

Mathematical Physics II

Numerical Methods using Python: Numerical Differentiation

In this topic we shall discuss how to get an approximate value of the first order derivative of a function $f(x)$. In this connection we shall cover **Forward** and **Backward Difference Formula** for Numerical Differentiation.

- **Forward Difference Formula:** From Taylor's Theorem we know that one can obtain the value of a function at a point $x + \Delta x$ if the function is known at x using the following relation:

$$f(x + \Delta x) = f(x) + \Delta x f'(x) + \frac{(\Delta x)^2}{2} f''(\theta);$$

where Δx is a small increment in x and $x < \theta < x + \Delta x$. Replacing Δx by h and rearranging the above relation one can get

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

If h is sufficiently small then one can approximate

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

This is known as Forward Difference Formula. Here the neglected term $-\frac{h}{2} f''(\theta)$ is referred as truncation error E_t .

- **Backward Difference Formula:** Similarly if the increment in x , $\Delta x = -h$ then

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

This is known as Backward Difference Formula.

References

1. 'Numerical Methods', E. Balagurusamy, TMH, 2016.

- **Example 1:** In the following pictures sample python programs using forward and backward difference formulae have been shown to solve the following problem.

Evaluate the first derivative at $x = -2.5$ and at $x = 2.5$ of the following table function:

x	-2.5	-1.5	-0.5	0.5	1.5	2.5
y	-23	-8	1.5	1	7.5	23.5

```

1#!/usr/bin/env python2
2# -*- coding: utf-8 -*-
3"""
4Created on Wed Jun  5 11:43:28 2019
5
6@author: sonali
7"""
8
9x=[-2.5, -1.5, -.5, 0.5, 1.5, 2.5]
10y=[-23, -8, 1.5, 1, 7.5, 23.5 ]
11h=x[1]-x[0]
12fprime=(y[1]-y[0])/h
13print 'The first derivative at x=-2.5 is'
14print fprime

```

Figure 1: Sample Python Code for numerical differentiation using Forward Difference Formula

```

Python 2.7.15+ (default, Nov 27 2018, 23:36:35)
Type "copyright", "credits" or "license" for more information.

IPython 5.5.0 -- An enhanced Interactive Python.
?          -> Introduction and overview of IPython's features.
%quickref  -> Quick reference.
help       -> Python's own help system.
object?    -> Details about 'object', use 'object??' for extra
details.

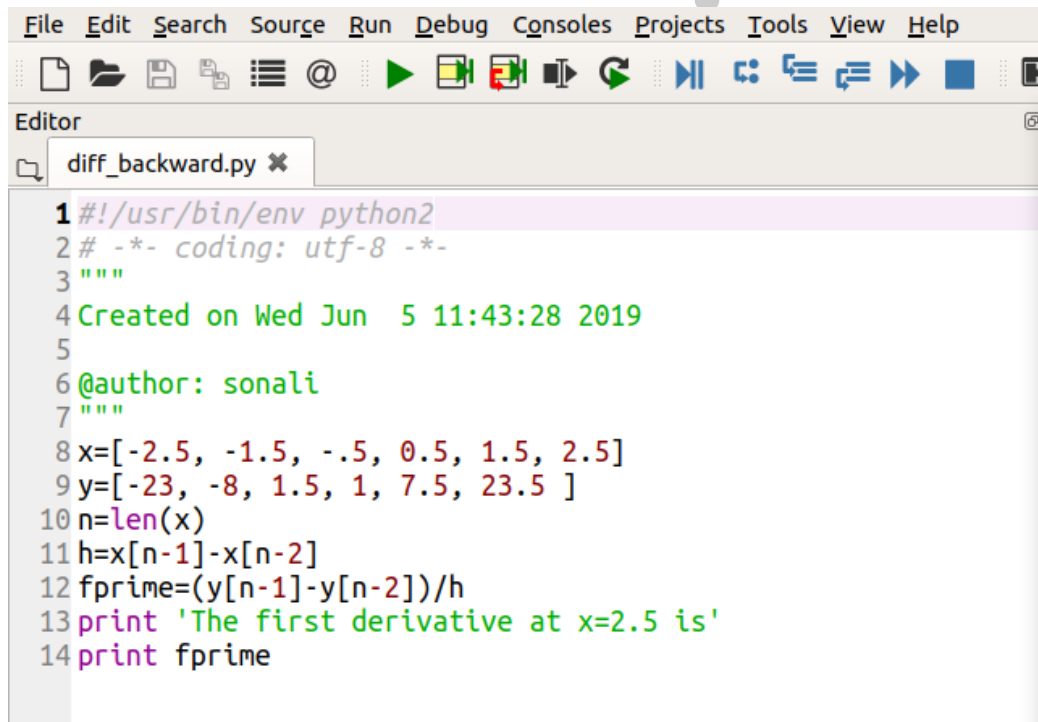
In [1]: runfile('/home/sonali/Documents/teaching_material/
diff_forward.py', wdir='/home/sonali/Documents/
teaching_material')
The first derivative at x=-2.5 is
15.0

In [2]:

