CHAPTER 7

NUMERICAL DIFFERENTIATION

The derivative of a function at x is defined as

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

To be able to find a derivative numerically, one could make Δx finite to give,

$$f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}.$$

Knowing the value of x at which you want to find the derivative of $f(x)$, we choose a value of Δx to find the value of $f'(x)$. To estimate the value of $f'(x)$, three such approximations are suggested as follows.

Forward Difference Approximation of the First Derivative

From differential calculus, we know

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

For a finite Δx,

$$f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

The above is the forward divided difference approximation of the first derivative. It is called forward because you are taking a point ahead of x. To find the value of $f'(x)$ at $x = x_i$, we may choose another point Δx ahead as $x = x_{i+1}$. This gives

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{\Delta x}$$

$$= \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

where

$$\Delta x = x_{i+1} - x_i$$

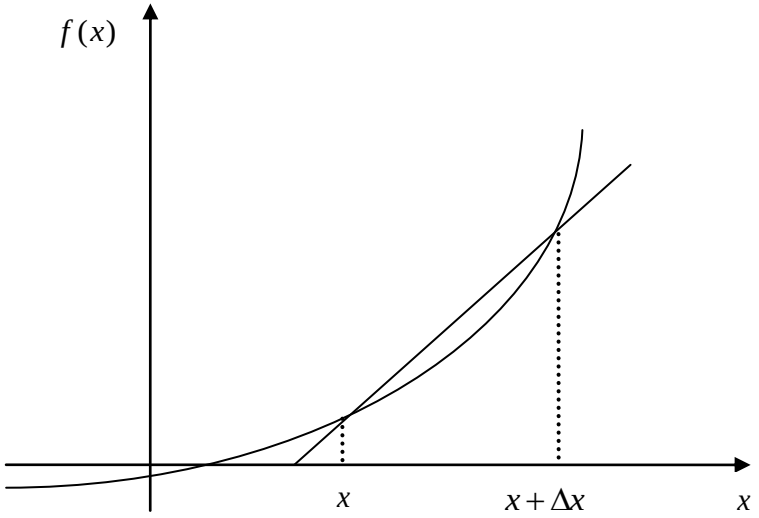


Figure 1 Graphical representation of forward difference approximation of first derivative

Example 1►
Let $f(x) = \ln x$ use forward difference two point formula to approximate $f'(1.8)$.
Solution
The formula $f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$ can be used to approximate $f'(1.8)$ using $\Delta x = 0.01$
$f'(1.8) = \frac{\ln(1.8+0.01) - \ln(1.8)}{0.01} = 0.5540180.$

Lagrange Polynomial

In this method, given $(x_0, y_0), \ldots, (x_n, y_n)$, one can fit a n^{th} order Lagrange polynomial given by

$$f_n(x) = \sum_{i=0}^{n} L_i(x) f(x_i)$$

where n in $f_n(x)$ stands for the n^{th} order polynomial that approximates the function $y = f(x)$ and

$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

$L_i(x)$ is a weighting function that includes a product of $n-1$ terms with terms of $j = i$ omitted.

Then to find the first derivative, one can differentiate $f_n(x)$ once, and so on for other derivatives.

For example, the second order Lagrange polynomial passing through $(x_0, y_0), (x_1, y_1),$ and (x_2, y_2) is

$$f_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

Differentiating the above equation gives

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

Appling this technique using the second Lagrange polynomial at x_0, $x_1 = x_0 + h$ and $x_2 = x_1 + h = x_0 + 2h$ produce the following formulas

Three point endpoint formula

$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3} f^{(3)}(\zeta).$

Where $x_0 \leq \zeta \leq x_0 + 2h$

Three point midpoint formula

$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] + \frac{h^2}{6} f^{(3)}(\zeta).$

Where $x_0 - h \leq \zeta \leq x_0 + 2h$

Example 2►

Use the most appropriate three-point formulas to determine approximations that will complete the following data:

x	0.1	0.3	0.5	0.7
$f(x) = xe^x$				
$f'(x)$				

Solution

First step:

x	0.1	0.3	0.5	0.7
$f(x) = xe^x$	0.110517	0.4049576	0.824606	1.4096269
$f'(x)$	End-Forward h = 0.2	Mid	Mid	End-Backward h = −0.2

