INTERPOLATION AND LEAST-SQUARES

CONTENT

	Page
1.1 INTRODUCTION	1
1.2 DIFFERENCE TABLE	4
1.3 NEWTON-GREGORY POLYNOMIALS	16
1.4 NEWTON'S DIVIDED DIFFERENCE	30
1.5 LAGRANGE POLYNOMIALS	38
1.6 2-D INTERPOLATION	49
1.7 LEAST SQUARES METHODS	54
1.8 SUMMARY.....	72

12 EXAMPLES INCLUDED

1.1 INTRODUCTION

- You may require estimates at points between the calculated discrete values.

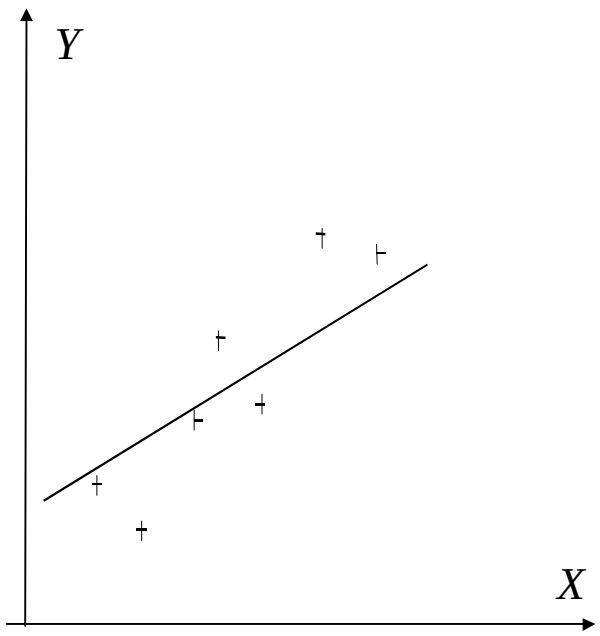
  For e.g. in numerical modelling of deep beam, plane stress elements are used. The displacements and strains are worked out at the internal points known as Gaussian points. These values are then *interpolated* to the corner nodes and mid-side nodes.

- You may require a simplified version of a complicated function.

- You may require to provide a statistical equation to a group of data.

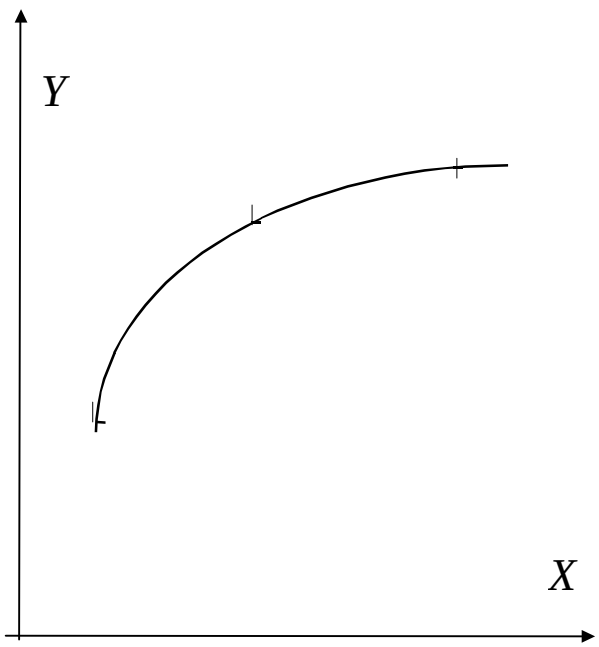
Basically, there are two approaches to numerical analysis of data, depending on the data themselves.

Firstly, where the data themselves inherit significant degree of error, we derive a single curve that represents the general trend of the data. This is a statistical approach.



This type of analysis is known as least-squares regression.

Secondly, where the data are known to be very accurate, we fit a curve that passes directly through each of the points. This is interpolation which we shall cover first.



Interpolation can be used to obtain intermediate values from discrete data points. Interpolation is also relevant to **Numerical Integration** and **Numerical Solution of O.D.E.**

These topics will be covered in later part of the course. In fact, interpolation forms the backbone of Numerical Methods.

1.2 DIFFERENCE TABLE

EXAMPLE 1: POLYNOMIAL FUNCTION

The difference table for a polynomial function e.g. $f(x) = x^3$ is shown below. What do you notice ?

x_i	$f(x_i)$	Df	D^2f	D^3f	D^4f
-3	-27				
		19			
-2	-8		-12		
		7		6	
-1	-1		-6		0
		1		6	
0	0		0		0
		1		6	
1	1		6		0
		7		6	
2	8		12		
		19			
3	27				

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

where Δ = forward difference operator

Note: For a 3rd degree polynomial, the 3rd order differences are constant.

Corollary:

- If the nth order differences are constant, we can approximate $f(x)$ by an nth degree polynomial function $P_n(x)$.

EXAMPLE 2: NON-POLYNOMIALS

The difference table for a non-polynomial function, e.g. $f(x) = 1/x$, is shown below. What can you infer from the difference columns ?

x	$f(x)$	Df	D^2f	D^3f
1.0	1.0000			
		-0.1667		
1.2	0.8333		0.0477	
		-0.1190		-0.0180
1.4	0.7143		0.0297	
		-0.0893		-0.0098
→1.6	0.6250		0.0199	
		-0.0694		-0.0061
1.8	0.5556		0.0138	
		-0.0556		
2.0	0.5000			

Note: 3rd order differences fluctuate wildly, although the values are small.

***Corollaries*:**

- For non-polynomial functions, the nth order of differences may be small as n increases, but the differences themselves will not be constant.

- If the nth order differences are constant, the underlying function must be a **polynomial** of degree n.

NOTATIONS FOR DIFFERENCES

Forward differences:

A polynomial function can be written in two forms:

(a) $P_n(x) = a_o + a_1 x + a_2 x^2 + \ldots + a_n x^n$

(evenly-spaced data)

(b) $P_n(x) = a_o + a_1 (x-x_o) + a_2 (x-x_o)(x-x_1) + \ldots$

$+ a_n x^n (x-x_o)(x-x_1) .. (x-x_{n-1})$

(unevenly-spaced data)

x	$f(x)$	1st	2nd	3rd	4th
x_{-2}	f_{-2}				
		Df_{-2}			
x_{-1}	f_{-1}		D^2f_{-2}		
		Df_{-1}		D^3f_{-2}	
x_o	f_o		D^2f_{-1}		D^4f_{-2}
		Df_o		D^3f_{-1}	
x_1	f_1		D^2f_o		
		Df_1			
x_2	f_2				

Note: $D f_{-2} = f_{-1} - f_{-2}$,

$$D^2 f_{-2} = D f_{-1} - D f_{-2}$$

$$D f_{-1} = f_o - f_{-1} ,$$

$$D^2 f_{-1} = D f_o - D f_{-1}$$

Generally,

$$Df_m = f_{m+1} - f_m$$

$$D^2 f_m = Df_{m+1} - Df_m$$

From Eg.2, if we choose the starting point

$$x_o = 1.6,$$

$$f_o = 0.6250$$

$$Df_o = -0.0694$$

$$D^2 f_o = 0.0138$$

EXAMPLE 3: EFFECT OF ERRORS IN *X*

x	$f(x)$	Df	D^2f	D^3f	D^4f
0	1				
		32			
2	33		160		
		192		133	
4	225		293		44
		485		177	
6	710		470		-66
		955		111	
8	1665		581		44
		1536		155	
10	3201		736		-11
		2272		144	
12	5473		880		0
		3152		144	
14	8625		1024		
		4176			
16	12801				

If one of the x data in the difference table is wrong, but we know that the underlying function is cubic degree beforehand, from the difference columns, we may be able to *undo* the error, and find the correct value for x.

(For comparison purpose, the actual function is $3x^3 + 2x^2 + 1$.)

- We would need at least one of the elements in the fourth order difference to be zero.

