Introduction

Numerical analysis is a branch of Mathematics that deals with devising efficient methods for obtaining numerical solutions to difficult Mathematical problems. Most of the Mathematical problems that arise in science and engineering are very hard and sometime impossible to solve exactly. Thus, an approximation to a difficult Mathematical problem is very important to make it easier to solve. Due to the immense development in the computational technology, numerical approximation has become more popular and a modern tool for scientists and engineers. As a result many scientific software are developed (for instance, MATLAB, Mathematical, Maple etc.) to handle more difficult problems in an efficient and easy way. These software contain functions that uses standard numerical methods, where a user can pass the required parameters and get the results just by a single command without knowing the details of the numerical method. Thus, one may ask why we need to understand numerical methods when such software are at our hands. In fact, there is no need of a deeper knowledge of numerical methods and their analysis in most of the cases in order to use some standard software as an end user. However, there are at least three reasons to gain a basic understanding of the theoretical background of numerical methods.

1. Learning different numerical methods and their analysis will make a person more familiar with the technique of developing new numerical methods. This is important when the available methods are not enough or not efficient for a specific problem to be solved.

2. In many circumstances, one has more methods for a given problem. Hence, choosing an appropriate method is important for producing an accurate result in lesser time.

3. With a sound background, one can use methods properly (especially when a method has its own limitations and/or disadvantages in some specific cases) and, most importantly, one can understand what is going wrong when results are not as expected.

Bracketing Methods

- The root is located within interval of lower and upper bound.
- Such methods are said to be convergent because they move closer to the truth as the computation progresses.

Nonlinear equations (finding the roots)

One of the most frequently occurring problems in scientific work is to find the roots of equations of the form

$$f(x) = 0 \qquad (1)$$

1. Fixed-point Iteration method

The idea of this method is to rewrite the equation (1) in the form:

$$x = g(x) \qquad (2)$$

Once the iteration function is chosen, then the method is defined as follows:

1. Choose an initial guess x_0;
2. Define the iteration methods as

$$x_{n+1} = g(x_n), \qquad n = 0, 1, \dots ....$$

Ex. Solve $f(x) = x^2 - 3x + 1$ by fixed-point iteration method.

Sol. First make $f(x) = 0$:

$$x^2 - 3x + 1 = 0$$

Second find iteration function:

$$x = 3 - \frac{1}{x} \rightarrow x_{n+1} = 3 - \frac{1}{x_n}$$

Third choose initial guess x_0:

$$X_0 = 1$$

$x_{0+1} = 3 - \frac{1}{x_0} = 3 - \frac{1}{1} = 2$ So $x_1 = 2$, $x_2 = 2.5$, $x_3 = 2.6$, $x_4 = 2.615$, $x_5 = 2.617$

The root is 2.617

Ex. Find a real root of the equation $x^3 + x^2 - 1 = 0$ on the interval [0, 1] with an accuracy of 10^{-4}?

Sol.

To find this root, we rewrite the given equation in the form

$$x = \frac{1}{\sqrt{x+1}}$$

$$X_0 = 0.75$$

Hence the iteration method gives:

n	x_n	$\sqrt{x_n + 1}$	$x_{n+1} = 1/\sqrt{x_n + 1}$
0	0.75	1.3228756	0.7559
1	0.7559	1.3251146	0.7546
2	0.7546	1.3246326	0.7549

At this stage,

$$|x_{n+1} - x_n| = 0.7549263 - 0.7546517 = 0.0002746,$$

Which is less than 0.0004. The iteration is therefore terminated and the root to the required accuracy is 0.7549.

2. Bisection Method

The bisection method is one of the bracketing methods for finding roots of an equation. For a given a function $f(x)$, guess an interval which might contain a root and perform a number of iterations, where, in each iteration the interval containing the root is get halved.

2.1. Intermediate value theorem for continuous functions:

If f is a continuous function and $f\ (a)$ and $f\ (b)$ have opposite signs, then at least one root lies in between a and b. If the interval (a, b) is small enough, it is likely to contain a single root.

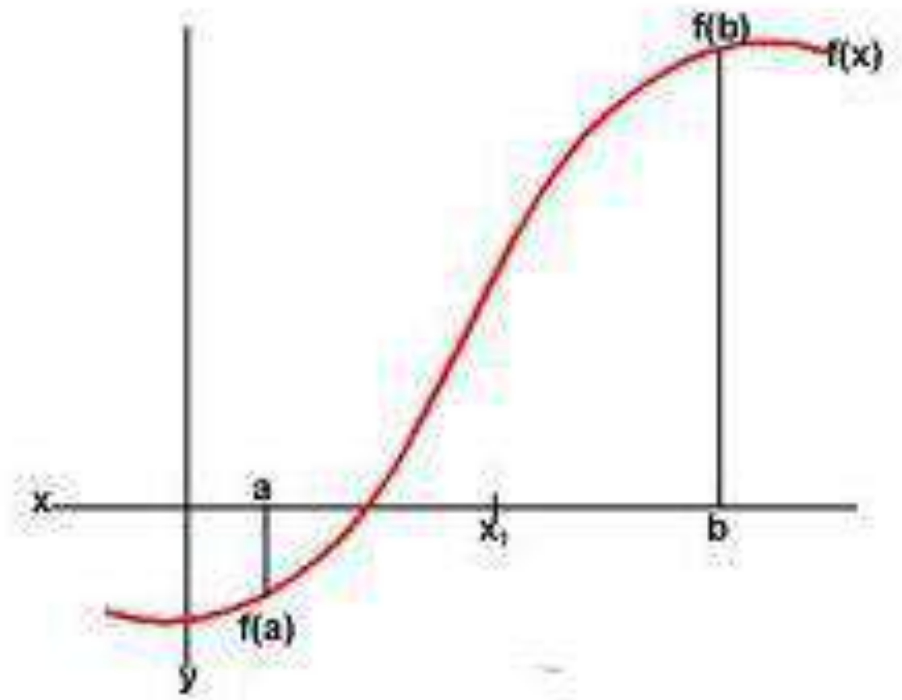

Figure (1) Bisection method

An interval $[a, b]$ must contain a zero of a continuous function f if the product$f(a) f(b) < 0$. Geometrically, this means that if $f(a) f(b) < 0$, then the curve f has to cross the x-axis at some point in between a and b.

2.2. Bisection Algorithm

Suppose we want to find the solution to the equation $(x) = 0$, where f is continuous. Given a function $f(x)$ continuous on an interval $[a0, b0]$ and satisfying$f(a) f(b) < 0$. For n = 0, 1, 2, … until termination do:

Find $x_n = \frac{1}{2}(a_n + b_n)$

If $f(x_n) = 0$, accept x_n as a solution and stop.

Else continue:

If $f(a_n)\, f(x_n) < 0$, a root lies in the interval (a_n, x_n).

Set $a_{n+1} = a_n$, $b_{n+1} = x_n$.

If $f(a_n)\, f(x_n) > 0$, a root lies in the interval (x_n, b_n).

Set $a_{n+1} = x_n$, $b_{n+1} = b_n$.

Ex. Solve $x^3 - 9x + 1$ for the root between $x = 2$ and $x = 4$, by bisection method?

Sol.

Given $f(x) = x^3 - 9x + 1$. Now $f(2) = -9$, $f(4) = 29$ so that $f(2)f(4) < 0$ and hence a root lies between 2 and 4.

Set $a_0 = 2$ and $b_0 = 4$. Then

$$x_0 = \frac{(a_0 + b_0)}{2} = \frac{2+4}{2} = 3 \quad \text{and} \quad f(x_0) = f(3) = 1.$$

Since $f(2)f(3) < 0$, a root lies between 2 and 3, hence we set $a_1 = a_0 = 2$ and $b_1 = x_0 = 3$. Then

$$x_1 = \frac{(a_1 + b_1)}{2} = \frac{2+3}{2} = 2.5 \quad \text{and} \quad f(x_1) = f(2.5) = -5.875$$

Since $f(2)f(2.5) > 0$, a root lies between 2.5 and 3, hence we set $a_2 = x_1 = 2.5$ and $b_2 = b_1 = 3$.

Then $x_2 = \dfrac{(a_2 + b_2)}{2} = \dfrac{2.5+3}{2} = 2.75$ and $f(x_2) = f(2.75) = -2.9531.$

The steps are illustrated in the following table.

n	x_n	$f(x_n)$
0	3	1.0000
1	2.5	-5.875
2	2.75	-2.9531
3	2.875	-1.1113
4	2.9375	-0.0901

Ex. Find a real root of the equation $f(x) = x^3 - x - 1 = 0$ by bisection method?

Sol.