Second step computations:

$$f'(0.1) = \frac{1}{2 \times 0.2}(-3 \times 0.110517 + 4 \times 0.4049576 - 0.824606) = 1.159797,$$

$$f'(0.3) = \frac{1}{2 \times 0.2}(0.824606 - 0.110517) = 1.7846009,$$

$$f'(0.5) = \frac{1}{2 \times 0.2}(1.4096269 - 0.4049576) = 2.51167325,$$

$$f'(0.7) = \frac{1}{2 \times -0.2}(-3 \times 1.4096269 + 4 \times 0.824606 - 0.4049576) = 3.34098975.$$

Third step complete the table:

x	0.1	0.3	0.5	0.7
$f(x) = xe^x$	0.110517	0.4049576	0.824606	1.4096269
$f'(x)$	1.159797	1.7846009	2.51167325	3.34098975

Example 3►

Use the most appropriate three points formulas to determine approximations that will complete the following data:

x	1.1	1.3	1.5	1.7
$f(x) = e^x$				
Approximation values of $f'(x)$				
Exact values of $f'(x)$				
Actual error				

Approximate each number within 5-decimal places.

Solution

First step:

x	1.1	1.3	1.5	1.7
$f(x) = e^x$	3.00417	3.66930	4.48169	5.47395
$f'(x)$	End-Forward h = 0.2	Mid	Mid	End-Backward h = −0.2

Second step: Computations:

$$f'(1.1) = \frac{1}{2 \times 0.2}(-3 \times 3.00417 + 4 \times 3.66930 - 4.48169) = 2.95750,$$

$$f'(1.3) = \frac{1}{2 \times 0.2}(4.48169 - 3.00417) = 3.69380,$$

$$f'(1.5) = \frac{1}{2 \times 0.2}(5.47395 - 3.66930) = 4.51163,$$

$$f'(1.7) = \frac{1}{2 \times -0.2}(-3 \times 5.47395 + 4 \times 4.48169 - 3.66930) = 5.41098.$$

Third step: Complete the table by computing the exact values of $f'(x) = e^x$ and the actual error:

x	1.1	1.3	1.5	1.7
$f(x) = e^x$	3.00417	3.66930	4.48169	5.47395
Approximation of $f'(x)$	2.95750	3.69380	4.51163	5.41098
Exact of $f'(x)$	3.00417	3.66930	4.48169	5.47395
Actual error	0.04667	0.02450	0.02994	0.06297

Example 4 ►

Given the data

x_i	1.8	1.9	2.0
$f(x_i)$	10.89	12.7	14.78

Use a 3-point formula to approximate $f'(2.0)$

Solution

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3}f^{(3)}(\zeta)$$

$\mathrm{h} = -0.1$

$$f'(2) = \frac{1}{2(-0.1)}[-3f(2) + 4f(1.9) - f(1.8)] + \frac{(-0.1)^2}{3}f^{(3)}(\zeta)$$

$$f'(2) = 22.15 + \frac{(-0.1)^2}{3}f^{(3)}(\zeta)$$

Exercise

1- Use forward difference two point formula to determine approximate that will complete the following tables

a)

x	0.5	0.6	0.7
$f(x)$	0.4797	0.5646	0.6442
$f'(x)$			

b)

x	0	0.2	0.4
$f(x)$	0.0	0.7414	0.13718
$f'(x)$			

2- Use the most appropriate three-point formulas to determine approximations that will complete the following data:

x	1.1	1.2	1.3	1.4
$f(x)$	9.0250	11.02318	13.46274	16.44465
$f'(x)$				

3- Use the most appropriate three-point formulas to determine approximations that will complete the following data:

x	8.1	8.3	8.5	8.7
$f(x)$	16.9441	17.56492	18.19056	18.82092
$f'(x)$				

4- Let $f(x) = \cos(\pi x)$. Use the three point formula and the values of $f(x)$ at $x = 0.25,\ 0.5\ and\ 0.75$ to approximate $f'(0.5)$. Compare this result to the exact value.