- Then we can perform a "reverse engineering" to back calculate the third order differences which should be constant.

- Working from the third order differences, we proceed to the second order differences and so forth, and finally zoom in on the wrong x.

- All these are only possible, if we already know the degree of the underlying function.

x	$f(x)$	Df	D^2f	D^3f	D^4f
				144	
			304		0
		496		144	
6	721		448		0
		944		144	
			592		0
				144	
					0

Notations for differences.

$$D^2 f_i = D(Df_i) = D(f_{i+1} - f_i)$$

$$= Df_{i+1} - Df_i$$

$$= f_{i+2} - f_{i+1} - (f_{i+1} - f_i)$$

\ $$D^2 f_i = f_{i+2} - 2f_{i+1} + f_i$$

Verify $D^3 f_i = f_{i+3} - 3f_{i+2} + 3f_{i+1} - f_i$

The coefficients can be obtained from the Pascal Triangle analogy:

				+1					
		+1		-2		+1			Δ^2
	+1		-3		+3		-1		Δ^3
+1		-4		+6		-4		+1	Δ^4

Forward Difference method

$$Df_i = f_{i+1} - f_i$$

$$D^2 f_i = D\,(Df_i) \qquad \text{etc. etc.}$$

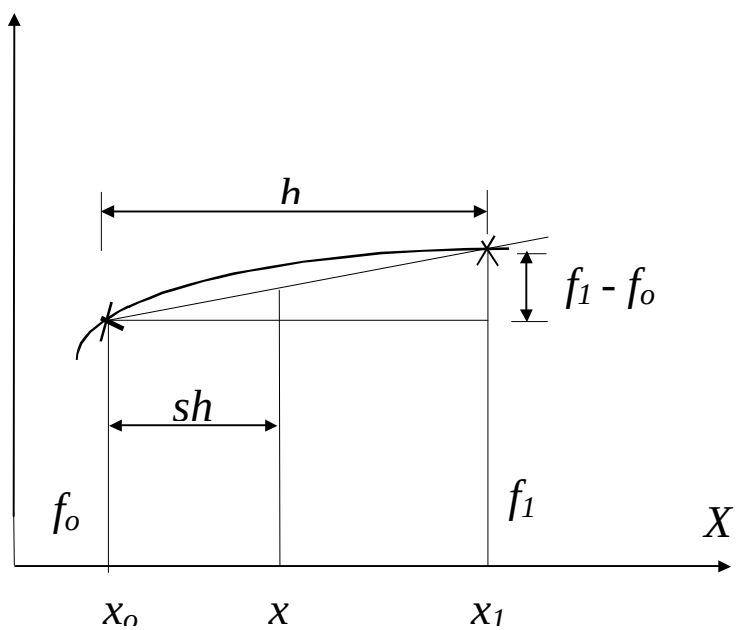
Homework:

Verify $D^4 f_i = f_{i+4} - 4f_{i+3} + 6f_{i+2} - 4\,f_{i+1} + f_i$

1.3 NEWTON-GREGORY POLYNOMIALS

It is noteworthy that the Newton-Gregory method applies to only evenly spaced data, i.e. *x* with uniform increment. For unevenly spaced data, we need to use Newton divided difference.

Linear Interpolation



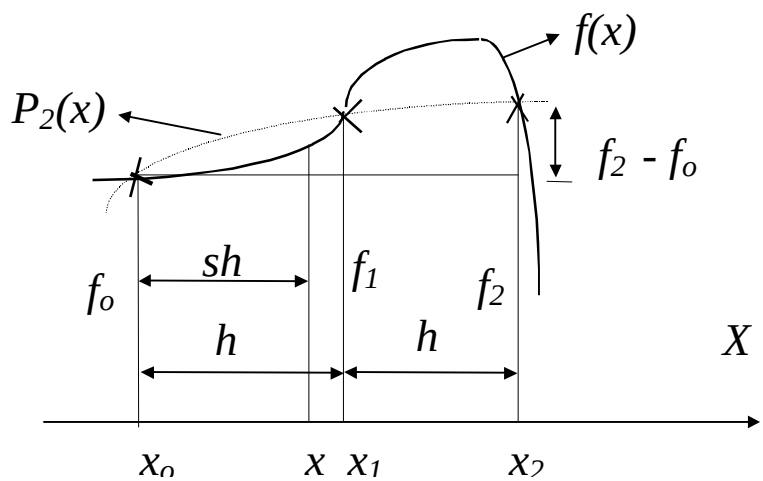
The curve $f(x)$ is approximated by a CHORD at two adjacent x-values, x_o and x_1.

Using Similar Triangle, $f(x)$ can be approximated by a linear function $P_1(x)$:

$$
\begin{aligned}
f(x) \approx \quad & P_1(x) \\
= \quad & f_o + (x - x_o)/h \quad (f_1 - f_o) \\
= \quad & f_o + s\, Df_o
\end{aligned}
$$

where $s = \dfrac{x - x_o}{h}$

Quadratic Interpolation (evenly-spaced data)



This time, $f(x)$ is approximated by a quadratic function $P_2(x)$, passing through three points (x_o, f_o), (x_1, f_1) and (x_2, f_2).

$$f(x) \;\; » \;\; P_2(x) \;\; = \;\; f_o + \; s\,Df_o + \frac{s(s-1)}{2}\,\Delta^2 f_o$$

where $\quad s \;=\; \dfrac{x - x_o}{h}$

At $x = x_o$, $s = 0$,

$P_2(x_o) = f_o$

At $x = x_1$, $s = 1$,

$P_2(x_1) = f_o + D f_o = f_1$

At $x = x_2$, $s = 2$,

$P_2(x_2) = f_o + 2D f_o + D^2 f_o$

$= f_1 + D f_1 = f_2$

(Note: $\Delta^2 f_o = \Delta f_1 - \Delta f_o$)

Newton-Gregory Forward Interpolation Formula

$$P_n(x) = f_o + s D f_o + \frac{s(s-1)}{2!} D^2 f_o + \ldots\ldots$$

$$= f_o + \binom{s}{1} D f_o + \binom{s}{2} D^2 f_o + \ldots\ldots$$

EXAMPLE 4: EXACT INTERPOLATION

In this example, we are trying to find a suitable polynomial function which *fits exactly* with the data in the table.

x	$f(x)$	Df	D^2f	D^3f	D^4f
0	0				
		1			
1	1		12		
		13		12	
2	14		24		0
		37		12	
3	51		36		0
		73		12	
4	124		48		
		121			
5	245				

Using cubic forward interpolation

$$P_3(x) = f_o + sD f_o + \frac{s(s-1)}{2!} D^2 f_o$$

$$+ \frac{s(s-1)(s-2)}{3!} D^3 f_o$$

Choose $x_o = 0$, $s = (x/1) = x$

$$P_3(x) = 0 + x.1 + \frac{x(x-1)}{2} . 12 +$$

$$\frac{x(x-1)(x-2)}{6} . 12$$

$$= 2x^3 - x$$

***Corollaries*:**

- If $f_n(x)$ can be exactly approximated by $P_n(x)$ (i.e. it requires n^{th} degree polynomial), then there is one and only one $P_n(x)$ that fits $f_n(x)$ - this comes from the *Uniqueness Theorem*.

- In this particular case, the starting point x_o can be *arbitrarily* chosen because $P_n(x) = f_n(x)$ for all values of x.

EXAMPLE 5: FINDING THE STARTING POINT

Find $f(3.2)$ in Eg. 4 using quadratic interpolation ($n = 2$). We need to locate x_o (starting point) if we use a lower degree of interpolation than the required one for exact matching.

