M2PHY 01 - CT05

Computational Methods in Physics

UNIT-2

Interpolation:

It is a type of estimation, a method of constructing new data points within the range of a discrete set of known data points.

We often have a set of data points, obtained by sampling or experimentation, representing the values of a function at limited number of independent variable, like follows:

x	x_1	x_2	x_3	...	x_n
$f(x)$	$f(x_1)$	$f(x_2)$	$f(x_3)$	...	$f(x_n)$

If the value of $f(x)$ is to be found at some point y in the interval $[x_1, x_n]$ and y is not one of the tabulated points, then the value is estimated by using the known values of $f(x)$ at surrounding points. This is called interpolation.

If y point is outside the interval $[x_1, x_n]$ then the estimation of $f(y)$ is called extrapolation.

Interpolation is the theoretical foundation which provides the derivation of differentiation and integration formulae and for sol^n of differential eq^{ns}.

Lagrange Interpolation:

The universal technique for interpolation is to fit a polynomial through the points surrounding the point 'y' where the value of the function is to be found.

This polynomial is an approximation of the function and is used to find $f(y)$.

Following process gives fitting of a second degree polynomial. Let the polynomial be of the form,

$$f(x) = C_1 (x-x_2)(x-x_3) + C_2 (x-x_1)(x-x_3) + C_3 (x-x_1)(x-x_2) \quad \text{—— (1)}$$

By putting $x = x_1$, x_2 and x_3 one by one, we can find the values of coefficients C_1, C_2 and C_3, as we know the values of function $f(x)$ at x_1, x_2 and x_3.

$$f(x_1) = C_1 (x_1 - x_2)(x_1 - x_3)$$

$$\Rightarrow \quad C_1 = \frac{f(x_1)}{(x_1-x_2)(x_1-x_3)} \quad \text{—— (2)}$$

Similarly, $f(x_2) = C_2 (x_2 - x_1)(x_2 - x_3)$

$$\Rightarrow \quad C_2 = \frac{f(x_2)}{(x_2-x_1)(x_2-x_3)} \quad \text{—— (3)}$$

and, $f(x_3) = C_3 (x_3 - x_1)(x_3 - x_2)$

$$\Rightarrow \quad C_3 = \frac{f(x_3)}{(x_3-x_1)(x_3-x_2)} \quad \text{—— (4)}$$

We can see that the coefficients of the polynomial $f(x)$ are directly obtained without solving simultaneous equations.

So, the polynomial can be expressed as,

By eqn (1) $\Rightarrow$

$$f(x) = c_1(x-x_2)(x-x_3) + c_2(x-x_1)(x-x_3) + c_3(x-x_1)(x-x_2)$$

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

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

or,

$$f(x) = \sum_{i=1}^{3} f(x_i) \prod_{\substack{j \neq i \\ j=1}}^{3} \frac{(x-x_j)}{(x_i-x_j)} \quad \text{—— (5)}$$

This polynomial is called the Lagrange Polynomial.

Algorithm: LAGRANGE INTERPOLATION

1. Read x, n
2. for $i = 1$ to $(n+1)$ in steps of 1 do
   Read x_i, f_i endfor
3. sum $\leftarrow 0$
4. for $i = 1$ to $(n+1)$ in steps of 1 do
5. prodfunc $\leftarrow 1$
6. for $j = 1$ to $(n+1)$ in steps of 1 do
7. If $(j \neq i)$ then
   prodfunc $\leftarrow$ prodfunc $\times (x - x_j)/(x_i - x_j)$
   endfor
8. sum $\leftarrow$ sum $+ f_i \times$ prodfunc
   endfor
9. Write x, sum
10. Stop

Example 1:

A table of x vs $f(x)$ is given below. Find the value of $f(x)$ at $x = 4$

x	1.5	3	6
$f(x)$	-0.25	2	20

Solution: Using Lagrange Polynomial,

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

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

$$= \frac{-0.25(x-3)(x-6)}{(1.5-3)(1.5-6)} + \frac{2(x-1.5)(x-6)}{(3-1.5)(3-6)}$$

$$+ \frac{20(x-1.5)(x-3)}{(6-1.5)(6-3)}$$

$$f(4) = \frac{-0.25(1)(-2)}{(-1.5)(-4.5)} + \frac{2(2.5)(-2)}{(1.5)(-3)} + \frac{20(2.5)(1)}{(4.5)(3)}$$

$$= 0.74 + 2.222 + 3.703$$

$$= 5.999 \simeq 6$$

Lagrange Polynomial generalised to n^{th} order:

$$f(x) = \sum_{i=1}^{n+1} f(x_i) \prod_{\substack{j \neq i \\ j=1}}^{n+1} \frac{(x-x_j)}{(x_i-x_j)} \qquad \text{——} (6)$$

DIFFERENCE TABLES

There is one more method to fit a polynomial using given data set values.

