Lecture 06
Numerical Differentiation

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Introduction

- ***Calculus*** is the mathematics of change. Because engineers and scientists must continuously deal with systems and processes that change, calculus is an essential tool of our profession. Standing at the heart of calculus is the mathematical concept of differentiation.
- According to the dictionary definition, to *differentiate* means to mark off by differences; distinguish; . . . to perceive the difference in or between.
- Mathematically, the *derivative*, which serves as the fundamental vehicle for differentiation, represents the rate of change of a dependent variable with respect to an independent variable.

Introduction

- Need for differentiation of a function arises quite often in engineering and scientific problems.
- If the function has a closed form representation in terms of standard calculus, then its derivative can be found exactly.
- However, in many situations, we may not know the exact function . What we know is only the values of the function at a discrete set of points. For instance, we are given the distance traveled by a moving object at some regular time intervals and asked to determine its velocity at a particular time.
- In some other instances, the function is known but it is so complicated that an analytic differentiation is difficult (if not impossible).

Introduction

- The method of obtaining the derivative of a function using a numerical technique is known as numerical differentiation.
- There are essentially two situations where numerical differentiation is required. They are:

1. The function values are known but the function is unknown. Such a function is called a tabulated function.
2. The function to be differentiated is complicated and, therefore, it is difficult to differentiate.

Differentiating Continuous Functions

- ✓ Forward Difference Formula

$$f'(x)=\frac{f(x+h)-f(x)}{h}$$

- ✓ Backward Difference Formula

$$f'(x)=\frac{f(x)-f(x-h)}{h}$$

- ✓ Central Difference Formula

$$f'(x)=\frac{f(x+h)-f(x-h)}{2h}$$

Example 3.1

Estimate approximate derivative of $f(x)=x^2$ at x=1, for h=0.2, 0.1, 0.05 and 0.01 using the forward, backward and central difference formula.

Solution:

Since $f(x)= x^2$,

$$f'(x)=2x$$

$$\text{so that } f'(1)= 2$$

So the correct value of the derivative is 2.

The forward difference formula is :

$$f'(x)=\frac{f(x+h)-f(x)}{h}$$

Example 3.1 (contd.)

In this case, x=1. Therefore,

$$f'(1)= \frac{f(1+h)-f(1)}{h}$$

So, when h= 0.2, we have

$$f'(1)= \frac{f(1+0.2)-f(1)}{0.2}$$

$$= \frac{f(1.2)-f(1)}{0.2}$$

$$= \frac{1.44-1}{0.2}$$

$$= 2.2$$

** **Do similar calculations for h= 0.1, 0.05 and 0.01 using forward difference formula.**

Example 3.1 (contd.)

Similarly, the computed derivatives when h= 0.1, 0.05 and 0.01 are computed and tabulated below:

h	f'(1)	Error
0.2	2.2	0.2
0.1	2.1	0.1
0.05	2.05	0.05
0.01	2.01	0.01

**The computed value of the derivate approaches the exact value as h decreases.

Example 3.1 (contd.)

- In a similar way, the backward difference formula is :

$$f'(x) = \frac{f(x) - f(x-h)}{h}$$

when x=1, the backward difference formula becomes,

$$f'(1) = \frac{f(1) - f(1-h)}{h}$$

when h=0.2, we have

$$f'(1) = \frac{f(1) - f(1-0.2)}{0.2}$$

$$= \frac{f(1) - f(0.8)}{0.2}$$

$$= \frac{1 - 0.64}{0.2}$$

$$= 1.8$$

** **Do similar calculations for h= 0.1, 0.05 and 0.01 using backward difference formula.**

Example 3.1 (contd.)

Similarly, the computed derivatives when h= 0.1, 0.05 and 0.01 are computed and tabulated below:

h	f'(1)	Error
0.2	1.8	- 0.2
0.1	1.9	- 0.1
0.05	1.95	- 0.05
0.01	1.99	- 0.01

** The computed value of the derivate approaches the exact value as h decreases.

Example 3.1 (contd.)

