qL^4}{256EI}. \qquad \text{.... (2)}$$

At $x_j=3L/4,$ $\quad y_1-4y_2+6y_3-4y_4+y_5=\dfrac{q(L/4)^4}{EI},$

$$\therefore\ y_1-4y_2+7y_3=\frac{qL^4}{256EI}. \qquad \text{.... (3)}$$

In matrix form: $\begin{bmatrix} 7 & -4 & 1 \\ -4 & 6 & -4 \\ 1 & -4 & 7 \end{bmatrix}\begin{Bmatrix} y_1 \\ y_2 \\ y_3 \end{Bmatrix}=\begin{bmatrix} qL^4/256EI \\ qL^4/256EI \\ qL^4/256EI \end{bmatrix}.$

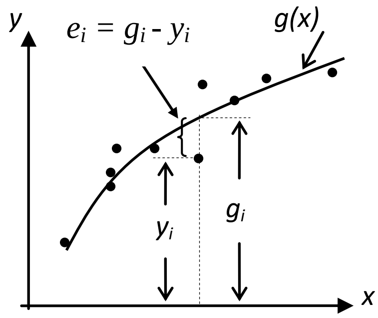
$$y_2=\frac{\begin{vmatrix} 7 & \frac{qL^4}{256EI} & 1 \\ -4 & \frac{qL^4}{256EI} & -4 \\ 1 & \frac{qL^4}{256EI} & 7 \end{vmatrix}}{\begin{vmatrix} 7 & -4 & 1 \\ -4 & 6 & -4 \\ 1 & -4 & 7 \end{vmatrix}}=\frac{\frac{qL^4}{256EI}\left[-\begin{vmatrix} -4 & -4 \\ 1 & 7 \end{vmatrix}+\begin{vmatrix} 7 & 1 \\ 1 & 7 \end{vmatrix}-\begin{vmatrix} 7 & 1 \\ -4 & -4 \end{vmatrix}\right]}{(-1)(-4)\begin{vmatrix} -4 & -4 \\ 1 & 7 \end{vmatrix}+6\begin{vmatrix} 7 & 1 \\ 1 & 7 \end{vmatrix}+(-1)(-4)\begin{vmatrix} 7 & 1 \\ -4 & -4 \end{vmatrix}}=\frac{\frac{96qL^4}{256EI}}{96}=\frac{qL^4}{256EI}.$$

$\therefore$ The deflection at midspan is $y_2\approx\dfrac{qL^4}{256EI}.$

8- Curve Fitting

Least-squares criterion (linear regression)

Let (x_1, y_1), (x_2, y_2), ….., (x_n, y_n) a set of observations to be modeled, $g(x)$ is the approximating model, and e is the local error (residual) between the observations and the model, that is $e_i = g_i - y_i$. In the least squares method, to get a good approximating model, the total error (which is the sum of the squares of the local errors around the regression line) $E = \sum_{i=1}^{n} e_i^2$ must be minimized.



Let $g(x) = a_o + a_1 x$ (1st order polynomial, i.e. a straight line),

$$E = \sum_{i=1}^{n} (g_i - y_i)^2 \quad \Rightarrow \quad E = \sum_{i=1}^{n} (a_o + a_1 x_i - y_i)^2 ,$$

The total error E is minimized if $\dfrac{\partial E}{\partial a_o} = 0$ and $\dfrac{\partial E}{\partial a_1} = 0$.

$$\frac{\partial E}{\partial a_o} = 2\sum_{i=1}^{n} (a_o + a_1 x_i - y_i) \quad \Rightarrow \quad 2\sum_{i=1}^{n} (a_o + a_1 x_i - y_i) = 0 ,$$

$$\sum_{i=1}^{n} a_o + \sum_{i=1}^{n} a_1 x_i - \sum_{i=1}^{n} y_i = 0 . \qquad \text{But} \quad \sum_{i=1}^{n} a_o = n.a_o ,$$

$$\therefore \quad n.a_o + \sum_{i=1}^{n} x_i a_1 = \sum_{i=1}^{n} y_i . \qquad \text{………….. (1)}$$

Similarly $\dfrac{\partial E}{\partial a_1} = 2\sum_{i=1}^{n} (a_o + a_1 x_i - y_i) x_i \quad \Rightarrow \quad 2\sum_{i=1}^{n} (a_o x_i + a_1 x_i^2 - x_i y_i) = 0 ,$

$$\sum_{i=1}^{n} x_i a_o + \sum_{i=1}^{n} x_i^2 a_1 - \sum_{i=1}^{n} x_i y_i = 0 , \quad \Rightarrow \quad \sum_{i=1}^{n} x_i a_o + \sum_{i=1}^{n} x_i^2 a_1 = \sum_{i=1}^{n} x_i y_i \qquad \text{…..... (2)}$$

In matrix form:

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{bmatrix} \begin{Bmatrix} a_o \\ a_1 \end{Bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \end{bmatrix} .$$

Generally, if $g(x) = a_o + a_1 x + a_2 x^2 + ...+ a_k x^k$ (kth order polynomial), we will have

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 & .... & \sum_{i=1}^{n} x_i^k \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 & \sum_{i=1}^{n} x_i^3 & .... & \sum_{i=1}^{n} x_i^{k+1} \\ \sum_{i=1}^{n} x_i^2 & \sum_{i=1}^{n} x_i^3 & \sum_{i=1}^{n} x_i^4 & .... & \sum_{i=1}^{n} x_i^{k+2} \\ .... & .... & .... & .... & .... \\ \sum_{i=1}^{n} x_i^k & \sum_{i=1}^{n} x_i^{k+1} & \sum_{i=1}^{n} x_i^{k+2} & .... & \sum_{i=1}^{n} x_i^{2k} \end{bmatrix} \begin{Bmatrix} a_o \\ a_1 \\ a_2 \\ \cdots \\ a_k \end{Bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \\ \sum_{i=1}^{n} x_i^2 y_i \\ .... \\ \sum_{i=1}^{n} x_i^k y_i \end{bmatrix}.$$

Statistical definitions

$\bar{y}$ is the mean of y.

E_m is the total sum of the squares around the mean of y, that is $E_m = \sum_{i=1}^{n} (y_i - \bar{y})^2$.

r^2 is the determination coefficient which is given by $r^2 = \dfrac{E_m - E}{E_m}$.

r is the correlation coefficient which is given by $r = \sqrt{r^2}$.

For a perfect fit $(E = 0) \quad \Rightarrow \quad r = r^2 = 1$, signifying that the approximating model $g(x)$ explains 100% of the variability of the data (observations).

