B.Sc.(H) Chem Semester-IV^{th} Generic Elective IV^{th} Numerical Method:- 9.

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Ex(1.1) The table gives the distance in kilometers for the given height in feet above the Mars surface:

x = height	100	150	200	250	300	350	400
y = distance	10.52	13.01	15.57	16.03	18.32	19.61	21.59

Find the value of y at x = 165 ft using Gregory-Newton Forward Difference Interpolation formula.

Sol^n: Construct Difference Table

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$	$\Delta^6 y$	
100	10.52							
		2.49						
150	13.01		0.07					
		2.56		-2.17				
200	15.57		-2.1		6.1			
		0.46		3.93		12.86		
250	16.03		1.83		-6.76		-1.58	
		2.29		-2.83		11.28		
300	18.32		-1.0		4.52			
		1.29		1.69				
350	19.61		0.69					
		1.98						
400	21.59							

Since we have to find the value of y at 165 ft; we take difference corresponding to x = 150 ft. as it is ...

closest to the point at which we have to find the value. 10.

Now proceeding further we get

$x_0 = 150$, $y_0 = 13.01$, $\Delta y_0 = 2.56$ $\Delta^2 y_0 = -2.1$, $\Delta^3 y_0 = 3.93$

$\Delta^4 y_0 = -6.76$, $\Delta^5 y_0 = 11.28$

Using Newton's forward interpolation formula

$$y = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0$$
$$+ \frac{u(u-1)(u-2)(u-3)}{4!}\Delta^4 y_0 + \frac{u(u-1)(u-2)(u-3)(u-4)}{5!}\Delta^5 y_0$$

Where $u = \frac{x - x_0}{h}$ $h = 50$, $x = 165$, $x_0 = 150$

$$u = \frac{160 - 150}{50} = \frac{15}{50} = 0.3$$

Putting all value in series we get

$$y(165) = 13.01 + 0.3(2.56) + \frac{(0.3)(-0.7)}{2}(-2.1) + \frac{(0.3)(-0.7)(-1.7)}{3.2} \times (3.93)$$
$$+ \frac{(0.3)(-0.7)(-1.7)(-2.7)}{4.3.2.}(-6.76) + \frac{(0.3)(-0.7)(-1.7)(-2.7)(-3.7)(11.28)}{5.4.3.2.}$$

$$y(165) = 13.01 + 0.768 + 0.2338 + \overset{+0.2205}{0.2714} + 0.3352$$

$$y(165) = 14.8389$$

Ex: Q) The following data represents the function $f(x) = e^x$

x	$f(x)$
1	2.718
1.5	4.4817
2.0	7.3891
2.5	12.1825

Estimate the value of f(2.25) using Newton's forward difference Interpolation and then compare with the exact value. 11.

Soln:

x	f(x)	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$
1	2.718			
		1.764		
1.5	4.4817		1.144	
		2.9074		0.742
2.0	7.3891		1.886	
		4.7934		
2.5	12.1825			

Newton divided forward difference interpolating polynomial is given by

$$P(x) = f(x_0) + \frac{(x-x_0)}{h}\Delta f(x_0) + \frac{(x-x_0)(x-x_1)}{2!\,h^2}\Delta^2 f(x_0) + \frac{(x-x_0)(x-x_1)(x-x_2)}{3!\,h^3}\Delta^3 f(x_0), \quad h = 0.5$$

$$P(x) = 2.718 + \frac{(x-1)}{0.5}(1.764) + \frac{(x-1)(x-1.5)}{2(0.5)^2}(1.144) + \frac{(x-1)(x-1.5)(x-2)}{6(0.5)^3}(0.742)$$

$$= \frac{1}{0.75}\left[0.742x^3 - 1.623x^2 + 3.178x - 0.258375\right]$$

$$P(x) = 0.9893x^3 - 2.164x^2 + 4.2374x - 0.3445$$

$$P(2.25) = 9.50675$$

Given $f(x) = e^x$ Exact value $f(2.25) = 9.487795$

Ex2-Q1: Find the value of $f(7.5)$ using Newton's backward interpolation formula from the given table:

x	1	2	3	4	5	6	7	8
y	1	8	27	64	125	216	343	512

Soln:- The backward difference table is

x	y	∇y	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$
1	1				
		7			
2	8		12		
		19		6	
3	27		18		0
		37		6	
4	64		24		0
		61		6	
5	125		30		0
		91		6	
6	216		36		0
		127		6	
7	343		42		
		169			
8	512				

Since the fourth & fifth order difference are zero, the equation of Newton backward interpolation becomes

$$f(x) = f_n + u\nabla f_n + \frac{u(u+1)}{2!}\nabla^2 f_n + \frac{u(u+1)(u+2)}{3!}\nabla^3 f_3$$