- The central difference formula is:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

when x=1, the central difference formula becomes,

$$f'(1) = \frac{f(1+h) - f(1-h)}{2h}$$

when h=0.2, we have

$$f'(1) = \frac{f(1+0.2) - f(1-0.2)}{0.4}$$

$$= \frac{f(1.2) - f(0.8)}{0.4}$$

$$= \frac{1.44 - 0.64}{0.4}$$

$$= 2$$

** **Do similar calculations for h= 0.1, 0.05 and 0.01 using central difference formula.**

Example 3.1 (contd.)

Similarly, the computed derivatives when h= 0.1, 0.05 and 0.01 are computed and tabulated below:

h	f'(1)	Error
0.2	2.0	0
0.1	2.0	0
0.05	2.0	0
0.01	2.0	0

** The derivate is exact for all values of h. This because we have quadratic approximation for a quadratic function .

Practice Problem

- **3.2** Compute the approximate derivatives of f(x)= sin x, at x=0.45 radians, for h= 0.030, 0.035 and 0.040 using the forward, backward and central difference formula. Compare the results with the exact value of the derivative.

- **3.3** Estimate approximate derivative of f(x)=ln x at x=1, for h=0.2, 0.1, 0.05 and 0.01 using the forward, backward and central difference formula. Compare the results with the exact value of the derivative.

Differentiating Tabulated Function

- Suppose that we are given a set of data points (x_i, f_i), i=0,1,….. , N which correspond to the values of an unknown function f(x) and we wish to estimate the derivatives at these points. Assume that the points are equally spaced with a step size of h.
- When function values are available in tabulated form, we may approximate this function by an interpolation polynomial and then differentiate it. We will use here the Newton-Gregory forward polynomial.

$$y = \sum_{j=0}^{n} \binom{s}{j} \Delta^j f_0$$

where $x=x_0 +sh$

Differentiating Tabulated Function

$$y = \sum_{j=0}^{n} \binom{s}{j} \Delta^j f_0$$

This equation can be written as :

$$y = f_0 + s\Delta f_0 + \frac{s\,(s-1)}{2!}\Delta^2 f_0 + \frac{s\,(s-1)\,(s-2)}{3!}\Delta^3 f_0 + \cdots\cdots$$

$$f'(x) = \frac{dy}{dx} = \frac{1}{h}\left[\Delta f_0 + \frac{2s-1}{2}\Delta^2 f_0 + \frac{3s^2-6s+2}{6}\Delta^3 f_0 + \cdots\cdots\right]$$

This formula can be used for computing the value of the first derivative f'(x) both for non-tabulated and tabulated values.

Differentiating Tabulated Function

However, for tabulated values of x, the formula takes a simple form, for setting $x=x_0$ and hence the equation becomes

$$f'(x_0)=\frac{dy}{dx}=\frac{1}{h}\left[\Delta f_0-\frac{1}{2}\Delta^2 f_0+\frac{1}{3}\Delta^3 f_0-\frac{1}{4}\Delta^4 f_0+\frac{1}{5}\Delta^5 f_0-\frac{1}{6}\Delta^6 f_0+\ldots\ldots\right]$$

Differentiating once again,

$$f''(x)=\frac{1}{h^2}\left[\Delta^2 f_0+(s-1)\Delta^3 f_0+\frac{12s^2-36s+22}{24}\Delta^4 f_0+\ldots\ldots\ldots\right]$$

From which we obtain by setting $x=x_0$ and $s=0$ the equation

$$f''(x_0)=\frac{1}{h^2}\left[\Delta^2 f_0-\Delta^3 f_0+\frac{11}{12}\Delta^4 f_0-\frac{5}{6}\Delta^5 f_0+\frac{137}{180}\Delta^6 f_0-\frac{7}{10}\Delta^7 f_0+\frac{363}{360}\Delta^8 f_0-\ldots..\right]$$

Example 3.4

From the following table of values of x and y, obtain dy/dx and d^2y/dx^2 for x=1.

x	**1.0**	**1.2**	**1.4**	**1.6**	**1.8**	**2.0**	**2.2**
y	2.7183	3.3201	4.0552	4.9530	6.0496	7.3891	9.0250