Example 1: Given the following data:

x	0	1	2	3	4	5
$f(x)$	2.1	7.7	13.6	27.2	40.9	61.6

Using the least squares criterion:

1- Fit a 1st order polynomial (straight line) to this data.

2- Fit a 2nd order polynomial (quadratic equation) to this data.

Solution:

1- Let the straight line is $g(x) = a_o + a_1 x$, then we have

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{bmatrix} \begin{Bmatrix} a_o \\ a_1 \end{Bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \end{bmatrix},$$

$n = 6, \quad \sum_{i=1}^{n} x_i = 0 + 1 + 2 + 3 + 4 + 5 = 15, \quad \sum_{i=1}^{n} x_i^2 = 0^2 + 1^2 + 2^2 + 3^2 + 4^2 + 5^2 = 55,$

$$\sum_{i=1}^{n} y_i = 2.1 + 7.7 + 13.6 + 27.2 + 40.9 + 61.6 = 153.1,$$

$$\sum_{i=1}^{n} x_i y_i = 0(2.1) + 1(7.7) + 2(13.6) + 3(27.2) + 4(40.9) + 5(61.6) = 588.1.$$

$$\therefore \begin{bmatrix} 6 & 15 \\ 15 & 55 \end{bmatrix} \begin{Bmatrix} a_o \\ a_1 \end{Bmatrix} = \begin{bmatrix} 153.1 \\ 588.1 \end{bmatrix}.$$

Use Cramer's rule:

$$a_o = \frac{\begin{bmatrix} 153.1 & 15 \\ 588.1 & 55 \end{bmatrix}}{\begin{bmatrix} 6 & 15 \\ 15 & 55 \end{bmatrix}} = \frac{153.1(55) - 15(588.1)}{6(55) - 15(15)} = \frac{-401}{105} = -3.819048,$$

$$a_1 = \frac{\begin{bmatrix} 6 & 153.1 \\ 15 & 588.1 \end{bmatrix}}{\begin{bmatrix} 6 & 15 \\ 15 & 55 \end{bmatrix}} = \frac{6(588.1) - 153.1(15)}{6(55) - 15(15)} = \frac{1232.1}{105} = 11.734286.$$

$$\therefore \; g(x) = -3.819048 + 11.734286x.$$

2- Let the 2nd order polynomial is $q(x) = b_o + b_1 x + b_2 x^2$, then we have

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 & \sum_{i=1}^{n} x_i^3 \\ \sum_{i=1}^{n} x_i^2 & \sum_{i=1}^{n} x_i^3 & \sum_{i=1}^{n} x_i^4 \end{bmatrix} \begin{Bmatrix} b_o \\ b_1 \\ b_2 \end{Bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \\ \sum_{i=1}^{n} x_i^2 y_i \end{bmatrix},$$

$$\sum_{i=1}^{n} x_i^3 = 0^3 + 1^3 + 2^3 + 3^3 + 4^3 + 5^3 = 225, \qquad \sum_{i=1}^{n} x_i^4 = 0^4 + 1^4 + 2^4 + 3^4 + 4^4 + 5^4 = 979,$$

$$\sum_{i=1}^{n} x_i^2 y_i = 0^2(2.1) + 1^2(7.7) + 2^2(13.6) + 3^2(27.2) + 4^2(40.9) + 5^2(61.6) = 2501.3.$$

$$\therefore \begin{bmatrix} 6 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 979 \end{bmatrix} \begin{Bmatrix} b_o \\ b_1 \\ b_2 \end{Bmatrix} = \begin{bmatrix} 153.1 \\ 588.1 \\ 2501.3 \end{bmatrix}.$$

Use Cramer's rule:

$$b_0 = \frac{\begin{vmatrix} 153.1 & 15 & 55 \\ 588.1 & 55 & 225 \\ 2501.3 & 225 & 979 \end{vmatrix}}{\begin{vmatrix} 6 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 979 \end{vmatrix}} = \frac{153.1\begin{vmatrix} 55 & 225 \\ 225 & 979 \end{vmatrix} + (-1)(588.1)\begin{vmatrix} 15 & 55 \\ 225 & 979 \end{vmatrix} + 2501.3\begin{vmatrix} 15 & 55 \\ 55 & 225 \end{vmatrix}}{6\begin{vmatrix} 55 & 225 \\ 225 & 979 \end{vmatrix} + (-1)(15)\begin{vmatrix} 15 & 55 \\ 225 & 979 \end{vmatrix} + 55\begin{vmatrix} 15 & 55 \\ 55 & 225 \end{vmatrix}} = 2.532143$$

$$b_1 = \frac{\begin{vmatrix} 6 & 153.1 & 55 \\ 15 & 588.1 & 225 \\ 55 & 2501.3 & 979 \end{vmatrix}}{\begin{vmatrix} 6 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 979 \end{vmatrix}} = \frac{-153.1\begin{vmatrix} 15 & 225 \\ 55 & 979 \end{vmatrix} + 588.1\begin{vmatrix} 6 & 55 \\ 55 & 979 \end{vmatrix} + (-1)(2501.3)\begin{vmatrix} 6 & 55 \\ 15 & 225 \end{vmatrix}}{6\begin{vmatrix} 55 & 225 \\ 225 & 979 \end{vmatrix} + (-1)(15)\begin{vmatrix} 15 & 55 \\ 225 & 979 \end{vmatrix} + 55\begin{vmatrix} 15 & 55 \\ 55 & 225 \end{vmatrix}} = 2.2075$$

$$b_2 = \frac{\begin{vmatrix} 6 & 15 & 153.1 \\ 15 & 55 & 588.1 \\ 55 & 225 & 2501.3 \end{vmatrix}}{\begin{vmatrix} 6 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 979 \end{vmatrix}} = \frac{153.1\begin{vmatrix} 15 & 55 \\ 55 & 225 \end{vmatrix} + (-1)(588.1)\begin{vmatrix} 6 & 15 \\ 55 & 225 \end{vmatrix} + 2501.3\begin{vmatrix} 6 & 15 \\ 15 & 55 \end{vmatrix}}{6\begin{vmatrix} 55 & 225 \\ 225 & 979 \end{vmatrix} + (-1)(15)\begin{vmatrix} 15 & 55 \\ 225 & 979 \end{vmatrix} + 55\begin{vmatrix} 15 & 55 \\ 55 & 225 \end{vmatrix}} = 1.905357$$

$$\therefore\ q(x) = 2.532143 + 2.2075x + 1.905357x^2.$$

Statistical comparison

x_i	y_i	$E_{m_i} = (y_i - \bar{y})^2$	For $g(x)$ $E_i = (g(x_i) - y_i)^2$	For $q(x)$ $E_i = (q(x_i) - y_i)^2$
0	2.1	548.340278	35.03512923	0.186747572
1	7.7	317.433611	0.046327396	1.113025
2	13.6	142.006944	36.59674063	0.938129782
3	27.2	2.83361111	17.50426612	0.804867356
4	40.9	236.646944	4.919949865	0.898429101
5	61.6	1302.00694	45.53034867	0.15715833
$\sum$	153.1	2549.3	139.6	4.1
$\bar{y} = \frac{\sum y_i}{n}$	$\bar{y} = \frac{153.1}{6}$ $= 25.51667$	$r^2 = \frac{E_m - E}{E_m}$	$r^2 = \frac{2549.3 - 139.6}{2549.3}$ $= 0.9452$	$r^2 = \frac{2549.3 - 4.1}{2549.3}$ $= 0.9984$

Since r^2, for $q(x)$, is closer to one, thus the quadratic equation $q(x)$ is better than the linear equation $g(x)$ in representing the given data.

