Lesson 18

Numerical Differentiation

18.1 Introduction

Given a continuous function $f(x)$ on an interval $[a,b]$, it can be differentiated on (a,b). However, when $f(x)$ is a complicated function or when it is given in a data set, we use numerical methods to find its derivatives. There are many ways of finding derivatives of a function when given in its data form. Important among these methods are methods based on interpolation, method based on finite difference operators. We discuss these methods through examples.

18.2 Methods based on Interpolation

If (x_i, f_i), $i = 0,1,2...$, N are the $(N+1)$ data points representing a function $y = f(x)$. The Lagrange interpolating polynomial for above set of data points is given by

$$P_N(x) = \sum_{k=0}^{N} l_k(x) f_k \tag{18.1}$$

where $l_k(x) = \dfrac{\pi(x)}{(x - x_k)\pi'(x_k)}$.

and $\pi(x) = (x - x_0)(x - x_1)...(x - x_N)$.

Differentiating (1) w.r.t. x, we obtain

$$P_N'(x) = \sum_{k=0}^{N} l_k'(x) f_k .$$

Case 1: Linear interpolation: For $(x_0, f_0), (x_1, f_1)$:

We have $P_1(x) = l_0(x) f_0 + l_1(x) f_1$

where $l_0(x) = \dfrac{x - x_1}{x_0 - x_1}$ and $l_1(x) = \dfrac{x - x_0}{x_1 - x_0}$.

$$P_1(x) = \frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1 .$$

The derivative of this is

$$P_1'(x) = \frac{1}{x_0 - x_1} f_0 + \frac{1}{x_1 - x_0} f \tag{18.2}$$

Case 2: Quadratic interpolation: For the data $\{(x_0, f_0),(x_1, f_1),(x_2, f_2)\}$, we have the interpolating polynomial as $P_2(x) = l_0(x) f_0 + l_1(x) f_1 + l_2(x) f_2$.

Its derivative is

$$P_2'(x) = l_0'(x) f_0 + l_1'(x) f_1 + l_2'(x) f_2$$

where $l_0'(x) = \dfrac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}$, $l_1'(x) = \dfrac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}$, $l_2'(x) = \dfrac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$.

$$\therefore P_2'(x) = \left[\frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} f_0 + \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} f_1 + \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} f_2 \right] \tag{18.3}$$

At $x = x_1$, $P_2'(x) = \dfrac{x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} f_0 + \dfrac{2x_1 - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} f_1 + \dfrac{x_1 - x_0}{(x_2 - x_0)(x_2 - x_1)} f_2$.

Similarly we can write $P_2'(x)$ at any nodal point or a non-nodal point.

In the same manner, $l_0''(x) = \dfrac{2}{(x_0 - x_1)(x_0 - x_2)}$, $l_1''(x) = \dfrac{2}{(x_1 - x_0)(x_1 - x_2)}$ and

$$l_2''(x) = \frac{2}{(x_2 - x_0)(x_2 - x_1)}$$

and the second derivative of $P_2(x)$ i.e.,

$$P_2''(x) = 2\left[\frac{f_0}{(x_0 - x_1)(x_0 - x_2)} + \frac{f_1}{(x_1 - x_0)(x_1 - x_2)} + \frac{f_2}{(x_2 - x_0)(x_2 - x_1)} \right] \tag{18.4}$$

This gives a way of finding an approximation to $f'(x)$ at every $x \in [x_0, x_N]$ by finding the interpolating polynomial $P_n(x)$ for the given set of data points.

Example 1: Find $f'(2)$ and $f''(2)$ for the below given data set.

x_i	2	2.2	2.6
f_i	0.69315	0.78846	0.95551

Solution:

We have

$$f'(x_0) = f'(2) = \frac{2x_0 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} f_0 + \frac{(x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)} f_1 + \frac{(x_0 - x_1)}{(x_2 - x_0)(x_2 - x_1)} f_2$$

$$= \frac{4 - 2.2 - 2.6}{(-0.2)(-0.6)}(0.69315) + \frac{2 - 2.6}{(0.2)(-0.4)}(0.78846) + \frac{2 - 2.2}{(0.6)(0.4)}(0.95551)$$

$$= 0.49619 .$$

$$f''(x_0) = 2\left[\frac{f_0}{(x_0 - x_1)(x_0 - x_2)} + \frac{f_1}{(x_1 - x_0)(x_1 - x_2)} + \frac{f_2}{(x_2 - x_0)(x_2 - x_1)}\right].$$

$$\therefore f''(2) = 2\left[\frac{0.69315}{(-0.2)(-0.6)} + \frac{0.78846}{(0.2)(-0.4)} + \frac{0.95551}{(0.6)(0.4)}\right]$$

$$= -0.19642 .$$

Thus $f'(2) = 0.49619$ and $f''(2) = -0.19642$.

In the above, we used Lagrange interpolation method. Similarly one can use Newton interpolation methods also.