Forward Interpolation

A quadratic curve will pass through 3 points (x_o, y_o), (x_1, y_1), and (x_2, y_2). To minimise errors, fit the mid point as close to $x = 3.2$ as possible. In this case we choose $x_1 = 3$, thus , $x_o = 2$.

$$\therefore \qquad s = \frac{3.2 - 2}{1.0} = 1.2$$

Thus, $f(3.2) \;\text{»}\; f_o + s\,D\,f_o + \dfrac{s(s-1)}{2} D^2 f_o$

$$= 14 + 1.2(37) + \frac{(1.2)(0.2)}{2}\, 36$$

$$= 62.72 \text{ (cf. to 62.336 from } f(x) = 2x^3 - x \text{)}$$

$$Error \;\; Term = \frac{s(s-1)(s-2)}{6}\, 12 = -0.384$$

Truncation Errors

Recall Newton-Gregory forward difference:

$$f(x) \;\text{»}\; f_o + sD f_o + \frac{s(s-1)}{2!}D^2 f_o + \;....\; +$$

$$\frac{s(s-1)...(s-n+1)}{n!}\, D^n f_o$$

Error involved in the case of a function *f(x)* that is at least *(n+1)* times continuously differentiable is

$$e_n(x) \qquad = \qquad f(x) - P_n(x)$$

$$= \frac{s\,(s-1)\,\Lambda\;\;(s-n+1)\,(s-n)}{(n+1)!}.h^{n+1} f^{\,n+1}(x)$$

where ξ lies between x_o and x_n.

Corollaries

- Error $e_n(x)$ is of the order of magnitude of the next difference not used in $P_n(x)$.

- One should choose x_o, x_1 ... x_n such that the value x at which one interpolates is *as well centred as possible among* x_o, ... x_n given in the Table.

- We can approximate the error term $f^{n+1}(x)$ by $\dfrac{\Delta^{n+1} f(x)}{h^{n+1}}$

EXAMPLE 6: FINDING BEST ESTIMATE

Find the best estimates and the associated truncation errors of $f(0.8)$ using Newton Gregory forward difference formula via:

(a) quadratic interplation.

(b) cubic interpolation.

x	$f(x)$	Df	D^2f	D^3f	D^4f
0.1	0.09983				
		0.37960			
0.5	0.47943		-0.07570		
		0.30390		-0.04797	
0.9	0.78333		-0.12367		0.01951
		0.18023		-0.02846	
1.3	0.96356		-0.15213		
		0.02810			
1.7	0.99166				

(a) Quadratic interpolation

3 points are required $(x_o, \ f_o)$, $(x_1, \ f_1)$ and $(x_2, \ f_2)$ for $n = 2$..

Choose $x_1 = 0.9 \Rightarrow x_o = 0.5$

$$s = \frac{x - x_o}{h} = \frac{0.8 - 0.5}{0.4} = 0.75$$

$$f(x) \;\; » \;\; f_o + sD f_o + \frac{s(s-1)}{2!} D^2 f_o + \;....$$

$$f(0.8) \;\; » 0.47943 + 0.30390(0.75) +$$

$$\frac{(-0.12367)(0.75)(-0.25)}{2!}$$

$$= 0.71895$$

$$e_2(x) = \frac{s(s-1)(s-2)}{3!}(-0.02846)$$

$$= -0.00111$$

(b) Cubic interpolation

4 points are required i.e. (x_o, f_o), (x_1, f_1), (x_2, f_2) and (x_3 , f_3).

Locate x = 0.8 between $x_1 = 0.5$ and $x_2 = 0.9$.

$$\Rightarrow \qquad x_o = 0.1$$

$$\therefore \quad s = \frac{0.8 - 0.1}{0.4} = 1.75$$

$$f(x) \quad » \quad f_o + sD f_o + \frac{s(s-1)}{2!} D^2 f_o +$$

$$\frac{s(s-1)\,(s-2)}{3!} D^3 f_o$$

$$f(0.8) = 0.09983 + 1.75\,(0.3796)$$

$$+\frac{(1.75)(0.75)(-0.0757)}{2}$$

$$+\frac{1.75\,(0.75)(-0.25)}{6}(-\,0.04797)$$

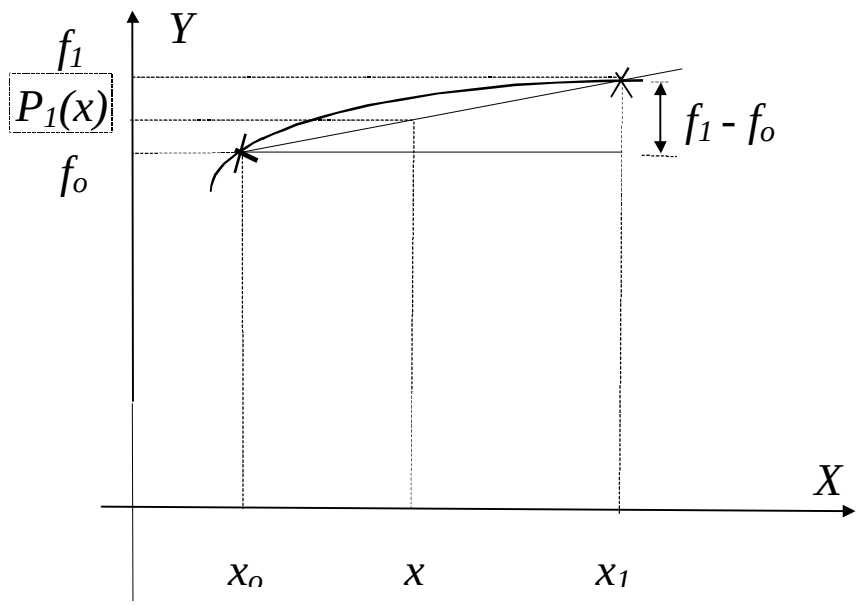
$$= 0.71707$$

$$e_3(x) = \frac{s(s-1)(s-2)(s-3)}{4!}(0.01951)$$

$$= 0.00033$$

1.4 NEWTON'S DIVIDED DIFFERENCE

Linear Interpolation



- Simplest form of divided difference.
- Identical with Newton-Gregory linear interpolation.
- The data need not be evenly spaced, but the formula can still be applied to evenly - spaced data.

$$\frac{f_1 - f_o}{x_1 - x_o} = \frac{P_1(x) - f_o}{x - x_o}$$

Rearranging, $$P_1(x) = f_o + \frac{(f_1 - f_o)}{(x_1 - x_o)}(x - x_o)$$

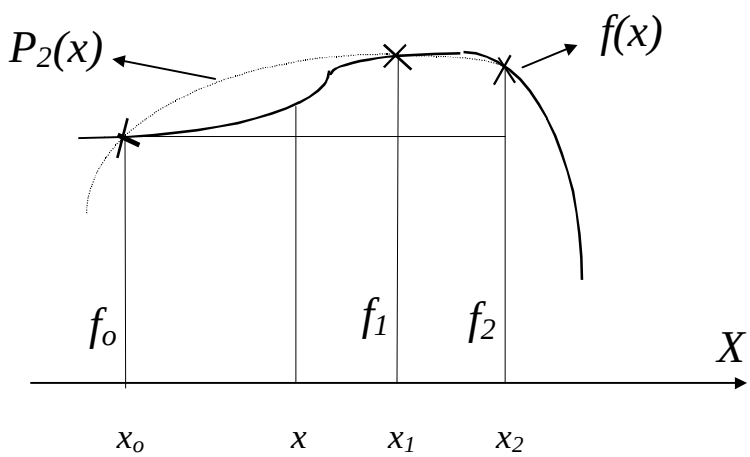
or symbolically $P_1(x) = f_o + f[x_o , x_1] (x - x_o)$

where $$f[x_o , x_1] = \frac{f_1 - f_o}{x_1 - x_o}$$

Quadratic Interpolation

To improve the accuracy of interpolation, we introduce some curvature into the line connecting the data points. In this case, three data points are required.

$$P_2(x) = b_o + b_1(x - x_o) + b_2(x - x_o)(x - x_1)$$



To determine the values of b_o, b_1 and b_2, we need to use the corresponding values of $f(x)$ at $x = x_o$, x_1 *and* x_2.

