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شعبة... طبيعة انجليزي

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Introduction to the computer

The computer was made to solve many problems. It initially solved mathematical and engineering problems. Then deal with the data for commercial purposes. Nowadays, it serves as a control tool in submarines, aircraft, and machinery production lines in factories. The computer does its work in all these areas by receiving data, processing it, and then outputting the output.

Computer components:

The computer consists of two main parts:

1- Hardware

2- Software A group of programs that control the work of the hard parts.

The computer is characterized as a machine for multiple uses, unlike other machines that are designed to do only one job. This is due to the ability of a computer to be programmed with multiple and different programs to do multiple tasks. As well as to connect many other devices and equipment.

Computer hardware:

There are four types of computer hardware:

1- Input units

2- Output units

3- Main memory

4- The unit of therapy and logic

Input and Output Units:

Input devices insert data from the outside into the computer's memory. There are many input devices, including keyboard, disk drive, magnetic disk drive, scanner, and mouse.

The output devices include: disk drive, magnetic drive, monitor, printer.

Features of the computer:

1- Its ability to perform in an automatic manner.

2- Its ability to be programmed.

Computers are divided according to their sizes into:

1- Small size microcomputer

2- Medium size minicomputer

3- Big size mainframe computer

There are many problems in engineering and science that can be expressed in the form of differential equations such as problems of vibrational motion and problems of currents and voltages in circuits of alternating currents...and so on. However, the exact solution to such equations using differential laws may be difficult or non-existent in some cases. Therefore, we resort to solving these equations in approximate ways, by solving them numerically, which are long and time-consuming methods. So we use computer software. We will discuss here some of the mathematical methods used in the programs to solve these equations numerically. As well as some interpolation methods, i.e. supplementing what is missing from the data, and fitting, which is the conclusion of the best line or curve to pass through a set of data.

Introduction to Differences

There is a branch of mathematics concerned with the differences between consecutive numbers in a series. The results of these differences are used in many applications, including calculating differential values that may be difficult to calculate by analytical methods. There are three types of differences:

1. Forward differences
2. Backward differences
3. Central differences

What is meant by forward differences?

Suppose we have the equation Yn = 3n – 1

Valid for values n = 1, 2, 3, ... , by substituting these values into the equation, we get the following values for the variable Y 2, 5, 8, 11, 14, ..

The forward differences between the consecutive numbers in the results are:

5 - 2 = 3, 8 - 5 = 3, 11-8 = 3, 14-11 = 3, ..

The series of numbers and the series of differences are usually written as:

2 5 8 11 19 results

3 3 3 3 Front First Teams

Also, suppose we have the equation: Yn = n2 – 3n –2

For the values n = 1, 2, 3, .. the results and forward differences are in the following picture:

- 4 – 4 – 2 2 8 16 results

  0 2 4 6 8 front first teams

  2 2 2 2 2nd front diff

The numbers in the second row are the differences in the numbers in the first row, and the numbers in the third row are the differences in the numbers in the second row. The numbers of the second row are called the first difference of the first row, and the numbers of the third row are called its second differences.

In general, if we assume that y1 , y2 , y3 , .. yn

are any consecutive numbers, the initial differences of which are given by the relationship

$\Delta yn = yn+1 - yn$

And its second differences are given by: $\Delta^2 y_n = \Delta y_{n+1} - \Delta y_n$

And its third difference is given by: $\Delta^3 y_n = \Delta^2 y_{n+1} - \Delta^2 y_n$

Thus, the table of numbers and their differences gives the first, second and third in the picture

y1 y2 y3 y4 y5

Δy1 Δy2 Δy3 Δy4 Δy5

Δ2y1 Δ2y2 Δ2y3 Δ2y4 Δ2y5

Δ3y1 Δ3y2 Δ3y3 Δ3y4 Δ3y5

Etc

Differentiation of a function related to the function of differences

To calculate the differential of the function F (x) at a known value of (x), there are three ways to do this in an approximate way, by measuring the differential in terms of the differences between the values of this function. This process is called numerically function calculus. These methods are:

1. Calculus in terms of the forward difference.
2. Differential calculus in terms of posterior difference.
3. Differential calculus in terms of central differences.

What is differential?

The differential of the function F(x) is defined in the following figure:

$$F^1(x) = \lim_{\Delta x \to o} \frac{f(x+\Delta x) - f(x)}{\Delta x} \qquad \rightarrow \qquad (1)$$

In order for this differential to be found numerically at a given value of x, Δx must be made very small but not equal to zero. Differential is calculated by one of the three previous methods.

1- Forward difference approximation of the first derivative:

We know that the differential of the function F'(x) is in the following form:

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

And by making Δx very small, then:

$$f^{1}(x) \cong \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

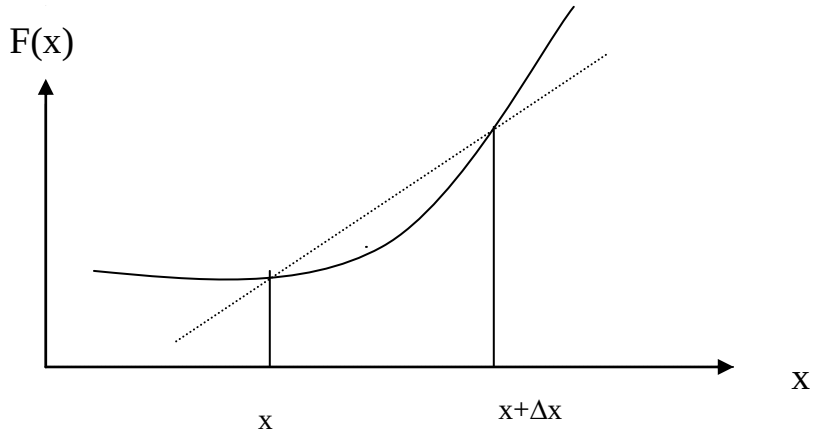


Illustration of the first differential in terms of the forward difference

So if we want to find the value of f'(x) at x = xi, we choose another point that is Δx forward at x = xi + 1 and thus:

$$f^{1}(x) \cong \frac{f(xi+\Delta x) - f(xi)}{\Delta x}$$

$$= \frac{f(x_{i+1}) - f(xi)}{x_{i+1} - x_i} \qquad \rightarrow \qquad (2)$$

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

2- Backward difference approximation of the first derivative

We know from the above that

$$f^1(x) = \lim_{\Delta x \to o} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

As the value of Δx is very small, then:

$$f^1(x) \cong \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

If Δx is chosen as a negative value (that is, a backward difference), then

$$f^1(x) \cong \frac{f(x-\Delta x) - f(x)}{-\Delta x}$$

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

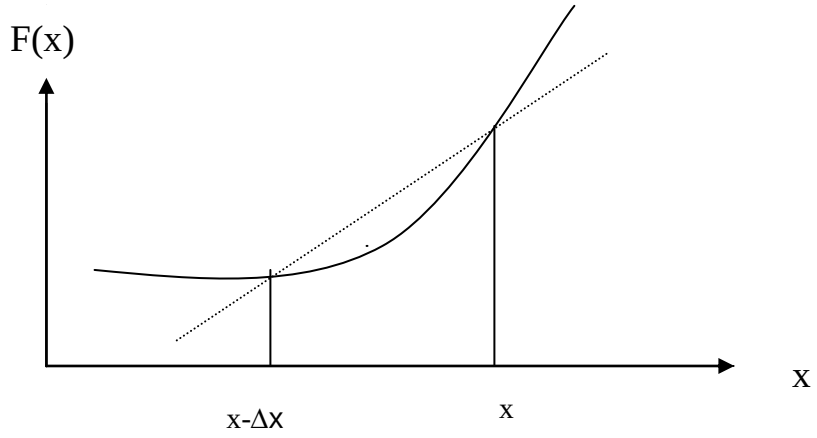


Illustration of the first differential in terms of the backward difference

If we want to find F'(x) at $x = x_i$, we can choose a point from which it returns by Δx, which is $x = x_{i-1}$ and thus:

$$f^{1}(x) \cong \frac{f(xi) - f(x_{i-1})}{\Delta x}$$

$$= \frac{f(xi) - f(x_{i-1})}{x_i - x_{i-1}} \qquad \rightarrow \qquad (3)$$

where Δx = x i – x i – 1

Example1

If the velocity of a missile is given by the following relationship:

$$v(t) = 2000\ln\left[\frac{14X10^4}{14X10^4 - 2100t}\right] - 9.8t \ , \qquad 0 \le t \le 30$$

Use forward differential calculus to determine acceleration at t=16s, use a difference of Δt=2s.

The solution:

From equation (2)

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

$\because t_i = 16,$
$\Delta t = 2$

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

$= 16 + 2 = 18$

$$\therefore a(16) = \frac{v(18) - v(16)}{2}$$

Substitute for V(16) , V(18)

$$V(18) = 2000In\left[\frac{14\times10^4}{14\times10^4 - 2100(18)}\right] - 9.8(18)$$

= 453.02 m/s

$$V(16) = 2000In\left[\frac{14\times10^4}{14\times10^4 - 2000(16)}\right] - 9.8(16)$$

= 392.07 m/s

And therefore:

$$a(16) = \frac{v(18) - v(16)}{2} = \frac{453.02 - 392.07}{2} = 30.475 \text{ m/s}^2$$

This is the approximate solution in terms of the speed difference

To find the true value of the acceleration at 16s., a(16), we differentiate the equation:

$$V(t) = 2000In\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t$$

This is as follows:

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

It is known that:

$$\frac{d}{dt}[In(t)] = \frac{1}{t} \quad , \quad \frac{d}{dt}\left(\frac{1}{t}\right) = -\frac{1}{t^2}$$

$$\therefore a(t) = 2000\left[\frac{14\times10^4 - 2100t}{14\times10^4}\right]\frac{d}{dt}\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9..8$$

$$= a(t) = 2000\left[\frac{14\times10^4 - 2100t}{14\times104}\right](-1)\left[\frac{14\times10^4}{(14\times104 - 2100t)^2}\right](-2100) - 9.8$$

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

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

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

By comparing the approximate value with the real value, the amount of error due to the approximation can be known.

Example 2:

If the speed of a missile is given by the relationship

$$V(t) = 2000In\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8 \qquad o \le t \le 30$$

Calculate using the backward difference approximation of the first differential the acceleration at t = 16s. , using a difference of $\Delta t = 2s$.

The solution:

For relationship (3)

$$a(t) = \frac{v(t_i) - V(t_{i-1})}{\Delta t}$$

$\because t_i = 16$

$\Delta t = 2$

$\therefore t_{i-1} = 16 - 2 = 14$

$$\therefore a(16) = \frac{V(16) - V(14)}{2}$$

$$\because V(16) = 2000In\left[\frac{14\times10^4}{14\times10^4 - 2100(16)}\right] - 9.8(16)$$

$$= 392.07m/s$$

$$\because V(14)2000In\left[\frac{14\times10^4}{14\times10^4 - 2100(14)}\right] - 9.8(14)$$

$$= 334.24m/s$$

$$\therefore a(16) = \frac{v(16) - v(14)}{2} = \frac{392.07 - 334.24}{2} = 28.915m/s^2$$

By knowing the true value of the differential, the error can be calculated.

Derivative of the forward difference approximation From Taylor series

Taylor's theorem states that if the value of the function F (x) is known at the point xi and all its derivatives at that point, provided that the derivatives are continuous between xi and x_{i+1}, then the value of the function at xi + 1 is given by the following relationship:

$$F(x_{i+1}) = f(x_i) + f^{1}(x_i)(x_{i+1} - x_i) + \frac{f^{11}(xi)}{2!}(x_{i+1} - x_i)^2 + ...$$

To make it easier, we make up for $\Delta x = x_{i+1} - x_i$

$$\therefore f(x_{i+1}) = f(x_i) + f^{1}(x_i)\Delta x + \frac{f^{11}(x_i)}{2!}(\Delta x)^2 + ...$$

$$\therefore f^{1}(x_i) = \frac{f(x_{i+1}) - f(x_i)}{\Delta x} - \frac{f^{11}(x_i)}{21}(\Delta x) - .....$$

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

Where o (Δx) shows that the approximation error is a function of (Δx). It is noted that we used the = sign here instead of the previous one. It is also noted that the solution resulting from the forward difference is greater than the true value by an amount proportional to (Δx) as shown in Example (1).

Derivative of the backward difference approximation From Taylor series

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

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

It is clear that the degree of accuracy is a function of Δx therefore, the accuracy increases with a decrease Δx .

Central difference approximation of the first derivative.

We use the central difference instead of the front difference or the back difference in order to reach greater accuracy in determining the differential numerically.

From the Taylor expansion, we know that in the case of forward derivative:

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

Also, in the case of background differences:

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

Subtracting Equation 2 from Equation 1

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

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

This equation is more accurate in the first calculus because the error is a function of the square of the small distance Δ x.

Example

If the speed of a missile is given by the relationship

$$V(t) = 2000In\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8 \qquad o \le t \le 30$$

Calculate the first differential using the central differences at t = 16s. , using a difference of Δt = 2s.

The solution:

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

$$\because t_i = 16$$
$$\because \Delta t = 2$$
$$\therefore t_{i+1} = 18$$
$$\therefore t_{i-1} = 14$$

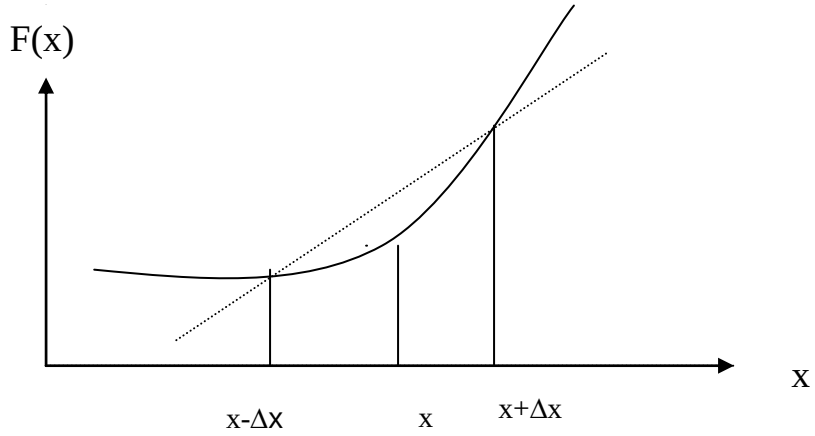
$$\therefore a(t) = \frac{v(18) - v(14)}{2*2}$$

$$v(18) = 2000\ln\left[\frac{14x10^4}{14x10^4 - 2100(18}\right] - 9.8(18) = 453.02m/s$$

$$v(14) = 2000\ln\left[\frac{14x10^4}{14x10^4 - 2100(14}\right] - 9.8(14) = 334.24m/s$$

$$\therefore a(16) = \left[\frac{453.02 - 334.24}{4}\right] = 29.659 m/s^2$$

A more accurate value than that obtained using the forward or backward differential.