Since $f(1)$ is negative and $f(2)$ positive, a root lies between 1 and 2 and therefore we take $x_0 = 3/2 = 1.5.$ Then

$f(x_0) = \frac{27}{8} - \frac{3}{2} = \frac{15}{8}$ is positive and hence $f(1)\, f(1.5) < 0$ and Hence the root lies between 1 and 1.5 and we obtain

$$x_1 = \frac{1+1.5}{2} = 1.25$$

$f(x_1) = -19/64,$ which is negative and hence $f(1)\, f(1.25) > 0$ and hence a root lies between 1.25 and 1.5. Also,

$$x_2 = \frac{1.25+1.5}{2} = 1.375$$

The procedure is repeated and the successive approximations are

$$x_3 = 1.3125, \quad x_4 = 1.34375, \quad x_5 = 1.328125, \text{ etc.}$$

H.W:

1. Find the real root of the equation $(x \log_{10} x - 1.2 = 0)$. Correct to five decimal places by the false-position method.
2. Solve the equation $(x^3 - 9x + 1 = 0)$ for the root lying between 2 and 3, correct to three significant figures.

References

[1] R. W Hamming, “Numerical methods for scientists and engineers (International series in pure & applied mathematics), McGraw-Hill; 2nd edition, ISBN-10: 0070258872.

[2] Steven Chapra, “Applied Numerical Methods with MATLAB for Engineers and Scientists”, McGraw-Hill; 4th edition, ISBN-13: 978-0073397962.

3. Newton-Raphson Method

Methods such as the bisection method and the false position method of finding roots of a nonlinear equation $f(x) = 0$ (require bracketing of the root by two guesses. Such methods are called bracketing methods. These methods are always convergent since they are based on reducing the interval between the two guesses so as to zero in on the root of the equation. In the Newton-Raphson method, the root is not bracketed. In fact, only one initial guess of the root is needed to get the iterative process started to find the root of an equation. The method hence falls in the category of open methods. Convergence in open methods is not guaranteed but if the method does converge, it does so much faster than the bracketing methods.

Algorithm of Newton method

The steps of the Newton-Raphson method to find the root of an equation $f(x) = 0$ are:

1. Evaluate $f'(x)$
2. Use an initial guess of the root, x_i, to estimate the new value of the root, x_{i+1}, as

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

3. Find the absolute relative approximate error $|\in_a|$ as

$$|\in_a| = \left|\frac{x_{i+1} - x_i}{x_{i+1}}\right| \times 100$$

4. Compare the absolute relative approximate error with the pre-specified relative error tolerance, if $|\epsilon_a| > \epsilon_s$ then go to Step 2, else stop the algorithm. Also, check if the number of iterations has exceeded the maximum number of iterations allowed.

Example: Use Newton-Raphson method to find a root of the equation $x^3 - 2x - 5 = 0$. ($\in_s$= 0.003)

Sol.

1. $f(x) = x^3 - 2x - 5$ and its derivative is $f\grave{}(x) = 3x^2 - 2$
2. $x_{n+1} = x_n - \frac{x_n^3 - 2x_n - 5}{3x_n^2 - 2}$

Choosing x_0 =2, we obtain $f(x_0) = -1$ and $\grave{f}(x_0) = 10$

$$x_1 = 2 - \left(-\frac{1}{10}\right) = 2.1$$

$$f(x_1) = (2.1)^3 - 2(2.1) - 5 = 0.061$$

And $\grave{f}(x_1) = 3(2.1)^2 - 2 = 11.23$

$$x_2 = 2.1 - \left(\frac{0.061}{11.23}\right) = 2.094568$$

The error will be $\in_a = \left|\frac{2.094568 - 2.1}{2.094568}\right| * 100 = 0.002$

So the root is 2.094568

Example: Find a root of the equation $x sinx + cos\, x = 0$.

Sol.

1. $f(x) = x sinx + cos\, x$ and $\grave{f}(x) = x\, cos\, x$
2. Hence the iteration formula is

$$x_{n+1} = x_n - \frac{x_n \sin x_n + \cos x_n}{x_n \cos x_n}$$

With $x_0 = \pi$, the successive iterates are given below:

N	Xn	F(xn)	Xn+1
0	3.1416	-1.0	2.8233
1	2.8233	-0.0662	2.7986
2	2.7986	-0.0006	2.7984
3	2.7984	0.0	2.7984

Drawbacks of the Newton-Raphson Method

1. Divergence at inflection points If the selection of the initial guess or an iterated value of the root turns out to be close to the inflection point of the function f(x) in the equation f(x)=0, Newton-Raphson method may start diverging away from the root.
2. Division by zero
3. Oscillations near local maximum and minimum Results obtained from the Newton-Raphson method may oscillate about the local maximum or minimum without converging on a root but converging on the local maximum or minimum. Eventually, it may lead to division by a number close to zero and may diverge.

4. Root jumping in some case where the function f(x) is oscillating and has a number of roots, one may choose an initial guess close to a root. However, the guesses may jump and converge to some other root.

4.Secant Method

A potential problem in implementing the Newton - Raphson method is the evolution of the derivative. Although this is not inconvenient for polynomials and many other functions, there are certain functions whose derivatives may be extremely difficult or inconvenient to evaluate. Graphical depiction of the Secant method, this technique is similar the Newton - Raphson technique in the sense that an estimate of the root is predicated by extrapolating a tangent of the function to the x axis. However, the secant method uses a difference rather than a derivative to estimate the slope.

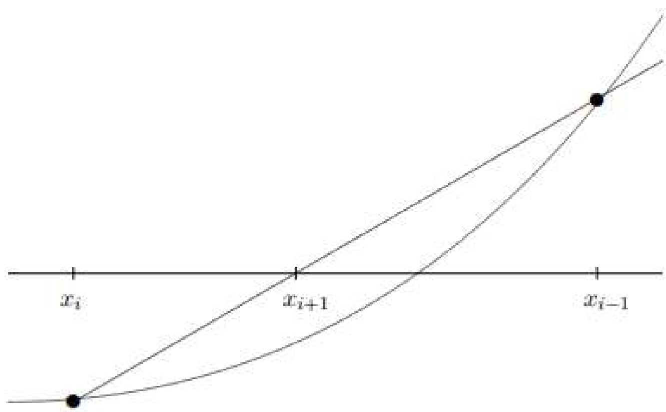

Figure (1) Secant method

The rule of secant method as follow:

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

Example: Use the secant method to estimate the root of $f(x) = e^{-x} - x$. Start with initial estimates of $x_{i-1} = 0$, $x_i = 1$.

Sol.

For i=0

$x_{-1} = 0, f(x_{-1}) = e^{-x_{-1}} - x_{-1} = e^0 - 0 = 1$

$x_0 = 1, f(x_0) = e^{-x_0} - x_0 = e^{-1} - 1 = -0.63212$

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

For i=1

$x_0 = 1, f(x_0) = e^{-x_0} - x_0 = e^{-1} - 1 = -0.63212$

$x_1 = 0.61270, f(x_1) = e^{-x_1} - x_1 = e^{-0.61270} - 0.61270 = -0.07081$

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

For i=2

$x_1 = 0.61270, f(x_1) = e^{-x_1} - x_1 = e^{-0.61270} - 0.61270 = -0.07081$

$x_2 = 0.56384, f(x_2) = e^{-x_2} - x_2 = e^{-0.56384} - 0.56384 = 0.00518$

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

For i=3

$x_2 = 0.56384, f(x_2) = e^{-x_2} - x_2 = e^{-0.56384} - 0.56384 = 0.00518$

$x_3 = 0.56717, f(x_3) = e^{-x_3} - x_3 = e^{-0.56717} - 0.56717 = -0.00004$

$$x_4 = x_3 - \frac{f(x_3)(x_2 - x_3)}{f(x_2) - f(x_3)} = 0.56717 - \frac{-0.00004(0.56384 - 0.56717)}{0.00518 - (-0.00004)}$$
$$= 0.56714$$

Solving simultaneous linear equations

➢ Gauss-Elimination Method

Gauss elimination is one of the oldest and most frequently used methods for solving systems of algebraic equations. It is attributed to the famous Gennan mathematician, Carl Friedrick Gauss (1777 -1855). This method is the generalization of the familiar method of eliminating one unknown between a pair of simultaneous linear equations. In this method the matrix A is reduced to the form U by using the elementary row operations which include:

1. Interchange any two rows.
2. Multiplying or dividing any row by a non-zero constant.
3. Adding or subtracting of one row to another row.

