

# python\_basics

November 15, 2022

## 1 Python:

### 1.1 basic features

<https://www.python.org/>

```
[1]: print("Hello, World!")
```

Hello, World!

```
[2]: a = 5  
     b = 2
```

```
[3]: a + b
```

```
[3]: 7
```

```
[4]: 1 + a * b
```

```
[4]: 11
```

```
[5]: a ** b
```

```
[5]: 25
```

```
[6]: # different in python 3: a//b  
     # for same behaviour run: from __future__ import division  
     a / b
```

```
[6]: 2.5
```

```
[7]: a / float(b)
```

```
[7]: 2.5
```

```
[8]: a % b
```

```
[8]: 1
```

```
[9]: min(a, b)
```

[9]: 2

```
[10]: a == b
```

[10]: False

```
[11]: a != b
```

[11]: True

```
[12]: a += 3
a
```

[12]: 8

```
[13]: # Python Lists
a = [1, "hello", 5.5]
a
```

[13]: [1, 'hello', 5.5]

```
[14]: len(a)
```

[14]: 3

```
[15]: a[2]
```

[15]: 5.5

```
[16]: a.append("how are you?")
a
```

[16]: [1, 'hello', 5.5, 'how are you?']

```
[17]: for x in a:
    print(x)
```

```
1
hello
5.5
how are you?
```

```
[18]: for i, x in enumerate(a):
    print("element {}: {}".format(i, x))
```

```
element 0: 1
element 1: hello
element 2: 5.5
element 3: how are you?
```

```
[19]: a[0] = 10
a
```

```
[19]: [10, 'hello', 5.5, 'how are you?']
```

```
[20]: # Python Tuples:
b = (-1, "bye", 'c')
b
```

```
[20]: (-1, 'bye', 'c')
```

```
[21]: b[-1]
```

```
[21]: 'c'
```

```
[22]: b[0] = 10
b
```

```
-----
TypeError                                Traceback (most recent call last)
Cell In [22], line 1
----> 1 b[0] = 10
      2 b

TypeError: 'tuple' object does not support item assignment
```

```
[23]: x, y = b
```

```
-----
ValueError                                Traceback (most recent call last)
Cell In [23], line 1
----> 1 x, y = b

ValueError: too many values to unpack (expected 2)
```

```
[30]: x
```

```
[30]: 'how are you?'
```

```
[31]: y
```

```
-----
NameError                                Traceback (most recent call last)
Cell In [31], line 1
----> 1 y
```

```
NameError: name 'y' is not defined
```

```
[32]: # Python Dictionaries (Keys, values)
a = {"name": "Mary", "age": 23, "sign": "capricorn"}
a
```

```
[32]: {'name': 'Mary', 'age': 23, 'sign': 'capricorn'}
```

```
[33]: a[1]
```

```
-----
KeyError                                Traceback (most recent call last)
Cell In [33], line 1
----> 1 a[1]

KeyError: 1
```

```
[34]: a["job"] = "student"
a
```

```
[34]: {'name': 'Mary', 'age': 23, 'sign': 'capricorn', 'job': 'student'}
```

```
[35]: # Python Functions
def f(a, b=4, c=5):
    if a > 2 and b < 10:
        return a
    elif c == 5:
        return b
    else:
        return a + b + c
```

```
[36]: f(4)
```

```
[36]: 4
```

```
[37]: f(4, 11)
```

```
[37]: 11
```

```
[38]: f(4, c=6, b=11)
```

```
[38]: 21
```