```

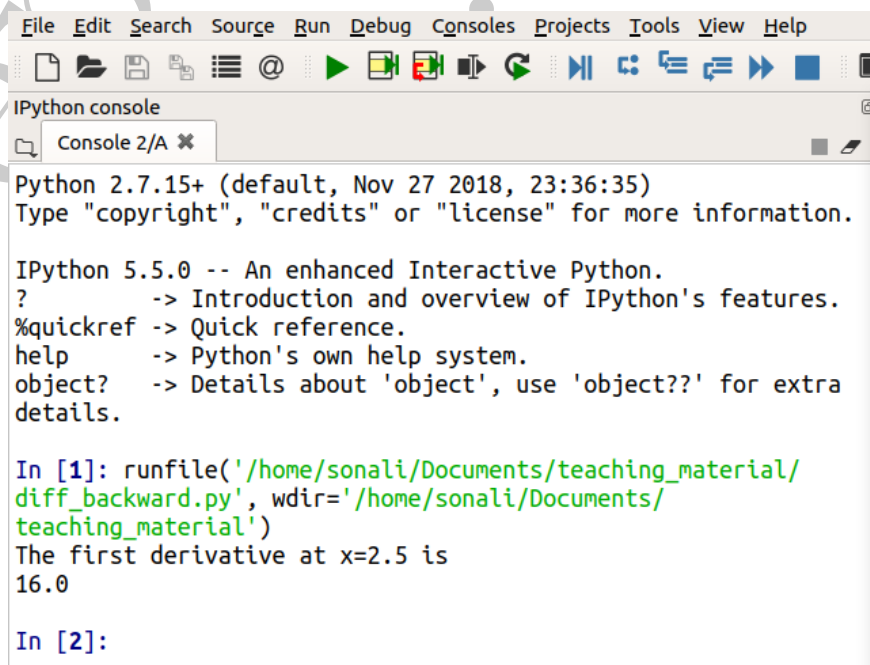
Figure 2: Output of the Python code using Forward Difference Formula

Now a sample code to determine the first derivative at $x = 2.5$ using backward difference formula follows as:



```
File Edit Search Source Run Debug Consoles Projects Tools View Help
diff_backward.py x
1#!/usr/bin/env python2
2# -*- coding: utf-8 -*-
3"""
4Created on Wed Jun  5 11:43:28 2019
5
6@author: sonali
7"""
8x=[-2.5, -1.5, -.5, 0.5, 1.5, 2.5]
9y=[-23, -8, 1.5, 1, 7.5, 23.5 ]
10n=len(x)
11h=x[n-1]-x[n-2]
12fprime=(y[n-1]-y[n-2])/h
13print 'The first derivative at x=2.5 is'
14print fprime
```

Figure 3: Sample Python Code for numerical differentiation using Backward Difference Formula



```
File Edit Search Source Run Debug Consoles Projects Tools View Help
IPython console
Console 2/A x
Python 2.7.15+ (default, Nov 27 2018, 23:36:35)
Type "copyright", "credits" or "license" for more information.

IPython 5.5.0 -- An enhanced Interactive Python.
?          -> Introduction and overview of IPython's features.
%quickref  -> Quick reference.
help       -> Python's own help system.
object?    -> Details about 'object', use 'object??' for extra
details.

In [1]: runfile('/home/sonali/Documents/teaching_material/
diff_backward.py', wdir='/home/sonali/Documents/
teaching_material')
The first derivative at x=2.5 is
16.0

In [2]:
```

Figure 4: Output of the Python code using Backward Difference Formula

- **Example 2:** In the following pictures sample python program is shown to calculate first derivative of function $f(x) = x^2 - 3x + 1$ at a point $x = 1$ with a specified accuracy 10^{-5} using forward difference formula along with its output.

```

1#!/usr/bin/env python2
2# -*- coding: utf-8 -*-
3"""
4Created on Wed May 29 11:32:19 2019
5
6@author: sonali
7"""
8
9def f(x):
10    return(x*x-3*x+1)
11x0=1
12h=0.1
13err=1000
14dfxold=1000
15while err>=0.00001:
16    dfx=(f(x0+h)-f(x0))/h
17    err=abs(dfxold-dfx)
18    dfxold=dfx
19    h=h/2.
20print 'The derivative at x=1 with specified accuracy is'
21print dfx
22
23

```

Figure 5: Sample Python Code for numerical differentiation of a function using Forward Difference Formula

```

Python 2.7.15+ (default, Nov 27 2018, 23:36:35)
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IPython 5.5.0 -- An enhanced Interactive Python.
?      -> Introduction and overview of IPython's features.
%quickref -> Quick reference.
help    -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra
details.

In [1]: runfile('/home/sonali/Documents/teaching_material/
differentiation.py', wdir='/home/sonali/Documents/
teaching_material')
The derivative at x=1 with specified accuracy is
-0.999993896476

In [2]:

```

Figure 6: Output of the Python code using Forward Difference Formula