Example 1: Find the solution to the following system of equations using the Gauss-elimination method.

$$2X_1 + 3X_2 - X_3 = 5$$

$$4X_1 + 4X_2 - 3X_3 = 3$$

$$-2X_1 + 3X_2 - X_3 = 1$$

Sol:

Rearrange equations as follow:

$$4X_1 + 4X_2 - 3X_3 = 3 \quad \ldots\ldots (1)$$

$$[2X_1 + 3X_2 - X_3 = 5 \ldots\ldots\ldots\ldots (2)] * (-2)$$

$$[-2X_1 + 3X_2 - X_3 = 1 \ldots\ldots\ldots (3)] * (2)$$

To eliminate X1 from equation (2) multiply it by (-2) and multiply equation (3) by (2) we get:

$$4X_1 + 4X_2 - 3X_3 = 3 \dots (1)$$

$$-4X_1 - 6X_2 + 2X_3 = -10 \dots (2)$$

$$-4X_1 + 6X_2 - 2X_3 = 2 \dots (3)$$

Now by summing equation (2) and equation (3) with equation (1) we get:

$$4X_1 + 4X_2 - 3X_3 = 3 \dots (1)$$

$$[0 - 2X_2 - 1X_3 = -7 \dots (4)] *5$$

$$0 + 10X_2 - 5X_3 = 5 \dots (5)$$

Now to eliminate X2 from fifth equation we multiply equation (2) by (5) we get:

$$4X_1 + 4X_2 - 3X_3 = 3 \dots (1)$$

$$0 - 10X_2 - 5X_3 = -35 \dots (4)$$

$$0 + 10X_2 - 5X_3 = 5 \dots (5)$$

Now by summing equation (5) with equation (4) only we get:

$$-10X_3 = -30 \dots (5)$$

So we get X3 = 3

Then by substitute the value of X3 in equation (4) or (5) we get:

X2 = 2

Then substitute the value of X3 and X2 in any general equations above we get:

$$X1 = 1$$

So the final values are X1 = 1, X2 = 2, X3 = 3

Example 2: Find the solution to the following system of equations using the Gauss-elimination method.

$$3X_1 + 2X_2 + X_3 = 3$$

$$2X_1 + X_2 + X_3 = 0$$

$$6X_1 + 2X_2 + 4X_3 = 6$$

Sol:

Rearrange equations as follow:

$$6X_1 + 2X_2 + 4X_3 = 6 \quad \ldots\ldots (1)$$

$$[3X_1 + 2X_2 + X_3 = 3 \ldots\ldots\ldots\ldots (2)] *(-2)$$

$$[2X_1 + X_2 + X_3 = 0 \ldots\ldots\ldots (3)] *(-3)$$

Now to eliminate X1 from equation (2) we multiply it by (-2) and to eliminate X1 from equation (3) we multiply it by (-3) we get:

$$6X_1 + 2X_2 + 4X_3 = 6 \quad \ldots\ldots (1)$$

$$-6X_1 - 4X_2 - 2X_3 = -6 \ldots\ldots\ldots\ldots (2)$$

$$-6X_1 - 3X_2 - 3X_3 = 0 \ldots\ldots\ldots (3)$$

Now by summing equation (2) and equation (3) with equation (1) we get:

$$6X_1 + 2X_2 + 4X_3 = 6 \quad \ldots\ldots (1)$$

$$0 - 2X_2 + 2X_3 = 0 \ldots\ldots\ldots\ldots (4)$$

$$0 - 1X_2 + 1X_3 = 6 \ldots\ldots\ldots (5)$$

It can see from the equation (4) & (5) we cannot eliminate X2 or X3. So the solution will stop here and we say that the equations are inconsistent.

- Gauss-Jordan elimination:

The steps of Jordan elimination as follow:

1. Form the augmented matrix corresponding to the system of linear equations.
2. Transform the augmented matrix to the matrix in reduced row echelon form via elementary row operations.
3. Solve the linear system corresponding to the matrix in reduced row echelon form.

Example 2: Solve the following system by using the Gauss-Jordan elimination method.

$$X + Y + Z = 5$$

$$2X + 3Y + 5Z = 8$$

$$4X + 5Z = 2$$

Sol:

1. Form the augmented matrix.

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 5 \\ 2 & 3 & 5 & 8 \\ 4 & 0 & 5 & 2 \end{array}\right]$$

2. Transform from augmented to reduced form matrix.

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 5 \\ 2 & 3 & 5 & 8 \\ 4 & 0 & 5 & 2 \end{array}\right] \xrightarrow{R_2-2R_1} \left[\begin{array}{ccc|c} 1 & 1 & 1 & 5 \\ 0 & 1 & 3 & -2 \\ 4 & 0 & 5 & 2 \end{array}\right]$$

$$\xrightarrow{R_3-4R_1} \left[\begin{array}{ccc|c} 1 & 1 & 1 & 5 \\ 0 & 1 & 3 & -2 \\ 0 & -4 & 1 & -18 \end{array}\right]$$

$$\xrightarrow{R_3+4R_2} \left[\begin{array}{ccc|c} 1 & 1 & 1 & 5 \\ 0 & 1 & 3 & -2 \\ 0 & 0 & 13 & -26 \end{array}\right]$$

$$\xrightarrow{\frac{1}{13}R_3} \left[\begin{array}{ccc|c} 1 & 1 & 1 & 5 \\ 0 & 1 & 3 & -2 \\ 0 & 0 & 1 & -2 \end{array}\right]$$

$$\xrightarrow{R_2-3R_3} \left[\begin{array}{ccc|c} 1 & 1 & 1 & 5 \\ 0 & 1 & 0 & 4 \\ 0 & 0 & 1 & -2 \end{array}\right]$$

$$\xrightarrow{R_1-R_3} \left[\begin{array}{ccc|c} 1 & 1 & 0 & 7 \\ 0 & 1 & 0 & 4 \\ 0 & 0 & 1 & -2 \end{array}\right]$$

$$\xrightarrow{R_1-R_2} \left[\begin{array}{ccc|c} 1 & 0 & 0 & 3 \\ 0 & 1 & 0 & 4 \\ 0 & 0 & 1 & -2 \end{array}\right]$$

3. Solve the linear system corresponding to the matrix in reduced row echelon form.

$$X = 3, Y = 4, Z = -2$$

Example 3: Solve the following system by using the Gauss-Jordan elimination method.

$$X + 2Y – 3Z = 2$$

$$6X + 3Y – 9Z = 6$$

$$7X + 14Y – 21Z = 13$$

Sol:

1. Form the augmented matrix.

$$\left[\begin{array}{ccc|c} 1 & 2 & -3 & 2 \\ 6 & 3 & -9 & 6 \\ 7 & 14 & -21 & 13 \end{array}\right]$$

2. Transform from augmented to reduced form matrix.

$$\left[\begin{array}{ccc|c} 1 & 2 & -3 & 2 \\ 6 & 3 & -9 & 6 \\ 7 & 14 & -21 & 13 \end{array}\right] \xrightarrow{R_2-6R_1} \left[\begin{array}{ccc|c} 1 & 2 & -3 & 2 \\ 0 & -9 & 9 & -6 \\ 7 & 14 & -21 & 13 \end{array}\right]$$

$$\xrightarrow{R_3-7R_1} \left[\begin{array}{ccc|c} 1 & 2 & -3 & 2 \\ 0 & -9 & 9 & -6 \\ 0 & 0 & 0 & -1 \end{array}\right]$$

We obtain a row whose elements are all zero’s except the last one on the right. Therefore, we conclude that the system of equations is inconsistent, i.e., it has no solutions.

Integration

Integration is the process of measuring the area under a function plotted on a graph. Why would we want to integrate a function? Among the most common examples are finding the velocity of a body from an acceleration function, and displacement of a body from a velocity function. Throughout many engineering fields, there are (what sometimes seems like) countless applications for integral calculus. Sometimes, the evaluation of expressions involving these integrals can become daunting, if not indeterminate. For this reason, a wide variety of numerical methods has been developed to simplify the integral. There some types of integration which are:

1. Trapezoidal rule.
2. Simpsons 1/3 rule.
3. Simpsons 3/8 rule.

➢ One segment Simpsons 1/3 rule

The trapezoidal rule was based on approximating the integrand by a first order polynomial, and then integrating the polynomial over interval of integration. Simpson's 1/3 rule is an extension of Trapezoidal rule where the integrand is approximated by a second order polynomial.