18.3 Methods based on Finite Differences

For a given equally spaced data set, we have learnt that $Ef(x) = e^{hD} f(x)$

i.e., $e^{hD} \equiv E \Rightarrow hD \equiv \log E$ (18.5)

where E is the shift operator, D is the differentiation operator, h being the constant step size. Using the relation between E, Δ and ∇, we write

$$hD \equiv \log E \equiv \left| \begin{array}{l} \log(1+\Delta) \equiv \Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \ldots \\ -\log(1-\nabla) \equiv \nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \ldots \end{array} \right. \tag{18.6}$$

Then $h\frac{df}{dx}(x_k) \equiv hDf(x_k) \equiv \left| \begin{array}{l} \Delta f_k - \frac{1}{2}\Delta^2 f_k + \frac{1}{3}\Delta^3 f_k - \ldots \\ \nabla f_k + \frac{1}{2}\nabla^2 f_k + \frac{1}{3}\nabla^3 f_k + \ldots \end{array} \right.$ (18.7)

In general we can write the higher order derivatives in terms of the higher order differences, the nth derivative operator $\frac{d^n}{dx^n}$ can be written as

$$h^n D^n \equiv \begin{cases} \Delta^n - \frac{n}{2}\Delta^{n+1} + \frac{n(3n+5)}{24}\Delta^{n+2} - \ldots \\ \nabla^n + \frac{n}{2}\nabla^{n+1} + \frac{n(3n+5)}{24}\nabla^{n+2} + \ldots \end{cases} \tag{18.8}$$

In particular, when $n = 2$ and at $x = x_k$,

$$h^2 \frac{d^2 f}{dx^2}(x_k) \equiv \begin{cases} \Delta^2 f_k - \Delta^3 f_k + \frac{11}{12}\Delta^4 f_k - \ldots \\ \nabla^2 f_k + \nabla^3 f_k + \frac{11}{12}\nabla^4 f_k + \ldots \end{cases} \tag{18.9}$$

Example 2: Find $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ at $x = 1.2$ using forward differential from the following table:

x:	1	1.2	1.4	1.6	1.8	2.0
$y(x)$:	2.7183	3.3201	4.0552	4.953	6.0496	7.3891

Solution:

Take $x_0 = 1.2$, $y_0 = 3.3201$, $h = 0.2$. We form the difference table for the given data set as:

$$\left.\frac{dy}{dx}\right|_{x=1.2} = \frac{1}{h}\left[\Delta f(1.2) - \frac{1}{2}\Delta^2 f(1.2) + \frac{1}{3}\Delta^3 f(1.2) - \ldots\right]$$

$$= \frac{1}{0.2}\left[0.7351 - \frac{1}{2}(0.1627) + \frac{1}{3}(0.0361) - \ldots\right]$$

≈ 3.3205.

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5
1.2	3.3201					
		0.7351				
1.4	4.0552		0.1627			
		0.8978		0.0361		
1.6	4.9530		0.1988		0.008	
		1.0966		0.0441		0.0001
1.8	6.0496		0.2429		0.0094	
		1.3395		0.0535		
2.0	7.3891		0.2964			
		1.6359				
2.4	9.025					

$$\left.\frac{d^2y}{dx^2}\right|_{x=1.2} = \frac{1}{h^2}\left[\Delta^2 f_k - \Delta^3 f_k + \ldots\right]$$

$$= \frac{1}{0.04}\left[0.1627 - 0.0361\right] \approx 3.165.$$

Example 3: Given: (x_i, y_i), $i = 1,2,3,4,5,6$ as:

x	3	4	5	6	7	8
y	0.205	0.24	0.259	0.262	0.25	0.224

Find the value of x for which y is minimum.

Solution:

The difference table is:

x	y	Δ	Δ^2	Δ^3
3	0.205			
		0.035		
4	0.24		-0.016	
		0.019		0.0
5	0.259		-0.016	
		0.003		0.001
6	0.262		-0.015	
		-0.012		0.001
7	0.25		-0.014	
		-0.026		
8	0.224			

Take $x_0 = 3$, $y_0 = 0.205$, $h = 1.0$.

Let us now obtain the interpolating polynomial using Newton's forward difference interpolation. It is $y(x) = y_0 + p\Delta y_0 + \frac{p(p-1)}{2}\Delta^2 y_0$ where $p = \frac{x - x_0}{h}$

or $y(x) = 0.205 + (0.035)\,p - \frac{(0.016)}{2}\,p(p-1)$.

The minimum value of $y(x)$ is obtained by solving $\frac{dy}{dp} = 0$

i.e., $(0.035) - \frac{(2p-1)}{2}(0.016) = 0$

$\Rightarrow 0.035 - 0.008(2p-1) = 0$

$\Rightarrow (2P-1) = \frac{0.035}{0.008}$

$\Rightarrow p = 2.6875$

Thus $x = x_0 + ph = 3 + 2.6875 = 5.6875$.

Hence minimum value of $y(x)$ is attained at $x = 5.6875$ and the minimum value is 0.2628.

Exercises

1. Find the value of $\cos 1.747$ using the below table:

x:	1.7	1.74	1.78	1.82
$\sin x$:	0.9916	0.9857	0.9781	0.9691

2. Given $\sin 0^o = 0, \sin 10^o = 0.1736, \sin 20^o = 0.3420, \sin 30^o = 0.5, \sin 40^o = 0.6428$.

Find

(i) $\sin 23^o$

(ii) $\cos 10^o$

(iii) $-\sin 20^o$ using the method based on the finite differences.

3. Find the value of x for which y is maximum from the below tabulated values for $y(x)$.

x:	1.2	1.3	1.4	1.5	1.6
y:	0.93	0.96	0.98	0.99	1.0

Keyword: Finite differences, Lagrange interpolation,

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Suggested Reading

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