The difference table is:

x	y= f(x)	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$	$\Delta^5 f$	$\Delta^6 f$
1.0	2.7183						
		0.6018					
1.2	3.3201		0.1333				
		0.7351		0.0294			
1.4	4.0552		0.1627		0.0067		
		0.8978		0.0361		0.0013	
1.6	4.9530		0.1988		0.0080		0.0001
		1.0966		0.0441		0.0014	
1.8	6.0496		0.2429		0.0094		
		1.3395		0.0535			
2.0	7.3891		0.2964				
		1.6359					
2.2	9.0250						

We have $x=x_0=1$, $h=0.2$ and $s=0$.

$$\mathbf{f'(x_0)= \frac{1}{h} [\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 - \frac{1}{4}\Delta^4 f_0 + \frac{1}{5}\Delta^5 f_0 - \frac{1}{6}\Delta^6 f_0 + \dots\dots]}$$

$$f'(1)= \frac{1}{0.2} [\, 0.6018 - \frac{1}{2} \times 0.1333 + \frac{1}{3} \times 0.0294 - \frac{1}{4} \times 0.0067 + \frac{1}{5} \times 0.0013 - \frac{1}{6} \times 0.0001]$$

$$= 2.7176$$

$$\mathbf{f''(x_0)= \frac{1}{h^2} [\Delta^2 f_0 - \Delta^3 f_0 + \frac{11}{12}\Delta^4 f_0 - \frac{5}{6}\Delta^5 f_0 + \frac{137}{180}\Delta^6 f_0 - \frac{7}{10}\Delta^7 f_0 + \frac{363}{360}\Delta^8 f_0 - \dots..]}$$

$$f''(1)= \frac{1}{(0.2)^2} [\, 0.1333 - 0.0294 + \frac{11}{12} \times 0.0067 - \frac{5}{6} \times 0.0013 + \frac{137}{180} \times 0.0001]$$

$$= 2.7259$$

Example 3.5

- From the following table find f'(1.4) using difference table. Compare the result with the correct result f'(1.4)= cosh(1.4)=2.1509

x	**1.2**	**1.3**	**1.4**	**1.5**	**1.6**
y	1.5095	1.6984	1.9043	2.1293	2.3756

Solution:

The difference table is:

x	**y= f(x)**	**Δ f**	**Δ^2f**	**Δ^3f**	**Δ^4f**
1.2	1.5095				
		0.1889			
1.3	1.6984		0.017		
		0.2059		0.0021	
1.4	1.9043		0.0191		0.0001
		0.2250		0.0022	
1.5	2.1293		0.0213		
		0.2463			
1.6	2.3756				

Method 1:

We have $x=x_0=1.4$, $h=0.1$ and $s= 0$.

$$\mathbf{f'(x_0)= \frac{1}{h} [\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 - \frac{1}{4}\Delta^4 f_0 + \frac{1}{5}\Delta^5 f_0 - \frac{1}{6}\Delta^6 f_0 + \dots\dots]}$$

$$f'(1.4)= \frac{1}{0.1} [\, 0.2250 - \frac{1}{2} \times 0.0213]$$

$$= \mathbf{2.1435}$$

Method 2:

$$f'(x)=\frac{dy}{dx}=\frac{1}{h}\left[\Delta f_0+\frac{2s-1}{2}\Delta^2 f_0+\frac{3s^2-6s+2}{6}\Delta^3 f_0+\frac{4s^3-18s^2+22s-6}{24}\Delta^4 f_0+\cdots\cdots\right]$$

$x=x_0+sh$

$s=\frac{x-x_0}{h}$

$=\frac{1.4-1.2}{0.1}$

$=2$

We have $x_0=1.2$, $h=0.1$ and $s=2$.

$$f'(x)=\frac{dy}{dx}=\frac{1}{h}\left[\Delta f_0+\frac{2s-1}{2}\Delta^2 f_0+\frac{3s^2-6s+2}{6}\Delta^3 f_0+\frac{4s^3-18s^2+22s-6}{24}\Delta^4 f_0+\cdots\cdots\right]$$

$$f'(1.4)=\frac{1}{0.1}\left[0.1889+\frac{2(2)-1}{2}\times 0.017+\frac{3(2)^2-6(2)+2}{6}\times 0.0021+\frac{4(2)^3-18(2)^2+22(2)-6}{24}\times 0.0001\right]$$

$$=2.15091$$

THANK YOU