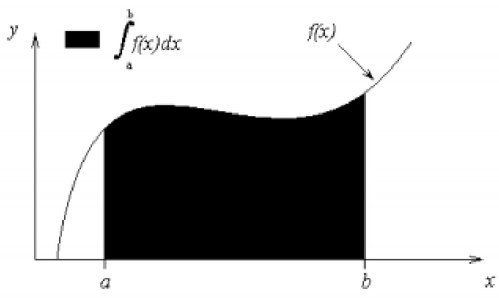

Figure (1) Function integration

For one segment Simpsons 1/3 rule we can applied the following law:

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

where $f_2(x)$ is a second order polynomial given by

$$f_2(x) = a_0 + a_1 x + a_2 x^2$$

Choose

$$(a, f(a)), \left(\frac{a+b}{2}, f\left(\frac{a+b}{2}\right)\right), \text{ and } (b, f(b))$$

as the three points of the function to evaluate a_0, a_1 and a_2.

$$f(a) = f_2(a) = a_0 + a_1 a + a_2 a^2$$

$$f\left(\frac{a+b}{2}\right) = f_2\left(\frac{a+b}{2}\right) = a_0 + a_1\left(\frac{a+b}{2}\right) + a_2\left(\frac{a+b}{2}\right)^2$$

$$f(b) = f_2(b) = a_0 + a_1 b + a_2 b^2$$

Solving the above three equations for unknowns, a_0, a_1 and a_2 give

$$a_0 = \frac{a^2 f(b) + abf(b) - 4abf\left(\frac{a+b}{2}\right) + abf(a) + b^2 f(a)}{a^2 - 2ab + b^2}$$

$$a_1 = -\frac{af(a) - 4af\left(\frac{a+b}{2}\right) + 3af(b) + 3bf(a) - 4bf\left(\frac{a+b}{2}\right) + bf(b)}{a^2 - 2ab + b^2}$$

$$a_2 = \frac{2\left(f(a) - 2f\left(\frac{a+b}{2}\right) + f(b)\right)}{a^2 - 2ab + b^2}$$

Then

$$I \approx \int_a^b f_2(x)dx$$

$$= \int_a^b \left(a_0 + a_1 x + a_2 x^2\right)dx$$

$$= \left[a_0 x + a_1\frac{x^2}{2} + a_2\frac{x^3}{3}\right]_a^b$$

$$= a_0(b-a) + a_1\frac{b^2 - a^2}{2} + a_2\frac{b^3 - a^3}{3}$$

Substituting values of a_0, a_1 and a_2 give

$$\int_a^b f_2(x)dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

Since for Simpson 1/3 rule, the interval $[a, b]$ is broken into 2 segments, the segment width

The segment width:

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

Hence the Simpson's 1/3 rule is given by:

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \ for\ one\ segment$$

Example 1: The distance covered by a rocket in meters from t = 8s to t = 30 s is given by:

$$x = \int_8^{30}\left(2000\ln\left[\frac{140000}{140000-2100t}\right] - 9.8t\right)dt$$

a) Use Simpson's 1/3 rule to find the approximate value of x.
b) Find the true error, E.
c) Find the absolute relative true error, ϵ

Sol:

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

a = 8, b = 30

$$f(8) = 2000\ln\left[\frac{140000}{140000-2100(8)}\right] - 9.8(8) = 177.27 m/s$$

$$f(30) = 2000\ln\left[\frac{140000}{140000-2100(30)}\right] - 9.8(30) = 901.67 m/s$$

$$\left(\frac{a+b}{2}\right) = 19$$

$$f(19) = 2000\ln\left(\frac{140000}{140000-2100(19)}\right) - 9.8(19) = 484.75 m/s$$

$$x = \frac{30-8}{6}[f(8) + 4f(19) + f(30)] = 11065.72m$$

b) The exact value of the above integral is:

$$x = \int_{8}^{30} \left(2000 \ln\left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

$$= 11061.34 \text{ m}$$

So the true error is:

$$E = Exact\ value - Approximate\ value = 11061.34 - 11065.72 = -4.38m$$

c) The absolute relative true error is:

$$\epsilon = \left| \frac{True\ error}{Exact\ value} \right| * 100 = \left| \frac{-4.38}{11061.34} \right| * 100 = 0.0396\%$$

➢ Multiple segment Simpsons 1/3 rule

Just like in multiple-segment trapezoidal rule, one can subdivide the interval [a,b] into n segments and apply Simpson's 1/3 rule repeatedly over every two segments. Note that n needs to be even. Divide interval [a,b] into n equal segments, so that the segment width is given by n:

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

Now:

$$\int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx$$

where

$$x_0 = a$$
$$x_n = b$$

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \dots\dots + \int_{x_{n-4}}^{x_{n-2}} f(x)dx + \int_{x_{n-2}}^{x_n} f(x)dx$$

Apply Simpson's 1/3rd Rule over each interval,

$$\int_a^b f(x)dx \cong (x_2 - x_0)\left[\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}\right] + (x_4 - x_2)\left[\frac{f(x_2) + 4f(x_3) + f(x_4)}{6}\right] + \dots$$

$$+ (x_{n-2} - x_{n-4})\left[\frac{f(x_{n-4}) + 4f(x_{n-3}) + f(x_{n-2})}{6}\right] + (x_n - x_{n-2})\left[\frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6}\right]$$

Since

$$x_i - x_{i-2} = 2h$$
$$i = 2, 4, \dots, n$$

then

$$\int_a^b f(x)dx \cong 2h\left[\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}\right] + 2h\left[\frac{f(x_2) + 4f(x_3) + f(x_4)}{6}\right] + \dots$$

$$+ 2h\left[\frac{f(x_{n-4}) + 4f(x_{n-3}) + f(x_{n-2})}{6}\right] + 2h\left[\frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6}\right]$$

$$= \frac{h}{3}\left[f(x_0) + 4\{f(x_1) + f(x_3) + \dots + f(x_{n-1})\} + 2\{f(x_2) + f(x_4) + \dots + f(x_{n-2})\} + f(x_n)\right]$$

$$= \frac{h}{3}\left[f(x_0) + 4\sum_{\substack{i=1 \\ i=odd}}^{n-1} f(x_i) + 2\sum_{\substack{i=2 \\ i=even}}^{n-2} f(x_i) + f(x_n) \right]$$

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 4\sum_{\substack{i=1 \\ i=odd}}^{n-1} f(x_i) + 2\sum_{\substack{i=2 \\ i=even}}^{n-2} f(x_i) + f(b) \right] \text{ for multiple}$$

Example 2: Use 4-segment Simpson's 1/3 rule to approximate the distance covered by a rocket in meters from t = 8 s to t = 30 s as given by:

$$x = \int_8^{30} \left(2000 \ln\left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

a) Use four segment Simpson's 1/3rd Rule to estimate x.
b) Find the true error, E.
c) Find the absolute relative true error, ϵ

Sol:

a) Using n segment Simpson's 1/3 rule,

n = 4, a = 8, b = 30

$$h = \frac{30 - 8}{4} = 5.5$$

$$f(8) = 2000 \ln\left[\frac{140000}{140000 - 2100(8)} \right] - 9.8(8) = 177.27 m/s$$

$$f(x_1) = f(a + h) = f(8 + 5.5) = f(13.5)$$

$$f(13.5) = 2000 \ln\left[\frac{140000}{140000 - 2100(13.5)} \right] - 9.8(13.5) = 320.25 m/s$$

$$f(x_2) = f(x_1 + h) = f(13.5 + 5.5) = f(19)$$

$$f(19)=2000\ln\left(\frac{140000}{140000-2100(19)}\right)-9.8(19)=484.75m/s$$

$$f(x_3)=f(x_2+h)=f(19+5.5)=f(24.5)$$

$$f(24.5)=2000\ln\left[\frac{140000}{140000-2100(24.5)}\right]-9.8(24.5)=676.05m/s$$

$$f(b)=f(x_3+h)=f(24.5+5.5)=f(30)$$

$$f(30)=2000\ln\left[\frac{140000}{140000-2100(30)}\right]-9.8(30)=901.67m/s$$

$$x=\frac{h}{3}\left[f(a)+4\sum_{\substack{i=1\\ i=odd}}^{n-1}f(x_i)+2\sum_{\substack{i=2\\ i=even}}^{n-2}f(x_i)+f(b)\right]$$

$$x=\frac{5.5}{3}\left[f(8)+4\big(f(x_1)+f(x_3)\big)+2\big(f(x_2)\big)+f(30)\right]$$

$$x=\frac{5.5}{3}[177.27+4(320.25+676.05)+2(484.75)+901.67]=11061.64m$$

b) The exact value of the above integral is:

$$x=\int_{8}^{30}\left(2000\ln\left[\frac{140000}{140000-2100t}\right]-9.8t\right)dt$$
$$=11061.34\text{ m}$$

So the true error is:

$$E=Exact\ value-Approximate\ value=11061.34-11061.64=-0.30m$$

c) The absolute relative true error is:

$$\epsilon = \left|\frac{True\ error}{Exact\ value}\right| * 100 = \left|\frac{-0.30}{11061.34}\right| * 100 = 0.0027\%$$

Differentiation

The derivative of a function at x is defined as

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

To be able to find a derivative numerically, one could make Δx finite to give,

$$f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

Knowing the value of x at which you want to find the derivative of $f(x)$, we choose a value of Δx to find the value of $f'(x)$. To estimate the value of $f'(x)$, three such approximations are suggested as follows.