Example 2: (Final 2014) The volume of water pumped by a pump is measured as a function of time as tabulated below:

Time, t, sec	0	1	5	8
Volume, V, m^3	2.1	7.7	13.6	27.2

Fit the equation $V = at + bt^3$ (where a and b are constants) to the above data using the least squares method.

Solution:

Since the required equation $V = at + bt^3$ is a 3rd order polynomial, thus, to make use of the general least squares matrix, we compare it with the general form of a 3rd order polynomial $g(t) = a_o + a_1 t + a_2 t^2 + a_3 t^3$. It is obvious that the first and third constants do not exist in the required equation, thus we cancel the first and third row and column of the general least squares (4×4) matrix,

$$\begin{bmatrix} n & \sum_{i=1}^{n} t_i & \sum_{i=1}^{n} t_i^2 & \sum_{i=1}^{n} t_i^3 \\ \sum_{i=1}^{n} t_i & \sum_{i=1}^{n} t_i^2 & \sum_{i=1}^{n} t_i^3 & \sum_{i=1}^{n} t_i^4 \\ \sum_{i=1}^{n} t_i^2 & \sum_{i=1}^{n} t_i^3 & \sum_{i=1}^{n} t_i^4 & \sum_{i=1}^{n} t_i^5 \\ \sum_{i=1}^{n} t_i^3 & \sum_{i=1}^{n} t_i^4 & \sum_{i=1}^{n} t_i^5 & \sum_{i=1}^{n} t_i^6 \end{bmatrix} \begin{Bmatrix} a_o \\ a_1 \\ a_2 \\ a_3 \end{Bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} V_i \\ \sum_{i=1}^{n} t_i V_i \\ \sum_{i=1}^{n} t_i^2 V_i \\ \sum_{i=1}^{n} t_i^3 V_i \end{bmatrix},$$

to get,

$$\begin{bmatrix} \sum_{i=1}^{n} t_i^2 & \sum_{i=1}^{n} t_i^4 \\ \sum_{i=1}^{n} t_i^4 & \sum_{i=1}^{n} t_i^6 \end{bmatrix} \begin{Bmatrix} a \\ b \end{Bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} t_i V_i \\ \sum_{i=1}^{n} t_i^3 V_i \end{bmatrix},$$

$\sum_{i=1}^{n} t_i^2 = 0^2 + 1^2 + 5^2 + 8^2 = 90$, $\sum_{i=1}^{n} t_i^4 = 4722$, $\sum_{i=1}^{n} t_i^6 = 277770$,

$\sum_{i=1}^{n} t_i V_i = 232.2$, and $\sum_{i=1}^{n} t_i^3 V_i = 13081.8$.

$$\therefore \begin{bmatrix} 90 & 4722 \\ 4722 & 277770 \end{bmatrix} \begin{Bmatrix} a \\ b \end{Bmatrix} = \begin{bmatrix} 293.3 \\ 15634.1 \end{bmatrix}.$$

Solving the above matrix, we get: $a = 2.829636 \approx 2.83$ and $b = 0.00818 \approx 0.008$.

$\therefore$ The required equation is $V = 2.83t + 0.008t^3$.

Example 3: If the curve $y = a + bx + \frac{c}{x}$ is to be used to represent the points $(1,4.5)$, $(2,4.75)$, and $(4,7.125)$, find the values of *a, b*, and *c* by using linear least squares regression.

Solution:

Since the given curve is not a polynomial, we cannot use the general least squares matrix, and we must use the general least squares derivation.

Let the approximating equation (model) $g(x) = a + bx + \frac{c}{x}$.

The local error is $e_i = g_i - y_i$ and the total error is $E = \sum_{i=1}^{n} e_i^2$ which must be minimized by letting $\frac{\partial E}{\partial a} = 0$, $\frac{\partial E}{\partial b} = 0$, and $\frac{\partial E}{\partial c} = 0$.

$$E = \sum_{i=1}^{n} (g_i - y_i)^2 \quad \Rightarrow \quad E = \sum_{i=1}^{n} (a + bx_i + \frac{c}{x_i} - y_i)^2 ,$$

$$\frac{\partial E}{\partial a} = 2\sum_{i=1}^{n} (a + bx_i + \frac{c}{x_i} - y_i), \quad \frac{\partial E}{\partial a} = 0 \quad \Rightarrow \quad 2\sum_{i=1}^{n} (a + bx_i + \frac{c}{x_i} - y_i) = 0,$$

$$\sum_{i=1}^{n} a + \sum_{i=1}^{n} bx_i + \sum_{i=1}^{n} \frac{c}{x_i} - \sum_{i=1}^{n} y_i = 0, \qquad \text{but} \quad \sum_{i=1}^{n} a = n.a ,$$

$$\therefore \quad n.a + \sum_{i=1}^{n} bx_i + \sum_{i=1}^{n} \frac{c}{x_i} = \sum_{i=1}^{n} y_i . \qquad \text{.............. (1)}$$

$$\frac{\partial E}{\partial b} = 2\sum_{i=1}^{n} (a + bx_i + \frac{c}{x_i} - y_i)x_i , \quad \frac{\partial E}{\partial b} = 0 \quad \Rightarrow \quad 2\sum_{i=1}^{n} (ax_i + bx_i^2 + c - x_i y_i) = 0,$$

$$\sum_{i=1}^{n} x_i a + \sum_{i=1}^{n} x_i^2 b + \sum_{i=1}^{n} c - \sum_{i=1}^{n} x_i y_i = 0, \qquad \text{but} \quad \sum_{i=1}^{n} c = n.c ,$$

$$\therefore \quad \sum_{i=1}^{n} x_i a + \sum_{i=1}^{n} x_i^2 b + n.c = \sum_{i=1}^{n} x_i y_i \qquad \text{.............. (2)}$$