Here $f_n = 512$, $\nabla f_n = 169$, $\nabla^2 f_n = 42$, $\nabla^3 f_n = 6$, $u = \frac{x - x_n}{h}$

$x = 7.5 \quad u = \frac{7.5 - 8}{1} = -0.5$

Substituting the value, we get

$$y_{7.5} = f(x) = 512 + (-0.5)169 + \frac{(-0.5)(0.5)}{2}(42) + \frac{(-0.5)(0.5)(1.5)}{3\cdot 2}(6)$$

$$= 421.875$$

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Ex :- 4. For the following data, obtain the backward difference polynomial using Gregory-Newton backward difference interpolation. Also interpolate at $x = 0.45$

x	$f(x)$
0.1	1.40
0.2	1.56
0.3	1.76
0.4	2.00
0.5	2.28

Soln :- The backward difference table is

x	$f(x)$	$\nabla f(x)$	$\nabla^2 f(x)$	$\nabla^3 f(x)$	
0.1	1.40				
		0.16			
0.2	1.56		0.04		
		0.20		0	
0.3	1.76		0.04		
		0.24		0	
0.4	2.00		0.04		
		0.28			
0.5	2.28				

Since the third & fourth order difference are zero the equation of Newton backward interpolation become

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

Here $f_n = 2.28$, $\nabla f_n = 0.28$, $\nabla^2 f_n = 0.04$

$u = \frac{x - x_n}{h}$ $x = 0.45$ $u = \frac{0.45 - 0.5}{0.1} = -0.5$

Substituting the value, we get

$$f(0.45) = f(x) = 2.28 + -(0.5)(0.28) + \frac{(-0.5)(0.5)(0.04)}{2.1}$$

$$= 2.135$$

Splines & Piecewise Interpolation :-

Introduction to splines :- In polynomial of higher degree, results of interpolation by computation becomes unreliable because of round off errors. In order to keep the degree of interpolating polynomial small and also to achieve accurate results piecewise interpolation is used. We divide the interval into various sub-interval. $x \in [a, b]$ to $[x_{i-1}, x_i]$ $i = 1, 2, \ldots n$ and approximate the function by some lower degree polynomial in each subinterval. i.e linear or quadratic or cubic interpolating polynomials to fit the data on each sub-interval.

or

An alternative approach is to apply lower-order polynomial in a piecewise fashion to ~~sub~~ subject to data points. Such connecting polynomial are called spline functions.

Ex) x_0 x_1 x_2 x_3 x_4 x_5 x_6

f_0 f_1 f_2 f_3 f_4 f_5 f_6 → Piecewise linear

→ " Quadratic

→ " Cubic

Linear Splines :- (Linear piece wise Interpolation)

For n data points (i = 1, 2 — n) there are n-1 interval. Each interval i has its own spline function, $s_i(x)$ For linear splines, each function is merely the straight line connecting the two points at each end of the interval, which is formulated as

$$s_i(x) = a_i + b_i (x - x_i) \quad \text{— (1)}$$

where a_i is the intercept, which is defined as

$$a_i = f_i$$

and b_i is the slope of the straight line connecting the points :

$$b_i = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

where f_i is shorthand for $f(x_i)$

Substituting a_i & b_i in eqn (1) it becomes

$$s_i(x) = f_i + \frac{f_{i+1} - f_i}{x_{i+1} - x_i}(x - x_i)$$

$s_i(x)$ give, linear spline in each sub-interval.

Ex:- (1.) Fit the data with first order splines. Evaluate the function at x=5

i	x_i	f_i
1	3.0	2.5
2	4.5	1.0
3	7.0	2.5
4	9.0	0.5

Soln: In the first interval [3, 4.5] we have

$$s_1(x) = 2.5 + \frac{1-2.5}{4.5-3}(x-3)$$

$$= 2.5 + \frac{-1.5}{1.5}(x-3) = -x+5.5$$

In the second interval [4.5, 7] we have

$$s_2(x) = 1.0 + \frac{2.5-1.0}{7.0-4.5}(x-4.5)$$

$$= 1.0 + \frac{1.5}{2.5}(x-4.5) = 0.6x-1.7$$

Since 5 lies in the interval [4.5, 7]

$$s_2(5) = 0.6(5)-1.7 = 1.3$$

In the third interval [7.0, 9.0] we have

$$s_3(x) = 2.5 + \frac{0.5-2.5}{9.0-7.0}(x-7)$$

$$s_3(x) = 2.5 + \frac{-2}{2}(x-7) = x+9.5$$

Hence, the piece wise interpolating polynomials are given as :-

$$s(x) = \begin{cases} -x+5.5 & 3 \le x \le 4.5 \\ 0.6x-1.7 & 4.5 \le x \le 7 \\ x+9.5 & 7 \le x \le 9 \end{cases}$$