At $x = x_o$ $\quad b_o = f_o$

At $x = x_1$ $\quad b_1 = \dfrac{f_1 - f_o}{x_1 - x_o} = f[x_o, x_1]$

At $x = x_2$,

$$b_2 = \frac{f_2 - f_o - \dfrac{(f_1 - f_o)(x_2 - x_o)}{x_1 - x_o}}{(x_2 - x_o)(x_2 - x_1)}$$

$$b_2 = \frac{(f_2 - f_o)(x_1 - x_o) - (f_1 - f_o)(x_2 - x_o)}{(x_2 - x_o)(x_2 - x_1)(x_1 - x_o)}$$

$$= \frac{(f_2 - f_1)(x_1 - x_o) - (f_1 - f_o)(x_2 - x_1)}{(x_2 - x_o)(x_2 - x_1)(x_1 - x_o)}$$

$$b_2 = \frac{\dfrac{(f_2 - f_1)}{x_2 - x_1} - \dfrac{(f_1 - f_o)}{x_1 - x_o}}{x_2 - x_o}$$

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

$$= f[x_o , x_1 , x_2]$$

Thus, if

$$P_n(x) = b_o + b_1 (x - x_o) + \ldots + b_n (x - x_o).(x - x_{n-1})$$

then $b_o = f_o$

$b_1 = f[x_o , x_1]$

$b_n = f[x_o , x_1 , \ldots x_n]$

EXAMPLE 7: NEWTON'S DIVIDED DIFFERENCE

To help us better understand the use of divided difference table, the following example is used:

x_i	f_i	$f[x_i,x_{i+1}]$	$f[x_i ,..x_{i+2}]$	$f[x_i ..x_{i+3}]$	$f[x_i ...x_{i+4}]$
3.2	22.000				
		8.400			
2.7	17.800		2.856		
		2.118		-0.528	
1.0	14.200		2.012		0.256
		6.342		0.086	
4.8	38.300		2.263		
		16.750			
5.6	51.700				

A polynomial of 3rd degree that fits in between $x_o = 3.2$ and $x_3 = 4.8$ is given by :

$$P_3(x) = 22 + 8.400(x - 3.2)$$

$$+ 2.856(x - 3.2)(x - 2.7)$$

$$-0.528(x - 3.2)(x - 2.7)(x - 1.0).$$

The 4th degree polynomial function would be :

$$P_4(x) = P3(x) + 0.256(x - x_o)(x - x_1)(x - x_2)(x - x_3)$$

$$P_4(x) = P3(x) + 0.256(x-3.2)(x-2.7)(x-1.)(x-4.8).$$

Corollaries:

- If the true underlying function is an nth degree polynomial, then the nth degree polynomial will yield exact results, based on $(n+1)$ data points.

- For an nth degree polynomial to approximate $(n+1)^{th}$ degree, the associated error term is:

$$e_n(x) = \frac{f^{n+1}(x)}{(n+1)!}(x - x_o)(x - x_1) \ldots (x - x_n)$$

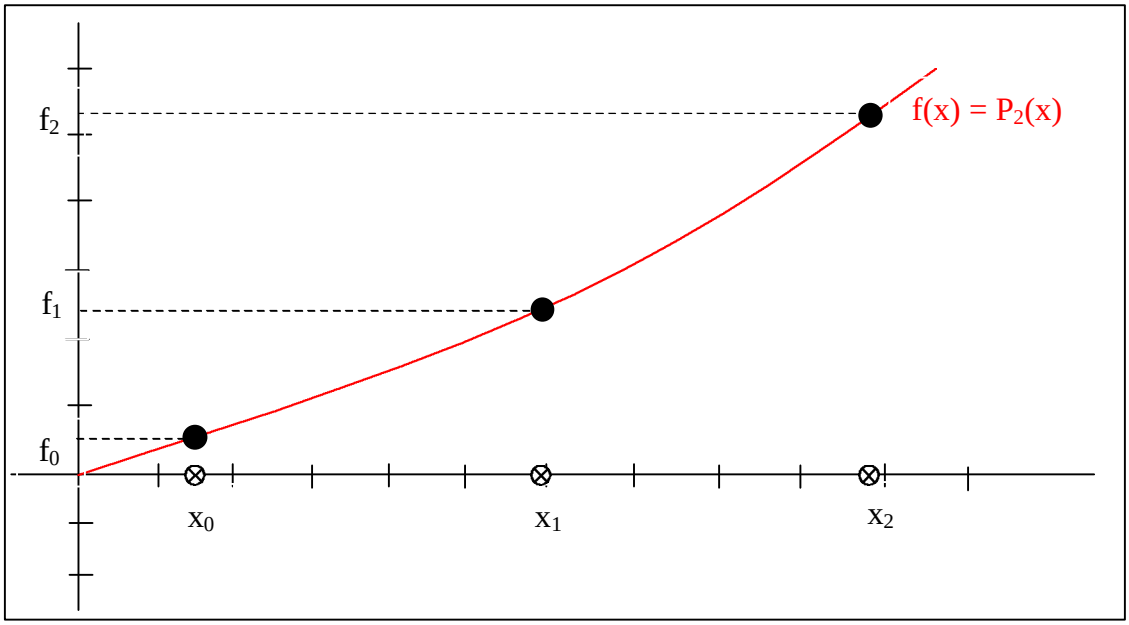
where $x_o < x < x_n$

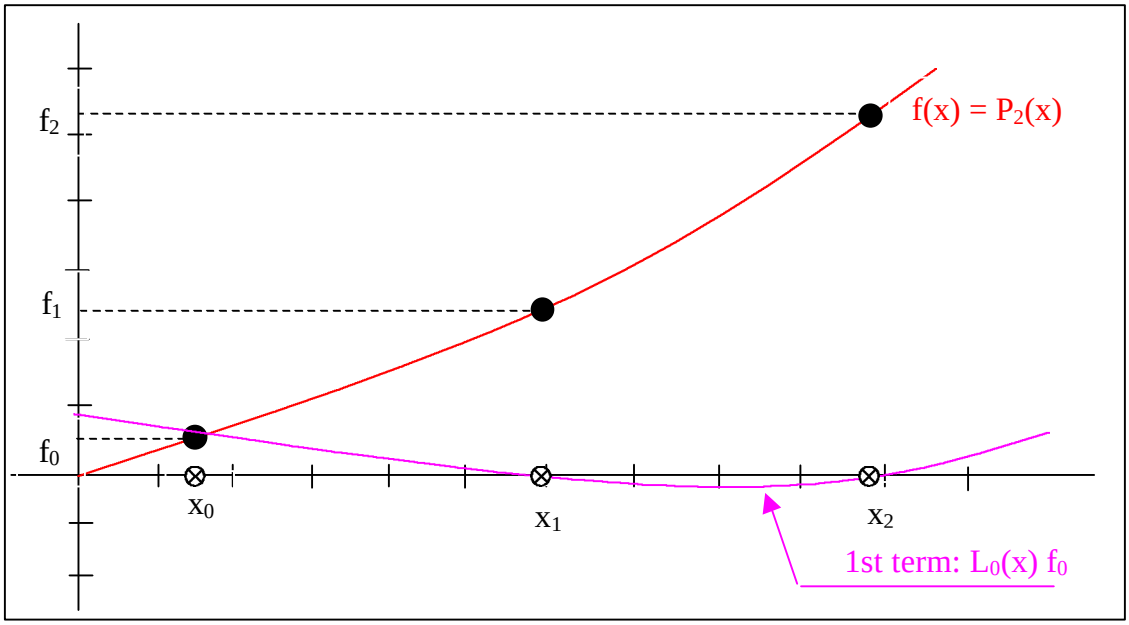
- For this formula to be useful, the function must be known and differentiable. Otherwise, we can approximate the error term by:

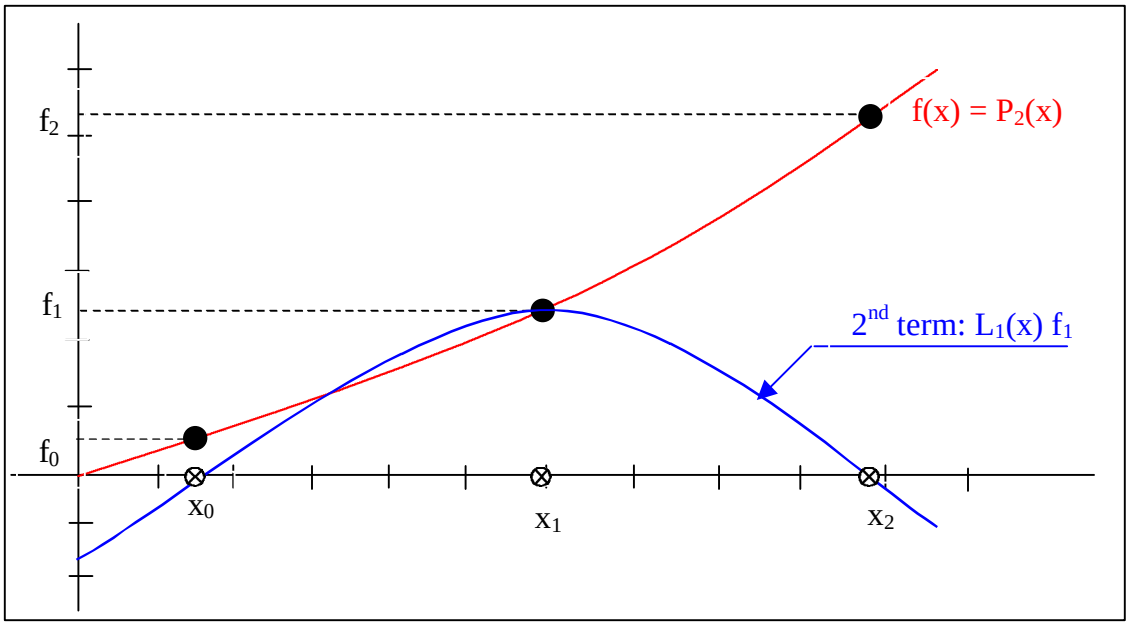
$$e_n(x) \approx f[x_o, x_1, x_2, \ldots x_{n+1}](x - x_o)(x - x_1)\ldots(x - x_n)$$

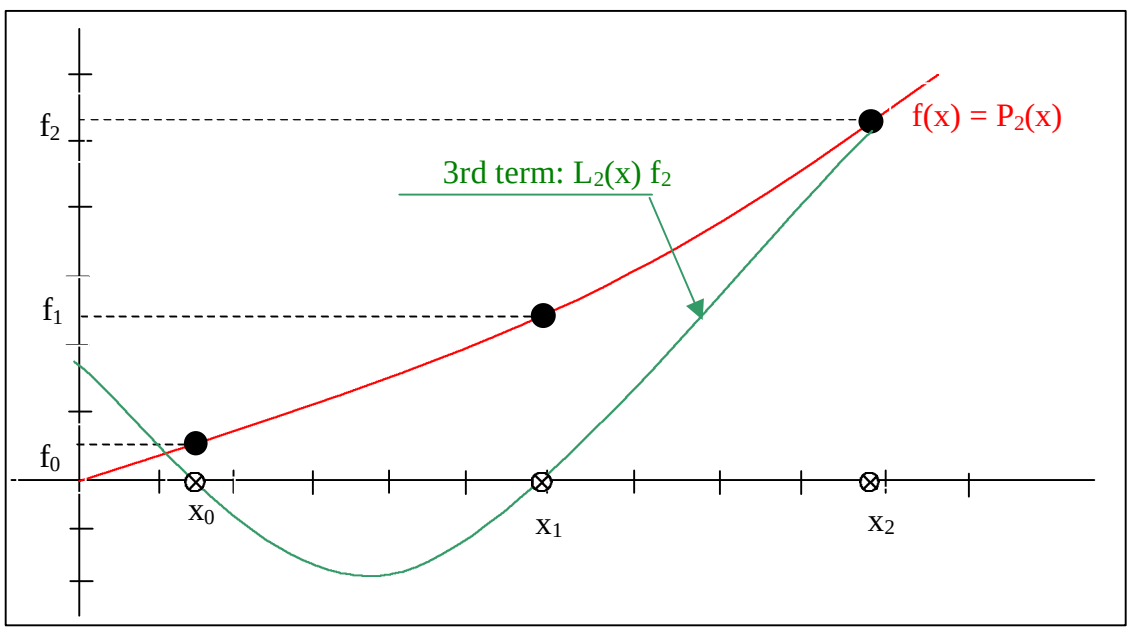
where $f[x_o, x_1, x_2 \ldots x_{n+1}]$ is the $(n+1)^{th}$ divided difference.