$$\frac{\partial E}{\partial c} = 2\sum_{i=1}^{n} (a + bx_i + \frac{c}{x_i} - y_i)\frac{1}{x_i}, \quad \frac{\partial E}{\partial c} = 0 \quad \Rightarrow \quad 2\sum_{i=1}^{n} (\frac{1}{x_i} a + b + \frac{1}{x_i^2} c - \frac{1}{x_i} y_i) = 0,$$

$$\sum_{i=1}^{n} \frac{1}{x_i} a + \sum_{i=1}^{n} b + \sum_{i=1}^{n} \frac{1}{x_i^2} c - \sum_{i=1}^{n} \frac{y_i}{x_i} = 0, \qquad \text{but} \quad \sum_{i=1}^{n} b = n.b ,$$

$$\therefore \quad \sum_{i=1}^{n} \frac{1}{x_i} a + n.b + \sum_{i=1}^{n} \frac{1}{x_i^2} c = \sum_{i=1}^{n} \frac{y_i}{x_i} . \qquad \text{.............. (3)}$$

In matrix form:

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} \frac{1}{x_i} \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 & n \\ \sum_{i=1}^{n} \frac{1}{x_i} & n & \sum_{i=1}^{n} \frac{1}{x_i^2} \end{bmatrix} \begin{Bmatrix} a \\ b \\ c \end{Bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \\ \sum_{i=1}^{n} \frac{y_i}{x_i} \end{bmatrix},$$

$n=3$, $\quad \sum_{i=1}^{n} x_i = 1+2+4=7$, $\quad \sum_{i=1}^{n} x_i^2 = 1^2+2^2+4^2=21$,

$\sum_{i=1}^{n} \frac{1}{x_i} = \frac{1}{1}+\frac{1}{2}+\frac{1}{4}=1.75$, $\quad \sum_{i=1}^{n} \frac{1}{x_i^2} = \frac{1}{1^2}+\frac{1}{2^2}+\frac{1}{4^2}=1.3125$,

$\sum_{i=1}^{n} y_i = 4.5+4.75+7.125=16.375$, $\quad \sum_{i=1}^{n} x_i y_i = 1(4.5)+2(4.75)+4(7.125)=42.5$,

$\sum_{i=1}^{n} \frac{y_i}{x_i} = \frac{4.5}{1}+\frac{4.75}{2}+\frac{7.125}{4}=8.65625$.

$$\therefore \begin{bmatrix} 3 & 7 & 1.75 \\ 7 & 21 & 3 \\ 1.75 & 3 & 1.3125 \end{bmatrix} \begin{Bmatrix} a \\ b \\ c \end{Bmatrix} = \begin{bmatrix} 16.375 \\ 42.5 \\ 8.65625 \end{bmatrix}.$$

Solving the above matrix, we get: $\quad a=0.5$, $b=1.5$, and $c=2.5$.

Non-polynomial models

Linear least-squares regression may be used to fit a non-polynomial model by transforming it to a polynomial model, such as

* $\quad y=\alpha e^{\beta x} \quad \Rightarrow \quad \ln y = \ln\alpha + \beta.x \quad \Rightarrow \quad y^* = a+\beta.x \quad$ (polynomial),

where $y^* = \ln y$ and $a=\ln\alpha$.

* $\quad y=\alpha x^{\beta} \quad \Rightarrow \quad \ln y = \ln\alpha + \beta\ln x \quad \Rightarrow \quad y^* = a+\beta x^* \quad$ (polynomial),

where $x^* = \ln x$, $y^* = \ln y$, and $a=\ln\alpha$.

* $\quad y=\dfrac{\alpha.x}{\beta+x} \quad \Rightarrow \quad \dfrac{1}{y}=\dfrac{\beta+x}{\alpha.x} \quad \Rightarrow \quad \dfrac{1}{y}=\dfrac{1}{\alpha}+\dfrac{\beta}{\alpha}.\dfrac{1}{x} \quad \Rightarrow \quad y^*=a+bx^*$ (polynomial),

where $x^*=\dfrac{1}{x}$, $y^*=\dfrac{1}{y}$, $a=\dfrac{1}{\alpha}$, and $b=\dfrac{\beta}{\alpha}$.

Example: The stress-strain data obtained from a compression test of a concrete cylinder is listed below. Perform a least-squares fit using the equation $\sigma = Ae^{B\varepsilon}$, where A and B are constants.

Strain ε $(\times 10^{-6})$	500	1000	1500	2000	2375
Stress σ (MPa)	15.5	24.6	29.3	30.3	30.6

Solution:

Since the given model $\sigma = Ae^{B\varepsilon}$ is a non-polynomial, thus we must first transform it to a polynomial form.

$$\sigma = Ae^{B\varepsilon} \quad \Rightarrow \quad \ln\sigma = \ln A + B\varepsilon \quad \Rightarrow \quad y = a + Bx \quad \text{(polynomial)},$$

where $x = \varepsilon$, $y = \ln\sigma$ and $a = \ln A$.

x, $(=\varepsilon)$, $(\times 10^{-6})$	500	1000	1500	2000	2375
y, $(=\ln\sigma)$	2.74084	3.202746	3.377588	3.411148	3.421

Now, use the least squares criterion,

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{bmatrix} \begin{Bmatrix} a \\ B \end{Bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \end{bmatrix},$$

$n = 5$, $\sum_{i=1}^{n} x_i = (500 + 1000 + 1500 + 2000 + 2375) \times 10^{-6} = 7375 \times 10^{-6}$,

$\sum_{i=1}^{n} x_i^2 = 1.314 \times 10^{-5}$, $\sum_{i=1}^{n} y_i = 16.153322$, and $\sum_{i=1}^{n} x_i y_i = 0.024587$.

$$\therefore \begin{bmatrix} 5 & 7375 \times 10^{-6} \\ 7375 \times 10^{-6} & 1.314 \times 10^{-5} \end{bmatrix} \begin{Bmatrix} a \\ B \end{Bmatrix} = \begin{bmatrix} 16.153322 \\ 0.024587 \end{bmatrix}.$$

Solving the above matrix, we get: $a = 2.734504$ and $B = 336.380242$.

But $a = \ln A \quad \Rightarrow \quad A = e^a \quad \Rightarrow \quad A = e^{2.734504} = 15.402102$.

$\therefore$ The required equation is $\sigma \approx 15.4e^{336.38\varepsilon}$.

