Chapter 5

Numerical Differentiation & Numerical integration

There are two reasons for approximating derivatives and integrals of a function f(x). One is when the function is very difficult to differentiate or integrate, or only the tabular values are available for the function. Another reason is to obtain solution of a differential or integral equation.

In section 1, we obtain numerical methods to find derivatives of a function. Rest of the chapter introduces various methods for numerical integration.

1- Numerical Differentiation

Numerical differentiation methods are obtained using one of the following techniques:

I. Methods based on Finite Difference Operators

II. Methods based on Interpolation (Lagrange and divided difference operator).

Through the first method, the numerical differentiation can be obtained by differentiating the Newton Gregory formula (forward or backward) then divide it by h for first derivative, h^2 for second derivative, etc.

Forward-difference: $f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$ when $h > 0$.

Backward-difference: $f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$ when $h < 0$.

We can simplify this considerably if we take k = 0, giving a derivative corresponding to $x = x_0$

$$\boxed{f'(x_0) \approx \tfrac{1}{h}\left\{\Delta f_0 - \tfrac{1}{2}\Delta^2 f_0 + \tfrac{1}{3}\Delta^3 f_0 - \tfrac{1}{4}\Delta^4 f_0 + \ldots - (-1)^n \tfrac{1}{n}\Delta^n f_0\right\} \qquad (1)}$$

(Same rule will be obtained for backward formula)

Examples

1. Using Newton's forward/backward differentiation method to find solution at x=0

Newton's forward differentiation table is as follows.

X	Y(X)	ΔY	$\Delta^2 Y$	$\Delta^3 Y$	$\Delta^4 Y$
0	**1**				
		-0.0025			
0.1	0.9975		**-0.005**		
		-0.0075		**0.0001**	
0.2	0.99		-0.0049		**-0.1**
		-0.0124		-0.0999	
0.3	0.9776		-0.1048		
		-0.1172			
0.4	0.8604				

The value of x at you want to find $f(x): x_0 = 0$

$h = x_1 - x_0 = 0.1 - 0 = 0.1$

$$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{1}{h} \cdot \left(\Delta Y_0 - \frac{1}{2} \cdot \Delta^2 Y_0 + \frac{1}{3} \cdot \Delta^3 Y_0 - \frac{1}{4} \cdot \Delta^4 Y_0\right)$$

$$\therefore \left[\frac{dy}{dx}\right]_{x=0} = \frac{1}{0.1} \cdot \left(-0.0025 - \frac{1}{2} \times -0.005 + \frac{1}{3} \times 0.0001 - \frac{1}{4} \times -0.1\right)$$

$$\therefore \left[\frac{dy}{dx}\right]_{x=0} = 0.25033$$

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2} \cdot \left(\Delta^2 Y_0 - \Delta^3 Y_0 + \frac{11}{12} \cdot \Delta^4 Y_0\right)$$

$$\therefore \left[\frac{d^2y}{dx^2}\right]_{x=0} = \frac{1}{0.01} \cdot \left(-0.005 - 0.0001 + \frac{11}{12} \times -0.1\right)$$

$$\therefore \left[\frac{d^2y}{dx^2}\right]_{x=0} = -9.67667$$

Solution for $Pn'(0) = 0.25033$

Solution for $Pn''(0) = -9.67667$

Example

Use the data in the table below to estimate y'(1.7).
Use h = 0.2 and find the result using 1, 2, 3 and 4 terms of the formula.

x	$y=e^x$	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
1.3	3.669				
		0.813			
1.5	4.482		0.179		
		0.992		0.041	
1.7	5.474		0.220		0.007
		1.212		0.048	
1.9	6.686		0.268		0.012
		1.480		0.060	
2.1	8.166		0.328		0.012
		1.808		0.072	
2.3	9.974		0.400		
		2.208			
2.5	12.182				

With one term : $y'(1.7) = \frac{1}{0.2}(1.212) = 6.060$

With two terms : $y'(1.7) = \frac{1}{0.2}(1.212 - \frac{1}{2}0.268) = 5.390$

With three terms : $y'(1.7) = \frac{1}{0.2}(1.212 - \frac{1}{2}0.268 + \frac{1}{3}0.060) = 5.490$

With four terms : $y'(1.7) = \frac{1}{0.2}(1.212 - \frac{1}{2}0.268 + \frac{1}{3}0.060 - \frac{1}{4}0.012) = 5.475$

H.W.
Use y = 1 + log x to determine y' at x = 0.15, 0.19 and 0.23 using
(a) one term, (b) two terms, (c) three terms.

Newton Backward differentiation formula

Formula

1. For $x = x_n$

$$\left[\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h} \cdot \left(\nabla Y_n + \frac{1}{2} \cdot \nabla^2 Y_n + \frac{1}{3} \cdot \nabla^3 Y_n + \frac{1}{4} \cdot \nabla^4 Y_n + \ldots\right)$$

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_n} = \frac{1}{h^2} \cdot \left(\nabla^2 Y_n + \nabla^3 Y_n + \frac{11}{12} \cdot \nabla^4 Y_n + \ldots\right)$$

2. For any value of x

$$\left[\frac{dy}{dx}\right] = \frac{1}{h} \cdot \left(\nabla Y_n + \frac{2t+1}{2} \cdot \nabla^2 Y_n + \frac{3t^2+6t+2}{6} \cdot \nabla^3 Y_n + \frac{4t^3+18t^2+22t+6}{24} \cdot \nabla^4 Y_n + \ldots\right)$$

$$\left[\frac{d^2y}{dx^2}\right] = \frac{1}{h^2} \cdot \left(\nabla^2 Y_n + (t+1) \cdot \nabla^3 Y_n + \frac{12t^2+36t+22}{24} \cdot \nabla^4 Y_n + \ldots\right)$$