Let $f(x) = b_1 + b_2(x - x_1) + b_3(x - x_1)(x - x_2)$ —— (1)

If we put $x = x_1, x_2$ and x_3, we get,

$$b_1 = f(x_1) \qquad \text{—— (2)}$$

$$b_2 = [f(x_2) - f(x_1)] / (x_2 - x_1) \qquad \text{—— (3)}$$

$$b_3 = \frac{[f(x_3) - f(x_1)] - [\{f(x_2) - f(x_1)\}(x_3 - x_1)/(x_2 - x_1)]}{(x_3 - x_1)(x_3 - x_2)}$$

$$b_3 = \frac{f(x_3) - f(x_2)}{(x_3 - x_2)(x_3 - x_1)} - \frac{f(x_2) - f(x_1)}{(x_2 - x_1)(x_3 - x_1)} \qquad \text{—— (4)}$$

The method of obtaining above coefficients b_1, b_2 and b_3 can also be expressed as difference table.

$f(x_1)$	$\Delta_d f_1 = b_2 = \frac{f(x_2) - f(x_1)}{(x_2 - x_1)}$	
$f(x_2)$		$\Delta_d^2 f_1 = b_3 = \frac{(\Delta_d f_2 - \Delta_d f_1)}{(x_3 - x_1)}$
$f(x_3)$	$\Delta_d f_2 = \frac{f(x_3) - f(x_2)}{(x_3 - x_2)}$	

The polynomial, eqn (1), may thus be written as,

$$f(x) = f(x_1) + \Delta_d f_1 (x - x_1) + \Delta_d^2 f_1 (x - x_1)(x - x_2) \qquad \text{—— (5)}$$

where $\Delta_d f_1$ and $\Delta_d^2 f_1$ are called <u>divided differences</u> and the table is called a <u>divided difference table</u>.

This may be generalised and for n tabulated points a (n-1) order polynomial may be fitted. The general polynomial formula is,

$$f(x) = f(x_1) + \Delta_d f_1 (x-x_1) + \Delta_d^2 f_1 (x-x_1)(x-x_2)$$
$$+ \Delta_d^3 f_1 (x-x_1)(x-x_2)(x-x_3) + \cdots + \Delta_d^{n-1} f_1 (x-x_1)(x-x_2)\ldots(x-x_{n-1})$$

where, $\Delta_d^{n-1} f_1 = (\Delta_d^{n-1} f_n - \Delta_d^{n-1} f_{n-1}) / (x_n - x_1)$

Example 2:

A table of polynomial function is given below. Fit a polynomial. Find the value of $f(x)$ at $x = 2.5$

x	-3	-1	0	3	5
$f(x)$	-30	-22	-12	330	3458

Solution:

The divided difference table is:

x	$f(x)$	$\Delta_d f$	$\Delta_d^2 f$	$\Delta_d^3 f$	$\Delta_d^4 f$
-3	-30				
		4			
			2		
-1	-22			4	
		10			5
			26		
0	-12			44	
		114			
			290		
3	330				
		1564			
5	3458				

Thus the polynomial is

$$f(x) = -30 + 4(x+3) + 2(x+3)(x+1) + 4(x+3)(x+1)(x) + 5(x+3)(x+1)(x)(x-3)$$

$$f(2.5) = 102.7$$

Difference Tables:

When the functions are tabulated at equal intervals, i.e., $(x_2 - x_1) = (x_3 - x_2) = \cdots = (x_n - x_{n-1}) = h$, a constant. For this case, the difference table for n points may be expressed as:

x_1	f_1				
		$\Delta f_1 = f_2 - f_1$			
x_1+h	f_2		$\Delta^2 f_1 = \Delta f_2 - \Delta f_1$		
		$\Delta f_2 = f_3 - f_2$		$\Delta^3 f_1 = \Delta^2 f_2 - \Delta^2 f_1$	
x_1+2h	f_3		$\Delta^2 f_2 = \Delta f_3 - \Delta f_2$		$\Delta^4 f_1 = \Delta^3 f_2 - \Delta^3 f_1$
		$\Delta f_3 = f_4 - f_3$		$\Delta^3 f_2 = \Delta^2 f_3 - \Delta^2 f_2$	
x_1+3h	f_4		$\Delta^2 f_3 = \Delta f_4 - \Delta f_3$		
		$\Delta f_4 = f_5 - f_4$			
$\vdots$		$\vdots$			
x_1+nh	f_{n+1}				

The elements in columns are obtained by taking two adjacent elements of the previous ~~sect~~ column and subtracting the upper element from the lower one.