9- Interpolation and Extrapolation

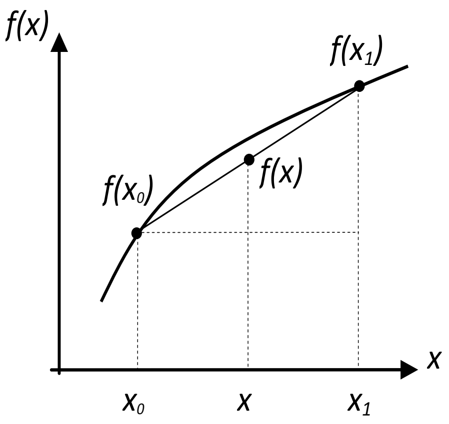
Introduction

By interpolation a functional value is approximated between the data points. While, by extrapolation a functional value is approximated beyond the data points.

The simplest form of interpolation is to connect two data points with a straight line then using similar triangles,

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

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



If $x_o=0$, then

$$f(x)=f(0)+x\frac{f(x_1)-f(x_o)}{h},$$

Or $$f(x)=f(0)+\frac{x}{h}\Delta f_o.$$

I- Interpolation with equally spaced data

1- Gregory-Newton forward interpolation formula

From Taylor series

$$f(x)=f(0)+xf'(0)+\frac{x^2}{2!}f''(0)+\frac{x^3}{3!}f'''(0)+\ldots\ldots.$$

Since $f'(0)=\frac{\Delta f_o}{h}-\frac{h}{2!}f''(0)-\frac{h^2}{3!}f'''(0)-\ldots\ldots,$

and $f''(0)=\frac{\Delta^2 f_o}{h^2}-hf'''(0)-\ldots\ldots,$

$$f(x)=f(0)+\frac{x}{h}\Delta f_o+\frac{x(x-h)}{2!h^2}\Delta^2 f_o+\frac{x(x-h)(x-2h)}{3!h^3}\Delta^3 f_o+\ldots\ldots \text{ (General formula)}$$

If $h=1$,

$$f(x)=f(0)+x\Delta f_o+\frac{x(x-1)}{2!}\Delta^2 f_o+\frac{x(x-1)(x-2)}{3!}\Delta^3 f_o+\ldots\ldots \text{ (Particular formula)}$$

2- Lagrange interpolation polynomial

The Lagrange interpolation polynomial is simply a reformulation of the Gregory-Newton polynomial that avoids the computation of divided differences. It can be represented as

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

where $L_i(x) = \prod_{\substack{i=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}$. ($\prod$ designates the " *product of* ")

Or

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

$$+ \ldots\ldots\ldots\ldots + \frac{(x-x_o)(x-x_1)\ldots(x-x_{n-1})}{(x_n-x_o)(x_n-x_1)\ldots(x_n-x_{n-1})} f(x_n) \ .$$

Example 1: Given the following data:

x	0	1	2	3
$f(x)$	- 7	- 3	6	25

Find $f(1.1)$ and $f(3.5)$.

Solution:

***Solution I*:** By Gregory-Newton interpolation formula,

Since $h = 1 \Rightarrow$ we can use the particular formula directly (rescaling is not required).

$x_o = 0 \Rightarrow$ Shifting is not required.

x	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$
0	- 7	4	5	5
1	- 3	9	10	
2	6	19		
3	25			

$$f(x) = f(0) + x\Delta f_o + \frac{x(x-1)}{2!}\Delta^2 f_o + \frac{x(x-1)(x-2)}{3!}\Delta^3 f_o + \ldots\ldots.$$

To get the most accurate interpolation we choose the first row, in the above forward differences table, as the base line (since it contains more entries).

$$f(x) = -7 + x(4) + \frac{x(x-1)}{2}(5) + \frac{x(x-1)(x-2)}{6}(5).$$

$$\therefore \qquad f(1.1) = -7 + 1.1(4) + \frac{1.1(1.1-1)}{2}(5) + \frac{1.1(1.1-1)(1.1-2)}{6}(5) = -2.4075.$$

$$f(3.5) = -7 + 3.5(4) + \frac{3.5(3.5-1)}{2}(5) + \frac{3.5(3.5-1)(3.5-2)}{6}(5) = 39.8125.$$

***Solution II*:** By Lagrange interpolation formula,

x	0	1	2	3
$f(x)$	- 7	- 3	6	25

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

$$f(x) = \frac{(x-1)(x-2)(x-3)}{(0-1)(0-2)(0-3)}(-7) + \frac{(x-0)(x-2)(x-3)}{(1-0)(1-2)(1-3)}(-3) + \frac{(x-0)(x-1)(x-3)}{(2-0)(2-1)(2-3)}(6) + \frac{(x-0)(x-1)(x-2)}{(3-0)(3-1)(3-2)}(25).$$

$$\therefore \qquad f(1.1) = \frac{(1.1-1)(1.1-2)(1.1-3)}{(0-1)(0-2)(0-3)}(-7) + \frac{(1.1-0)(1.1-2)(1.1-3)}{(1-0)(1-2)(1-3)}(-3) + \frac{(1.1-0)(1.1-1)(1.1-3)}{(2-0)(2-1)(2-3)}(6) + \frac{(1.1-0)(1.1-1)(1.1-2)}{(3-0)(3-1)(3-2)}(25) = -2.4075.$$

$$f(3.5) = \frac{(3.5-1)(3.5-2)(3.5-3)}{(0-1)(0-2)(0-3)}(-7) + \frac{(3.5-0)(3.5-2)(3.5-3)}{(1-0)(1-2)(1-3)}(-3) + \frac{(3.5-0)(3.5-1)(3.5-3)}{(2-0)(2-1)(2-3)}(6) + \frac{(3.5-0)(3.5-1)(3.5-2)}{(3-0)(3-1)(3-2)}(25) = 39.8125.$$

Example 2: Approximate the functional value at x = 4.31.

x	1	2	3	4	5
$f(x)$	6	10	46	138	430

Solution:

By Gregory-Newton interpolation formula,

Since $h=1 \Rightarrow$ Rescaling is not required. (we can use the particular formula directly)

$x_o \neq 0 \Rightarrow$ Shifting is required.

x	$x_{shifted}$	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
1	0	6	4	32	24	120
2	1	10	36	56	144	
3	2	46	92	200		
4	3	138	292			
5	4	430				

$$f(x) = f(0) + x\Delta f_o + \frac{x(x-1)}{2!}\Delta^2 f_o + \frac{x(x-1)(x-2)}{3!}\Delta^3 f_o + \dots\dots$$

$$f(x) = 6 + x(4) + \frac{x(x-1)}{2}(32) + \frac{x(x-1)(x-2)}{6}(24) + \frac{x(x-1)(x-2)(x-3)}{24}(120).$$

At $x_{old} = 4.31 \quad \Rightarrow \quad x_{new} = 4.31 - 1 = 3.31,$

$$\therefore \quad f(x_{new}) = 6 + 3.31(4) + \frac{3.31(3.31-1)}{2}(32) + \frac{3.31(3.31-1)(3.31-2)}{6}(24) +$$
$$+ \frac{3.31(3.31-1)(3.31-2)(3.31-3)}{24}(120) = 197.16857.$$

$$\therefore \quad f(4.31) = 197.16857.$$

Example 3: Given the following data. Find $y(0.23)$.

x	0.2	0.4	0.6	0.8	1.0
y	0.916	0.836	0.74	0.624	0.4

Solution:

By Gregory-Newton interpolation formula,

Since $h \neq 1 \Rightarrow$ Either we use the general formula or we can use the particular formula after rescaling the given points.