& $s_2(5) = 1.3$

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Ex) Q.) Obtain the piecewise linear interpolating polynomial for the function f(x) defined by the given data.

x	f(x)
0	1
1	2
2	5
3	10

and interpolate at $x=0.5$ and 1.5

Soln:- In the first interval $[0,1]$ we have

$$s_1(x) = 1 + \frac{2-1}{1-0}(x-0) = x+1$$

In the second interval $[1,2]$ we have

$$s_2(x) = 2 + \frac{5-2}{2-1}(x-1)$$

$$= 3x-1$$

In the third interval $[2,3]$ we have

$$s_3(x) = 5 + \frac{10-5}{3-2}(x-2)$$

$$= 5x-5$$

Hence, the piecewise interpolation polynomials are given as

$$s(x) = \begin{cases} x+1 & 0 \le x \le 1 \\ 3x-1 & 1 \le x \le 2 \\ 5x-5 & 2 \le x \le 3 \end{cases}$$

Since 0.5 lies in [0,1]

$s_1(0.5) = 0.5+1 = 1.5$

Since 1.5 lies in [1,2]

$s_2(1.5) = 3(1.5)-1 = 3.5$

Cubic Splines:- (Only Method):- The objective in cubic splines is to draw a third order polynomial for each interval between knots as represented generally by $s_i(x) = a_i + b_i(x-x_i) + c_i(x-x_i)^2 + d_i(x-x_i)^3$

Thus, for n data points ($i = 1,2,\ldots n$) there are n-1 interval and 4(n-1) unknown coefficient to evaluate. Consequently, 4(n-1) conditions are required for their evaluation. For example if we have 4 data points then we have to determine 4(4-1) = 12 unknown using these relations i.e.

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ h_1 & 2(h_1+h_2) & h_2 & 0 \\ 0 & h_2 & 2(h_2+h_3) & h_3 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 3\{f[x_3,x_2] - f[x_2,x_1]\} \\ 3\{f[x_4,x_3] - f[x_3,x_2]\} \\ 0 \end{bmatrix} \quad (1)$$

where $f[x_i, x_j] = \dfrac{f_i - f_j}{x_i - x_j}$ the system is tridiagonal & Linear efficient to solve. The other coefficient can be determined by i.e. $b_i = \dfrac{f_{i+1} - f_i}{h_i} - \dfrac{h_i}{3}(2c_i + c_{i+1}) \quad (2)$

& $d_i = \dfrac{c_{i+1} - c_i}{3h_i} \quad (3) \qquad a_i = f_i$.

Let us take an example:

Ex: (1.1): Fit the data with cubic spline. Evaluate the function at $x=5$

i	x_i	f_i
1	3.0	2.5
2	4.5	1.0
3	7.0	2.5
4	9.0	0.5

Soln: The first step is to generate the set of simultaneous equation using matrix ① and determine c coefficient

we have ~~$x_1=1, x_2=1, x_3=3, x_4$~~ $x_1=3, x_2=4.5, x_3=7, x_4=9$

$f_1=2.5, f_2=1, f_3=2.5, f_4=0.5$

$h_1=4.5-3=1.5, h_2=7-4.5=2.5, h_3=9-7=2$

These can be substituted to yield

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1.5 & 8 & 2.5 & 0 \\ 0 & 2.5 & 9 & 2 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 4.8 \\ -4.8 \\ 0 \end{bmatrix}$$

$c_1=0, c_4=0, c_2=0.839543726, c_3=-0.76653$

Now using eqn ② & ③ we can determine b's & d's

$b_1=-1.419771863$ $d_1=0.186565272$ $a_1=f_1=2.5$

$b_2=-0.160456274$ $d_2=-0.214144487$ $a_2=f_2=1.0$

$b_3=0.022053232$ $d_3=0.127756654$ $a_3=f_3=2.5$

Now substituting these values in cubic spline eqn for different interval we get cubic spline for each interval

$s_1(x) = 2.5 - 1.419771863(x-3) + 0.186565272(x-3)^3$

$s_2(x) = 1.0 - 0.160456274(x-4.5) + 0.839543726(x-4.5)^2$

$\quad - 0.214144487(x-4.5)^3$

$s_3(x) = 2.5 + 0.622053232(x-7.0) + 0.766539924(x-7.0)^2$

$\quad + 0.127756654(x-7.0)^3$

Since 5 lies in the interval $[4.5, 7]$

so, $s_2(5) = 1.0 - 0.160456274(5-4.5) + 0.839543726(5-4.5)^2$

$\quad - 0.214144487(5-4.5)^3$

$= 1.102889734$

* The problem related to cubic spline is not in the syllabus, this problem is solved just for understand the method.