An n^{th} order polynomial fitted through the points $(f_1, f_2, \ldots, f_{n+1})$ may be expressed in terms of differences by generalising eq^ns 1 and 5 as:

By eqn (1) and (5)

$$f(x) = b_1 + b_2(x-x_1) + b_3(x-x_1)(x-x_2) + \cdots + b_n(x-x_1)\cdots(x-x_n)$$

$$f(x) = f_1 + \frac{\Delta f_1}{h}(x-x_1) + \frac{\Delta^2 f_1}{\lfloor 2\, h^2}(x-x_1)(x-x_2) + \frac{\Delta^3 f_1}{\lfloor 3\, h^3}(x-x_1)$$

$$(x-x_2)(x-x_3) + \cdots + \frac{\Delta^n f_1}{\lfloor n\, h^n}(x-x_1)(x-x_2)\cdots(x-x_n) \quad \text{(6)}$$

This polynomial of eqn (6) may be expressed by putting $(x = x_1 + uh)$ where u is a number between 0 and 1.

$$x = x_1 + uh$$

$$hu = x - x_1 \Rightarrow x - x_1 = hu$$

$$x - x_2 = (x_1 + hu) - (x_1 + h)$$

$$= x_1 + hu - x_1 - h = h(u-1)$$

$$x - x_3 = x - (x_2 + h) = x - x_2 - h$$

$$= h(u-1) - h = h(u-2)$$

$$\vdots$$

$$x - x_n = h\{u-(n-1)\}$$

putting this in eqn (6), we get

$$f(x_1 + uh) = f_1 + \Delta f_1 u + \frac{\Delta^2 f_1}{\lfloor 2} u(u-1)$$

$$+ \frac{\Delta^3 f_1}{\lfloor 3} u(u-1)(u-2) + \cdots + \frac{\Delta^n f_1}{\lfloor n} u(u-1)(u-2)\cdots(u-\overline{n-1}) \quad \text{(7)}$$

This is called the Newton - Gregory Forward Interpolation formula.

Example 3 :

Using the table given below, find $f(0.16)$.

x	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$
0.1	1.005			
		0.015		
			0.010	
0.2	1.020			0.001
		0.025		
0.3	1.045		0.011	
		0.036		
0.4	1.081			

using Newton-Gregory Forward Formula,

$$f(x_1+uh) = f_1 + \Delta f_1 u + \frac{\Delta^2 f_1}{\lfloor 2} u(u-1) + \frac{\Delta^3 f_1}{\lfloor 3} u(u-1)(u-2)$$

here $x = 0.16 = x_1 + uh$

$= 0.1 + 0.06$

$\Rightarrow uh = 0.06$

$h = 0.1 \quad \Rightarrow u = 0.6$

$$f(0.16) = 1.005 + (0.015)(0.6) + \frac{(0.010)}{2}(0.6)(0.6-1)$$

$$+ \frac{(0.001)}{6}(0.6)(0.6-1)(0.6-2)$$

$= 1.005 + 0.0090 - 0.0012 + 0.000056$

$\simeq 1.0128$

FORWARD AND BACKWARD Difference Tables:

The forward difference formula is suitable when one wants to interpolate near the top of a set of tabulated values.

If $f(x)$ at $x = x_1 + \frac{3h}{2}$ is needed then the first two forward differences are sufficient and can be found from Forwad Difference table.

If the value of function is needed at $x = x_1 + \frac{9h}{2}$, then it would be convenient to calculate the differences from the bottom of the table - Backward difference.