$x_o \neq 0 \Rightarrow$ Shifting is required.

x	$x_{rescaled}$	$x_{shifted}$	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
0.2	1	0	0.916	- 0.08	- 0.016	- 0.004	- 0.084
0.4	2	1	0.836	- 0,096	- 0.02	- 0.088	
0.6	3	2	0.74	- 0.116	- 0.108		
0.8	4	3	0.624	- 0.224			
1.0	5	4	0.4				

$$y(x) = y(0) + x\Delta y_o + \frac{x(x-1)}{2!}\Delta^2 y_o + \frac{x(x-1)(x-2)}{3!}\Delta^3 y_o + \dots\dots$$

$$y(x) = 0.916 + x(-0.08) + \frac{x(x-1)}{2}(-0.016) + \frac{x(x-1)(x-2)}{6}(-0.004) + \frac{x(x-1)(x-2)(x-3)}{24}(-0.084)$$

At $x_{old} = 0.23 \quad \Rightarrow \quad x_{new} = \frac{0.23}{0.2} - 1 = 0.15,$

$$y(x_{new}) = 0.916 + 0.15(-0.08) + \frac{0.15(0.15-1)}{2}(-0.016) + \frac{0.15(0.15-1)(0.15-2)}{6}(-0.004) +$$
$$+ \frac{0.15(0.15-1)(0.15-2)(0.15-3)}{24}(-0.084) = 0.907216.$$

$$\therefore \quad y(0.23) = 0.907216.$$

II- Interpolation with unequally spaced data

For unequally spaced data (h is different), the Lagrange interpolation polynomial may be used.

Example 1: (Final 2014) The accompanying table gives the velocity, of a moving body, at various times. Estimate the velocity at $t = 7$ s.

Time, t, s	1	2	3	8
Velocity, v, m/s	2	4.1	6.4	36.5

Solution:

Since h is different, we use Lagrange interpolation polynomial.

$$v(t)=\frac{(t-t_1)(t-t_2)\ldots(t-t_n)}{(t_o-t_1)(t_o-t_2)\ldots(t_o-t_n)}v(t_o)+\frac{(t-t_o)(t-t_2)\ldots(t-t_n)}{(t_1-t_o)(t_1-t_2)\ldots(t_1-t_n)}v(t_1)+\ldots$$

$$v(t)=\frac{(t-2)(t-3)(t-8)}{(1-2)(1-3)(1-8)}(2)+\frac{(t-1)(t-3)(t-8)}{(2-1)(2-3)(2-8)}(4.1)+\frac{(t-1)(t-2)(t-8)}{(3-1)(3-2)(3-8)}(6.4)+$$
$$+\frac{(t-1)(t-2)(t-3)}{(8-1)(8-2)(8-3)}(36.5).$$

$$\therefore \quad v(7)=\frac{(7-2)(7-3)(7-8)}{(1-2)(1-3)(1-8)}(2)+\frac{(7-1)(7-3)(7-8)}{(2-1)(2-3)(2-8)}(4.1)+$$
$$+\frac{(7-1)(7-2)(7-8)}{(3-1)(3-2)(3-8)}(6.4)+\frac{(7-1)(7-2)(7-3)}{(8-1)(8-2)(8-3)}(36.5)=26.5 \text{ m/s}.$$

Example 2: (Final 2015) The ratio of the work done in a project, as a function of time, is found as below. Estimate this ratio at $t = 2$ month.

Time, t, (month)	3	4	5
Work, W, (%)	5	14	37

Solution:

Since $h=1 \Rightarrow$ We can use the particular Gregory-Newton interpolation formula directly without rescaling.

$t_o \neq 0 \Rightarrow$ Shifting is required.

t	$t_{shifted}$	W	ΔW	$\Delta^2 W$
3	0	5	9	14
4	1	14	23	
5	2	37		

$$W(t)=W(0)+t\Delta W_o+\frac{t(t-1)}{2!}\Delta^2 W_o+\ldots\ldots \quad \Rightarrow \quad W(t)=5+t.(9)+\frac{t(t-1)}{2!}.(14)$$

$$\therefore \quad W(t)=5+9t+7t(t-1).$$

At $t_{old} = 2 \quad \Rightarrow \quad t_{new} = 2 - 3 = -1,$

$$W(t_{new}) = 5 + 9(-1) + 7[-1(-1-1)] = 10\% \qquad \text{Not O.k. .}$$

If a function cannot be well approximated by a polynomial, a useful device can be adopted by plotting a (log – log) graph. This reduces a large variety of functions to essentially straight lines or to smooth curves which are easy to interpolate.

$\therefore$ Use a (log – log) graph ,

$t^* = \ln t$	1.099	1.386	1.609
$W^* = \ln W$	1.609	2.639	3.611

Now, since *h* is different, we use Lagrange interpolation polynomial.

$$W^*(t^*) = \frac{(t^* - t^*_1)(t^* - t^*_2)\ldots(t^* - t^*_n)}{(t^*_o - t^*_1)(t^*_o - t^*_2)\ldots(t^*_o - t^*_n)} W^*(t^*_o) + \frac{(t^* - t^*_o)(t^* - t^*_2)\ldots(t^* - t^*_n)}{(t^*_1 - t^*_o)(t^*_1 - t^*_2)\ldots(t^*_1 - t^*_n)} W^*(t^*_1) + \ldots$$

$$W^*(t^*) = \frac{(t^* - 1.386)(t^* - 1.609)}{(1.099 - 1.386)(1.099 - 1.609)}(1.609) + \frac{(t^* - 1.099)(t^* - 1.609)}{(1.386 - 1.099)(1.386 - 1.609)}(2.639) + $$
$$+ \frac{(t^* - 1.099)(t^* - 1.386)}{(1.609 - 1.099)(1.609 - 1.386)}(3.611).$$

At $t = 2 \quad \Rightarrow \quad t^* = \ln 2 = 0.693,$

$$W^*(t^*) = \frac{(0.693 - 1.386)(0.693 - 1.609)}{(1.099 - 1.386)(1.099 - 1.609)}(1.609) + \frac{(0.693 - 1.099)(0.693 - 1.609)}{(1.386 - 1.099)(1.386 - 1.609)}(2.639) + $$
$$+ \frac{(0.693 - 1.099)(0.693 - 1.386)}{(1.609 - 1.099)(1.609 - 1.386)}(3.611) = 0.576664.$$

But $W^* = \ln W \quad \Rightarrow \quad W = e^{W^*} = e^{0.576664} = 1.78.$

$\therefore \; W(2) = 1.78\%.$

10- Matrices and Determinants for Solving Simultaneous Algebraic Equations

Introduction

The solution of set of algebraic equations is an important step in wide variety of engineering problems, such as the structural analysis, network analysis, numerical solution of differential equations, ….etc. There are various methods to solve a set of algebraic equations, such as Cramer's rule, Gauss elimination, Gauss-Jordan elimination, and matrix inverse.