An illustration of the first differential in terms of the central difference

Chapter Two

Forward differences

Forward differences

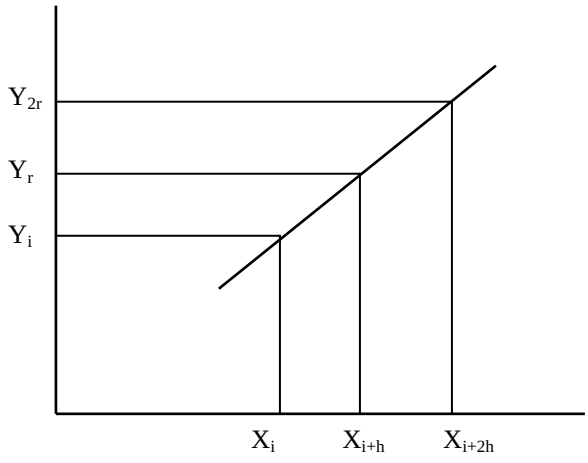
Forward differences are used when dealing with the beginnings of a data series. Assuming that there are known values at specific points of the independent variable xi [the values of x_i are called indices], each value is assigned to y_i as the dependent variable. Assuming that the indices x_i are on equal dimensions such that $x_{i+h} - x_i = h$, the resulting differences in values for the dependent variable yi are given by the relationship:

$$\Delta y_i = y_{i+1} - y_i \qquad \rightarrow (1)$$

Putting the following formulas for ease,

$y_{i+1} = y_r$, $y_{i+2} = y_{2r}$, $y_{i+3} = y_{3r}$ …

The relationship between yi and xi can be drawn in the following figure:



Therefore, equation (1) takes the following form:

$\Delta y_i = y_r - y_i \qquad \rightarrow (1)$

It is called the primary forward difference equation.

We note that we calculated the initial forward differences Δy_i in terms of the values of the dependent variable, (yi) (i) in this case it expresses the order of the number in the data series expressing the results.

The differences of the first forward differences are called the second forward differences, and they are calculated as follows:

$\Delta^2 y_i = \Delta(\Delta y_i) = \Delta y_{i+1} - \Delta y_i$

$= \Delta y_r - \Delta y_i$

$= (y_{2r} - y_r) - (y_r - y_i)$

$= y_{2r} - y_r - y_r + y_i$

$= y_{2r} - 2y_r + y_i \qquad \rightarrow (3)$

The third forward difference can also be calculated:

$\Delta^3 y_i = \Delta(\Delta^2 y_i)$

$= \Delta(y_{2r} - 2y_r + y_i)$

$= \Delta y_{2r} - 2\Delta y_r + \Delta y_i$

$= (y_{3r} - y_{2r}) - 2(y_{2r} - y_r) + (y_r - y_i)$

$= y_{3r} - y_{2r} - 2y_{2r} + 2y_r + y_r - y_i$

$\Delta^3 y_i = y_{3r} - 3y_{2r} + 3y_r - y_i \qquad \rightarrow (4)$

لا تنسى بأن $r = i + 1$ أو $i = r - 1$

Similarly, the fourth forward difference can be calculated:

$\Delta^4 y_i = \Delta (\Delta^3 y_i)$

$= \Delta(y_{3r} – 3y_{2r} + 3y_r – y_i)$

$= \Delta y_{3r} - 3\Delta y_{2r} + 3\Delta y_r - \Delta y_i$

$= (y_{4r} – y_{3r}) – 3(y_{3r} – y_{2r}) + 3(y_{2r} - y_r) – (y_r – y_i)$

$= y_{4r} – y_{3r} – 3y_{3r} + 3y_{2r} + 3y_{2r} – 3y_r – y_r + y_i$

$\Delta^4 y_i = y_{4r} – 4y_{3r} + 6y_{2r} – 4y_r + y_i \quad \rightarrow (5)$

From the above, a general law can be developed for calculating the forward nth difference at any point (i) in the series, in the following form:

$\Delta^n y_i = \Delta^{n-1} y_{i+1} - \Delta^{n-1} y_i$

For example, $\Delta^3 yi$, which is the third forward difference at point i, can be found as follows:

$\Delta^3 y_i = \Delta^2 y_{i+1} - \Delta^2 y_i \quad \rightarrow (1)$

Applying the law to the first term of the right-hand side, we find $\Delta^2 y_{i+1} = \Delta y_{i+2} - \Delta y_{i+1}$ ……*

**Applying the law to the second term on the right side, we find

$\Delta^2 y_i = \Delta y_{i+1} - \Delta y_i$ ……**

From the equation (*), we get:

$\Delta^2 y_{i+1} = (y_{i+3} – y_{i+2}) – (y_{i+2} – y_{i+1})$

$= y_{i+3} – y_{i+2} – y_{i+2} + y_{i+1}$

$= y_{i+3} - 2y_{i+2} + y_{i+1}$

From the equation (**), we get:

$\Delta^2 y_i = (y_{i+2} - y_{i+1}) - (y_{i+1} - y_i)$

$= y_{i+2} - y_{i+1} - y_{i+1} + y_i$

$= y_{i+2} - 2y_{i+1} + y_i$

Substituting in equation (1) for $\Delta^2 y_i$, $\Delta^2 y_{i+1}$, then:

$\Delta^3 y_i = (y_{i+3} - 2y_{i+2} + y_{i+1}) - (y_{i+2} - 2y_{i+1} + y_i)$

$= y_{i+ 3} - 2y_{i+2} + y_{i+1} - y_{i+2} + 2y_{i+1} - y_i$

$= y_{i+3} - 3y_{i+2} + 3y_{i+1} - y_i$

If we want to calculate the third difference at point i = o, for example, which is the first point in the series of results, then:

$\Delta^3 y_o = y_3 - 3y_2 + 3y_1 - y_o$

And that's by substituting for i = o in the previous $\Delta^3 yi$.

Also, the third difference at the fourth point, for example i = 3, then

$\Delta^3 y_3 = y_6 - 3y_5 + 3y_4 - y_3$

Also, $\Delta^3 y_8$ at the ninth point is

$\Delta^3 y_8 = y_{11} - 3y_{10} + 3y_9 - y_8$

And so on ....

Example:

prove that

$\Delta^4 y_o = y_4 - 4y_3 + 6y_2 - 4y_1 + y_o$

The solution:

from the definition

$\Delta^4 y_o = \Delta^3 y_1 - \Delta^3 y_0 \qquad \rightarrow (1)$

Whereas, $\Delta^3 yo$ is obtained which is equal to:

$\Delta^3 y_o = y_3 - 3y_2 + 3y_1 - y_o$

Then $\Delta^3 y1$ is of the same form by increasing the lower evidence (as it progresses) by 1 .

$\Delta^3 y_1 = y_4 - 3y_3 + 3y_2 - y_1$

Compensation in (1)

$\Delta^4 y_o = y_4 - 3y_3 + 3y_2 - y_1 - y_3 - 3y_2 - 3y_1 + y_o$

$= y_4 - 4y_3 + 6y_2 - 4y_1 + y_o$

which is required,,,,

Example: To calculate the forward variances

Suppose we have the equation $y_n = n^2 - 3n - 2$ valid for the values of n = 1, 2, 3, 4 , ... Find the first forward difference and the second forward difference at n = 3

The solution:

For values of n = 1 , 2 , 3 , 4 , 5 , ... y_n has the following results

y_1 y_2 y_3 y_4 y_5

-4 -4 -2 2 8

The equation for the first forward *difference is*

$\Delta y_i = y_r - y_i$

$\Delta y_3 = y_4 - y_3$

$= 2 - (-2) = 4$

The equation of the second forward *difference*

$\Delta^2 y_i = y_{2r} - 2y_r + y_i$

$\Delta^2 y_3 = y_5 - 2y_4 + y_3$

$= 8 - 2\,(2) + (-2) = 8 - 4 - 2 = 2$

To verify this solution, we write the results series and the first two front difference series, respectively, as follows:

y_1	y_2	y_3	y_4	y_5	
-4	-4	-2	2	8	Results
	0	2	4	6	*first* forward *difference*
		2	2	2	*second* forward *difference*

From it, it is clear that the first forward difference at y_3 is

$2 - (-2) = 4$

And that the second forward difference at y_3 is

6 – 4 = 2

The first, second and third forward differences and can be calculated by the following general rule:

$$\Delta^k y_i = \sum_{i=0}^{k} (-1)^i \binom{k}{i} y_{k-1}$$

This law gives the i term in the k . difference

That is, k is the order of the difference (first, second, third, ...) and i is the order of the term inside it.

The term is a and is given as in the following table for values of k from 1 to 5, and values of I from 0 to .5

i / k	0	1	2	3	4	5
1	1	1				
2	1	2	1			
3	1	3	3	1		
4	1	4	6	4	1	
5	1	5	10	10	5	1

for example

$$\frac{4^{(3)}}{3!} = \frac{4*3*2}{3*2*1} = 4, \ldots\ldots \frac{3^{(1)}}{1!} = \frac{3}{1} = 3, \ldots\ldots\ldots \frac{3^{(2)}}{2!} = \frac{3*2}{2*1} = 3$$

Example: using the law $\Delta^k y_i = \sum_{i=0}^{k} (-1)^i \binom{k}{i} y_{k-1}$

Calculate the first forward difference Δy_i

We put in the law k = 1, i changes from 0 to 1.

First: by setting k=1 , i=0

$$\therefore \Delta y_0 = (-1)^0 \binom{1}{0} y_{1-0} = y_1$$

Then by setting k=1 , i=1

$$\therefore \Delta y_1 = (-1)^1 \binom{1}{1} y_0 = -y_0$$

Adding the two previous equations,

$$\therefore \Delta y_i = y_1 - y_0$$

This is the first forward difference.

Second forward difference

To calculate the second forward difference, the general law takes the following form:

$$\Delta^2 y_i = \sum_{i=0}^{2} (-1)^i \binom{2}{i} y_{2-i}$$

With i=0 it is

$$\Delta^2 y_0 = (-1)^0 \binom{2}{0} y_{2-0} = y_2$$

With i=1 it is

$$\Delta^2 y_1 = (-1)^1 \binom{2}{1} y_{2-1} = -2y_1$$

With i=2 it is

$$\Delta^2 y_2 = (-1)^2 \binom{2}{2} y_{2-2} = y_0$$

Adding the previous three equations, we get

$$\Delta^2 y_i = y_2 - 2y_1 + y_0$$

In the same way, the third forward difference can be calculated

Where the common law takes the following form:

$$\Delta^3 y_i = \sum_{i=0}^{3} (-1)^i \binom{3}{i} y_{3-i}$$

Putting i = 0 we get

$$\Delta^3 y_0 = (-1)^0 \binom{3}{0} y_{3-0} = y_3$$

Putting i = 1 we get

$$\Delta^3 y_1 = (-1)^1 \binom{3}{1} y_{3-1} = -3y_2$$

Putting i = 2 we get

$$\Delta^3 y_2 = (-1)^2 \binom{3}{2} y_{3-2} = 3y_1$$

Putting i = 3 we get

$$\Delta^3 y_3 = (-1)^3 \binom{3}{3} y_{3-3} = -y_0$$

Sum up the previous four equations

$$\therefore \Delta^3 y_i = y_3 - 3y_2 + 3y_1 - y_0$$

The fourth forward difference can also be calculated,

Where the common law takes the following form:

$$\Delta^4 y_i = \sum_{i=0}^{4} (-1)^i \binom{4}{i} y_{4-i}$$

Putting i = 0 we get

$$\Delta^4 y_0 = (-1)^0 \binom{4}{0} y_{4-0} = y_4$$

Putting i = 1 we get

$$\Delta^4 y_1 = (-1)^1 \binom{4}{1} y_{4-1} = -4y_3$$

Putting i = 2 we get

$$\Delta^4 y_2 = (-1)^2 \binom{4}{2} y_{4-2} = 6y_2$$

Putting i = 3 we get

$$\Delta^4 y_3 = (-1)^3 \binom{4}{3} y_{4-3} = -\frac{24}{6} y_1 = -4y_1$$

Putting i = 4 we get

$$\Delta^4 y_4 = (-1)^4 \binom{4}{4} y_{4-4} = y_0$$

Adding the previous five equations, we get

$$\Delta^4 y_i = y_4 - 4y_3 + 6y_2 - 4y_1 + y_0$$

The previous law can take the following form to calculate the forward difference

$$\Delta^k y_i = \sum_{m=0}^{k} (-1)^m \binom{k}{m} y_{i+k-m}$$

Where i expresses the term number in the original data series for which the forward difference is to be calculated, and it can take the values 0, 1, 2 .... for the first, second, third term ..... respectively.

K expresses the rank of the front teams and takes the values 1, 2, 3, ... for the first, second, third, ... and so on. m

The term number in the resulting difference equation takes values from 0 to k+1.

Therefore, for the first frontal teams we have

k=1

m=0, 1

So the first term from the first difference law we get by setting m=0 and k=1

$$\Delta y_i = (-1)^0 \binom{1}{0} y_{i+1-0}$$

$$= \Delta y_i = 1*1* y_{i+1} = y_{i+1}$$

The second term of the first difference law is obtained by setting m=1 and k=1

$$\Delta y_i = (-1)^1 \binom{1}{1} y_{i+1-1}$$

$$\Delta y_i = -1*1* y_i = -y_i$$

The law of the first forward difference is the sum of the previous two terms

$$\Delta y_i = y_{i+1} - yi$$

Second forward difference law

In this case, k = 2 is set, so m = 0, 1, 2

We get the first term by putting m = 0 into the law $\Delta^2 y_i = \sum_m^2 (-1)^m \binom{2}{m} y_{i+2-m}$

We get the first term by putting m = 0 into the law, so it takes the following form

$$\Delta^2 y_i = (-1)^0 \binom{2}{0} y_{i+2-0} = 1*1* y_{i+2} = y_{i+2}$$

Putting m = 1 we get the second term

$$\Delta^2 y_i = (-1)^1 \binom{2}{1} y_{i+2-1} = -1*2* y_{i+1} = -2y_{i+1}$$

Putting m = 2, we get the third term

$$\Delta^2 y_i = (-1)^2 \binom{2}{2} y_{i+2-2} = 1*1* y_{i+2-2} = y_i$$

$$\Delta^2 y_i = y_{i+2} - 2y_{i+1} + y_i$$

$$\Delta^2 y_i = y_{2r} - 2y_r + y_i$$

Chapter Three

Backward differences

Backward differences

~~~~~~~~~~

We need to deal with backward differences when we're dealing with the end of the data series. If we assume that for every value of xi there is a value yi of the dependent variable, and assuming that the indices xi are on equal dimensions so that $x_i - x_{i-1} = h$, then the differences of the resulting values of the dependent variable y_i are given by:

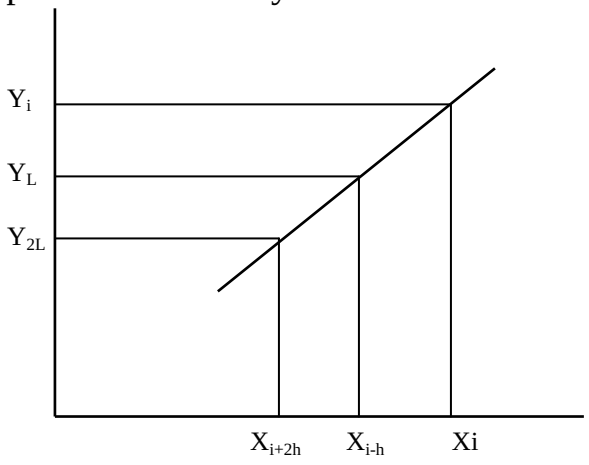
$$\nabla y_i = y_i - y_{i-1} \qquad \rightarrow (1)$$

This is called the first backward difference

Putting the following dye for ease

$Y_{i-1} = y_L$, $y_{i-2} = y_{2L}$, $y_{i-3} = y_{3L}$, …

The relationship between xi and yi can be drawn as follows:



So we take equation (1) the following form:
~~~~~~~~~~

$\nabla y_i = y_i - y_L$ → (2)

It is called the backward -primary difference equation. i, as in the aforementioned frontal differences, expresses the order of the number in the series of results.