FORWARD Diff. Table

x_1	$f1$	$\Delta f1$	$\Delta^2 f1$
x_1+h	$f2$	$\Delta f2$	$\Delta^2 f2$
x_1+2h	$f3$	$\Delta f3$	$\Delta^2 f3$
x_1+3h	$f4$	$\Delta f4$	$\Delta^2 f4$
x_1+4h	$f5$	$\Delta f5$	
x_1+5h	$f6$		

BACKWARD Diff. Table

x_1	$f1$	$\nabla f2$	$\nabla^2 f3$	$\nabla^3 f4$
x_1+h	$f2$	$\nabla f3$	$\nabla^2 f4$	$\nabla^3 f5$
x_1+2h	$f3$	$\nabla f4$	$\nabla^2 f5$	$\nabla^3 f6$
x_1+3h	$f4$	$\nabla f5$	$\nabla^2 f6$	
x_1+4h	$f5$	$\nabla f6$		
x_1+5h	$f6$			

We can see in Backward diff. table

$\nabla f_6 = f_6 - f_5 = \Delta f_5$. So, using this

$$f(x) = f_6 + \frac{\nabla f_6}{h}(x - x_6) + \frac{\nabla^2 f_6}{2h^2}(x - x_6)(x - x_5)$$

Finding ∇f_6 and $\nabla^2 f_6$ would be easier from the bottom of the table.

If interpolation is required near the centre of a set of tabulated values, a difference of average of the backward and forward difference is taken. It is called a central difference.

Example 4: The population of a city in a census taken once in ten years is given below: Estimate the population in the years 1925, 1975 and 1984.

Year	1921	1931	1941	1951	1961	1971	1981
Population in thousands	35	42	58	84	120	165	220

Soln: By preparing the difference table:

year	Population	Δf	$\Delta^2 f$	$\Delta^3 f$
1921	35			
		7		
1931	42		9	
		16		1
1941	58		10	
		26		0
1951	84		10	
		36		-1
1961	120		9	
		45		1
1971	165		10	
		55		
1981	220			

As $\Delta^3 f$ is almost zero we can fit a quadratic and use only upto second differences.

(i) 1925 is near the top of the table and we use the forward difference formula,

$$f(x) = f_1 + \frac{\Delta f_1}{h}(x-x_1) + \frac{\Delta^2 f_1}{2h^2}(x-x_1)(x-x_2)$$

$$= f_1 + \Delta f_1 u + \frac{\Delta^2 f_1}{2} u(u-1)$$

where $x - x_1 = uh$

$x_1 = 1921, \quad h = 10, \quad x = 1925$

$\Rightarrow x - x_1 = uh$

$u = \frac{x - x_1}{h} = \frac{4}{10} = 0.4$

$$f(1925) = 35 + 7(0.4) + \frac{9}{2}(0.4)(0.4-1)$$

$$= 36.7 \simeq 37 \text{ (rounded)}$$

(ii) 1975 is near the end of the table so we apply backward difference formula,

$$f(x) = f_7 + \frac{\nabla f_7}{h}(x - x_7) + \frac{\nabla^2 f_7}{2h^2}(x-x_7)(x-x_6)$$

$$f(x) = f_7 + \nabla f_7 u + \frac{\nabla^2 f_7}{2} u(u+1)$$

as $uh = x - x_7 \Rightarrow u = \frac{x - x_7}{h} = \frac{1975 - 1981}{10}$

$u = -0.6$

$$f(1975) = 220 + 55(-0.6) + \frac{10}{2}(-0.6)(-0.6+1)$$

$$= 195.8 \simeq 196 \text{ (rounded)}$$

(iii) 1984 is outside the tabulated values, so we can not interpolate.

Truncation Error in Interpolation

When we fit a polynomial of a finite order to a set of tabulated values there is error in interpolation, which is called the truncation error.

The error term is similar to the remainder term in a Taylor series expansion of the function.

The error terms are:

(i) For Newton-Gregory forward difference interpolation formula:

$$E_n = \frac{h^{n+1} f^{n+1}(a)}{\lfloor n+1} u(u-1)(u-2)\cdots(u-n)$$

where $f^{n+1}(a)$ is the $(n+1)$th derivative of the function $f(x)$ being interpolated ~~be~~ and a is a value between x_1 and x_n.

(ii) For Lagrange formula:

$$E_n = \frac{f^{n+1}(a)}{\lfloor n+1} (x-x_1)(x-x_2)\cdots(x-x_{n+1})$$

To estimate the error ~~is~~ we need to find $f^{n+1}(a)$ at the unknown point a.

To find $f^{n+1}(a)$, we require $f(x)$. Thus

$$f^{n+1}(a) \simeq \frac{\Delta^{n+1} f_1}{h^{n+1}}$$

(iii): In Newton's Forward formula

$$E_n = \frac{\Delta^{n+1} f_1}{\lfloor n+1} u(u-1)\cdots(u-n)$$

which would be the $(n+1)^{th}$ term in the interpolation formula if an $(n+1)$ order polynomial has been used.

The error term may be used to fix the order of interpolation polynomial automatically in the algorithm for forward difference interpolation.

In Lagrange interpolation this is not possible as differences are not computed.

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