1. Cramer's Rule

$$C.X = R \qquad \Rightarrow \qquad X_k = \frac{|C_k|}{|C|}.$$

Example: Solve the following set of algebraic equations

$$2x + 4y - 2z - 2 = 0,$$
$$x + z - 3 = 0,$$
$$2x + y - z - 1 = 0.$$

Solution:

$$2x + 4y - 2z = 2,$$
$$x + z = 3,$$
$$2x + y - z = 1.$$

In matrix form:

$$\begin{bmatrix} 2 & 4 & -2 \\ 1 & 0 & 1 \\ 2 & 1 & -1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix}.$$

Using Cramer's rule to solve the above matrix, gives

$$x = \frac{\begin{vmatrix} 2 & 4 & -2 \\ 3 & 0 & 1 \\ 1 & 1 & -1 \end{vmatrix}}{\begin{vmatrix} 2 & 4 & -2 \\ 1 & 0 & 1 \\ 2 & 1 & -1 \end{vmatrix}} = \frac{2\begin{vmatrix} 0 & 1 \\ 1 & -1 \end{vmatrix} + (-1)(4)\begin{vmatrix} 3 & 1 \\ 1 & -1 \end{vmatrix} + (-2)\begin{vmatrix} 3 & 0 \\ 1 & 1 \end{vmatrix}}{2\begin{vmatrix} 0 & 1 \\ 1 & -1 \end{vmatrix} + (-1)(4)\begin{vmatrix} 1 & 1 \\ 2 & -1 \end{vmatrix} + (-2)\begin{vmatrix} 1 & 0 \\ 2 & 1 \end{vmatrix}}$$

$$= \frac{2[0(-1)-1(1)] - 4[3(-1)-1(1)] - 2[3(1)-0(1)]}{2[0(-1)-1(1)] - 4[1(-1)-1(2)] - 2[1(1)-0(2)]} = \frac{8}{8} = 1.$$

Similarly,

$$y = \frac{\begin{vmatrix} 2 & 2 & -2 \\ 1 & 3 & 1 \\ 2 & 1 & -1 \end{vmatrix}}{\begin{vmatrix} 2 & 4 & -2 \\ 1 & 0 & 1 \\ 2 & 1 & -1 \end{vmatrix}} = \frac{2\begin{vmatrix} 3 & 1 \\ 1 & -1 \end{vmatrix} + (-1)(2)\begin{vmatrix} 1 & 1 \\ 2 & -1 \end{vmatrix} + (-2)\begin{vmatrix} 1 & 3 \\ 2 & 1 \end{vmatrix}}{8}$$

$$= \frac{2[3(-1)-1(1)] - 2[1(-1)-1(2)] - 2[1(1)-3(2)]}{8} = \frac{8}{8} = 1.$$

$$z = \frac{\begin{vmatrix} 2 & 4 & 2 \\ 1 & 0 & 3 \\ 2 & 1 & 1 \end{vmatrix}}{\begin{vmatrix} 2 & 4 & -2 \\ 1 & 0 & 1 \\ 2 & 1 & -1 \end{vmatrix}} = \frac{2\begin{vmatrix} 0 & 3 \\ 1 & 1 \end{vmatrix} + (-1)(4)\begin{vmatrix} 1 & 3 \\ 2 & 1 \end{vmatrix} + 2\begin{vmatrix} 1 & 0 \\ 2 & 1 \end{vmatrix}}{8}$$

$$= \frac{2[0(1)-3(1)] - 4[1(1)-3(2)] + 2[1(1)-0(2)]}{8} = \frac{16}{8} = 2.$$

2. Gauss Elimination

Example: Solve the following system of algebraic equations

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

$$x + z = 3,$$

$$2x + y - z = 1.$$

Solution:

In matrix form:

$$\begin{bmatrix} 2 & 4 & -2 \\ 1 & 0 & 1 \\ 2 & 1 & -1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix}.$$

Use Gauss elimination method to solve the above matrix:

Step 1;

$$\begin{matrix} \\ (-1)(R_1/2) + R_2 \rightarrow \\ (-2)(R_1/2) + R_3 \rightarrow \end{matrix} \begin{bmatrix} 2 & 4 & -2 \\ 0 & -2 & 2 \\ 0 & -3 & 1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 2 \\ 2 \\ -1 \end{bmatrix}.$$

Step 2;

$$\begin{matrix} \\ \\ (3)(R_2/-2) + R_3 \rightarrow \end{matrix} \begin{bmatrix} 2 & 4 & -2 \\ 0 & -2 & 2 \\ 0 & 0 & -2 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 2 \\ 2 \\ -4 \end{bmatrix}.$$

Note: R_1, R_2 and R_3 mean the first, second and third row, respectively.

From $R_3 \Rightarrow -2z = -4 \Rightarrow z = 4/2 \Rightarrow z = 2$.

Use back substitution:

From $R_2 \Rightarrow -2y + 2z = 2 \Rightarrow y = z - 1 \Rightarrow y = 2 - 1 \Rightarrow y = 1$.

From $R_1 \Rightarrow 2x + 4y - 2z = 2 \Rightarrow x = 1 - 2y + z \Rightarrow x = 1 - 2(1) + 2 \Rightarrow x = 1$.