➢ Forward Difference Approximation of the First Derivative

From differential calculus, we know

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

For a finiteΔx,

$$f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

The above is the forward divided difference approximation of the first derivative. It is called forward because you are taking a point ahead of x. To find the value of $f'(x)$ at $x = x_i$, we may choose another point Δx ahead as $x = x_{i+1}$. This gives

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

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

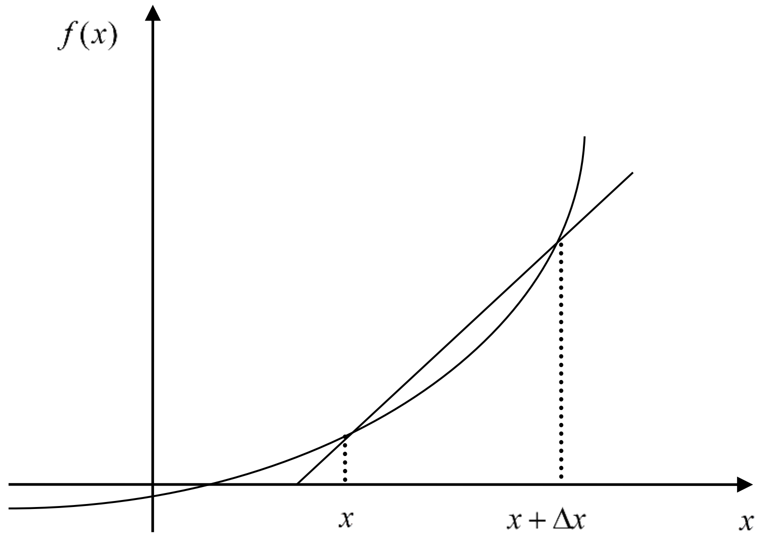

Figure (1) graphical representation of forward difference approximation

Example 1: The velocity of a rocket is given by

$$\nu(t) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t,\ 0 \le t \le 30$$

Where ν is given in m/s and t is given in seconds. At $t = 16\,\text{s}$,

a) Use the forward difference approximation of the first derivative of $\nu(t)$ to calculate the acceleration. Use a step size of $\Delta t = 2\,\text{s}$.

b) Find the exact value of the acceleration of the rocket.

c) Calculate the absolute relative true error for part (b).

Sol:

(a) $$a(t_i) \approx \frac{\nu(t_{i+1}) - \nu(t_i)}{\Delta t}$$

$t_i = 16$

$\Delta t = 2$

$t_{i+1} = t_i + \Delta t$

$= 16 + 2$

=18

$$a(16) \approx \frac{\nu(18) - \nu(16)}{2}$$

$$\nu(18) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(18)}\right] - 9.8(18)$$

$$= 453.02 \text{ m/s}$$

$$\nu(16) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(16)}\right] - 9.8(16)$$

$$= 392.07 \text{ m/s}$$

Hence

$$a(16) \approx \frac{\nu(18) - \nu(16)}{2}$$

$$= \frac{453.02 - 392.07}{2}$$

$$= 30.474 \text{ m/s}^2$$

(b) The exact value of $a(16)$ can be calculated by differentiating

$$\nu(t) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t}\right] - 9.8t$$

as

$$a(t) = \frac{d}{dt}[\nu(t)]$$

Knowing that

$$\frac{d}{dt}[\ln(t)] = \frac{1}{t} \text{ and } \frac{d}{dt}\left[\frac{1}{t}\right] = -\frac{1}{t^2}$$

$$a(t) = 2000\left(\frac{14 \times 10^4 - 2100t}{14 \times 10^4}\right)\frac{d}{dt}\left(\frac{14 \times 10^4}{14 \times 10^4 - 2100t}\right) - 9.8$$

$$= 2000\left(\frac{14 \times 10^4 - 2100t}{14 \times 10^4}\right)(-1)\left(\frac{14 \times 10^4}{(14 \times 10^4 - 2100t)^2}\right)(-2100) - 9.8$$

$$= \frac{-4040 - 29.4t}{-200 + 3t}$$

$$a(16) = \frac{-4040 - 29.4(16)}{-200 + 3(16)}$$

$$= 29.674 \text{ m/s}^2$$

(c) The absolute relative true error is

$$|\in_t| = \left|\frac{\text{True Value} - \text{Approximate Value}}{\text{True Value}}\right| \times 100$$

$$= \left|\frac{29.674 - 30.474}{29.674}\right| \times 100$$

$$= 2.6967\%$$

➢ Backward Difference Approximation of the First Derivative

We know

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

For a finite Δx,

$$f'(x) \approx \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

If Δx is chosen as a negative number,

$$f'(x) \approx \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

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

This is a backward difference approximation as you are taking a point backward from x. To find the value of $f'(x)$ at $x = x_i$, we may choose another point Δx behind as $x = x_{i-1}$. This gives

$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{\Delta x}$$

$$= \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

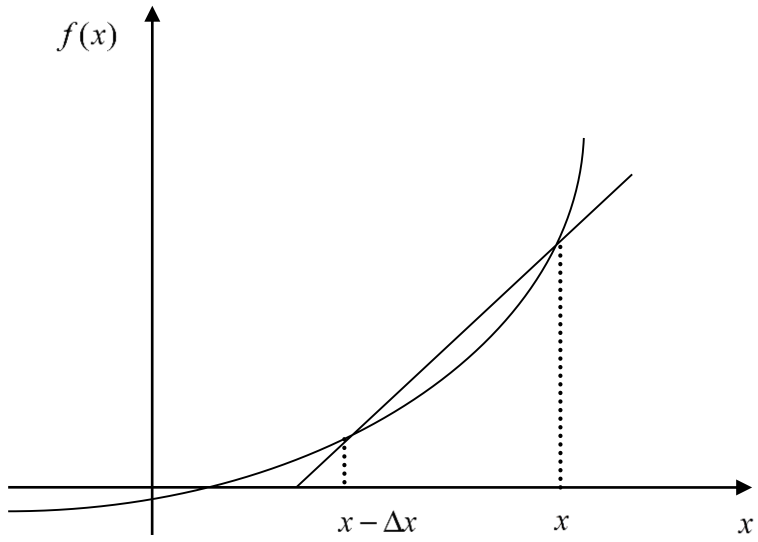

Figure (2) graphical representation of backward difference approximation

Example 2: The velocity of a rocket is given by

$$v(t) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t, 0 \le t \le 30$$

(a) Use the backward difference approximation of the first derivative of $v(t)$ to calculate the acceleration at $t = 16\,\text{s}$. Use a step size of $\Delta t = 2\,\text{s}$.

(b) Find the absolute relative true error for part (a).

Sol:

a) $a(t) \approx \dfrac{v(t_i) - v(t_{i-1})}{\Delta t}$

$t_i = 16$

$\Delta t = 2$

$$t_{i-1} = t_i - \Delta t$$

$$= 16 - 2$$

= 14

$$a(16) \approx \frac{\nu(16) - \nu(14)}{2}$$

$$\nu(16) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(16)}\right] - 9.8(16)$$

$$= 392.07 \text{ m/s}$$

$$\nu(14) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(14)}\right] - 9.8(14)$$

$$= 334.24 \text{ m/s}$$

$$a(16) \approx \frac{\nu(16) - \nu(14)}{2}$$

$$= \frac{392.07 - 334.24}{2}$$

$$= 28.915 \text{ m/s}^2$$

(b) The exact value of the acceleration at $t = 16\text{s}$ from Example 1 is

$$a(16) = 29.674 \text{ m/s}^2$$

The absolute relative true error for the answer in part (a) is

$$|\in_t| = \left|\frac{29.674 - 28.915}{29.674}\right| \times 100$$

$$= 2.5584\%$$

➢ Finite Difference Approximation of Higher Derivatives

One can also use the Taylor series to approximate a higher order derivative. For example, to approximate $f''(x)$, the Taylor series is

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2\Delta x) + \frac{f''(x_i)}{2!}(2\Delta x)^2 + \frac{f'''(x_i)}{3!}(2\Delta x)^3 + \ldots \qquad (3)$$

Where

$$x_{i+2} = x_i + 2\Delta x$$

$$f(x_{i+1}) = f(x_i) + f'(x_i)(\Delta x) + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 \ldots \qquad (4)$$

Where

$$x_{i-1} = x_i - \Delta x$$

Subtracting 2 times Equation (4) from Equation (3) gives

$$f(x_{i+2}) - 2f(x_{i+1}) = -f(x_i) + f''(x_i)(\Delta x)^2 + f'''(x_i)(\Delta x)^3 \ldots$$

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

$$f''(x_i) \approx \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{(\Delta x)^2} + O(\Delta x) \qquad (5)$$

Example 3: The velocity of a rocket is given by

$$\nu(t) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t, 0 \le t \le 30$$

Use the forward difference approximation of the second derivative of $\nu(t)$ to calculate the jerk at $t = 16\,\text{s}$. Use a step size of $\Delta t = 2\,\text{s}$.