The differences in the first backward differences are called the second background differences:

$\nabla^2 y_i = \nabla (\nabla y_i)$

$= \nabla (y_i - y_L)$

$= \nabla y_i - \nabla y_L$

$= (y_i - y_L) - (y_L - y_{2L})$

$= y_i - y_L - y_L + y_{2L}$

$= y_i - 2y_L + y_{2L}$ → (3)

Notes that:$L = i - 1$, $2L = i - 2$, $3L = i - 3$, …..

The third backward difference can also be calculated

$\nabla^3 y_i = \nabla (\nabla^2 y_i)$

$= \nabla (y_i - 2y_L + y_{2L})$

$= \nabla y_i - 2\nabla y_L + \nabla y_{2L}$

$= (y_i - y_L) - 2 (y_L - y_{2L}) + (y_{2L} - y_{3L})$

$= y_i - y_L - 2y_L + 2y_{2L} + y_{2L} - y_{3L}$

$= y_i - 3y_L + 3y_{2L} - y_{3L}$ → (4)

The fourth backward difference can also be calculated:

$$\nabla^4 y_i = \nabla\ (\nabla^3 y_i)$$

$$= \nabla\ (\ y_i - 3y_L + 3y_{2L} - y_{3L}\ )$$

$$= \nabla y_i - 3\nabla y_L + 3\nabla y_{2L} - \nabla y_{3L}$$

$$= (\ y_i - y_L\ ) - 3\ (\ y_L - y_{2L}\ ) + 3\ (\ y_{2L} - y_{3L}\ ) - (\ y_{3L} - y_{4L}\ )$$

$$= y_i - y_L - 3y_L + 3y_{2L} + 3y_{2L} - 3y_{3L} - y_{3L} - y_{4L}$$

$$= y_i - 4y_L + 6y_{2L} - 4y_{3L} + y_{4L} \qquad \rightarrow (5)$$

Examples of calculating backward variances:

Suppose we have the equation $y_n = n^2 - 3n - 2$

Valid for n = 1, 2, 3, 4 , ... find the first backward difference and the second backward difference at n = 3

The solution:

For the values n = 1, 2, 3, 4, 5, the results for y_n have the following sequence:

y_1	y_2	y_3	y_4	y_5
-4	-4	-2	2	8

The equation for the first backward difference is

$$\nabla y_i = y_i - y_L$$

$$= y_3 - y_2$$

$$= -2 - (\ -4)$$

$$= 2$$

The second backward difference equation is

$\nabla^2 y_i = y_i - 2y_L + y_{2L}$

where, i=3, L = i-1 = 2, 2L = i -2 = 1

$= y_3 - 2y_2 + y_1$

$= -2 -2 (-4) + (-4)$

$= -2 + 8 - 4$

$= 2$

To verify this solution, we write the results series and the first backward difference series, then the second backward difference series as follows

y_1	y_2	y_3	y_4	y_5	
-4	-4	-2	2	8	Output
	0	2	4	6	First backward differences
		2	2	2	second backward differences

From it it is clear that the first backward difference at y_3 is

$- 2 -(-4) = - 2 + 4 = 2$

and that the second backward difference at y_3 is

$2 - 0 = 2$

Deduce backward variance formulas from the law:

$$\nabla^k y_i = \sum_{m=0}^{k} (-1)^m \binom{k}{m} y_{i-m}$$

where i expresses the term number in the original data series for which the backward difference is to be calculated, and it can take the values 0, 1, 2 .... for the first, second, third term ..... respectively.

K expresses the rank of the backward difference and takes the values 1, 2, 3, ... for the first, second, third, ... and so on.

m is the number of the term in the resulting difference equation (formula) and takes the values from 0 to k+1.

Example 1: Derive the formula for the first posterior difference from the relationship $\nabla^k y_i = \sum_{m=0}^{k} (-1)^m \binom{k}{m} y_{i-m}$

The solution:

Since what is required is to deduce the first posterior difference formula, k = 1 and therefore m takes the values 0, 1.

Substituting k = 1 and m = 0 into the relationship

$$\nabla^k y_i = \sum_{m=0}^{k} (-1)^m \binom{k}{m} y_{i-m}$$

then

$$\nabla\ y_i = (-1)^0 \binom{1}{0} y_{i-0} = 1*1*y_i = y_i$$

Substituting for k=1 and m=1 we get

$$\nabla\ y_i = (-1)^1 \binom{1}{1} y_{i-1} = -1*1*\ y_{i-1} = -y_{i-1}$$

Thus, the final formula for the first back difference is as follows:

$$\nabla\ y_i = y_i - y_{i-1}$$

You can write in the image:

$$\nabla\ y_i = y_i - y_L$$

Example 2

Derive the formula for the second back difference from the relationship

$$\nabla^k y_i = \sum_{m=0}^{k} (-1)^m \binom{k}{m} y_{i-m}$$

The solution:

Since what is required is to derive the formula for the second back difference, then

k=2, so m takes values of 0, 1, 2.

Substituting k=2 and m=0 into the relationship,

$$\nabla^k y_i = \sum_{m=0}^{k} (-1)^m \binom{k}{m} y_{i-m}$$

we get

Substituting for k=2 and m=0

$$\nabla^2 y_i = (-1)^0 \binom{2}{0} y_{i-0} = y_i$$

Substituting for k=2 and m=1

$$\nabla^2 y_i = (-1)^1 \binom{2}{1} y_{i-1} = -2y_{i-1}$$

Substituting for k=2 and m=2

$$\nabla^2 y_i = (-1)^2 \binom{2}{2} y_{i-2} = y_{i-2}$$

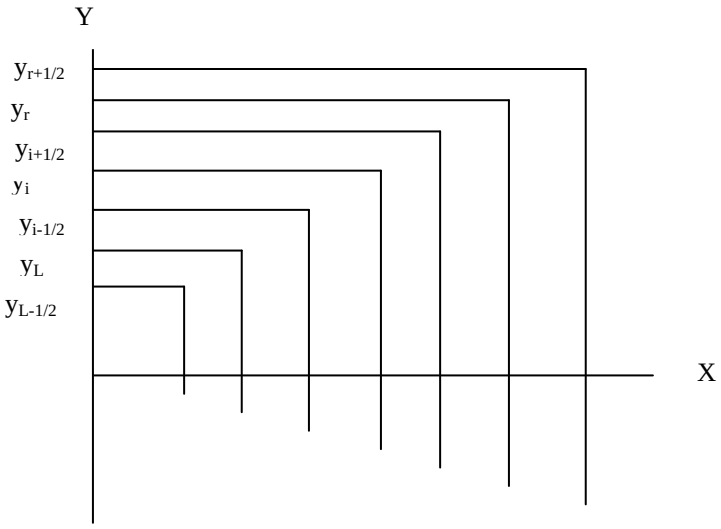
$$\therefore \nabla^2 y_i = y_i - 2y_{i-1} + y_{i-2}$$

This can be written in the formula

$$\nabla^2 y_i = y_i - 2y_L + y_{2L}$$

Chapter Four
Central Differences

Central Differences (Mean Central Differences)



The first central difference:

$$\delta yi = y_{i+\frac{1}{2}} - y_{i-\frac{1}{2}} \qquad \rightarrow ❻$$

The second central difference:

$$\delta^2 yi = \delta(\delta yi)$$

$$= \delta(y_{i+\frac{1}{2}} - y_{i-\frac{1}{2}})$$

$$= \delta y_{i+\frac{1}{2}} - \delta y_{i-\frac{1}{2}} \qquad \rightarrow ❼$$

$$= y_r - y_i - (y_i - y_L)$$

$$= y_r - 2y_i + y_L$$

The third difference:

$$\delta^3 y_i = \delta(\delta^2 y_i)$$
$$= \delta\left(y_r - 2y_i + y_L\right)$$
$$= \delta y_r - 2\delta y_i + s y_L$$
$$= \left(y_{r+\frac{1}{2}} - y_{i+\frac{1}{2}}\right) - 2\left(y_{i+\frac{1}{2}} - y_{i-\frac{1}{2}}\right) + \left(y_{i-\frac{1}{2}} - y_{L-\frac{1}{2}}\right) \quad \rightarrow ❽$$
$$= y_{r+\frac{1}{2}} - y_{i+\frac{1}{2}} - 2y_{i+\frac{1}{2}} + 2y_{i-\frac{1}{2}} + y_{i-\frac{1}{2}} - y_{L-\frac{1}{2}}$$
$$= y_{r+\frac{1}{2}} - 3y_{i+\frac{1}{2}} + 3y_{i-\frac{1}{2}} - y_{L-\frac{1}{2}}$$

Similarly the fourth, fifth, ... central difference can be calculated.

Deduce central difference formulas

The formulas for central differences can be deduced from the following relationships:

First: Formulas for central differences with even orders (second difference, fourth difference, sixth difference, ...)

The even-order central difference formulas are derived from the following relationship:

$$\delta^{2k} y_i = \sum_m^{2k} (-1)^m \binom{2k}{m} y_{i+k-m}$$

Where i expresses the number of the term in the original data series for which the central difference is to be calculated, and it can take the values 0, 1, 2 .... for the first, second, third terms ..... in order.

K expresses the rank of the central teams and takes the values 1, 2, 3, ... for the first, second, third, ... and so on.

m is the number of the term in the resulting difference equation (formula) and takes the values from 0 to 2k.

Example 1:

Derive the second central difference formula from the relationship

$$\delta^{2k} y_i = \sum_{m}^{2k} (-1)^m \binom{2k}{m} y_{i+k-m}$$

Solution: To calculate the second central difference, k = 1 and therefore m takes the values 0, 1, 2.

We get the following relations

With k=1 and m=0

$$\delta^2 y_i = (-1)^0 \binom{2}{0} y_{i+1-0} = y_{i+1}$$

With k=1 and m=1

$$\delta^2 y_i = (-1)^1 \binom{2}{1} y_{i+1-1} = -2y_i$$

With k=1 and m=2

$$\delta^2 y_i = (-1)^2 \binom{2}{2} y_{i+1-2} = y_{i-1}$$

$$\therefore \delta^2 y_i = y_{i+1} - 2y_i + y_{i-1}$$

$$\delta^2 y_i = y_r - 2y_i + y_L$$

In the same way, the formula for the fourth and sixth central difference can be deduced.

Second: Forms of central differences with odd ranks (first difference, third difference, fifth difference, ...)

The odd-order central difference formulas are derived from the following relationship:

$$\delta^{2k+1} y_{i+\frac{1}{2}} = \sum_{m}^{2k+1} (-1)^m \binom{2k+1}{m} y_{i+k+1-m}$$

Example:

Derive the first central difference formula from the relationship

$$\delta^{2k+1} y_{i+\frac{1}{2}} = \sum_{m}^{2k+1} (-1)^m \binom{2k+1}{m} y_{i+k+1-m}$$

Solution: To calculate the first central difference, k = 0 and therefore m takes the values 0, 1.

We get the following relations:

With k=0 and m=0 .

.

$$\delta y_{i+\frac{1}{2}} = (-1)^0 \binom{1}{0} y_{i+0+1-0} = y_{i+1}$$

With k=0 and m=1 .

$$\delta y_{i+\frac{1}{2}} = (-1)1 \binom{1}{1} y_{i+0+1-1} = -y_i$$

Adding the previous terms

$$\therefore \delta y_{i+\frac{1}{2}} = y_{i+1} - y_i$$

Subtract ½ from the evidence

$$\therefore \delta y_i = y_{i+\frac{1}{2}} - y_{i-\frac{1}{2}}$$

Example:

Derive the formula for the third central difference from the relationship

$$\delta^{2k+1} y_{i+\frac{1}{2}} = \sum_{m}^{2k+1} (-1)^m \binom{2k+1}{m} y_{i+k+1-m}$$

Solution: To calculate the third central difference, k = 1 and therefore m takes the values 0,1,2,3

We get the following relations:

With k=1 and m=0 .

we get

$$\delta^3 y_{i+\frac{1}{2}} = (-1)^0 \binom{3}{0} y_{i+1+1-0} = y_{i+2}$$

With k=1 and m=1 .

$$\delta^3 y_{i+\frac{1}{2}} = (-1)^1 \binom{3}{1} y_{i+1+1-1} = -3y_{i+1}$$

With k=1 and m=2 .

$$\delta^3 y_{i+\frac{1}{2}} = (-1)^2 \binom{3}{2} y_{i+1+1-2} = 3y_i$$

With k=1 and m=3 .

$$\delta^3 y_{i+\frac{1}{2}} = (-1)^3 \binom{3}{3} y_{i+1+1-3} = -y_{i-1}$$

Add the previous limits

$$\delta^3 y_{i+\frac{1}{2}} = y_{i+2} - 3y_{i+1} + 3y_i - y_{i-1}$$

$$\therefore \delta^3 y_{i+\frac{1}{2}} = y_{2r} - 3y_r + 3y_i - y_L$$

Subtracting ½ of the evidence

$$\delta^3 y_i = y_{r+\frac{1}{2}} - 3y_{i+\frac{1}{2}} + 3y_{i-\frac{1}{2}} - y_{L-\frac{1}{2}}$$

The mean value of the function

From the previous figure, we find that it is the mean of yr + yi, that is :,

$$y_{i+\frac{1}{2}} = \frac{1}{2}(y_r + y_i)$$

We also find that:

$$y_{i-\frac{1}{2}} = \frac{1}{2}(y_i + y_L)$$

If we take μ (the middle operator) or the mean operator, then:

$$\mu y_{i+\frac{1}{2}} = \frac{1}{2}(y_r + y_i) \qquad \rightarrow ❻$$

like that

$$\mu y_i = \frac{1}{2}(y_{i+\frac{1}{2}} + y_{i-\frac{1}{2}})$$

If we add this effect to the equation for the first difference:

$$\delta y_i = y_{i+\frac{1}{2}} - y_{i-\frac{1}{2}}$$

$$\therefore \mu\delta y_i = \mu y_{i+\frac{1}{2}} - \mu y_{i-\frac{1}{2}}$$

$$= \frac{1}{2}[(y_r + y_i) - (y_i + y_L)] \qquad \rightarrow ❼$$

$$= \frac{1}{2}y_r + \frac{1}{2}y_i - \frac{1}{2}y_i - \frac{1}{2}y_L$$

$$\therefore \mu\delta yi = \frac{1}{2}(y_r - y_L)$$

By adding this effect to the second mean difference equation:

$$\mu\,\delta^2 y_i = \mu\ \delta\ (\delta\ y_i)$$

$$= \mu\,(\,y_r - 2y_i + y_L\,)$$

$= \mu y_r - 2\mu y_i + \mu y_L)$

$= \frac{1}{2} (y_{r+\frac{1}{2}} + y_{i+\frac{1}{2}}) - 2 * \frac{1}{2} (y_{i+\frac{1}{2}} + y_{i-\frac{1}{2}}) + \frac{1}{2} (y_{i-\frac{1}{2}} + y_{L-\frac{1}{2}})$

$= \frac{1}{2} y_{r+\frac{1}{2}} + \frac{1}{2} y_{i+\frac{1}{2}} - y_{i+\frac{1}{2}} - y_{i-\frac{1}{2}} + \frac{1}{2} y_{i-\frac{1}{2}} + 1/2\, y_{L-1/2}$

$= \frac{1}{2} y_{r+\frac{1}{2}} - \frac{1}{2} y_{i+\frac{1}{2}} - \frac{1}{2} y_{i-\frac{1}{2}} + \frac{1}{2} y_{L-\frac{1}{2}}$

$\mu \delta^2 y_i = \frac{1}{2} (y_{r+\frac{1}{2}} - y_{i+\frac{1}{2}} - y_{i-\frac{1}{2}} + y_{L-\frac{1}{2}}) \quad \rightarrow 3$

By adding this indicator to the third average difference equation:

$\therefore \mu \delta^3 y_i = \mu y_{r+\frac{1}{2}} - 3\mu y_{i+\frac{1}{2}} + 3\mu y_{l-\frac{1}{2}} - \mu y_{L-1/2}$

$= \frac{1}{2} (y_{2r}+y_r) - 3/2(y_r+y_i) + 3/2(y_i+y_L) - \frac{1}{2} (y_L+y_{2L})$

$= \frac{1}{2} \{ y_{2r} + y_r - 3y_r - 3y_i + 3y_i + 3y_L - y_L - y_{2L}\}$

$= \frac{1}{2} \{ y_{2r} - 2\, y_r + 2y_L - y_{2L}\}$

Chapter Five

Interpolation

What is meant by Conclusion or Interpolation?

