TRINITY COLLEGE FOR WOMEN
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Department of Physics

COMPUTATIONAL METHODS
19PPH08-ODD Semester

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Curve Fitting – Fitting a straight line

By Least squares

- The straight line equation y = f(x) = ax+b
- The normal equations are, $a\sum x^2 + b\sum x = \sum xy$ and $a\sum x + nb = \sum y$
- Example: Fit a straight line to the following data

x	0	5	10	15	20	25
y	12	15	17	22	24	30

Solution:

Let the equation of straight line to best fit be

y=ax+b

The Normal equation are

$$a\sum x + nb = \sum y$$

$$a\sum x^2 + b\sum x = \sum xy$$

Substitute the values in normal equations

75a+6b=120

1375a+75b=1805

Solve the equations, we get

a=0.697

b=11.287

Therefore the straight line equation is

Y=0.697x +11.237

x	y	xy	x^2
0	12	0	0
5	15	75	25
10	17	170	100
15	22	330	225
20	24	480	400
25	30	750	625
$\sum x=75$	$\sum y=120$	$\sum xy=1805$	$\sum x^2=1375$

Interpolation

for equal intervals

- Linear interpolation : $f(x) = f(x_1) + (x - x_1) \cdot \frac{f(x_2) - f(x_1)}{x_2 - x_1}$

Example: The table below gives square roots for integers determine the square root of 2.5.

x	1	2	3	4	5
f(x)	1	1.4142	1.7321	2	2.2361

Solution

The given value of 2.5 lies between the points 2 and 3 in the given values.

Therefore we are using linear interpolation formula $f(x) = f(x_1) + (x - x_1) \cdot \frac{f(x_2) - f(x_1)}{x_2 - x_1}$

where,

x=2.5 , x1=2 , f(x1)=1.4142, x2=3 , f(x2)=1.7321

$$f(2.5) = 1.4142 + (2.5 - 2)\,\frac{1.7321 - 1.4142}{3 - 2}$$

f(2.5) =1.5731

Truncation error

Example: Find the truncation error in the result of the following function for x= $\frac{1}{5}$, $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \frac{x^5}{5!} + \frac{x^6}{6!}$, when we use first four terms.

Solution

Given x= $\frac{1}{5}$= 0.5

We take first four terms for calculation therefore the remining two is the value of error. Therefore

Truncation error for first four terms $= \frac{x^4}{4!} + \frac{x^5}{5!}$

$$= \frac{0.5^4}{4!} + \frac{0.5^5}{5!}$$

$$= 0.694222 \text{ x } 10^{-4}$$

Newton-Raphson method

Roots of nonlinear equations

- Newton-Raphson method f(x_{n+1}) $= x_n - \dfrac{f(x_n)}{f'(x_n)}$

Example: Find the root of the equation f(x) = $x^2 - 3x + 2$ in the vicinity of x = 0 by using Newton-Raphson method.

Solution

Newton-Raphson method f(x_{n+1}) $= x_n - \dfrac{f(x_n)}{f'(x_n)}$

Given :

For first approximation x_0 = 0, f(x) = $x^2 - 3x + 2$, f'(x) = 2x−3

$$f(x_1) = x_0 - \frac{f(x_0)}{f'(x_0)} = 0 - \frac{{x_0}^2 - 3x_0 + 2}{(2x_0 - 3)} = -\frac{2}{-3} = \frac{2}{3} = 0.6667$$

Similarly in second approximation x_1 = 0.6667, f(x) = $x^2 - 3x + 2$, f'(x) = 2x−3

$$f(x_1) = x_0 - \frac{f(x_1)}{f'(x_1)} = 0.6667 - \frac{0.4444}{-1.6667} = 0.9333$$

Continue the approximation, we get the answer 1.0 for sixth and seventh approximation. Therefore the root close to the point at **x = 0 is 1.0**

Simpson’s 3/8 Rule

Numerical Integration

- Simpson’s 3/8 rule $\int_{x_0}^{x_n} f(x)dx = \frac{3h}{8}$ [f(a) + f(b) + 3 f(x_1) + 3 f(x_2)]

Example: Evaluate the following intervals using Simpson’s 3/8 rule: $\int_1^2 (x^3 + 1)$ dx

Solution:

Simpson’s 3/8 rule $\int_{x_0}^{x_n} f(x)dx = \frac{3h}{8}$ [f(a) + f(b) + 3 f(x_1) + 3 f(x_2)]

Given: a = 1, b = 2, f(x_1) = f (a + h) , f(x_2) = f (a + 2h), h = $\frac{b-a}{2}$ = 0.5

$\int_1^2 (x^3 + 1)$ dx = $\frac{3(0.5)}{8}$ [f(1) + f(2) + 3 f(1+) + 3 f(x_2)]

= 0.1875 [2 + 9 + 3.375 + 27]

$\int_1^2 (x^3 + 1)$ dx = 7.7578

Two Point formula

Numerical Differentiation - first order

- **First order forward difference two point formula f'(x) = $\frac{f(x+h)-f(x)}{h}$**

Example: estimate approximate derivative of f(x) = x^2 at x=1 for h= 0.2 and 0.1 using first order forward difference formula and compare with the exact answer.

Solution:

First order forward difference two point formula f'(x) = $\frac{f(x+h)-f(x)}{h}$

Given: f(x) = x^2 at x=1 for

i) If h= 0.2

$$f'(1) = \frac{f(1+0.2)-f(1)}{0.2} = \frac{f(1.2)-f(1)}{0.2} = \frac{1.2^2-1^2}{0.2} = 2.2$$

ii) If h= 0.1

$$f'(1) = \frac{f(1+0.1)-f(1)}{0.1} = \frac{f(1.1)-f(1)}{0.1} = \frac{1.1^2-1^2}{0.1} = 2.1$$

III) Exact answer

f(x) = x^2

f'(x) = 2x = 2 X 1 = 2

h	f'(x)	Error
0.2	2.2	0.2
0.1	2.1	0.1

Euler's Method

Numerical Solution to ordinary differential equations

- **The Euler's formula $y_{n+1} = y_n + \text{f h}(x_{n,} y_n)$**

Example: Given the equation $\frac{dy}{dx} = 3x^2 + 1$ with y(1) = 2 estimate y(2) by Euler's method using h=0.5.

Solution:

The Euler's formula $y_{n+1} = y_n + \text{f h}(x_{n,} y_n)$

Given: y(1) = 2, f(x) = = $3x^2 + 1$, $x_0 = 1$, y_0= 2, h= 0.5

$y_1(0.5) = y_0 + \text{o.5 f } (x_0, y_0)$

$= 2 + 0.5\ (3x_0^2 + 1)$

$= 2 + 0.5\ (4)$

$y_1(0.5) = 4$ and $x_1 = 1.5$

$y_2(1.0) = y_1 + 0.5\text{ f } (x_1, y_1)$

$= 4 + 0.5\ (3x_1^2 + 1)$

$= 4 + 0.5\ (7.75)$

$y_2(1.0) = 7.875$, $x_1 = 2$

Gauss Elimination Method

Solution of Linear equations

Example: Using Gauss Jordan method and solve the following linear equations

$5x + 4y = 15$ and $3x + 7y = 12$

Solution:

Write the equations in augmented matrix form

$$\begin{pmatrix} 5 & 4 & 15 \\ 3 & 7 & 12 \end{pmatrix}$$

Change the element I first row and first column as one

$$\rightarrow \begin{pmatrix} 1 & 4/5 & 3 \\ 3 & 7 & 12 \end{pmatrix} R_1 \qquad R_1/5$$

Make all the other components in the first column equal to zero

$$\begin{pmatrix} 1 & 4/5 & 3 \\ 0 & 7 - \frac{3 X 4}{5} & 12 - 3 X 3 \end{pmatrix} R_2 \qquad R_2 - 3R_1; \rightarrow \begin{pmatrix} 1 & 4/5 & 3 \\ 0 & {}^{23}/_{5} & 3 \end{pmatrix}$$

Make the element in the second row and second column as one

$$\begin{pmatrix} 1 & 4/5 & 3 \\ 0 & 1 & \frac{15}{23} \end{pmatrix} R_2 \qquad R_2 / \frac{23}{5} \rightarrow$$

By using back substitution method

$y = \frac{15}{23} = \mathbf{0.6522}$ and $x + \frac{4}{5}y = 3$; $x = 3 - \frac{4}{5}(0.6522)$

x = 2.4782 and

y = 0.6522

THANK YOU

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