Sol:

$$j(t_i) \approx \frac{v(t_{i+2}) - 2v(t_{i+1}) + v(t_i)}{(\Delta t)^2}$$

$$t_i = 16$$

$$\Delta t = 2$$

$$\begin{aligned} t_{i+1} &= t_i + \Delta t \\ &= 16 + 2 \\ &= 18 \end{aligned}$$

$$\begin{aligned} t_{i+2} &= t_i + 2(\Delta t) \\ &= 16 + 2(2) \\ &= 20 \end{aligned}$$

$$j(16) \approx \frac{v(20) - 2v(18) + v(16)}{(2)^2}$$

$$v(20) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(20)}\right] - 9.8(20)$$

$$= 517.35 \, \text{m/s}$$

$$v(18) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(18)}\right] - 9.8(18)$$

$$= 453.02 \, \text{m/s}$$

$$v(16) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(16)}\right] - 9.8(16)$$

$$= 392.07 \, \text{m/s}$$

$$j(16) \approx \frac{517.35 - 2(453.02) + 392.07}{4}$$

$$= 0.84515 \text{ m/s}^3$$

The exact value of $j(16)$ can be calculated by differentiating

$$v(t) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t}\right] - 9.8t$$

Twice as

$$a(t) = \frac{d}{dt}[v(t)]$$

And

$$j(t) = \frac{d}{dt}[a(t)]$$

Knowing that

$$\frac{d}{dt}[\ln(t)] = \frac{1}{t}$$

And

$$\frac{d}{dt}\left[\frac{1}{t}\right] = -\frac{1}{t^2}$$

$$a(t) = 2000\left(\frac{14 \times 10^4 - 2100t}{14 \times 10^4}\right)\frac{d}{dt}\left(\frac{14 \times 10^4}{14 \times 10^4 - 2100t}\right) - 9.8$$

$$= 2000\left(\frac{14 \times 10^4 - 2100t}{14 \times 10^4}\right)(-1)\left(\frac{14 \times 10^4}{(14 \times 10^4 - 2100t)^2}\right)(-2100) - 9.8$$

$$= \frac{-4040 - 29.4t}{-200 + 3t}$$

Similarly it can be shown that

$$j(t) = \frac{d}{dt}[a(t)]$$

$$= \frac{18000}{(-200 + 3t)^2}$$

$$j(16) = \frac{18000}{[-200 + 3(16)]^2}$$
$$= 0.77909\,\text{m/s}^3$$

The absolute relative true error is

$$|\in_t| = \left|\frac{0.77909 - 0.84515}{0.77909}\right| \times 100$$

$$= 8.4797\%$$

The formula given by Equation (5) is a forward difference approximation of the second derivative and has an error. So we will get more accuracy from central difference approximation rule as follow:

$$f(x_{i+1}) = f(x_i) + f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 + \frac{f''''(x_i)}{4!}(\Delta x)^4 + \ldots \qquad (6)$$

Where

$$x_{i+1} = x_i + \Delta x$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 - \frac{f'''(x_i)}{3!}(\Delta x)^3 + \frac{f''''(x_i)}{4!}(\Delta x)^4 - \ldots \qquad (7)$$

Where

$$x_{i-1} = x_i - \Delta x$$

Adding Equations (6) and (7), gives

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + f''(x_i)(\Delta x)^2 + f''''(x_i)\frac{(\Delta x)^4}{12} + \ldots$$

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{(\Delta x)^2} - \frac{f''''(x_i)(\Delta x)^2}{12} + \ldots$$

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

Example 4: The velocity of a rocket is given by

$$\nu(t) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t,\ 0 \le t \le 30,$$

(a) Use the central difference approximation of the second derivative of $\nu(t)$ to calculate the jerk at $t = 16\,\text{s}$. Use a step size of $\Delta t = 2\,\text{s}$.

Sol:

The second derivative of velocity with respect to time is called jerk. The second order approximation of jerk then is

$$j(t_i) \approx \frac{\nu(t_{i+1}) - 2\nu(t_i) + \nu(t_{i-1})}{(\Delta t)^2}$$

$$t_i = 16$$

$$\Delta t = 2$$

$$\begin{aligned} t_{i+1} &= t_i + \Delta t \\ &= 16 + 2 \\ &= 18 \end{aligned}$$

$$t_{i+2} = t_i - \Delta t$$
$$= 16 - 2$$
$$= 14$$

$$j(16) \approx \frac{\nu(18) - 2\nu(16) + \nu(14)}{(2)^2}$$

$$\nu(18) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(18)}\right] - 9.8(18)$$

$$= 453.02 \text{ m/s}$$

$$\nu(16) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(16)}\right] - 9.8(16)$$

$$= 392.07 \text{ m/s}$$

$$\nu(14) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(14)}\right] - 9.8(14)$$

$$= 334.24 \text{ m/s}$$

$$j(16) \approx \frac{\nu(18) - 2\nu(16) + \nu(14)}{(2)^2}$$

$$= \frac{453.02 - 2(392.07) + 334.24}{4}$$

$$= 0.77969 \text{ m/s}^3$$

The absolute relative true error is

$$|\in_t| = \left|\frac{0.77908 - 0.77969}{0.77908}\right| \times 100$$

$$= 0.077992\%$$

Interpolation

Many times, data is given only at discrete points such as (x_0, y_0), (x_1, y_1), ..., (x_{n-1}, y_{n-1}), (x_n, y_n). So, how then does one find the value of y at any other value of x. Well, a continuous function $f(x)$ may be used to represent the $n+1$ data values with $f(x)$ passing through the $n+1$ points (Figure 1). Then one can find the value of y at any other value of x. This is called interpolation. If x falls outside the range of x for which the data is given, it is no longer interpolation but instead is called extrapolation. A polynomial is a common choice for an interpolating function because polynomials are easy to

(A) evaluate,

(B) differentiate, and

(C) integrate, relative to other choices such as a trigonometric and exponential series.

Polynomial interpolation involves finding a polynomial of order n that passes through the $n + 1$ data points. One of the methods used to find this polynomial is called the Lagrangian method of interpolation. Other methods include Newton's divided difference polynomial method and the direct method.

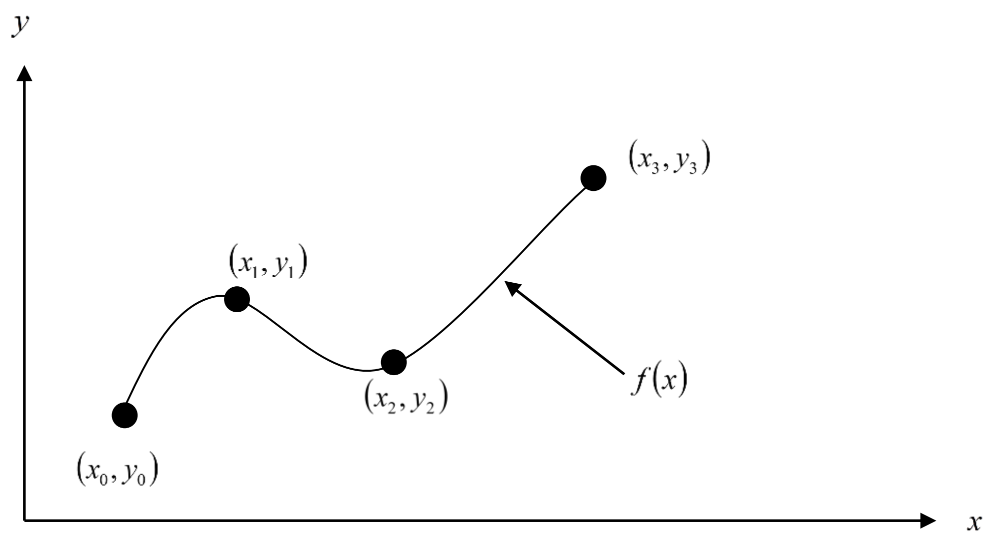

Figure (1) Interpolation of discrete data.

The Lagrangian interpolating polynomial is given by:

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

Where n in $f_n(x)$ stands for the n^{th} order polynomial that approximates the function $y = f(x)$ given at $n+1$ data points as $(x_0, y_0), (x_1, y_1), \ldots\ldots, (x_{n-1}, y_{n-1}), (x_n, y_n)$, and:

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

$L_i(x)$ is a weighting function that includes a product of $n-1$ terms with terms of $j = i$ omitted.

Example 1: The upward velocity of a rocket is given as a function of time in Table below.

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

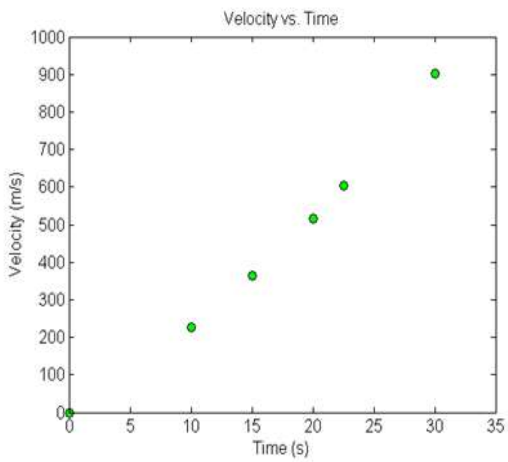

Figure (2) Graph of velocity vs. time data for the rocket example

Determine the value of the velocity at $t = 16$ seconds using a first order Lagrange polynomial.