1- Definition of Interpolation

Interpolation is the process of finding a value y when a given value x is not present in the given points table.

This process is called the issue of completion. Two types of issues must be distinguished:

First issue:

The required point is inside the points of the table and thus the process in this case is called an internal interpolation.

The second issue:

That the required point is outside the points of the table, and thus the process is called in this case an external extrapolation.

Assuming that there is a function y= f(x) defined only at certain points (x0,y0), (x1,y1), (x2,y2), ...(xn,yn) how can we find the value of the function at any value other than x those values? This can be done using a continuous function f (x) representing that data such that the function f(x) passes through n+ 1 point, where n is the degree of the function used. Thus, the value of the function can be calculated at any point, and this is called Interpolation. Of course, if x is outside the range of f(X), setting the value of the function at x in this case is called extrapolation.

We then come to choose the type of function that should be used to represent the data.

It is common for polynomial functions to be used for the following adjectives:

(1)Ease of computation.

(2)Ease of differentiation.

(3)Ease of integration.

By comparing it with sin or exponential functions.

How to work polynomial Interpolation

A polynomial can be done to represent a function in a number of ways, including:

1. Direct method of Interpolation.
2. Newton's divided difference method.
3. Lagrange interpolation method.
4. Sterling method

First: The direct method of making a polynomial:

The direct method is based on that, assuming that we have (n+1) points, a polynomial of degree (n) can be done as follows**:**

$Y= a_0 + a_1 x + a_2 x^2 +\ldots. a_n x^n \rightarrow ❻$

across the data so that an ... , a1, a0 are n+1 real constants. Since we have n +1 values of y and n+1 values of x, we can do n+ 1 equation. Then, n+1 constants are calculated, which are a0, a1,a2..an. By knowing these constants, the

function expressing the data number ❻ is known. By substituting the value of x in it, the value of y to be calculated is known.

But what degree of polynomial will we use? Is it possible to use a polynomial of the first degree (which is called a linear equation), or of the second degree (a quadratic equation), or of the third degree (cubic), and what is the difference in the accuracy of the result? This can be illustrated by an example

Example 1: The vertical velocity of a rocket is given as in the following table as a function of time

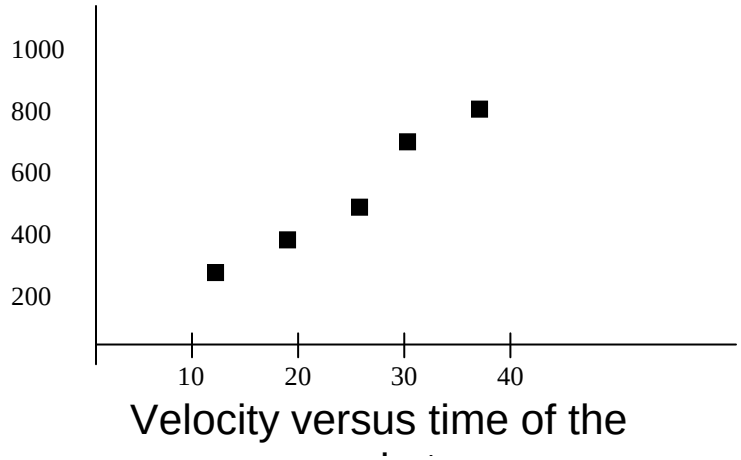
ts	0	10	15	20	22.5	30
$V_{m/s}$	0	227.04	362.78	517.35	602.97	901.67

Determine the missile's velocity at t=l6s using the direct method and a first-order polynomial

Solution: Since we are required to use an equation of first degree (linear equation), the velocity equation is in the next picture

$V(t) = a_0 + a_1 t$

And its graph is as follows:



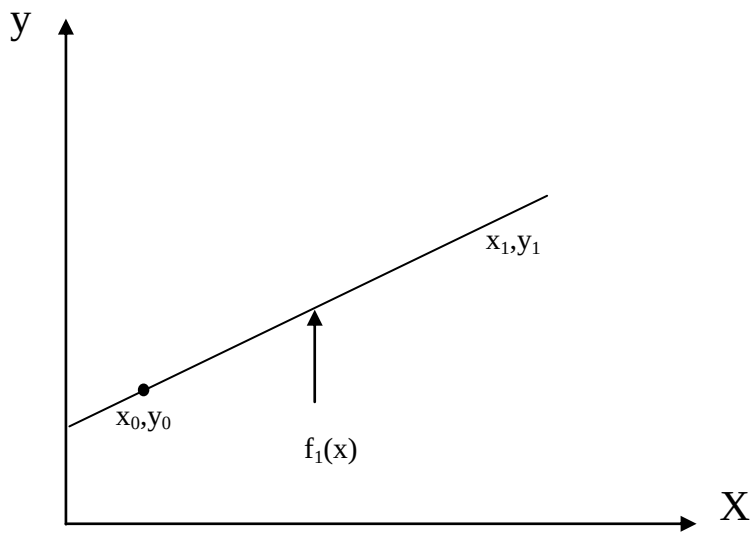
Velocity versus time of the

Since we are required to use an equation of the first degree (linear equation).

The equation for velocity is in the following image:

$v(t) = a_0 + a_1 t$

Its graph is as follows:



Draw a straight line to represent the data for the missile

Since the equation is of first degree n = 1 we choose n + 1 Points any two points. These two points must surround the required point in order for that point to be within the scope of application of the deduced equation.

Since the required point t = 16s lΔ, the two points must be

t1 = 20 , t0 = 15

and where we have

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

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

We have two equations

$V(15) = a_0 + a_1(15) = 362.78$

$V(20) = a_0 + a_1(20) = 517.35$

The two equations can be written in matrix form:

$$\begin{bmatrix} 1 & 15 \\ 1 & 20 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} 362.78 \\ 517.35 \end{bmatrix}$$

By solving the above two equations, you get:

$a_0 = -100.91$

$a_1 = 30.913$

Thus, the proposed equation is:

$v(t) = -100.91 + 30.913 \qquad 15 \leq t \leq 20$

To calculate the velocity at t= 16s, we substitute in this equation the value of t

$\therefore V(16) = 393.7$ m/ s

Example 2:
The velocity of a missile is given vertically as in the following table:

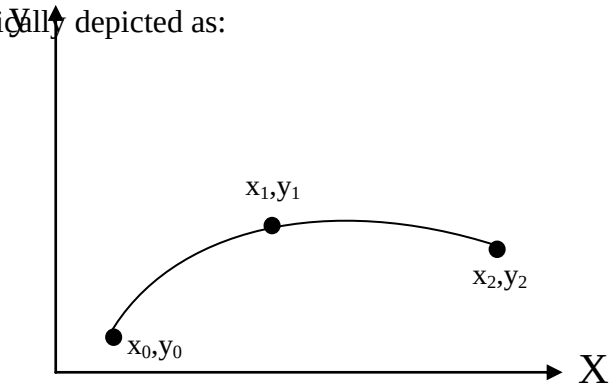
t= s	0	10	15	20	22.5	30
v(t) m/s	0	227.04	362.78	517.35	602.97	901.67

Determine the missile's velocity at t = 16 s using the direct method and a quadratic polynomial.

Solution: To make an equation of the second degree (a quadratic equation) that will be of the following form:

$$v(t) = a_0 + a_1 t + a_2 t^2$$

It is graphically depicted as:



Since we want to deduce the missile's velocity at t = 16 s, we choose three points (n + 1) that include the value (16 s). These points are:

T_0=10 , t_1 = 15 , t_2 = 20

The following equations are given for each point:

$v(10) = a_0 + a_1(10) + a_2(10)^2 = 227.04$

$v(15) = a_0 + a_1(15) + a_2(15)^2 = 362.78$

$v(20) = a_0 + a_1(20) + a_2(20)^2 = 517.35$

We put these equations in matrix form as follows:

$$\begin{bmatrix} 1 & 10 & 100 \\ 1 & 15 & 225 \\ 1 & 20 & 400 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 227.04 \\ 362.78 \\ 517.35 \end{bmatrix}$$

This matrix can be solved by the Gaussian method for forward elimination and backward substitution or by the LU method. Then we get:

$a_0 = 12.001$, $a_1 = 17.740$, $a_2 = 0.37637$

And the required equation is:

$v(t) = 12.001 + 17.790t + 0.37637\, t^2 \quad 10 \leq t \leq 20$

Substituting the value of t = 16s into this equation, we get v(16):

$v(16) = 12.001 + 17.790\,(16) + 0.37637\,(16)^2$

$= 392.19 \quad m/s$

From the two previous examples it is possible to calculate : $|\in_c|$ the absolute relative approximate error arising from the transition from a first degree equation to a second degree equation:

$$|\in_c| = \left|\frac{392.19 - 393.70}{392.19}\right| \times 100$$

$$= 0.38502\%$$

Newton's Divided Difference Interpolating Polynomral Method

To illustrate this method, we will start with linear and quadratic interpolation, then, the general form of the Newton's Divided Difference Polynomial method will be presented.

1.3.1. Linear interpolation

Given (x_0, y_0), (x_1, y_1), fit a linear interpolant through the data. Note taht $y_0 = f(x_0)$ and $y_1 = f(x_1)$, assuming a linear interpolant means:

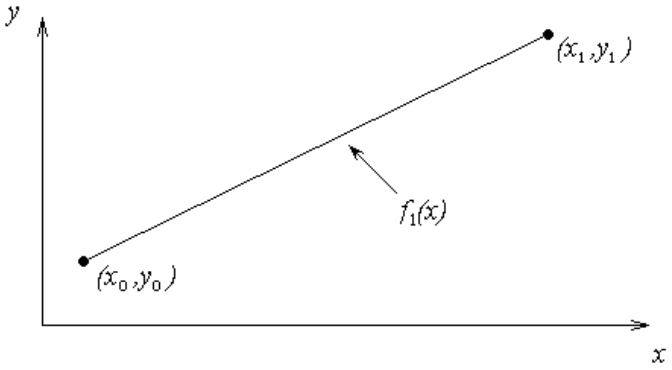
$$f_1(x) = b_0 + b_1(x - x_0)$$

Since at $x = x_0$: $f_1(x_0) = f(x_0) = b_0 + b_1(x_0 - x_0) = b_0$,

and at $x = x_1$: $f_1(x_1) = f(x_1) = b_0 + b_1(x_1 - x_0) = f(x_0) + b_1(x_1 - x_0)$

Then

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



so

$$b_0 = f(x_0)$$

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

And the linear interpolant,

$$f_1(x) = b_0 + b_1(x - x_0)$$

Becomes:

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

1.3.2. Quadratic interpolation

Given (x_0, y_0), (x_1, y_1), and (x_2, y_2), fit a quadratic interpolant through the data. Note that $y = f(x)$, $y_0 = f(x_0)$, $y_1 = f(x_1)$, and $y_2 = f(x_2)$, assume the quadratic interpolant $f_2(x)$ given by

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

At $x = x_0$

$$f(x_0) = f_2(x_0) = b_0 + b_1(x_0 - x_0) + b_2(x_0 - x_0)(x_0 - x_1)$$

$$= b_0$$

$$b_0 = f(x_0)$$

At $x = x_1$

$$f(x_1) = f_2(x_1) = b_0 + b_1(x_1 - x_0) + b_2(x_1 - x_0)(x_1 - x_1)$$

$$f(x_1) = f(x_0) + b_1(x_1 - x_0)$$

then

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

At $x = x_2$

$$f(x_2) = f_2(x_2) = b_0 + b_1(x_2 - x_0) + b_2(x_2 - x_0)(x_2 - x_1)$$

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

then

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

Hence the quadratic interpolant is given by

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

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

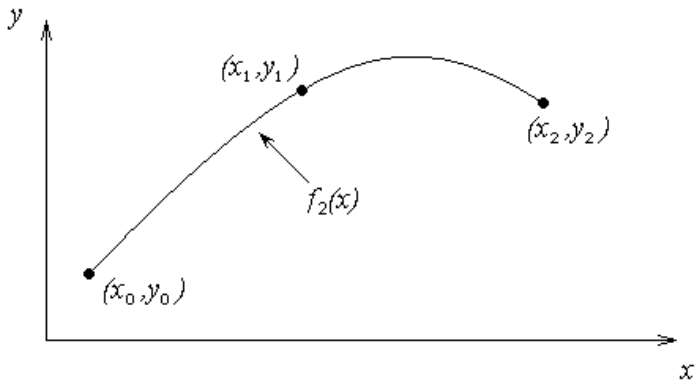


Figure Quadratic interpolation

1.3.3. General Form of Newton's Divided Difference Polynomial

In the two previous cases, we found how linear and quadratic interpolation is derived by Newton's Divided Difference polynomial method. Let us analyze the quadratic polynomial interpolant formula

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

where

$$b_0 = f(x_0)$$

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

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

Note that b_0, b_1, and b_2 are **finite divided differences**. b_0, b_1, and b_2 are first, second, and third finite divided differences, respectively. Denoting first divided difference by

$$f[x_0] = f(x_0)$$

the second divided difference by

$$f[x_1, x_0] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

and the third divided difference by

$$f[x_2, x_1, x_0] = \frac{f[x_2, x_1] - f[x_1, x_0]}{x_2 - x_0}$$

$$= \frac{\dfrac{f(x_2) - f(x_1)}{x_2 - x_1} - \dfrac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}$$

where $f[x_0]$, $f[x_1, x_0]$, and $f[x_2, x_1, x_0]$ are called bracketed functions of their variables enclosed in square brackets.