3. Gauss-Jordan Elimination

Example: Solve the following system

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

$$x + z = 3,$$

$$2x + y - z = 1.$$

Solution:

In matrix form:

$$\begin{bmatrix} 2 & 4 & -2 \\ 1 & 0 & 1 \\ 2 & 1 & -1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix}.$$

Use Gauss-Jordan elimination method to solve the above matrix:

Step 1;

$$\begin{matrix} R_1/2 & \rightarrow \\ (-1)R_1 + R_2 & \rightarrow \\ (-2)R_1 + R_3 & \rightarrow \end{matrix} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -2 & 2 \\ 0 & -3 & 1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 1 \\ 2 \\ -1 \end{bmatrix}.$$

Step 2;

$$\begin{matrix} (-2)R_2 + R_1 & \rightarrow \\ R_2/-2 & \rightarrow \\ (3)R_2 + R_3 & \rightarrow \end{matrix} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & -2 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 3 \\ -1 \\ -4 \end{bmatrix}.$$

Step 3;

$$\begin{matrix} (-1)R_3 + R_1 & \rightarrow \\ (1)R_3 + R_2 & \rightarrow \\ R_3/-2 & \rightarrow \end{matrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix}.$$

$$\therefore \quad \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix}.$$

4. Matrix Inverse

$$C.X = R \qquad \Rightarrow \qquad C^{-1}.C.X = C^{-1}.R.$$

But, $\quad C^{-1}.C = I \qquad \Rightarrow \qquad X = C^{-1}.R.$

Example: Solve the following system

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

$$x + z = 3,$$

$$2x + y - z = 1.$$

Solution:

In matrix form:

$$\begin{bmatrix} 2 & 4 & -2 \\ 1 & 0 & 1 \\ 2 & 1 & -1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix}.$$

Use matrix inverse method to solve the above matrix:

To find C^{-1};

$$\left[\begin{matrix} 2 & 4 & -2 \\ 1 & 0 & 1 \\ 2 & 1 & -1 \end{matrix}\right]\left[\begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}\right].$$

$$\begin{matrix} R_1/2 \rightarrow \\ (-1)R_1 + R_2 \rightarrow \\ (-2)R_1 + R_3 \rightarrow \end{matrix} \quad \left[\begin{matrix} 1 & 2 & -1 \\ 0 & -2 & 2 \\ 0 & -3 & 1 \end{matrix}\right]\left[\begin{matrix} 1/2 & 0 & 0 \\ -1/2 & 1 & 0 \\ -1 & 0 & 1 \end{matrix}\right].$$

$$\begin{matrix} (-2)R_2 + R_1 \rightarrow \\ R_2/(-2) \rightarrow \\ (3)R_2 + R_3 \rightarrow \end{matrix} \quad \left[\begin{matrix} 1 & 0 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & -2 \end{matrix}\right]\left[\begin{matrix} 0 & 1 & 0 \\ 1/4 & -1/2 & 0 \\ -1/4 & -3/2 & 1 \end{matrix}\right].$$

$$\begin{matrix} (-1)R_3 + R_1 \rightarrow \\ (1)R_3 + R_2 \rightarrow \\ R_3/(-2) \rightarrow \end{matrix} \quad \left[\begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}\right]\left[\begin{matrix} -1/8 & 1/4 & 1/2 \\ 3/8 & 1/4 & -1/2 \\ 1/8 & 3/4 & -1/2 \end{matrix}\right].$$

$$\therefore \qquad C^{-1} = \begin{bmatrix} -1/8 & 1/4 & 1/2 \\ 3/8 & 1/4 & -1/2 \\ 1/8 & 3/4 & -1/2 \end{bmatrix}.$$

$$X = C^{-1}.R \qquad \Rightarrow \qquad \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{bmatrix} -1/8 & 1/4 & 1/2 \\ 3/8 & 1/4 & -1/2 \\ 1/8 & 3/4 & -1/2 \end{bmatrix} \begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix}.$$

$$\therefore \quad x = -\frac{1}{8}\times 2 + \frac{1}{4}\times 3 + \frac{1}{2}\times 1 = -\frac{1}{4} + \frac{3}{4} + \frac{1}{2} = 1,$$

$$y = \frac{3}{8}\times 2 + \frac{1}{4}\times 3 - \frac{1}{2}\times 1 = \frac{3}{4} + \frac{3}{4} - \frac{1}{2} = 1,$$

$$z = \frac{1}{8}\times 2 + \frac{3}{4}\times 3 - \frac{1}{2}\times 1 = \frac{1}{4} + \frac{9}{4} - \frac{1}{2} = 2.$$

Note; we can find C^{-1} by another procedure, as follows,

$$C^{-1} = \frac{adjointC}{|C|}, \qquad \text{where,} \qquad adjointC = [cofactorC]^T.$$

$$|C| = \begin{vmatrix} 2 & 4 & -2 \\ 1 & 0 & 1 \\ 2 & 1 & -1 \end{vmatrix} = 2\begin{vmatrix} 0 & 1 \\ 1 & -1 \end{vmatrix} + (-1)(4)\begin{vmatrix} 1 & 1 \\ 2 & -1 \end{vmatrix} + (-2)\begin{vmatrix} 1 & 0 \\ 2 & 1 \end{vmatrix}$$

$$= 2[0(-1) - 1(1)] - 4[1(-1) - 1(2)] - 2[1(1) - 0(2)] = -2 + 12 - 2 = 8.$$

$$cofactorC = \begin{bmatrix} +\begin{vmatrix} 0 & 1 \\ 1 & -1 \end{vmatrix} & -\begin{vmatrix} 1 & 1 \\ 2 & -1 \end{vmatrix} & +\begin{vmatrix} 1 & 0 \\ 2 & 1 \end{vmatrix} \\ -\begin{vmatrix} 4 & -2 \\ 1 & -1 \end{vmatrix} & +\begin{vmatrix} 2 & -2 \\ 2 & -1 \end{vmatrix} & -\begin{vmatrix} 2 & 4 \\ 2 & 1 \end{vmatrix} \\ +\begin{vmatrix} 4 & -2 \\ 0 & 1 \end{vmatrix} & -\begin{vmatrix} 2 & -2 \\ 1 & 1 \end{vmatrix} & +\begin{vmatrix} 2 & 4 \\ 1 & 0 \end{vmatrix} \end{bmatrix} = \begin{bmatrix} -1 & 3 & 1 \\ 2 & 2 & 6 \\ 4 & -4 & -4 \end{bmatrix}.$$

$$adjointC = [cofactorC]^T = \begin{bmatrix} -1 & 2 & 4 \\ 3 & 2 & -4 \\ 1 & 6 & -4 \end{bmatrix}.$$

$$\therefore \qquad C^{-1} = \frac{1}{8}\times \begin{bmatrix} -1 & 2 & 4 \\ 3 & 2 & -4 \\ 1 & 6 & -4 \end{bmatrix} = \begin{bmatrix} -1/8 & 1/4 & 1/2 \\ 3/8 & 1/4 & -1/2 \\ 1/8 & 3/4 & -1/2 \end{bmatrix}.$$