Sol:

For first order polynomial interpolation (also called linear interpolation), the velocity is given by:

$$v(t) = \sum_{i=0}^{1} L_i(t)v(t_i)$$

$$= L_0(t)v(t_0) + L_1(t)v(t_1)$$

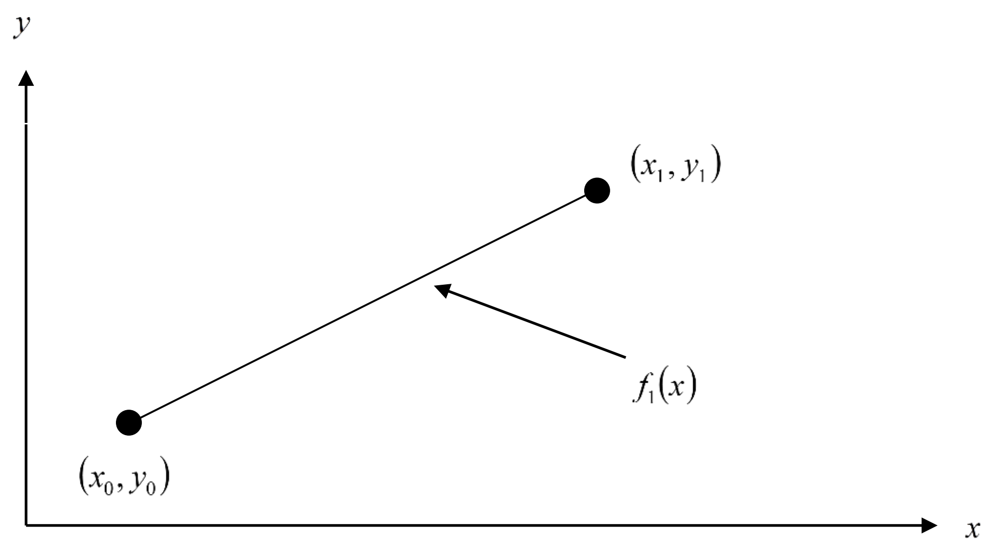

Figure (3) linear interpolation.

Since we want to find the velocity at $t = 16$, and we are using a first order polynomial, we need to choose the two data points that are closest to $t = 16$ that also bracket $t = 16$ to evaluate it. The two points are $t_0 = 15$ and $t_1 = 20$. Then:

$$t_0 = 15, \; v(t_0) = 362.78$$

$$t_1 = 20, \; v(t_1) = 517.35$$

$$L_0(t) = \prod_{\substack{j=0 \\ j \neq 0}}^{1} \frac{t - t_j}{t_0 - t_j}$$

$$= \frac{t - t_1}{t_0 - t_1}$$

$$L_1(t) = \prod_{\substack{j=0 \\ j \neq 1}}^{1} \frac{t - t_j}{t_1 - t_j}$$

$$= \frac{t - t_0}{t_1 - t_0}$$

Hence

$$v(t) = \frac{t - t_1}{t_0 - t_1} v(t_0) + \frac{t - t_0}{t_1 - t_0} v(t_1)$$

$$= \frac{t-20}{15-20}(362.78) + \frac{t-15}{20-15}(517.35), \quad 15 \le t \le 20$$

$$v(16) = \frac{16-20}{15-20}(362.78) + \frac{16-15}{20-15}(517.35)$$

$$= 0.8(362.78) + 0.2(517.35)$$

$$= 393.69 \text{ m/s}$$

We can see that $L_0(t) = 0.8$ and $L_1(t) = 0.2$ are like weightages given to the velocities at $t = 15$ and $t = 20$ to calculate the velocity at $t = 16$.

Example 2: The upward velocity of a rocket is given as a function of time in Table below.

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

a) Determine the value of the velocity at $t = 16$ seconds with second order polynomial interpolation using Lagrangian polynomial interpolation.

b) Find the absolute relative approximate error for the second order polynomial approximation.

Sol:

a) For second order polynomial interpolation (also called quadratic interpolation), the velocity is given by:

$$v(t) = \sum_{i=0}^{2} L_i(t)v(t_i)$$

$$= L_0(t)v(t_0) + L_1(t)v(t_1) + L_2(t)v(t_2)$$

Since we want to find the velocity at $t = 16$, and we are using a second order polynomial, we need to choose the three data points that are closest to $t = 16$ that also bracket $t = 16$ to evaluate it. The three points are $t_0 = 10, t_1 = 15, and\ t_2 = 20$.

Then

$$t_0 = 10,\ \ v(t_0) = 227.04$$

$$t_1 = 15,\ \ v(t_1) = 362.78$$

$$t_2 = 20,\ \ v(t_2) = 517.35$$

Gives

$$L_0(t) = \prod_{\substack{j=0 \\ j\neq 0}}^{2} \frac{t - t_j}{t_0 - t_j}$$

$$= \left(\frac{t - t_1}{t_0 - t_1}\right)\left(\frac{t - t_2}{t_0 - t_2}\right)$$

$$L_1(t) = \prod_{\substack{j=0 \\ j\neq 1}}^{2} \frac{t - t_j}{t_1 - t_j}$$

$$= \left(\frac{t - t_0}{t_1 - t_0}\right)\left(\frac{t - t_2}{t_1 - t_2}\right)$$

$$L_2(t) = \prod_{\substack{j=0 \\ j\neq 2}}^{2} \frac{t - t_j}{t_2 - t_j}$$

$$= \left(\frac{t - t_0}{t_2 - t_0}\right)\left(\frac{t - t_1}{t_2 - t_1}\right)$$

Hence

$$v(t)=\left(\frac{t-t_1}{t_0-t_1}\right)\left(\frac{t-t_2}{t_0-t_2}\right)v(t_0)+\left(\frac{t-t_0}{t_1-t_0}\right)\left(\frac{t-t_2}{t_1-t_2}\right)v(t_1)+\left(\frac{t-t_0}{t_2-t_0}\right)\left(\frac{t-t_1}{t_2-t_1}\right)v(t_2),\ t_0\le t\le t_2$$

$$v(16)=\frac{(16-15)(16-20)}{(10-15)(10-20)}(227.04)+\frac{(16-10)(16-20)}{(15-10)(15-20)}(362.78)$$
$$+\frac{(16-10)(16-15)}{(20-10)(20-15)}(517.35)$$

$$=(-0.08)(227.04)+(0.96)(362.78)+(0.12)(517.35)$$

$$=392.19\text{ m/s}$$

b) The absolute relative approximate error $|\in_a|$ for the second order polynomial is calculated by considering the result of the first order polynomial (Example 1) as the previous approximation.

$$|\in_a|=\left|\frac{392.19-393.69}{392.19}\right|\times 100$$

$$=0.38410\%$$

Solving Ordinary Differential Equation

Runge-Kutta method

The Runge-Kutta method is a numerical technique used to solve an ordinary differential equation of the form.

$$\frac{dy}{dx} = f(x, y), y(0) = y_0$$

Runge-Kutta 2nd order method

Euler's method is given by

$$y_{i+1} = y_i + f(x_i, y_i)h \qquad (1)$$

Where

$$x_0 = 0$$

$$y_0 = y(x_0)$$

$$h = x_{i+1} - x_i$$

To understand the Runge-Kutta 2nd order method, we need to derive Euler's method from the Taylor series.

$$y_{i+1} = y_i + \left.\frac{dy}{dx}\right|_{x_i, y_i} (x_{i+1} - x_i) + \frac{1}{2!}\left.\frac{d^2y}{dx^2}\right|_{x_i, y_i} (x_{i+1} - x_i)^2 + \frac{1}{3!}\left.\frac{d^3y}{dx^3}\right|_{x_i, y_i} (x_{i+1} - x_i)^3 + \ldots$$

$$= y_i + f(x_i, y_i)(x_{i+1} - x_i) + \frac{1}{2!} f'(x_i, y_i)(x_{i+1} - x_i)^2 + \frac{1}{3!} f''(x_i, y_i)(x_{i+1} - x_i)^3 + \ldots \qquad (2)$$

As you can see the first two terms of the Taylor series

$$y_{i+1} = y_i + f(x_i, y_i)h$$

are Euler's method and hence can be considered to be the Runge-Kutta 1st order method.