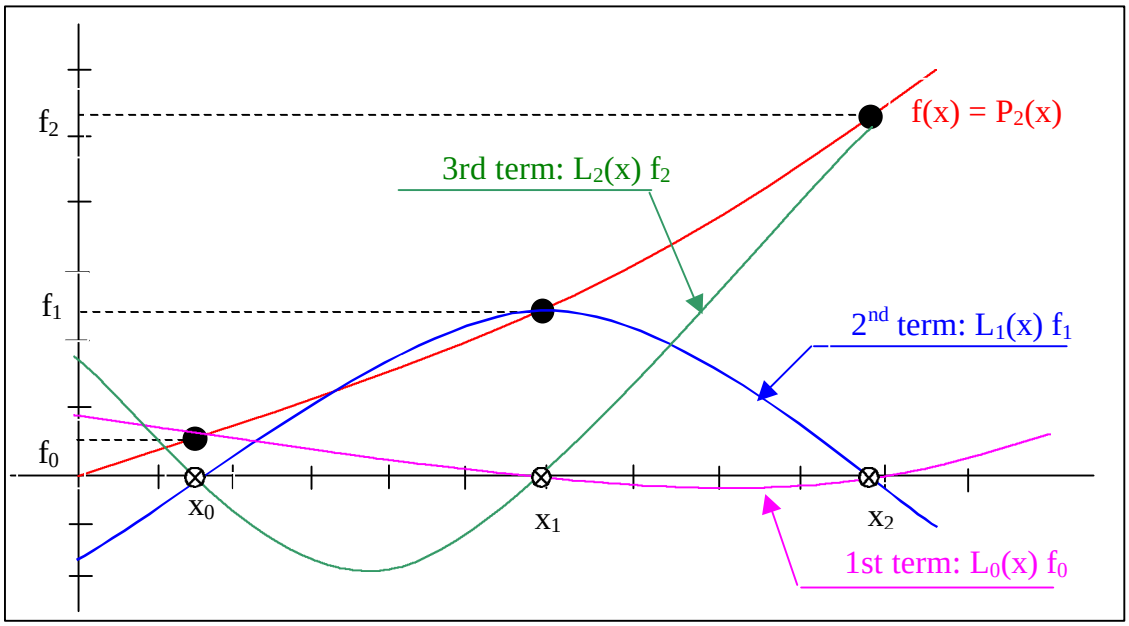
1.5 LAGRANGIAN POLYNOMIALS






f(x) = P2(x)
2nd term: L1(x) f1
f2
f1
f0
x0
x1
x2


f(x) = P2(x)
3rd term: L2(x) f2
f2
f1
f0
x0
x1
x2

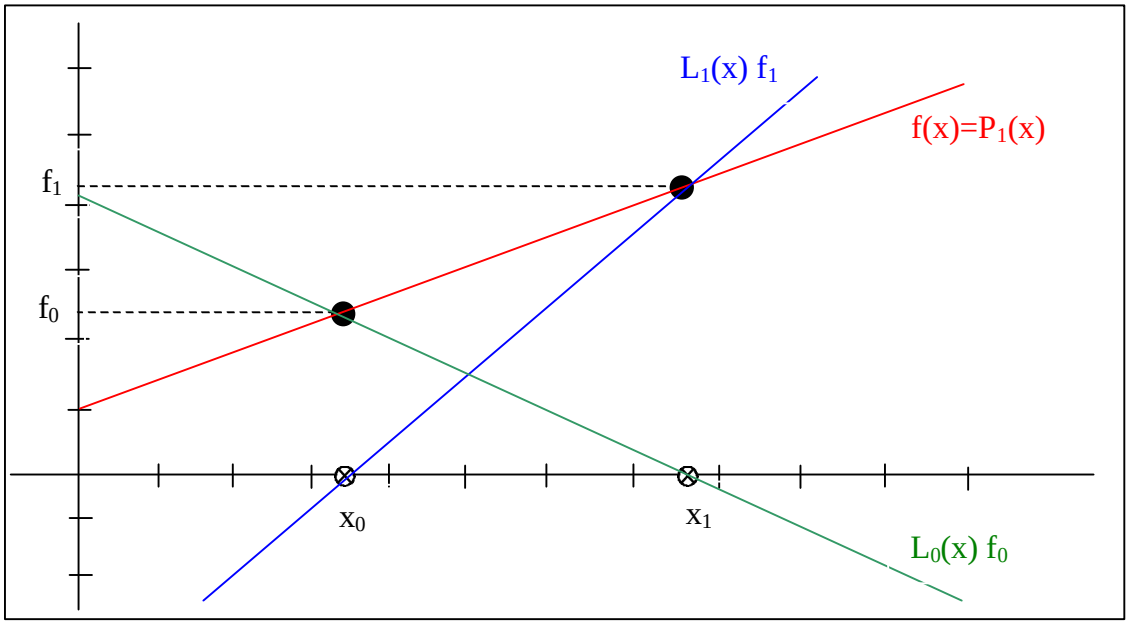


The rationale underlying Lagrange formulation can be understood by realising that each term $L_i(x)$ will be 1 at $x = x_i$ and 0 at all other sample points.

Figure above shows a second-degree case where each of the terms passes through one of the data points and is zero at the other two points.

Summation of 3 terms is the unique $P_2(x)$ that pass through the 3 points exactly.

Consider the linear polynomial $P_1(x)$:



$$P_1(x) = \frac{(x - x_1)}{(x_o - x_1)} f_o + \frac{(x - x_o)}{(x_1 - x_o)} f_1$$

when $x = x_o$, $P_1(x_o) = 1 . f_o + 0 . f_1 = f_o$

when $x = x_1$, $P_1(x_1) = 0 . f_o + 1 . f_1 = f_1$

where $L_o(x) = \dfrac{x - x_1}{x_o - x_1}$

$$L_1(x) = \frac{x - x_o}{x_1 - x_o}$$

$$\Rightarrow P_1(x) = L_o(x) \,.\, f_o + L_1(x) \,.\, f_1$$

Lagrange formulation can be derived from Divided difference as shown for 1st degree case:

$$P_1(x) = f(x_o) + (x - x_o)\, f[x_1, x_o] \quad .. (1.5.1)$$

But $f[x_1, x_o] = \dfrac{f_1 - f_o}{x_1 - x_o}$

$$= \frac{f_1}{x_1 - x_o} + \frac{f_o}{x_o - x_1} \quad (1.5.2)$$

Substituting Eq (1.5.2) into Eq (1.5.1),

$$P_1(x) = f(x_o) + \frac{(x - x_o)}{(x_1 - x_o)} f_1 + \frac{(x - x_o)}{(x_o - x_1)} f_o$$

$$P_1(x) = \frac{(x - x_1)}{(x_o - x_1)} f_o + \frac{(x - x_o)}{(x_1 - x_o)} f_1$$

The 2nd degree Lagrangian formula is:

$$P_2(x) = \frac{(x - x_1)(x - x_2)}{(x_o - x_1)(x_o - x_2)} f_o + \frac{(x - x_o)(x - x_2)}{(x_1 - x_o)(x_1 - x_2)} f_1$$

$$+ \frac{(x - x_o)(x - x_1)}{(x_2 - x_o)(x_2 - x_1)} f_2$$

$$P_2(x) = L_o(x) \cdot f_o + L_1(x) \cdot f_1 + L_2(x) \cdot f_2$$

The Lagrangian Polynomials are:

- straight forward to apply.
- can be used for unevenly spaced data.
- can be used for randomly ordered data (i.e. no sequencing)

Disadvantages are that:

- more arithmetic is involved.
- need to start all over again if new data is introduced.

EXAMPLE 8: LAGRANGIAN POLYNOMIAL

Using Lagrangian Polynomials, find $P_2(3)$.

x	f(x)
3.2	22.000
2.7	17.800
1.0	14.200

$P_2(3) =$

$$\frac{(3-2.7)(3-1.0)}{(3.2-2.7)(3.2-1.0)}\,22.000 + \frac{(3-3.2)(3-1.0)}{(2.7-3.2)(2.7-1.0)}\,17$$

$$+\frac{(3-3.2)(3-2.7)}{(1-3.2)(1-2.7)}\,14.200 = 20.149$$

Truncation error for Lagrange Polynomials.

As with Newton's divided difference, Lagrange has an estimated error of:

$$e_n(x) = f[x_o, x_1, x_2, \ldots x_n, x_{n+1}] \prod_{i=0}^{n} (x - x_i)$$

EXAMPLE 9: LAGRAGIAN ERROR

x	f_i	$f[x_i, x_{i+1}]$	$f[x_i, \ldots x_{i+2}]$	$f[x_i, \ldots x_{i+3}]$
3.2	22.000			
		8.400		
2.7	17.800		2.856	
		2.118		-0.528
1.0	14.200		2.012	
		6.342		
4.8	38.300			

Suppose in Eg.8, 1 pair of data (4.8, 38.300) is missing. What would be the error involved in estimating *f(3)* from the Table in Eg.8?

$$e_2(x) = -0.528(x - 3.2)(x - 2.7)(x - 1.0)$$

$$\backslash \quad Error = 0.528(3 - 3.2)(3 - 2.7)(3 - 1.0)$$

$$= 0.06336$$

Using Lagrangian method

we have,

x	f
3.2	22.000
2.7	17.800
1.0	14.200
4.8	38.300

$$P_3(3) = \frac{(3-2.7)(3-1.0)(3-4.8)22}{(3.2-2.7)(3.2-1.0)(3.2-4.8)}$$

$$+\frac{(3-3.2)(3-1.0)(3-4.8)17.8}{(2.7-3.2)(2.7-1.0)(2.7-4.8)}$$

$$+\frac{(3-3.2)(3-2.7)(3-4.8)14.2}{(1-3.2)(1-2.7)(1-4.8)}$$

$$+\frac{(3-3.2)(3-2.7)(3-1.0)38.3}{(4.8-3.2)(4.8-2.7)(4.8-1.0)}$$

$$P_3(x) = 13.5 + 7.17983 + (-0.17909) + (-0.35996) =$$

Error=

$$P_3(3) - P_2(3) = 20.2120 - 20.1486 = 0.06336$$

1.6 2-D INTERPOLATION

Consider the following triangle:

$$
\begin{array}{ccccccccccc}
 & & & & & 1 & & & & & \\
 & & & & x & & y & & & & \\
 & & & x^2 & & xy & & y^2 & & & \\
 & & x^3 & & x^2y & & x\,y^2 & & y^3 & & \\
 & x^4 & & x^3y & & x^2y^2 & & x\,y^3 & & y^4 & \\
x^5 & & x^4y & & x^3y^2 & & x^2\,y^3 & & x\,y^4 & & y^5
\end{array}
$$

Suppose z is a polynomial function of two variables x,y such that x is of 2nd degree and y is of 3rd degree, then

$$z = f(x,y)$$

$$= a_o + a_1x + a_2y + a_3x^2 + a_4xy + a_5y^2 + a_6\,x^2y + a_7x\,y^2 + a_8\,y^3 + a_9\,x^2y^2 + a_{10}xy^3 + a_{11}x^2y^3$$

The technique is to hold a variable (say, x) constant first and then z is reduced to a single variable problem, i.e. $z = f(c,y)$ where c is a constant.