We can write:

$$f_2(x) = f[x_0] + f[x_1, x_0](x - x_0) + f[x_2, x_1, x_0](x - x_0)(x - x_1)$$

This leads to the general form of the Newton's divided difference polynomial for $(n+1)$ data points, $(x_0, y_0), (x_1, y_1), ..., (x_{n-1}, y_{n-1}), (x_n, y_n)$ as

$$f_n(x) = b_0 + b_1(x - x_0) + ... + b_n(x - x_0)(x - x_1)...(x - x_{n-1})$$

where

$$b_0 = f[x_0]$$

$$b_1 = f[x_1, x_0]$$

$$b_2 = f[x_2, x_1, x_0]$$

$$\vdots$$

$$b_{n-1} = f[x_{n-1}, x_{n-2}, ..., x_0]$$

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

where the definition of the m^{th} divided difference is

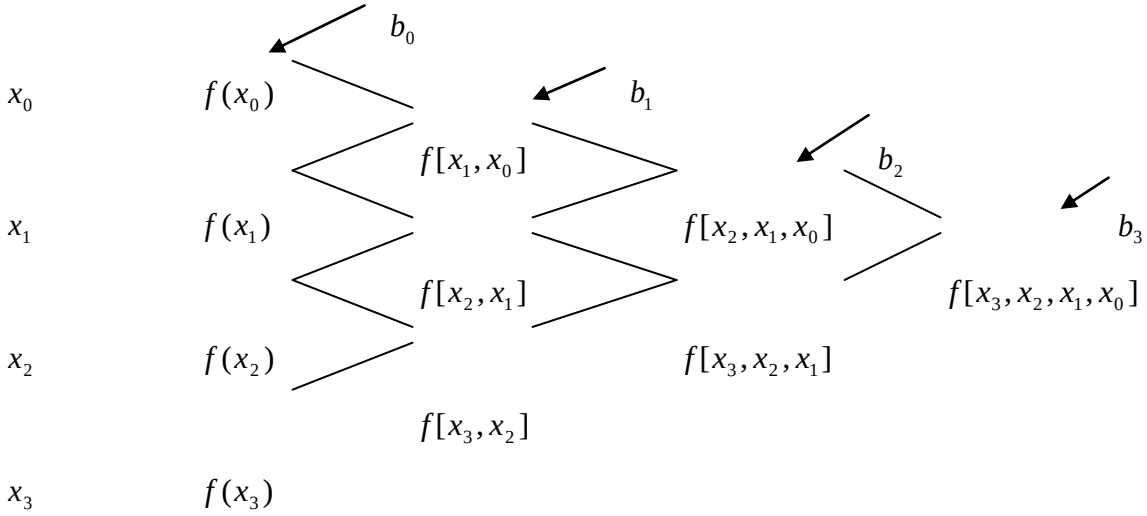
$$b_m = f[x_m, ..., x_0]$$

$$= \frac{f[x_m, ..., x_1] - f[x_{m-1}, ..., x_0]}{x_m - x_0}$$

From the above definition, it can be seen that the divided differences are calculated recursively.

For an example of a third order polynomial, given (x_0, y_0), (x_1, y_1), (x_2, y_2), and (x_3, y_3),

$$f_3(x) = f[x_0] + f[x_1, x_0](x - x_0) + f[x_2, x_1, x_0](x - x_0)(x - x_1) + f[x_3, x_2, x_1, x_0](x - x_0)(x - x_1)(x - x_2)$$



Example

Use the same previous data of the upward velocity of a rocket, to determine the value of the velocity at t=16 s using third order polynomial interpolation using Newton's Divided Difference polynomial.

Example 1:

The vertical missile velocity is given as a function of time, as shown in the following table:

T= s	0	10	15	20	22.5	3-
s	0	227.04	362.78	517.35	602.97	901.67

Determine the value of the velocity at t = 16s using an equation of the first degree using the Newton's divided difference method.

Example 2:

It gives a vertical missile velocity as in the previous table Determine the missile's velocity at t = 16 s using a quadratic equation using Newton's divisive difference method.

Chapter Six

CURVE FITTING

6.1 Linear Regression and Matrix Algebra

Error is inherent in data. When data exhibits substantial error rigorous techniques must be used to fit the "best" curve to the data. Otherwise prediction of intermediate values, or the derivatives of values, may yield unsatisfactory results.

Visual inspection may be used to fit the "best" line through data points, but this method is very subjective. Some criterion must be devised as a basis for the fit. One criterion would be to derive a curve that minimizes the discrepancy between the data points and the curve. Least-squares regression is one technique for accomplishing this objective.

It is easiest to interpolate between data points, and to develop correlation, when the dependent variable is linearly related to the independent variable. While individual variables may not be linearly related, they may be grouped together or mathematically manipulated, such as having their log or square root taken, to yield a linear relationship. We wish to fit the "best" straight line to the set of paired data points: (x_1,Y_1), (x_2,Y_2), …,(x_i,Y_i). The mathematical expression for the calculated values is:

$$y_i = a_1 + a_2 x_i$$

where y_i is the calculated (linear) value approximating the experimental value Y_i. The model error, or residual, e_i can be represented as

$$e_i = Y_i - a_1 - a_2 x_i$$

where e_i is discrepancy between the measured value Y_i and the approximated value y_i as predicted by the linear equation.

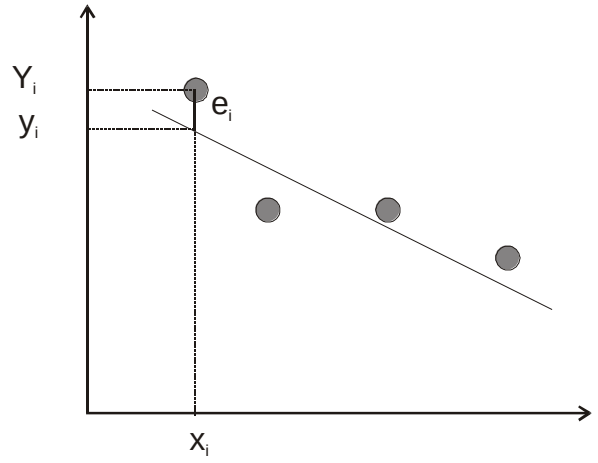


Figure Relationship between the model equation and the data

We wish to find values for a_1 and a_2 to give the "best" fit for all the data. One strategy would be to select values for a_1 and a_2 to yield a straight line that minimizes the sum of the errors e_i's. Since error is undesirable regardless of sign this criterion is inadequate because negative errors can cancel positive errors. The problem may be fixed if one selects a_1 and a_2 such that the absolute value of the sum of errors is minimized. However one may show that this criterion does not yield a unique "best" fit. A third criterion for fitting the "best" line is the minimax criterion. With this technique one selects a line that minimizes the maximum distance that an individual data point deviates from the calculated line. Unfortunately this strategy gives an undue influence to an outliner, a single point with a large error.

A strategy that overcomes the shortcomings of these previous approaches is to minimize the sum of the squares of the errors or residuals, between the measured Y_i's and the y_i's calculated from the linear model. This criterion has a number of advantages. A unique line results for a given data set. This criterion also leads to the to the most likely a_1 and a_2 from a statistical standpoint.

Regression analysis is used to determine the constants in a relationship between variables. We only consider the simple case where y is a linear function of x. In other words we wish to find an equation $y = a_1 + a_2x$ to best fit the obtained experimental data x_i and Y_i. At the values x_i, the experimental values Y_i are subject to random errors. Let's define

$$e_i = Y_i - y_i$$

to be the difference between the experimental and predicted values. The least-squares criterion requires that S defined by Eq. (5.1-1) be a minimum

$$S = e_1^2 + e_2^2 + ... + e_N^2 = \sum_{i=1}^{N} e_i^2 \qquad (1)$$

or

$$S = \sum_{i=1}^{N} \{Y_i - [a_1 + a_2 (x_i)]\}^2 \qquad (2)$$

Setting the derivative of this sum with respect to each coefficient equal to zero will result in a minimum for the sum. Thus the coefficients a_1 and a_2 must satisfy the conditions

$$\frac{\partial S}{\partial a_1} = \sum_{i=1}^{N} \{-2\}\{Y_i - [a_1 + a_2 (x_i)]\} = 0 \qquad (a)$$

$$\frac{\partial S}{\partial a_2} = \sum_{i=1}^{N} \{-2(x_i)\}\{Y_i - [a_1 + a_2 (x_i)]\} = 0 \qquad (b)$$

We have two equations in the two unknowns a_1 and a_2, so we may solve for a unique set of coefficients. Dividing Eqs. (5.1-3.a) and (5.1-3.b) by (-2) and rearranging

$$a_1 N + a_2 \sum_{i=1}^{N} x_i = \sum_{i=1}^{N} Y_i \qquad (a)$$

$$a_1 \sum_{i=1}^{N} x_i + a_2 \sum_{i=1}^{N} x_i x_i = \sum_{i=1}^{N} x_i Y_i \qquad (b)$$

The system can be expressed in the matrix notation

$$A.a = B \qquad (a)$$

or

$$\begin{bmatrix} N & \sum_{i=1}^{N} x_i \\ \sum_{i=1}^{N} x_i & \sum_{i=1}^{N} x_i x_i \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} Y_i \\ \sum_{i=1}^{N} x_i Y_i \end{bmatrix} \qquad (b)$$

The column vector a can be easily solved using the matrix capability of Matlab

$$a = A\backslash B \qquad (6)$$

Example The following data represent the concentration of reactant A in a constant volume reactor. (Ref. Module 3: Linear Regression by Bequette[4])

Time (min)	0	1	2	3	4	5
C_A, kmol/m^3	8.47	5.00	2.95	1.82	1.05	0.71

If the reaction is first order, A --> B, determine the reaction rate constant k where $r_A(\text{kmol/m}^3\cdot\text{min}) = kC_A$.

Solution:

The material balance for reactant A in a constant volume batch reactor is

$$\frac{dC_A}{dt} = -kC_A$$

Separating variables and integrating:

$$\frac{dC_A}{C_A} = -kdt$$

$$\ln C_A = \ln C_{Ao} - kt$$

where C_{Ao} is the initial concentration of A.

For this example: N = 6, y = ln C_A, a_1 = ln C_{Ao}, and x = t. The calculated values C_{Ao} and k can be obtained from the solution of Eqs. (6) by using the matrix algebra capability of Matlab.

The coefficient matrix A and the column vector B can be determined by defining a new matrix w

$$w = \begin{bmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \vdots \\ 1 & t_N \end{bmatrix}$$

and the transpose of w

$$w^T = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ t_1 & t_2 & \cdots & t_N \end{bmatrix}$$

so that

$$A = w^T * w \text{ and } B = w^T * Y$$

Matrix A can be obtained by the following Matlab statements:

```
>>  f1=ones(6,1);

>>  f2=[0; 1; 2; 3; 4; 5];

>> w=[f1 f2]

w =
    1     0
    1     1
    1     2
    1     3
    1     4
    1     5

>> A=w'*w      Note: w' is the Matlab notation for the transpose of w

A =
    6    15
   15    55
```

The right hand vector B is obtained by the following Matlab statements:

```
>> Ca=[8.47; 5; 2.95; 1.82; 1.05; 0.71];

>> Y=log(Ca)

Y =
  2.1365e+000
  1.6094e+000
  1.0818e+000
  5.9884e-001
  4.8790e-002
 -3.4249e-001

>> B=w'*Y

B =
  5.1329e+000
  4.0523e+000
```

The solution vector a is then

```
>> a=A\B

a =
  2.1098e+000
 -5.0171e-001
```

and the linear relationship between the variables is

$$\ln C_A = 2.1098 - 0.50171t$$

The same values for the parameters can also be obtained by using polyfit, a function provided by Matlab, to find the best linear fit of the data.

```
% Matlab program for Example 5.1-1
% Least square curve fitting of ln(Ca) = ln(Cao) - kt
%
t=[0 1 2 3 4 5];
Ca=[8.47 5 2.95 1.82 1.05 0.71];
Y=log(Ca);
ap=polyfit(t,Y,1)
```

```
ap =
  -0.5017    2.1098
```

You should notice that the first element in vector ap is the coefficient of the highest degree term. This is the convention used by Matlab in any polynomial functions. The experimental data and the best fitted line can be plotted by the following Matlab statements

```
>> ycal=polyval(ap,t)

ycal =
  2.1098e+000
  1.6081e+000
  1.1063e+000
  6.0463e-001
  1.0291e-001
 -3.9880e-001
```

```
>> plot(t,ycal,t,Y,'o')
>> ylabel ('ln Ca'); xlabel ('t, min')
```

The parameters ap(1) and ap(2) are converted back to the physical parameters:

```
>> Cao_cal=exp(ap(2))
Cao_cal =
  8.2464e+000
k=-ap(1)
k =
  5.0171e-001
```

The experimental data and the fitted model can also be compared on a time-concentration plot by the following Matlab statements. The results are presented in Figure 5.1-2

```
>> t1=0:0.25:5;
>> Ca_cal=Cao_cal*exp(-k*t1);
>> plot(t1,Ca_cal,t,Ca,'o')
>> ylabel('Ca');xlabel('t,min')
```

A crude measure of the how well the data is fitted by a straight line is given by the linear correlation coefficient r, which is defined for two variables t and Y as

$$r = \frac{N\sum_{i=1}^{N} t_i Y_i - \sum_{i=1}^{N} t_i \sum_{i=1}^{N} Y_i}{(C_t C_Y)^{1/2}}$$

where

$$C_t = \sum_{i=1}^{N} t_i^2 - \left(\sum_{i=1}^{N} t_i\right)^2 \qquad C_Y = N\sum_{i=1}^{N} Y_i^2 - \left(\sum_{i=1}^{N} Y_i\right)^2$$

Values of r may range from (-1) to (1). The positive value indicates a positive correlation, i.e., the dependent variable is increasing with the independent variable. If |r| is exactly 1, the data is perfectly represented by the straight line.

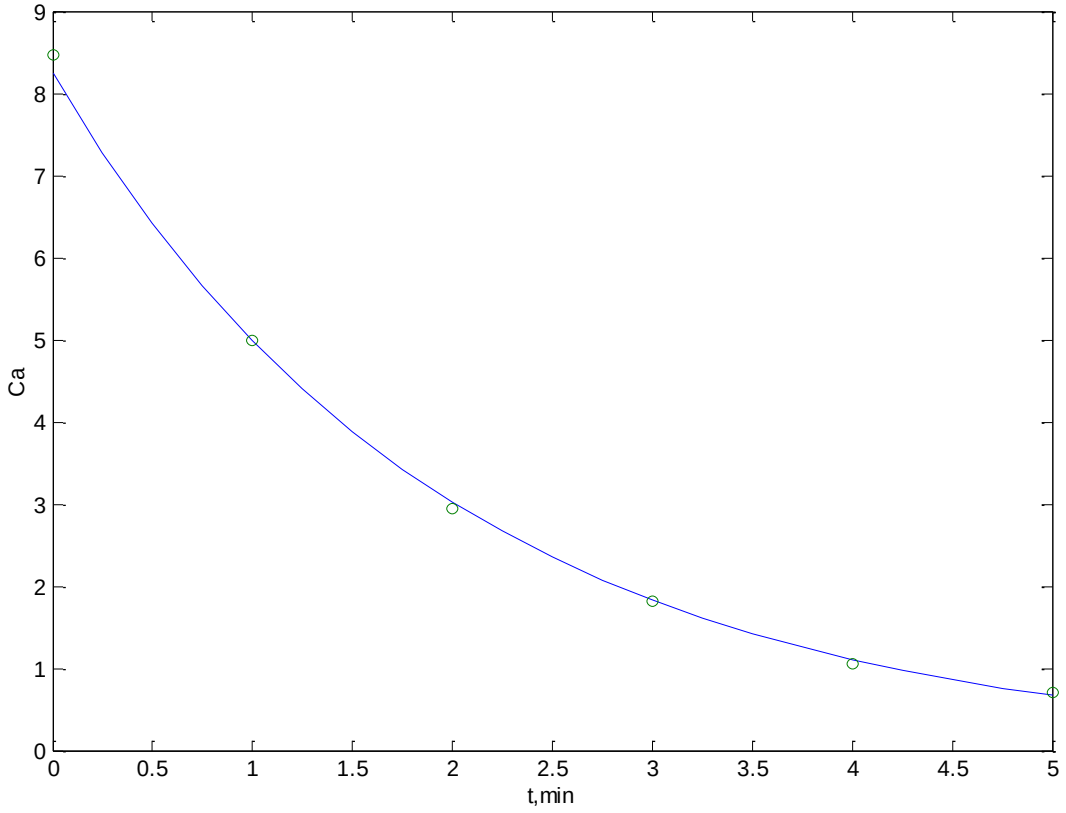


Figure Experimental and fitted concentration as a function of time

The correlation coefficient for the straight line

$$Y = \ln C_A = 2.1098 - 0.50171t$$

can be evaluated by the following Matlab statements:

% corre.m

```
% Evaluate the linear correlation coefficient r of two vector t and Y
%
t = [0; 1; 2; 3; 4; 5];
Ca = [8.47; 5; 2.95; 1.82; 1.05; 0.71];
Y = log(Ca);
N = length(t);
sumt = sum(t); sumY= sum(Y);
sumts = t'*t; sumYs = Y'*Y; sumtY = t'*Y;
ct = N*sumts - sumt*sumt;
cy = N*sumYs - sumY*sumY;
r = (N*sumtY - sumt*sumY)/sqrt(ct*cy)
```

The linear correlation coefficient for this example is

```
r = -9.9915e-001
```

6.2.General Linear Least Squares

We wish to fit the "best" curve to the set of paired data points: (x_1,Y_1), (x_2,Y_2), …,(x_N,Y_N). The mathematical expression for the calculated values is:

$$y_i = a_1 f_1(x_i) + a_2 f_2(x_i) + \ldots + a_n f_n(x_i) \qquad (6.2\text{-}1)$$

where y_i is the calculated value approximating the experimental value Y_i. The above expression is a general linear least squares model since the unknown parameters a_1, a_2, …, a_n are linear combination of the known functions $f_1(x_i)$, $f_2(x_i)$, …, $f_n(x_i)$. The model error, or residual, e_i can be represented as

$$e_i = Y_i - y_i = Y_i - [a_1 f_1(x_i) + a_2 f_2(x_i) + \ldots + a_n f_n(x_i)] \qquad (6.2\text{-}2)$$

where e_i is discrepancy between the measured value Y_i and the approximated value y_i as predicted by the model equation.