Examples

1. Using Newton's Backward Difference formula to find solution at x=2.2

Newton's backward differentiation table is

x	y	∇y	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$
1.4	4.0552				
		0.8978			
1.6	4.953		0.1988		
		1.0966		0.0441	
1.8	6.0496		0.2429		**0.0094**
		1.3395		**0.0535**	
2	7.3891		**0.2964**		
		1.6359			
2.2	**9.025**				

$h = x_1 - x_0 = 1.6 - 1.4 = 0.2$

$$\left[\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h} \cdot \left(\nabla y_n + \frac{1}{2} \cdot \nabla^2 y_n + \frac{1}{3} \cdot \nabla^3 y_n + \frac{1}{4} \cdot \nabla^4 y_n\right)$$

$$\therefore \left[\frac{dy}{dx}\right]_{x=2.2} = \frac{1}{0.2} \times \left(1.6359 + \frac{1}{2} \times 0.2964 + \frac{1}{3} \times 0.0535 + \frac{1}{4} \times 0.0094\right)$$

$$\therefore \left[\frac{dy}{dx}\right]_{x=2.2} = 9.02142$$

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_n} = \frac{1}{h^2} \cdot \left(\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12} \cdot \nabla^4 y_n\right)$$

$$\therefore \left[\frac{d^2y}{dx^2}\right]_{x=2.2} = \frac{1}{0.04} \cdot \left(0.2964 + 0.0535 + \frac{11}{12} \times 0.0094\right)$$

$$\therefore \left[\frac{d^2y}{dx^2}\right]_{x=2.2} = 8.96292$$

$\therefore \; Pn'(2.2) = 9.02142$ and $Pn''(2.2) = 8.96292$

First derivative by Lagrange interpolation formula

Formula

Langrange's formula

1. Find equation using Langrange's formula

$$f(x) = \frac{(x - x_1)(x - x_2)...(x - x_n)}{(x_0 - x_1)(x_0 - x_2)...(x_0 - x_n)} \times y_0 + \frac{(x - x_0)(x - x_2)...(x - x_n)}{(x_1 - x_0)(x_1 - x_2)...(x_1 - x_n)} \times y_1$$

$$+ \frac{(x - x_0)(x - x_1)(x - x_3)...(x - x_n)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)...(x_2 - x_n)} \times y_2 + ... + \frac{(x - x_0)(x - x_1)...(x - x_{n-1})}{(x_n - x_0)(x_n - x_1)...(x_n - x_{n-1})} \times y_n$$

2. Now, differentiate f(x) with respect to x to get f'(x) and f''(x)

3. Now, substitute value of x in f'(x) and f''(x)

1. Example: Using Langrange's formula to find solution at x=5

Solution:
The value of table for x and y

x	2	4	9	10
y	4	56	711	980

Langrange's Interpolating Polynomial
Langrange's formula is

$$f(x) = \frac{(x - x_1)(x - x_2)(x - x_3)}{(x_0 - x_1)(x_0 - x_2)(x_0 - x_3)} \times y_0 + \frac{(x - x_0)(x - x_2)(x - x_3)}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)} \times y_1 + \frac{(x - x_0)(x - x_1)(x - x_3)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)} \times y_2 + \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_3 - x_0)(x_3 - x_1)(x_3 - x_2)} \times y_3$$

$$f(x) = \frac{(x - 4)(x - 9)(x - 10)}{(2 - 4)(2 - 9)(2 - 10)} \times 4 + \frac{(x - 2)(x - 9)(x - 10)}{(4 - 2)(4 - 9)(4 - 10)} \times 56 + \frac{(x - 2)(x - 4)(x - 10)}{(9 - 2)(9 - 4)(9 - 10)} \times 711 + \frac{(x - 2)(x - 4)(x - 9)}{(10 - 2)(10 - 4)(10 - 9)} \times 980$$

$$f(x) = \frac{(x - 4)(x - 9)(x - 10)}{(-2)(-7)(-8)} \times 4 + \frac{(x - 2)(x - 9)(x - 10)}{(2)(-5)(-6)} \times 56 + \frac{(x - 2)(x - 4)(x - 10)}{(7)(5)(-1)} \times 711 + \frac{(x - 2)(x - 4)(x - 9)}{(8)(6)(1)} \times 980$$

$$f(x) = \frac{x^3 - 23x^2 + 166x - 360}{-112} \times 4 + \frac{x^3 - 21x^2 + 128x - 180}{60} \times 56 + \frac{x^3 - 16x^2 + 68x - 80}{-35} \times 711 + \frac{x^3 - 15x^2 + 62x - 72}{48} \times 980$$

$$f(x) = (x^3 - 23x^2 + 166x - 360) \times -0.0357 + (x^3 - 21x^2 + 128x - 180) \times 0.9333 + (x^3 - 16x^2 + 68x - 80) \times -20.3143 + (x^3 - 15x^2 + 62x - 72) \times 20.4167$$

$$f(x) = (- + 0.82x^2 - 5.93x + 12.86) + (0.93x^3 - 19.6x^2 + 119.47x - 168) + (-20.31x^3 + 325.03x^2 - 1381.37x + 1625.14) + (20.42x^3 - 306.25x^2 + 1265.83x - 1470)$$

$f(x) = x^3 - 2x$

$f(x) = x^3 - 2x$

Now, differentiate with x

$f'(x) = 3x^2 - 2$

$f''(x) = 6x$

Now, substitute $x = 5$

$f'(5) = 3 \times 5^2 - 2 = 73$

$f''(5) = 6 \times 5 = 30$

Remark: to compute the derivative using divided difference formula, same procedure will be followed as in Lagrange case