## 2 NumPy: multi-dimensional arrays and scientific computing

<https://www.numpy.org/>

```
[39]: import numpy as np
```

```
[40]: a = np.array([0, 2, 4, 6, 8, 10, 12, 14, 16])  
a
```

```
[40]: array([ 0,  2,  4,  6,  8, 10, 12, 14, 16])
```

```
[41]: a.ndim
```

```
[41]: 1
```

```
[42]: a.shape
```

```
[42]: (9,)
```

```
[43]: a[2]
```

```
[43]: 4
```

```
[44]: a[2:]
```

```
[44]: array([ 4,  6,  8, 10, 12, 14, 16])
```

```
[45]: a[:4]
```

```
[45]: array([0, 2, 4, 6])
```

```
[46]: a[2:7]
```

```
[46]: array([ 4,  6,  8, 10, 12])
```

```
[47]: a[2:7:2]
```

```
[47]: array([ 4,  8, 12])
```

```
[48]: a[-1]
```

```
[48]: 16
```

```
[49]: a[::-1]
```

```
[49]: array([16, 14, 12, 10,  8,  6,  4,  2,  0])
```

```
[50]: a[[0, 4, 5]]
```

```
[50]: array([ 0,  8, 10])
```

```
[51]: b = a > 3  
b
```

```
[51]: array([False, False,  True,  True,  True,  True,  True,  True,  True])
```

```
[52]: a[b]
```

```
[52]: array([ 4,  6,  8, 10, 12, 14, 16])
```

```
[53]: a = np.array([[0, 1, 2, 3], [4, 5, 6, 7], [8, 9, 10, 11]])  
a
```

```
[53]: array([[ 0,  1,  2,  3],  
          [ 4,  5,  6,  7],  
          [ 8,  9, 10, 11]])
```

```
[54]: a.ndim
```

```
[54]: 2
```

```
[55]: a.shape
```

```
[55]: (3, 4)
```

```
[56]: a[1, 2]
```

```
[56]: 6
```

```
[57]: a[0]
```

```
[57]: array([0, 1, 2, 3])
```

```
[58]: a[:, 1:3]
```

```
[58]: array([[ 1,  2],  
          [ 5,  6],  
          [ 9, 10]])
```

```
[59]: a.T
```

```
[59]: array([[ 0,  4,  8],  
          [ 1,  5,  9],  
          [ 2,  6, 10],  
          [ 3,  7, 11]])
```

```
[60]: a + 10
```

```
[60]: array([[10, 11, 12, 13],
           [14, 15, 16, 17],
           [18, 19, 20, 21]])
```

```
[61]: a ** 2
```

```
[61]: array([[ 0,  1,  4,  9],
           [16, 25, 36, 49],
           [64, 81, 100, 121]])
```

```
[62]: a * [10, 20, 30, 40]
```

```
[62]: array([[ 0, 20, 60, 120],
           [40, 100, 180, 280],
           [80, 180, 300, 440]])
```

```
[63]: np.sin(a)
```

```
[63]: array([[ 0.          ,  0.84147098,  0.90929743,  0.14112001],
           [-0.7568025 , -0.95892427, -0.2794155 ,  0.6569866 ],
           [ 0.98935825,  0.41211849, -0.54402111, -0.99999021]])
```

```
[64]: np.mean(a)
```

```
[64]: 5.5
```

```
[65]: a.mean(axis=1)
```

```
[65]: array([1.5, 5.5, 9.5])
```

```
[66]: np.max(a)
```

```
[66]: 11
```

```
[67]: np.max(a, axis=1)
```

```
[67]: array([ 3,  7, 11])
```

```
[68]: np.arange(10)
```

```
[68]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

```
[69]: np.linspace(2, 4, 5)
```

```
[69]: array([2. , 2.5, 3. , 3.5, 4. ])
```

```
[70]: np.zeros((2, 3))
```

```
[70]: array([[0., 0., 0.],
            [0., 0., 0.]])
```

```
[71]: np.full((2, 3), 2.5)
```

```
[71]: array([[2.5, 2.5, 2.5],
            [2.5, 2.5, 2.5]])
```

### 3 matplotlib: plotting

<https://matplotlib.org/>

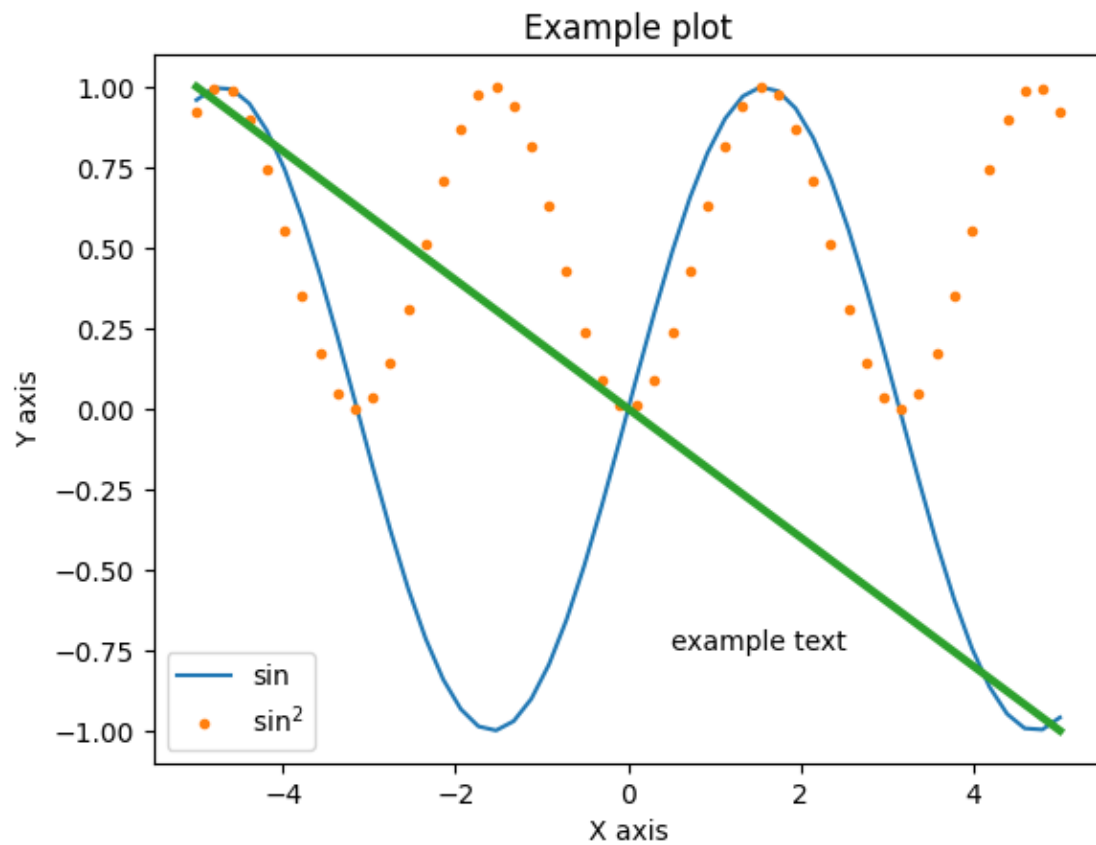
```
[72]: import matplotlib.pyplot as plt
```