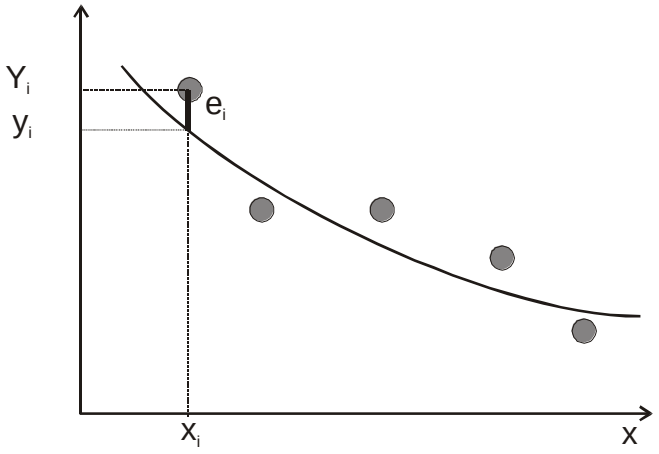


Figure Relationship between the model equation and the data

We wish to find values for the parameters a_1 to a_n to give the "best" fit for all the data. Regression analysis is used to determine the constants in a relationship between functions. The least-squares criterion requires that S defined by Eq. (5.2-3) be a minimum

$$S = e1^2 + e2^2 + ... + eN^2 = \sum_{i=1}^{N} e_i^2 \qquad (6.2\text{-}3)$$

or

$$S = \sum_{i=1}^{N} \{ Y_i - [a_1 f_1(x_i) + a_2 f_2(x_i) + \ldots + a_n f_n(x_i)]\}^2 \qquad (6.2\text{-}4)$$

Setting the derivative of this sum with respect to each coefficient equal to zero will result in a minimum for the sum. Thus the coefficients $a1$, $a2$, and $a3$ must satisfy the conditions

$$\frac{\partial S}{\partial a_1} = \sum_{i=1}^{N} \{-2\}\{ Y_i - [a_1 f_1(x_i) + a_2 f_2(x_i) + \ldots + a_n f_n(x_i)]\}(- f_1(x_i)) = 0 \qquad (6.2\text{-}5.a)$$

$$\frac{\partial S}{\partial a_2} = \sum_{i=1}^{N} \{-2\}\{ Y_i - [a_1 f_1(x_i) + a_2 f_2(x_i) + \ldots + a_n f_n(x_i)]\} (- f_2(x_i)) = 0 \qquad (6.2\text{-}5.b)$$

$$\ldots = \ldots$$

$$\frac{\partial S}{\partial a_n} = \sum_{i=1}^{N} \{-2\}\{ Y_i - [a_1 f_1(x_i) + a_2 f_2(x_i) + \ldots + a_n f_n(x_i)]\} (- f_n(x_i)) = 0 \qquad (6.2\text{-}5.n)$$

We can divide equations (5.2-5.a – 5.2-5.n) by (–2) and rearrange them to obtain the following set

$$a1 \sum_{i=1}^{N} f_1(x_i)\ f_1(x_i) + a2 \sum_{i=1}^{N} f_1(x_i)\ f_2(x_i) + \ldots + a_n \sum_{i=1}^{N} f_1(x_i) f_n(x_i) = \sum_{i=1}^{N} f_1(x_i) Y_i \qquad (6.2\text{-}6.a)$$

$$a1 \sum_{i=1}^{N} f_2(x_i)\ f_1(x_i) + a2 \sum_{i=1}^{N} f_2(x_i)\ f_2(x_i) + \ldots + a_n \sum_{i=1}^{N} f_2(x_i) f_n(x_i) = \sum_{i=1}^{N} f_2(x_i) Y_i \qquad (6.2\text{-}6.b)$$

$$\ldots \qquad \ldots \qquad \ldots \qquad = \ldots$$

$$a1 \sum_{i=1}^{N} f_n(x_i)\ f_1(x_i) + a2 \sum_{i=1}^{N} f_n(x_i)\ f_2(x_i) + \ldots + a_n \sum_{i=1}^{N} f_n(x_i) f_n(x_i) = \sum_{i=1}^{N} f_n(x_i) Y_i \qquad (6.2\text{-}6.n)$$

The system can be expressed in the matrix notation

$$A.a = B \qquad (6.2\text{-}7.a)$$

or

$$\begin{bmatrix} \sum_{i=1}^{N} f_1 f_1 & \sum_{i=1}^{N} f_1 f_2 & \cdots & \sum_{i=1}^{N} f_1 f_n \\ \vdots & \vdots & \vdots & \vdots \\ \sum_{i=1}^{N} f_2 f_1 & \sum_{i=1}^{N} f_2 f_2 & & \sum_{i=1}^{N} f_2 f_n \\ \sum_{i=1}^{N} f_n f_1 & \sum_{i=1}^{N} f_n f_2 & & \sum_{i=1}^{N} f_n f_n \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} f_1 Y_i \\ \sum_{i=1}^{N} f_2 Y_i \\ \vdots \\ \sum_{i=1}^{N} f_n Y_i \end{bmatrix} \qquad (6.2\text{-}7.b)$$

The column vector **a** can be easily solved using the matrix capability of Matlab

$$\mathbf{a} = \mathbf{A}\backslash\mathbf{B} \qquad (6.1\text{-}6)$$

Example 6.2-1

The following data represent the growth in height of a boy from 11 to 21 years of age.

Elapsed time (year)	0 (age 11)	1.4	3.2	4.8	8.0	10.0 (age 21)
Growth (cm)	0	2.25	15.0	26.25	33.0	35.0

Determine a best fit using $f_1(t_i) = \sin\frac{\pi t}{20}$, $f_2(t_i) = \sin\frac{3\pi t}{20}$, and $f_3(t_i) = \sin\frac{5\pi t}{20}$

Solution

The model equation is $y = a_1 \sin\frac{\pi t}{20} + a_2 \sin\frac{3\pi t}{20} + a_3 \sin\frac{5\pi t}{20}$

$\mathbf{a} = [a_1 \ a_2 \ a_3]^{\mathrm{T}}$, $n = 3$, $N = 5$

$$\mathbf{Y} = [2.25\ 15.0\ 26.25\ 33.0\ 35.0]^{\mathrm{T}}$$

The functions $f_1(t_i)$, $f_2(t_i)$, and $f_3(t_i)$ can be evaluated

i	t_i	$f_1(t_i)$	$f_2(t_i)$	$f_3(t_i)$
1	1.4	0.218	0.613	0.891
2	3.2	0.482	0.998	0.588
3	4.8	0.685	0.771	–0.588
4	8.0	0.951	–0.588	0.00
5	10.0	1.00	–1.00	1.00

$$\text{Let } \mathbf{W} = \begin{bmatrix} f_1(t_1) & f_2(t_1) & f_3(t_1) \\ f_1(t_2) & f_2(t_2) & f_3(t_2) \\ \vdots & \vdots & \vdots \\ f_1(t_N) & f_2(t_N) & f_3(t_N) \end{bmatrix} = \begin{bmatrix} 0.218 & 0.613 & 0.891 \\ 0.482 & 0.998 & 0.588 \\ 0.685 & 0.771 & -0.588 \\ 0.951 & -0.588 & 0.00 \\ 1.00 & -1.00 & 1.00 \end{bmatrix}$$

$$\text{then } \mathbf{W^T} = \begin{bmatrix} f_1(t_1) & f_1(t_2) & \cdots & f_1(t_N) \\ f_2(t_1) & f_2(t_2) & \cdots & f_2(t_N) \\ \vdots & \vdots & & \vdots \\ f_n(t_1) & f_n(t_2) & \cdots & f_n(t_N) \end{bmatrix} = \begin{bmatrix} 0.218 & 0.482 & 0.685 & 0.951 & 1.00 \\ 0.613 & 0.998 & 0.771 & -0.588 & -1.00 \\ 0.891 & 0.588 & -0.588 & 0.00 & 1.00 \end{bmatrix}$$

The matrix $\mathbf{A}$ is then evaluated

$$\mathbf{A} = \mathbf{W^T W} = \begin{bmatrix} \sum_{i=1}^{N} f_1 f_1 & \sum_{i=1}^{N} f_1 f_2 & \sum_{i=1}^{N} f_1 f_3 \\ \sum_{i=1}^{N} f_2 f_1 & \sum_{i=1}^{N} f_2 f_2 & \sum_{i=1}^{N} f_2 f_3 \\ \sum_{i=1}^{N} f_3 f_1 & \sum_{i=1}^{N} f_3 f_2 & \sum_{i=1}^{N} f_3 f_3 \end{bmatrix} = \begin{bmatrix} 2.653 & -0.416 & 1.075 \\ -0.416 & 3.312 & -0.321 \\ 1.075 & -0.320 & 2.484 \end{bmatrix}$$

The right hand vector **B** can also be evaluated from $\mathbf{W}^{\mathbf{T}}$

$$\mathbf{B} = \begin{bmatrix} \sum_{i=1}^{N} f_1 Y_i \\ \sum_{i=1}^{N} f_2 Y_i \\ \vdots \\ \sum_{i=1}^{N} f_n Y_i \end{bmatrix} = \mathbf{W}^{\mathbf{T}}\mathbf{Y}$$

$$\mathbf{B} = \begin{bmatrix} 0.218 & 0.482 & 0.685 & 0.951 & 1.00 \\ 0.613 & 0.998 & 0.771 & -0.588 & -1.00 \\ 0.891 & 0.588 & -0.588 & 0.00 & 1.00 \end{bmatrix} \begin{bmatrix} 2.25 \\ 15.0 \\ 26.25 \\ 33.0 \\ 35.0 \end{bmatrix} = \begin{bmatrix} 92.08 \\ -17.816 \\ 30.389 \end{bmatrix}$$

The parameters a_1, a_2, and a_3 are calculated

$a_1 = 35.94$, $a_2 = -1.2067$, and $a_3 = -3.5077$

The model equation is then

$$y = 35.94\sin\frac{\pi t}{20} - 1.2067\sin\frac{3\pi t}{20} + -3.5077\sin\frac{5\pi t}{20}$$

Example 6.2-2

Fit a second order polynomial to the following data

x_i	0.05	0.15	0.46	0.70	0.82	1.17
Y_i	0.956	0.832	0.571	0.378	0.306	0.104

Solution

The model equation is $y = a_1 + a_2\, x + a_3\, x^2$

Therefore $f_1(x_i) = 1$, $f_2(x_i) = x_i$ and $f_3(t_i) = x_i^2$, $\mathbf{a} = [a_1 \;\; a_2 \;\; a_3]^T$, $n = 3$, $N = 6$

$$\mathbf{Y} = \begin{bmatrix} 0.956 \\ 0.832 \\ 0.571 \\ 0.378 \\ 0.306 \\ 0.104 \end{bmatrix}$$

Let $\mathbf{W} = \begin{bmatrix} 1 & 0.05 & 0.05^2 \\ 1 & 0.15 & 0.15^2 \\ 1 & 0.46 & 0.46^2 \\ 1 & 0.70 & 0.70^2 \\ 1 & 0.82 & 0.82^2 \\ 1 & 1.17 & 1.17^2 \end{bmatrix}$

then

$$\mathbf{A} = \mathbf{W^T W} = \begin{bmatrix} 6 & 3.35 & 2.7679 \\ 3.35 & 2.7679 & 2.5968 \\ 2.7679 & 2.5968 & 2.6114 \end{bmatrix}$$

The right hand vector **B** can also be evaluated from $\mathbf{W^T}$

$$\mathbf{B} = \mathbf{W^T Y} = \begin{bmatrix} 3.147 \\ 1.07246 \\ 0.67527 \end{bmatrix}$$

The parameters a_1, a_2, and a_3 are calculated

$a_1 = 0.998$, $a_2 = -1.054$, and $a_3 = 0.248$

The second polynomial is given as

$$y = 0.998 - 1.054x + 0.248x^2$$

Chapter Seven

Errors Measurement

Errors and Uncertainty in Experimental Data

Causes and Types of Errors

Conducting research in any science course is dependent upon obtaining measurements. No measure is ever exact due to errors in instrumentation and measuring skills. If you were to obtain the mass of an object with a digital balance, the reading gives you a measure with a specific set of values. We can assume that the actual measure lies either slightly above or slightly below that reading. The range is the uncertainly of the measurement taken. More accurate instruments have a smaller range of uncertainty. Whenever you take a measurement, the last recorded digit is your estimate. We call digits in a measurement significant figures.

All measurements have inherent uncertainty. We therefore need to give some indication of the reliability of measurements and the uncertainties in the results calculated from these measurements. When processing your experimental results, a discussion of uncertainties should be included. When writing the conclusion to your lab report you should evaluate your experiment and its results in terms of the various types of errors. To better understand the outcome of experimental data an estimate of the size of the systematic errors compared to the random errors should be considered. Random errors are due to the accuracy of the equipment and systematic errors are due to how well the equipment was used or how well the experiment was controlled. We will focus on the types of experimental uncertainty, the expression of experimental results, and a simple method for estimating experimental uncertainty when several types of measurements contribute to the final result.

1. **Random errors**: Precision (Errors inherent in apparatus.)

A random error makes the measured value both smaller and larger than the true value. Chance alone determines if it is smaller or larger. Reading the scales of a balance, graduated cylinder, thermometer, etc. produces random errors. In other words, you can weigh a dish on a balance and get a different answer each time simply due to random errors. They cannot be avoided; they are part of the measuring process. Uncertainties are measures of random errors. These are errors incurred as a result of making measurements

on imperfect tools which can only have certain degree of accuracy. They are predictable, and the degree of error can be calculated. Generally they can be estimated to be half of the smallest division on a scale. For a digital reading such as an electronic balance the last digit is rounded up or down by the instrument and so will also have a random error of ± half the last digit.

2. **Systematic errors**: Accuracy (Errors due to "incorrect" use of equipment or poor experimental design.)