EXAMPLE 10: 2-D INTERPOLATION

Estimate $f(1.6,0.33)$ using quadratic interpolation for x and cubic interpolation for y.

y / x	0.1	0.2	0.3	0.4	0.5
0.5	.165	.428	.687	.942	1.190
1.0	.271	.640	1.003	1.359	1.703
1.5	.447	.990	1.524	2.045	2.549
2.0	.738	1.568	2.384	3.177	3.943
2.5	1.216	2.520	3.800	5.044	6.241

$x = 1.0$

y	z	Dz	D^2z	D^3z
0.2	0.640			
		0.363		
0.3	1.003		-0.007	
		0.356		-0.005
0.4	1.359		-0.012	
		0.344		
0.5	1.703			

$x = 1.5$

y	z	Dz	D^2z	D^3z
0.2	0.990			
		0.534		
0.3	1.524		-0.013	
		0.521		-0.004
0.4	2.045		-0.017	
		0.504		
0.5	2.549			

$x = 2.0$

y	z	Dz	D^2z	D^3z
0.2				
0.3				
0.4				
0.5				

$y = 0.33$

x	z	Dz	D^2z
1.0	1.111		
		0.571	
1.5	1.682		0.372
		0.943	
2.0	2.625		

From previous tables, when $y = 0.33$

$$s_y = \frac{0.33 - 0.2}{0.1} = 1.3$$

$$\therefore \; z(1.0, 0.33) = 0.64 + 1.3(0.363)$$

$$+ \frac{1.3\,(0.3)(-0.007)}{2} + \frac{1.3\,(0.3)(-0.7)(-0.005)}{6}$$

$$= 1.111$$

When $x = 1.6$, $s_x = \dfrac{1.6 - 1.0}{0.5} = 1.2$

$$z\,(1.6, 0.33)$$

$$= 1.111 + 1.2\,(0.571) + \frac{1.2\,(0.2)(0.372)}{2}$$

$$= 1.841$$

1.7 LEAST SQUARES METHOD

1.7.1 INTRODUCTION

In engineering problems, very often a relationship is found to exist between two (or more) variables.

We wish to model the relationship by determining a function that "best" represents a set of data obtained from experiment, test or observation.

In plotting values of a quantity Y against values of X, we obtain pairs of numbers (x_1, y_1), (x_2, y_2), ..., (x_n, y_n) which could be represented as points in the x - y plane.

For example, the curve that "best" fits these points could then be used to predict other points or to estimate coefficients related to the physical problems being studied.
e.g. the slope $\frac{\Delta s}{\Delta e} \Rightarrow E$

Which is better ?

Interpolation or Least-squares ?

Given n points, we can find a polynomial $y = f(x)$ of sufficiently high degree to fit exactly the n points such that

$$f(x_1) = y_1, \quad f(x_2) = y_2, \ldots\ldots, \quad f(x_n) = y_n$$

e.g. using one of the interpolation formulae, a polynomial of 4th degree can pass through 5 given points exactly.

But exact fitting implies that the data themselves are error free.

An exact fitting might not be appropriate:

(a) Experimental data are generally subject to some errors.

(b) A high degree polynomial with many turning points may not be smooth enough to represent the underlying physical law.

(c) Prior knowledge of physical laws may indicate some function other than a polynomial.

$\therefore$ In practice, the given points would generally not lie exactly on the graph, i.e. the equation $y = f(x)$ represents the ideal line with the minimum scatter.

1.7.2 ERRORS IN OBSERVATIONS

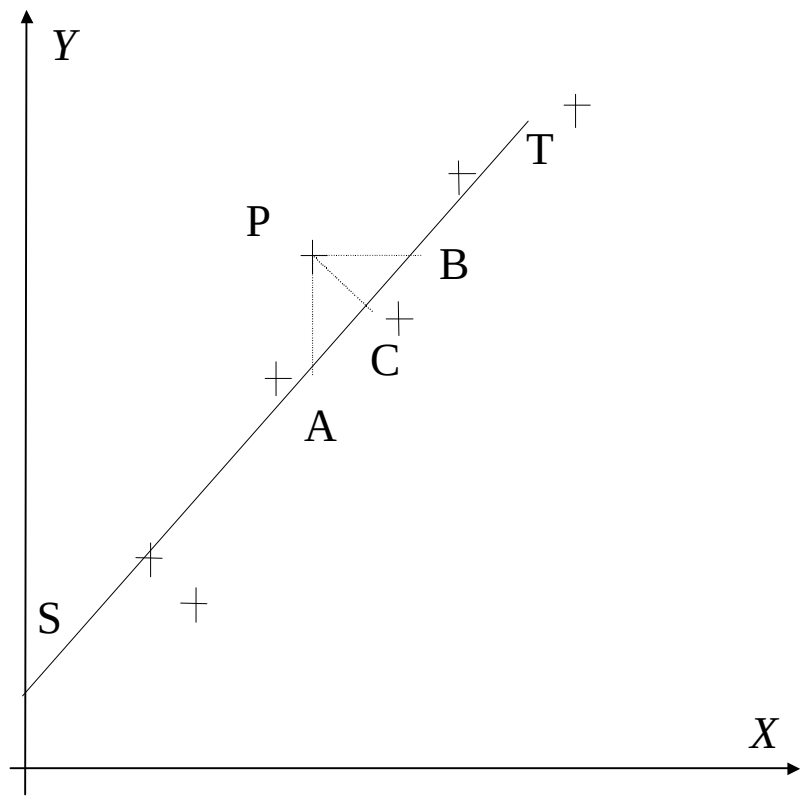
Data for X and Y may have errors as follows:

(a) the X is exact, but the Y is in error.
e.g. in studying temperature in a mass of fresh concrete, the temperature y_i is measured at pre-determined times x_i. Errors occur in reading y_i.

(b) the Y is exact, but the X is in error.
e.g. in a pile load-test, settlements x_i are measured at known loads y_i.

(c) both the X and Y are in errors
e.g. in a pile load-test using a hydraulic jack, read the load y_i and settlement x_i at various intervals.

Fig. 1 shows some points to be fitted by a line ST.



If $P(x_i, y_i)$ is one of the given points and is the true line governing the relation between X and Y, with $y = a_o + a_1 x$ then,

In case (a), the error represents the distance PA

In case (b), the error represents the distance PB

In case (c), the usual supposition is to treat the error as the distance PC which is perpendicular to ST.

1.7.3 FITTING THE STRAIGHT LINE

Simplest method: plot the points and fit a line by eye using a straight edge.

Disadvantage: different persons would most likely plot different lines.

Some criteria need to be applied with regard to the errors in the observations.

Consider the errors in Y only.

In Fig.1, point A on ST has the ordinate

$$y(x_i) = a_o + a_1 x_i$$

For point P, the error or deviation is

$$e_i = y_i - y(x_i) = y_i - a_o - a_1 x_i$$

Consider the error for all given points for $i = 1$ to n:

If we impose the condition

$$\sum_{i=0}^{n} e_i = 0$$

then $$\sum_{i=0}^{n} (y_i - a_o - a_1 x_i) = 0$$

==> $$a_o n + a_1 S x_i = S y_i$$

1 equation is insufficient for computing

a_o & a_1.

$\therefore$ the condition $\Sigma e_i = 0$ is usually not adopted.

1.7.4 PRINCIPLE OF LEAST SQUARES

This is widely adopted in practice.