The true error in the approximation is given by

$$E_t = \frac{f'(x_i, y_i)}{2!} h^2 + \frac{f''(x_i, y_i)}{3!} h^3 + \ldots \qquad (3)$$

So what would a 2nd order method formula look like. It would include one more term of the Taylor series as follows.

$$y_{i+1} = y_i + f(x_i, y_i)h + \frac{1}{2!} f'(x_i, y_i)h^2 \qquad (4)$$

Let us take a generic example of a first order ordinary differential equation

$$\frac{dy}{dx} = e^{-2x} - 3y, y(0) = 5$$

$$f(x, y) = e^{-2x} - 3y$$

Now since y is a function of x,

$$f'(x, y) = \frac{\partial f(x, y)}{\partial x} + \frac{\partial f(x, y)}{\partial y}\frac{dy}{dx} \qquad (5)$$

$$= \frac{\partial}{\partial x}\left(e^{-2x} - 3y\right) + \frac{\partial}{\partial y}\left[\left(e^{-2x} - 3y\right)\right]\left(e^{-2x} - 3y\right)$$

$$= -2e^{-2x} + (-3)\left(e^{-2x} - 3y\right)$$

$$= -5e^{-2x} + 9y$$

The 2nd order formula for the above example would be

$$y_{i+1} = y_i + f(x_i, y_i)h + \frac{1}{2!} f'(x_i, y_i)h^2$$

$$= y_i + \left(e^{-2x_i} - 3y_i\right)h + \frac{1}{2!}\left(-5e^{-2x_i} + 9y_i\right)h^2$$

However, we already see the difficulty of having to find $f'(x, y)$ in the above method. What Runge and Kutta did was write the 2nd order method as

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)h \qquad (6)$$

where

$$k_1 = f(x_i, y_i)$$

$$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h) \qquad (7)$$

This form allows one to take advantage of the 2nd order method without having to calculate $f'(x, y)$.

So how do we find the unknowns a_1, a_2, p_1 and q_{11}. Without proof (see Appendix for proof), equating Equation (4) and (6), gives three equations.

$$a_1 + a_2 = 1$$

$$a_2 p_1 = \frac{1}{2}$$

$$a_2 q_{11} = \frac{1}{2}$$

Since we have 3 equations and 4 unknowns, we can assume the value of one of the unknowns. The other three will then be determined from the three equations. Generally the value of a_2 is chosen to evaluate the other three constants. The three values generally used for a_2 are $\frac{1}{2}$, 1 and $\frac{2}{3}$, and are known as Heun's Method, the midpoint method and Ralston's method, respectively.

<u>Heun's Method</u>

Here $a_2 = \frac{1}{2}$ is chosen, giving

$$a_1 = \frac{1}{2}$$

$$p_1 = 1$$

$$q_{11} = 1$$

Resulting in

$$y_{i+1} = y_i + \left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)h \tag{8}$$

Where

$$k_1 = f\left(x_i, y_i\right) \tag{9a}$$

$$k_2 = f\left(x_i + h, y_i + k_1 h\right) \tag{9b}$$

Example 1: A ball at 1200 K is allowed to cool down in air at an ambient temperature of 300 K. Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\,(\theta^4 - 81\times10^8)$$

Where θ is in K and t in seconds. Find the temperature at $t = 480$ seconds using Runge-Kutta 2nd order method. Assume a step size of $h = 240$ seconds.

Sol:

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

$$f(t,\theta) = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

Per Heun's method given by Equations (8) and (9)

$$\theta_{i+1} = \theta_i + \left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)h$$

$$k_1 = f(t_i, \theta_i)$$

$$k_2 = f(t_i + h, \theta_i + k_1 h)$$

$$i = 0, t_0 = 0, \theta_0 = \theta(0) = 1200$$

$$k_1 = f(t_0, \theta_o)$$

$$= f(0,1200)$$

$$= -2.2067\times10^{-12}\left(1200^4 - 81\times10^8\right)$$

$$= -4.5579$$

$$k_2 = f(t_0 + h, \theta_0 + k_1 h)$$

$$= f(0 + 240, 1200 + (-4.5579)240)$$

$$= f(240, 106.09)$$

$$= -2.2067\times10^{-12}\left(106.09^4 - 81\times10^8\right)$$

$$= 0.017595$$

$$\theta_1 = \theta_0 + \left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)h$$

$$= 1200 + \left(\frac{1}{2}(-4.5579) + \frac{1}{2}(0.017595)\right)240$$

$$= 1200 + (-2.2702)240$$

$$= 655.16\,\mathrm{K}$$

$$i = 1, t_1 = t_0 + h = 0 + 240 = 240, \theta_1 = 655.16\mathrm{K}$$

$$k_1 = f(t_1, \theta_1)$$

$$= f(240, 655.16)$$

$$= -2.2067 \times 10^{-12}\left(655.16^4 - 81 \times 10^8\right)$$

$$= -0.38869$$

$$k_2 = f(t_1 + h, \theta_1 + k_1 h)$$

$$= f(240 + 240, 655.16 + (-0.38869)240)$$

$$= f(480, 561.87)$$

$$= -2.2067 \times 10^{-12}\left(561.87^4 - 81 \times 10^8\right)$$

$$= -0.20206$$

$$\theta_2 = \theta_1 + \left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)h$$

$$= 655.16 + \left(\frac{1}{2}(-0.38869) + \frac{1}{2}(-0.20206)\right)240$$

$$= 655.16 + (-0.29538)240$$

$$= 584.27\,\mathrm{K}$$

$$\theta_2 = \theta(480) = 584.27\,\mathrm{K}$$

Example 2: A ball at 1200 K is allowed to cool down in air at an ambient temperature of 300 K. Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right), \theta(0) = 1200\,\text{K}$$

where θ is in K and t in seconds. Find the temperature at $t = 480$ seconds using Runge-Kutta 4th order method. Assume a step size of $h = 240$ seconds.

Sol:

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

$$f(t,\theta) = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

$$\theta_{i+1} = \theta_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

For $i = 0$, $t_0 = 0$, $\theta_0 = 1200\text{K}$

$$k_1 = f(t_0, \theta_0)$$

$$= f(0,1200)$$

$$= -2.2067\times10^{-12}\left(1200^4 - 81\times10^8\right)$$

$$= -4.5579$$

$$k_2 = f\left(t_0 + \frac{1}{2}h, \theta_0 + \frac{1}{2}k_1 h\right)$$

$$= f\left(0 + \frac{1}{2}(240), 1200 + \frac{1}{2}(-4.5579)\times 240\right)$$

$$= f(120, 653.05)$$

$$= -2.2067\times10^{-12}\left(653.05^4 - 81\times10^8\right)$$

$$= -0.38347$$

$$k_3 = f\left(t_0 + \frac{1}{2}h, \theta_0 + \frac{1}{2}k_2 h\right)$$

$$= f\left(0+\frac{1}{2}(240),1200+\frac{1}{2}(-0.38347)\times 240\right)$$

$$= f(120,1154.0)$$

$$= -2.2067\times 10^{-12}\left(1154.0^4 - 81\times 10^8\right)$$

$$= -3.8954$$

$$k_4 = f(t_0+h, \theta_0 + k_3 h)$$

$$= f(0+240,1200+(-3.894)\times 240)$$

$$= f(240,265.10)$$

$$= -2.2067\times 10^{-12}\left(265.10^4 - 81\times 10^8\right)$$

$$= 0.0069750$$

$$\theta_1 = \theta_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$$= 1200 + \frac{1}{6}(-4.5579 + 2(-0.38347) + 2(-3.8954) + (0.069750))240$$

$$= 1200 + (-2.1848)\times 240$$

$$= 675.65\,\text{K}$$

θ_1 is the approximate temperature at

$$t = t_1$$

$$= t_0 + h$$

$$= 0 + 240$$

$$= 240$$

$$\theta_1 = \theta(240)$$

$$\approx 675.65\,\text{K}$$

For $i = 1, t_1 = 240, \theta_1 = 675.65\,\text{K}$

$$k_1 = f(t_1, \theta_1)$$

$$= f(240,675.65)$$

$$= -2.2067\times 10^{-12}\left(675.65^4 - 81\times 10^8\right)$$

$= -0.44199$

$k_2 = f\left(t_1 + \frac{1}{2}h, \theta_1 + \frac{1}{2}k_1 h\right)$

$= f\left(240 + \frac{1}{2}(240), 675.65 + \frac{1}{2}(-0.44199)240\right)$

$= f(360, 622.61)$

$= -2.2067 \times 10^{-12}\left(622.61^4 - 81 \times 10^8\right)$

$= -0.31372$

$k_3 = f\left(t_1 + \frac{1}{2}h, \theta_1 + \frac{1}{2}k_2 h\right)$

$= f\left(240 + \frac{1}{2}(240), 675.65 + \frac{1}{2}(-0.31372) \times 240\right)$

$= f(360, 638.00)$

$= -2.2067 \times 10^{-12}\left(638.00^4 - 81 \times 10^8\right)$

$= -0.34775$

$k_4 = f(t_1 + h, \theta_1 + k_3 h)$

$= f(240 + 240, 675.65 + (-0.34775) \times 240)$

$= f(480, 592.19)$

$= 2.2067 \times 10^{-12}\left(592.19^4 - 81 \times 10^8\right)$

$= -0.25351$

$\theta_2 = \theta_1 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$

$= 675.65 + \frac{1}{6}(-0.44199 + 2(-0.31372) + 2(-0.34775) + (-0.25351)) \times 240$

$= 675.65 + \frac{1}{6}(-2.0184) \times 240$

$= 594.91\text{K}$

θ_2 is the approximate temperature at

$$t = t_2$$
$$= t_1 + h$$
$$= 240 + 240$$
$$= 480$$

$$\theta_2 = \theta(480)$$
$$\approx 594.91\text{K}$$