A systematic error makes the measured value always smaller or larger than the true value, but not both. An experiment may involve more than one systematic error and these errors may nullify one another, but each alters the true value in one way only. Accuracy (or validity) is a measure of the systematic error. If an experiment is accurate or valid then the systematic error is very small. Accuracy is a measure of how well an experiment measures what it was trying to measure. These are difficult to evaluate unless you have an idea of the expected value (e.g. a text book value or a calculated value from a data book). Compare your experimental value to the literature value. If it is within the margin of error for the random errors then it is most likely that the systematic errors are smaller than the random errors. If it is larger then you need to determine where the errors have occurred. Assuming that no heat is lost in a calorimetry experiment is a systematic error when a Styrofoam cup is used as a calorimeter. Thus, the measured value for heat gain by water will always be too low. When an accepted value is available for a result determined by experiment, the percent error can be calculated.

Examples of Systemic errors:

- Leaking gas syringes.
- Calibration errors in pH meters.
- Calibration of a balance
- Changes in external influences such as temperature and atmospheric pressure affect the measurement of gas volumes, etc.
- Personal errors such as reading scales incorrectly.
- Unaccounted heat loss.
- Liquids evaporating.
- Spattering of chemicals

Categories of Systematic Errors and how to eliminate them:

a. Personal errors: These errors are the result of ignorance, carelessness, prejudices, or physical limitations on the experimenter. This type of error can be greatly reduced if you are familiar with the experiment you are doing. Be sure to thoroughly read over every lab before you come to class and be familiar with the equipment you are using. **Be Prepared**!!!

b. Instrumental Errors: Instrumental errors are attributed to imperfections in the tools with which the analyst works. For example, volumetric equipment such as burets, pipets, and volumetric flasks frequently deliver or contain volumes slightly different from those indicated by their graduations. Calibration can eliminate this type of error.

c. Method Errors: This type of error many times results when you do not consider how to control an experiment. For any experiment, ideally you should have only one manipulated (independent) variable. Many times this is very difficult to accomplish. The more variables you can control in an experiment the fewer method errors you will have.

Estimating and Reducing Errors through Proper Measurement Technique

- Scientists make a lot of measurements. They measure the masses, lengths, times, speeds, temperatures, volumes, etc.

- When they report a number as a measurement the number of digits and the number of decimal places tell you how exact the measurement is
  - For example: 121 is less exact than 121.5
  - The difference between these two numbers is that a more precise tool was used to measure the 121.5.
  - If a scientist reports a number as 121.5 they are saying that they were able to measure that quantity up to the tenths place.
  - If a scientist reports a number as 121 they are saying that they were able to measure that quantity up to the ones place.

- The total number of digits and the number of decimal points tell you how precise a tool was used to make the measurement.

- Reporting measurements:

a. There are 3 parts to a measurement:

1. The measurement
2. The uncertainty
3. The unit

b. Example: 5.2 ± 0.5 cm

1. Which means you are reasonably sure the actual length is somewhere between 4.7 and 5.7

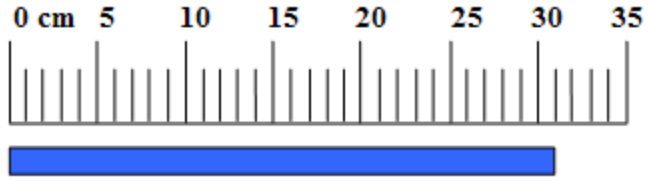
c. No measurement should be written without all three parts.

d. The last digit in your measurement should be an estimate

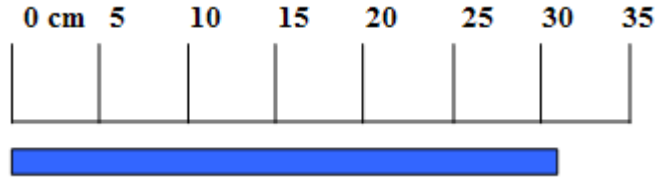
1. If the smallest marks on your tool are .001 apart (as they are on a meter stick that has millimeters marked) then your last digit should be in the ten-thousandths place (i.e. 0.0010)*

**This is true for measurements that donít fluctuate. If the tool you use fluctuates then your estimated digit will probably not be smaller than the smallest hash mark on the tool but should indicate how sure you are of the exactness of your measurement. See below for how to deal with this situation.*

2. Logic:



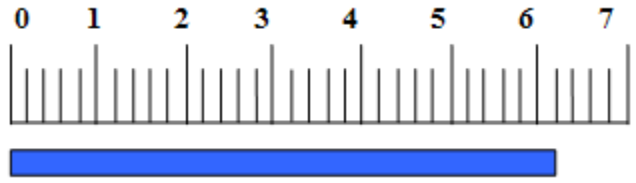
In the above, you would report the length of the bar as 31.0 ± 0.5 cm (assuming the big marks are centimeters). The bar appears to line up with the 31st mark and you know itís more than 1/2 way from the 30 mark and less than 1/2 way from the 32nd mark. So you can be reasonably sure the actual length of the bar is between 30.5 and 31.5 cm.



In the above, you would report the length of the bar as 31 ± 2 cm. You know the bar is longer than 30 cm and the last digit is your best guess. You are reasonably sure the actual bar length is between 30 and 33 cm.

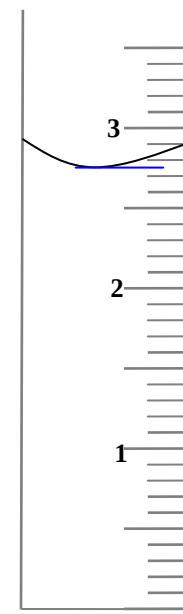
e. The uncertainty is 1/2 the amount between the smallest hash marks. Notice in the above 2 examples that this is the case.

1. This rule may change depending on the book you look at or the teacher you work with.
2. Some uncertainties are determined by the manufacturer. (e.g. electronic balances, probes)
3. Some uncertainties are determined based on what you, as the experimenter decide:



In this case, the divisions between the mark = 0.2 cm which makes estimating a digit trickier. If you say the measurement is right on the 6.2 mark than according to the above rules you should report the measurement as 6.20 cm. However, the uncertainty, according to the rules above is 1/2 the distance between the smallest two marks, or 0.2/2 = 0.1. It doesn't make sense to say 6.20 ± 0.1 cm because your uncertainty is so much bigger than the estimated digit (the zero). So, we need to go back to the most important idea of reporting uncertainties. We need to report a measurement that we are reasonably sure of. I am reasonably sure that the blue bar is bigger than 6.1 cm and less than 6.3, in which case you would report the measurement as 6.2 ± 0.1 cm, but you could also argue that the blue bar is bigger than 6.15 and less than 6.25 cm. In which case, you would report 6.20 ± 0.05 cm. This is where you, as the experimenter, have to make the decision. Consider what another experimenter would get if he/she measured the blue bar again. Consider the implications of stating a too precise number.

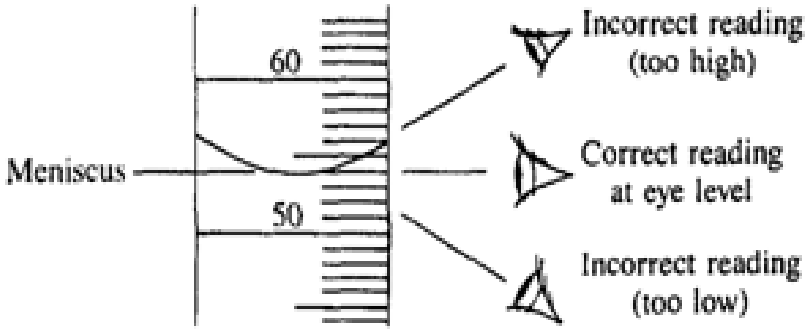
f. from data provided by the manufacture (printed on the apparatus). Temperature probes for example state that the uncertainty is 0.2^{o}C.



g. from the last significant figure in a measurement (as for a digital balance). Since our digital balances measure to .01 g, (or 0.001 g) we assume that the unseen digit is rounded either up or down, so the uncertainty is ± 0.01 g (± 0.001 g)

h. Measurements can sometimes be difficult to determine. The following are some important techniques.

1. When measuring liquids that have a curve at the surface, measure from the bottom of the meniscus. The meniscus is the curve formed at the surface of a liquid due to attraction of the liquid for the sides of the container (adhesion). Measuring from the bottom ñ you should get 2.75 ± 0.05 mL (assuming the marks represent milliliters).



Reading a meniscus. Read the bottom of the meniscus while holding at eye level.

2. Sometimes the measurement on an electronic balance will fluctuate. Start with the numbers that are not fluctuating and then make your best guess as to what the next digit would be. Say for example you are weighing something on a balance and you get the following readings:

1. 12.345
2. 12.320
3. 12.349
4. 12.357
5. 12.327

This should be reported as a measurement of 12.34 ± 0.05. If you use a balance containing a shield the fluctuations will be greatly reduced.

Remember: when reporting measurements, you need to do 3 things

1. give the measurement (the magnitude)

2. tell how good a tool you used to measure it (this is given by the number of significant figures and uncertainty)

3. State the units

Dealing with Uncertainties

Now you know the kinds of errors, random and systematic, that can occur with physical measurements and you should also have a very good idea of how to estimate the magnitude of the random error that occurs when making measurements. Now we can deal with the question, "what do we do with the uncertainties when we add or subtract two measurements? Or divide/multiply two measurements?"

When you mathematically manipulate a measurement you must take into consider the precision. If you add two measurements the result CANNOT be more precise than your measures. It just doesn't make sense. Here's an example.

Let's say you make the following measurements for the mass of a copper weight in a small cylinder:

- Mass of empty container: 2.3 g
- Mass of container with copper: 22.54 g

What is the mass of the copper? 22.54 - 2.3 = 20.24 g
Answer to report: 20.2 g

Why 20.2 g and not 20.24 g?

Since you only measured the container to the tenths place then the 3 is really an estimate. Perhaps the actual value was 2.2 or 2.4 g, then the mass of copper could be (22.54-2.3 or 22.54-2.4) 20.34 or 20.14 g. As you can see the difference in the tenths place is far more significant than the hundredths place. So the mass you should report is 20.2 g

Remember that when making measurements there are three parts to a measurement:

- The measurement
- The uncertainty
- The unit

To take into consideration precision

1. For single measurements
    a. For the measurement ñ use significant figures
    b. For the uncertainty ñ use error propagation
    c. It doesn't make sense to talk about a unit's precision
    d. Once you have the determined the value and uncertainty, make sure the significant figures and uncertainty match.

Resource: Significant figures & Uncertainties

The uncertainty of a calculated value, and therefore the possible random error, can be estimated from uncertainties of individual measurements which are required for that particular calculation. In a calorimetry experiment, for example, the uncertainty in the amount of heat produced depends on the uncertainties in the mass, temperature and specific heat measurements. The estimation of an overall uncertainty from component parts is called Error Propagation.

2. For a set of the trials for which you are finding the average
    a. Use the average and standard deviation for both the measurement and the uncertainty.

Another measure of uncertainty or precision arises when an experiment is repeated many times, yielding several results from which an average value can be calculated. The precision is a measure of how close the results are to the average value. The uncertainty (here called experimental uncertainty) is a measure of how far apart the results are from the average.

This usually is calculated either as the average (and percent average) deviation or as the standard deviation compared to the average of the final results. The average value should always be the average of the final results calculated from each trial, rather than the average of the raw data or results of intermediate calculations. This uncertainty of an experiment is a measure of random error. If the uncertainty is low, then the random error is small.

**You should never take the average of beginning measurements (raw data) or intermediate data. Only final results should be averaged.

Example 1: Standardization of NaOH by titration

The following concentrations, in mol / dm^3, were calculated from the results of three trials:

0.0945, 0.0953, 0.1050

The average value is 0.0983 and the standard deviation is 0.0058

Since uncertainties are meaningful only to one sig. fig., the results should be reported as follows:

Concentration = 0.098 ± 0.006 mol / dm^3

Significant Figures and Rounding Answers:

Every physical measurement is subject to a degree of uncertainty that, at best, can be decreased only to an acceptable level. When numerical data are collected, the values cannot be determined exactly, regardless of the nature of the scale or instrument or the care taken by the operator. If the mass of an object is determined with a digital balance reading to 0.1 g, the actual value lies in a range above and below the reading. This range is the uncertainty of the measurement. Remember every time you take a measurement, the last digit recorded represents a guess. If the same object is measured on a balance reading to 0.001 g the uncertainty is reduced, but can never be completely eliminated.

The term precision is used to describe the reproducibility of results. It can be defined as the agreement between the numerical values of two or more measurements that have been made in an identical fashion.

The terms precision and reliability are inversely related to uncertainty. Where uncertainty is relatively low, precision is relatively high. Every measurement you make in the lab should tell you the magnitude (size) of the object and the precision (reliability) of the instrument used to make the measurement. The number of subdivisions on the instrument can indicate the precision of the instrument.

Error Propagation

In data collection, estimated uncertainties should be indicated for all measurements. These uncertainties may be estimated in different ways:

1. from the smallest division (as for a measuring cylinder)
2. from the last significant figure in a measurement (as for a digital balance)
3. from data provided by the manufacture (printed on the apparatus)

The amount of uncertainty attached to a reading is usually expressed in the same units as the reading. This is then called the Absolute uncertainty. eg. 25.4 ± 0.1 s. The symbol for absolute uncertainty is dx, where x is the measurement:

In the example: x =25.4 and dx = 0.1

The absolute uncertainty is often converted to show a Percentage or Fractional uncertainty. For the above example, this would be: 25.4 ± 0.4% s (0.1 s / 25.4s x 100% = 0.4%). The symbol for fractional uncertainty is: dx/x

**Note that uncertainties are themselves approximate and are not given to more than one significant figure, so the percentage uncertainty here is 0.4%, not 0.39370%.

Multiple Readings

If more than one reading of a measurement is made, then the uncertainty increases with each reading.