In fitting a straight line to the points (x_1, y_1), ..., (x_n, y_n) in which the errors are taken in the Y, the straight line $y = a_o + a_1 x$ should be fitted through the given points so that the sum of the squares of the distances of these points from the straight line is a *minimum*

i.e. $$\sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left(y_i - a_o - a_1 x_i\right)^2$$

is a minimum, where y_i is the observed data and $a_o + a_1 x_i$ is the idealised straight line.

Normal Equations

Let SSE represent the sum of squares of errors

$$\text{SSE} = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left(y_i - a_o - a_1 x_i\right)^2$$

For SSE to be minimum :

$$\frac{\P\, SSE}{\P\, a_o} = -2 \sum \left(y_i - a_o - a_1 x_i\right) = 0$$

$$\frac{\P\, SSE}{\P\, a_1} = -2 \sum x_i \left(y_i - a_o - a_1 x_i\right) = 0$$

i.e. $a_o n + a_1 \sum x_i = \sum y_i$ (i)

$a_o \sum x_i + a_1 \sum x_i^2 = \sum x_i y_i$ (ii)

(i) and (ii) are normal equations for the determination of the Least-squares straight line. All Σ are for $i = 1$ to n.

EXAMPLE 11: LEAST-SQUARES LINEAR

Using the method of least squares, fit a straight line to six points (0,3), (1,2), (2,2), (3,1), (4,1), (5,0). Assume that the errors are in the *Y*.

X	Y	X^2	XY
0	3	0	0
1	2	1	2
2	2	4	4
3	1	9	3
4	1	16	4
5	0	25	0
$\Sigma = 15$	9	55	13

The normal equations:

$$a_o\ n\ +\ a_1 \sum x_i = \sum y_i$$

$$a_o\ \sum x_i + a_1\ \sum x_i^2 = \sum\ x_i\ y_i$$

$$6\ a_o\ +\ 15\ a_1\ =\ 9$$

$$15\ a_o\ +\ 55\ a_1\ =\ 13$$

===> $a_o\ =\ \frac{20}{7}\ ,\quad a_1\ =\ -\ \frac{19}{35}$

Thus, the required line : $y\ =\ \frac{20}{7}\ -\ \frac{19}{35}x$

or $35y\ +\ 19x\ =\ 100$

1.7.5 LEAST SQUARES PROCEDURE FOR POLYNOMIALS

The sum of squares of errors

SSE

$$= \sum_{i=1}^{n} e_i^2 = \sum \left(y_i - a_o - a_1 x_i - \text{K} - a_m x_i^m \right)^2$$

where there are *(m+1)* unknowns in the coefficients *a*.

For minimum SSE:

$$\frac{\P\, SSE}{\P\, a_o} = -2 \sum \left(y_i - a_o - a_1 x_i - \text{K} - a_m x_i^m \right) = 0$$

$$\frac{\P\, SSE}{\P\, a_1} = -2 \sum x_i \left(y_i - a_o - a_1 x_i - \text{K} - a_m x_i^m \right) = 0$$

$$\frac{\P\, SSE}{\P\, a_m} = -2 \sum x_i^m \left(y_i - a_o - a_1 x_i - \text{K} - a_m x_i^m \right) = 0$$

==> Normal equations for finding the polynomial of degree m :

$$a_o n + a_1 \sum x_i + \text{K} + a_m \sum x_i^m = \sum y_i$$

$$a_o \sum x_i + a_1 \sum x_i^2 + \text{K} + a_m \sum x_i^{m+1} = \sum x_i y_i$$

$$a_o \sum x_i^2 + a_1 \sum x_i^3 + \text{K} + a_m \sum x_i^{m+2} = \sum x_i^2 y_i$$

$$\begin{array}{ccccccc} & \cdot & & & \cdot & & \\ & \cdot & & & \cdot & & \\ & \cdot & & & \cdot & & \\ a_o \sum x_i^m & + & a_1 \sum x_i^{m+1} & + \text{K} + & a_m \sum x_i^{2m} & = & \sum x_i^m y_i \end{array}$$

Observe the pattern of the coefficient matrix :

$$
\begin{array}{ccccc}
n & Sx_i & Sx_i^2 & ..... & Sx_i^m \\
Sx_i & Sx_i^2 & Sx_i^3 & ..... & Sx_i^{m+1} \\
Sx_i^2 & Sx_i^3 & Sx_i^4 & ..... & Sx_i^{m+2} \\
. & & & & . \\
. & & & & \\
. & & & & . \\
Sx_i^m & Sx_i^{m+1} & Sx_i^{m+1} & ..... & Sx_i^{2m}
\end{array}
$$

Solving a large set of equations poses practical difficulties for the unknowns a_o, a_1, ..., a_m.

Generally, these equations are <u>ill-conditioned</u>, i.e. the answers are very sensitive to round-off errors.

EXAMPLE 12: LEAST-SQUARES QUADRATIC

Using the method of least squares, fit a curve $y = a_o + a_1x + a_2x^2$ to the data :

x_i	-2	-1	0	1	2	3	5	7
y_i	9	6	3	-1	-2	-3	-1	3

From the data:

$$Sx = 15, \quad Sy = 14, \quad Sx^2 = 93, \quad Sx^3 = 495,$$

$$Sx^4 = 3142, \quad Sxy = -22, \quad Sx^2y = 128, \quad n=8$$

Normal equations :

$$a_o n + a_1 \sum x + a_2 \sum x^2 = \sum y$$

$$a_o \sum x + a_1 \sum x^2 + a_2 \sum x^3 = \sum xy$$

$$a_o \sum x^2 + a_1 \sum x^3 + a_2 \sum x^4 = \sum x^2 y$$

$$8\,a_o + 15\,a_1 + 93\,a_2 = 14$$

$$15\,a_o + 93\,a_1 + 495\,a_2 = -22$$

$$93\,a_o + 495\,a_1 + 3141\,a_2 = 128$$

Solving for a_o, a_1, a_2,

==> $$y = 2.133 - 2.864x + 0.429\,x^2$$

1.7.6 WEIGHTED LEAST SQUARES

In some cases, the data points may not be all equally reliable, e.g. some measurements tend to be less reliable towards one or both ends of a range of measurements.

One way to overcome the biasedness is to attach different weights to the terms in the summation,

$$SSE = \sum_{i=1}^{n} w_i \, e_i^2$$

Minimising SSE implies that normal equations are modified by the weights w_i.

For example, taking the errors in the Y, and fitting the data with straight line

$$y = a_o + a_1 x$$

$$SSE = \sum_{i=1}^{n} w_i \left(y_i - a_o - a_1 x_i\right)^2$$

$$\frac{\partial SSE}{\partial a_o} = -2 \sum w_i \left(y_i - a_o - a_1 x_i\right) = 0$$

$$\frac{\partial SSE}{\partial a_1} = -2 \sum w_i \, x_i \left(y_i - a_o - a_1 x_i\right) = 0$$

Normal equations:

$$a_o \sum w_i + a_1 \sum w_i x_i = \sum w_i y_i$$

$$a_o \sum w_i x_i + a_1 \sum w_i x_i^2 = \sum w_i x_i y_i$$

The effect of attaching weights is that w_i appears in the respective sums.

A similar effect occurs in fitting with higher polynomials.

1.8 SUMMARY

$$f(x) \quad » \quad P_n(x)$$

$$e_n(x) = (x - x_o)(x - x_1) \ldots (x - x_n) \frac{f^{n+1}(x)}{(n+1)!}$$

applies to both sets of data.

But $e_n(x) = \begin{pmatrix} s \\ n+1 \end{pmatrix} h^{n+1} f^{n+1}(x)$ applies only to evenly spaced data.

For two dimensional interpolation e.g. $z = f(x,y)$, the trick is to hold one variable at a time. The usual procedure for centering the data (whether in the x- or y- directions) still applies.

TKH/jam
2 Jan 2001