Example 3:
For example: 10.0 cm^3 of acid is delivered from a 10cm^3 pipette (± 0.1 cm^3), repeated 3 times. The total volumes delivered is

- 10.0 ± 0.1 cm^3
- 10.0 ±. 0.1 cm^3
- 10.0 ± 0.1 cm^3

Total volume delivered = 30.0 ± 0.3 cm^3

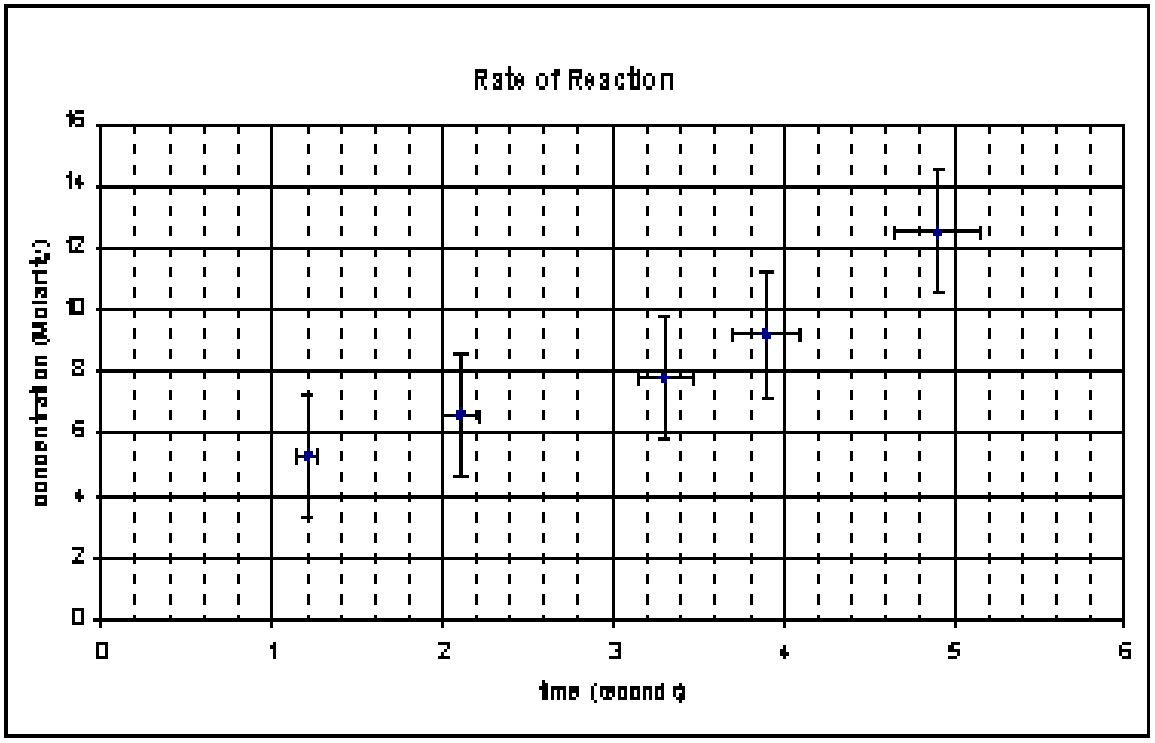
Example 4:
When using a burette ($\pm$ 0.02 cm^3), you subtract the initial volume from the final volume. The volume delivered is:

Final volume = 38.46 $\pm$ 0.05 cm^3
Initial volume = 12.15 $\pm$ 0.05 cm^3
Total volume delivered = 26.31 $\pm$ 0.04 cm^3

Basic rules for propagation of uncertainties

	Rule	Example
1	When adding or subtracting uncertain values, add the absolute uncertainties	Initial temp. = 34.50^{o}C (± 0.05) Final Temp. = 45.21^{o}C (± 0.05) ΔT= 45.21 -34.5 =10.71^{o}C (± 0.05 + 0.05 = ± 0.1^{o}C) ΔT should be reported as 10.7 ± 0.1^{o}C
2	When multiplying or dividing add the percentage uncertainties	Mass = 9.24 g (±0.005g) Volume = 14.1cm3 (±0.05cm3)
	a Make calculations	Density = 9.24/14.1 =0.655 g/cm3
	b Convert absolute uncertainties to percentage/fractional/ relative uncertainties	Mass: 0.005/9.24x100 = 0.054% Vol: 0.05/14.1 x 100 = 0.35 %
	c Add percentage uncertainties	0.054 + 0.35 = 0.40 % Density = 0.655 g/cm^3 (± 0.40%)
	d Convert total uncertainty back to absolute uncertainty	0.655 *0.4/100 = 0.00262 Density = 0.655 ± 0.003 g/cm3
3	Multiplying or dividing by a pure (whole) number: multiply or divide the uncertainty by that number.	4.95 ± 0.05 x 10 = 49.5 ±0.5
4	Powers: … When raising to the nth power, multiply the % uncertainty by n. … When extracting the nth root, divide the % uncertainty by n.	(4.3 ± .5 cm)^3 = 4.33 ± (.5/4.3)*3 = 79.5 cm^3 (± 0.349%) = 79.5 ± 0.3 cm^3

5	Formulas: Follow the order of operations: find uncertainties for numbers added and subtracted. Use that new uncertainty when calculating uncertainty for multiplication and division portion of formula, etc. This can be very complex. See example below.
	Graphing Graphing is an excellent way to average a range of values. When a range of values is plotted each point should have error bars drawn on it. The size of the bar is calculated from the uncertainty due to random errors. Any line that is drawn should be within the error bars of each point. If it is not possible to draw a line of "best" fit within the error bars then the systematic errors are greater than the random errors.



Example of Error Propagation with Formula

1. A student performs an experiment to determine the specific heat of a sample of metal. 212.01 g of the metal at 95.5^{o}C was placed into 150.25 g of 25.2 ^{o}C water in the calorimeter. The temperature of the water went to 27.5^{o}C. Given: CH_2O = 4.18 J/g-^{o}C. The thermometer was marked in 1 ^{o}C increments and the balance was digital.

a. Calculate the specific heat of the metal Cm using the following equation:

b. Calculate the uncertainty in the

i. Temperature

(absolute uncertainty is ‡ distance between smallest mark, for this thermometer which measures to the nearest *f*C, uncertainty is 0.5^{o}C)

1. Tf = 27.5 ± 0.5 ^{o}C
2. Ti (H2O) = 25.2 ± 0.5 ^{o}C
3. Ti (metal) = 95.5 ± 0.5 oC
4. ΔT (H_2O) = (27.5-25.2) ± (0.5 + 0.5) = 4.3 ± 1 ^{o}C % =1/4.3*100 =23%
5. ΔT (metal) = (95.5-27.5) ± (0.5 + 0.5) = 68 ± 1 ^{o}C % =1/68*100 =1.5%

ii. Mass

(absolute uncertainty for electronic balance half of smallest decimal place)

1. H_2O = 150.25 ± 0.05 g %=.033%
2. metal = 212.01 ± 0.05 g %=.024%

iii. specific heat capacity

1. assume there is no uncertainty in numbers used as constants. So no uncertainty in water's specific heat capacity.
2. (metal) add % uncertainties for all quantities involved in the calculation of the heat capacity

0.033 + 23 + .024 + 1.5 = 24.6 %

0.1002 J/g-^{o}C (±24.6%) = .10 ± .02 J/g-^{o}C

c. Calculate the percent error if the literature value is 0.165 J/g-^{o}C.

d. Comment on the error. Is the uncertainty greater or less than the percent error? Is the error random or systemic? Explain

Since percent error is much greater than the uncertainty and the literature value does not fall in the range of uncertainty (.10 ± 0.02 J/g-^{o}C), than systematic errors is a problem. Random error is estimated by the uncertainty and since this is smaller than the percent error, systematic errors are at work and are making the measured data inaccurate.

Measuring Errors

In any numerical analysis, errors will arise during the calculations. To be able to deal with the issue of errors, we need to

(A) identify where the error is coming from, followed by

(B) quantifying the error, and lastly

(C) minimize the error as per our needs.

In this chapter, we will concentrate on item (B), that is, how to quantify errors.

Q: What is true error?

A: True error denoted by E_t is the difference between the true value (also called the exact value) and the approximate value.

True Error = True value – Approximate value

Example 1

The derivative of a function $f(x)$ at a particular value of x can be approximately calculated by

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

of $f'(2)$ For $f(x) = 7e^{0.5x}$ and $h = 0.3$, find

a) the approximate value of $f'(2)$

b) the true value of $f'(2)$

c) the true error for part (a)

Solution

a) $f'(x) \approx \dfrac{f(x+h) - f(x)}{h}$

For $x = 2$ and $h = 0.3$,

$$f'(2) \approx \frac{f(2+0.3) - f(2)}{0.3}$$

$$= \frac{f(2.3) - f(2)}{0.3}$$

$$= \frac{7e^{0.5(2.3)} - 7e^{0.5(2)}}{0.3}$$

$$= \frac{22.107 - 19.028}{0.3}$$

$$= 10.265$$

b) The exact value of $f'(2)$ can be calculated by using our knowledge of differential calculus.

$$f(x) = 7e^{0.5x}$$

$$f'(x) = 7 \times 0.5 \times e^{0.5x}$$

$$= 3.5e^{0.5x}$$

So the true value of $f'(2)$ is

$$f'(2) = 3.5e^{0.5(2)}$$

$$= 9.5140$$

c) True error is calculated as

E_t = True value – Approximate value

$$= 9.5140 - 10.265$$

$$= -0.75061$$

The magnitude of true error does not show how bad the error is. A true error of $E_t = -0.722$ may seem to be small, but if the function given in the Example 1 were $f(x) = 7 \times 10^{-6} e^{0.5x}$, the true error in calculating $f'(2)$ with $h = 0.3$, would be

$E_t = -0.75061 \times 10^{-6}$. This value of true error is smaller, even when the two problems are similar in that they use the same value of the function argument, $x = 2$ and the step size, $h = 0.3$. This brings us to the definition of relative true error.

Q: What is relative true error?

A: Relative true error is denoted by $\in_t$ and is defined as the ratio between the true error and the true value.

$$\text{Relative True Error} = \frac{\text{True Error}}{\text{True Value}}$$

Example 2

The derivative of a function $f(x)$ at a particular value of x can be approximately calculated by

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

For $f(x) = 7e^{0.5x}$ and $h = 0.3$, find the relative true error at $x = 2$.

Solution

From Example 1,

E_t = True value – Approximate value

$= 9.5140 - 10.265$

$= -0.75061$

Relative true error is calculated as

$$\in_t = \frac{\text{True Error}}{\text{True Value}}$$

$$= \frac{-0.75061}{9.5140}$$

$$= -0.078895$$

Relative true errors are also presented as percentages. For this example,

$$\in_t = -0.0758895 \times 100\%$$

$$= -7.58895\%$$

Absolute relative true errors may also need to be calculated. In such cases,

$$|\in_t| = |-0.075888|$$

$$= 0.0758895$$

$$= 7.58895\%$$

Q: What is approximate error?

A: In the previous section, we discussed how to calculate true errors. Such errors are calculated only if true values are known. An example where this would be useful is when one is checking if a program is in working order and you know some examples where the true error is known. But mostly we will not have the luxury of knowing true values as why you would want to find the approximate values if you know the true values. So when we are solving a problem numerically, we will only have access to approximate values. We need to know how to quantify error for such cases.

Approximate error is denoted by E_a and is defined as the difference between the present approximation and previous approximation.

Approximate Error = Present Approximation – Previous Approximation

Example 3

The derivative of a function $f(x)$ at a particular value of x can be approximately calculated by

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

For $f(x) = 7e^{0.5x}$ and at $x = 2$, find the following

a) $f'(2)$ using $h = 0.3$

b) $f'(2)$ using $h = 0.15$

c) approximate error for the value of $f'(2)$ for part (b)

Solution

a) The approximate expression for the derivative of a function is

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

For $x = 2$ and $h = 0.3$,

$$f'(2) \approx \frac{f(2+0.3) - f(2)}{0.3}$$

$$= \frac{f(2.3) - f(2)}{0.3}$$

$$= \frac{7e^{0.5(2.3)} - 7e^{0.5(2)}}{0.3}$$

$$= \frac{22.107 - 19.028}{0.3}$$

$$= 10.265$$

b) Repeat the procedure of part (a) with $h = 0.15$,

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

For $x = 2$ and $h = 0.15$,

$$f'(2) \approx \frac{f(2+0.15)-f(2)}{0.15}$$

$$= \frac{f(2.15)-f(2)}{0.15}$$

$$= \frac{7e^{0.5(2.15)} - 7e^{0.5(2)}}{0.15}$$

$$= \frac{20.50 - 19.028}{0.15}$$

$$= 9.8799$$

c) So the approximate error, E_a is

$$E_a = \text{Present Approximation} - \text{Previous Approximation}$$

$$= 9.8799 - 10.265$$

$$= -0.38474$$

The magnitude of approximate error does not show how bad the error is . An approximate error of $E_a = -0.38300$ may seem to be small; but for $f(x) = 7 \times 10^{-6} e^{0.5x}$, the approximate error in calculating $f'(2)$ with $h = 0.15$ would be $E_a = -0.38474 \times 10^{-6}$. This value of approximate error is smaller, even when the two problems are similar in that they use the same value of the function argument, $x = 2$, and $h = 0.15$ and $h = 0.3$. This brings us to the definition of relative approximate error.

Q: What is relative approximate error?

A: Relative approximate error is denoted by $\in_a$ and is defined as the ratio between the approximate error and the present approximation.

$$\text{Relative Approximate Error} = \frac{\text{Approximate Error}}{\text{Present Approximation}}$$

Example 4

The derivative of a function $f(x)$ at a particular value of x can be approximately calculated by

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

For $f(x) = 7e^{0.5x}$, find the relative approximate error in calculating $f'(2)$ using values from $h = 0.3$ and $h = 0.15$.

Solution

From Example 3, the approximate value of $f'(2) = 10.263$ using $h = 0.3$ and $f'(2) = 9.8800$ using $h = 0.15$.

$$E_a = \text{Present Approximation} - \text{Previous Approximation}$$
$$= 9.8799 - 10.265$$
$$= -0.38474$$

The relative approximate error is calculated as

$$\in_a = \frac{\text{Approximate Error}}{\text{Present Approximation}}$$
$$= \frac{-0.38474}{9.8799}$$
$$= -0.038942$$

Relative approximate errors are also presented as percentages. For this example,

$$\in_a = -0.038942 \times 100\%$$
$$= -3.8942\%$$

Absolute relative approximate errors may also need to be calculated. In this example

$$|\in_a| = |-0.038942|$$
$$= 0.038942 \text{ or } 3.8942\%$$

Q: While solving a mathematical model using numerical methods, how can we use relative approximate errors to minimize the error?

A: In a numerical method that uses iterative methods, a user can calculate relative approximate error $\in_a$ at the end of each iteration. The user may pre-specify a minimum acceptable tolerance called the pre-specified tolerance, $\in_s$. If the absolute relative approximate error $\in_a$ is less than or equal to the pre-specified tolerance $\in_s$, that is, $|\in_a| \leq \in_s$, then the acceptable error has been reached and no more iterations would be required.

Alternatively, one may pre-specify how many significant digits they would like to be correct in their answer. In that case, if one wants at least m significant digits to be correct in the answer, then you would need to have the absolute relative approximate error, $|\in_a| \leq 0.5 \times 10^{2-m}$ %.

Example 5

If one chooses 6 terms of the Maclaurin series for e^x to calculate $e^{0.7}$, how many significant digits can you trust in the solution? Find your answer without knowing or using the exact answer.

Solution

$$e^x = 1 + x + \frac{x^2}{2!} + \text{.....}$$

Using 6 terms, we get the current approximation as

$$e^{0.7} \cong 1 + 0.7 + \frac{0.7^2}{2!} + \frac{0.7^3}{3!} + \frac{0.7^4}{4!} + \frac{0.7^5}{5!}$$

$$= 2.0136$$

Using 5 terms, we get the previous approximation as

$$e^{0.7} \cong 1 + 0.7 + \frac{0.7^2}{2!} + \frac{0.7^3}{3!} + \frac{0.7^4}{4!}$$

$$= 2.0122$$

The percentage absolute relative approximate error is

$$|\in_a| = \left|\frac{2.0136 - 2.0122}{2.0136}\right| \times 100$$

$$= 0.069527\%$$

Since $|\in_a| \le 0.5 \times 10^{2-2}\%$, at least 2 significant digits are correct in the answer of

$$e^{0.7} \cong 2.0136$$

Q: But what do you mean by significant digits?

A: Significant digits are important in showing the truth one has in a reported number. For example, if someone asked me what the population of my county is, I would respond, "The population of the Hillsborough county area is 1 million". But if someone was going to give me a $100 for every citizen of the county, I would have to get an exact count. That count would have been 1,079,587 in year 2003. So you can see that in my statement that the population is 1 million, that there is only one significant digit, that is, 1, and in the statement that the population is 1,079,587, there are seven significant digits. So, how do we differentiate the number of digits correct in 1,000,000 and 1,079,587? Well for that, one may use scientific notation. For our data we show

$$1{,}000{,}000 = 1 \times 10^6$$

$$1{,}079{,}587 = 1.079587 \times 10^6$$

to signify the correct number of significant digits.

Example 5

Give some examples of showing the number of significant digits.

Solution

a) 0.0459 has three significant digits

b) 4.590 has four significant digits

c) 4008 has four significant digits

d) 4008.0 has five significant digits

e) 1.079×10^{3} has four significant digits

f) 1.0790×10^{3} has five significant digits

g) 1.07900×10^{3} has six significant digits