```
[73]: #!/matplotlib notebook
      %matplotlib inline
```

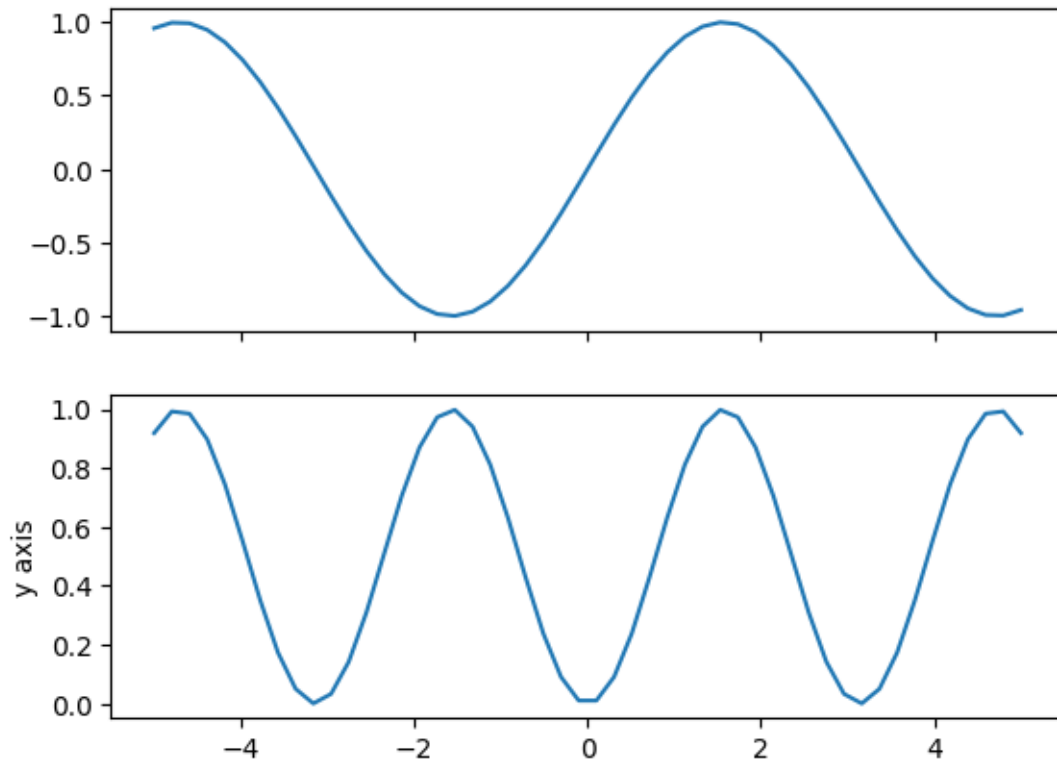
```
[74]: x = np.linspace(-5, 5, 50)
      y = np.sin(x)
      y2 = y ** 2
      y3 = -x / 5
```

```
[75]: plt.figure()
      plt.plot(x, y, label='sin')
      plt.plot(x, y2, '.', label='$\sin^2$')
      plt.plot(x, y3, linewidth=3)
      plt.annotate('example text', xy=(0.5, -0.75))
      plt.xlabel("X axis")
      plt.ylabel("Y axis")
      plt.title("Example plot")
      plt.legend()
      plt.show()
```

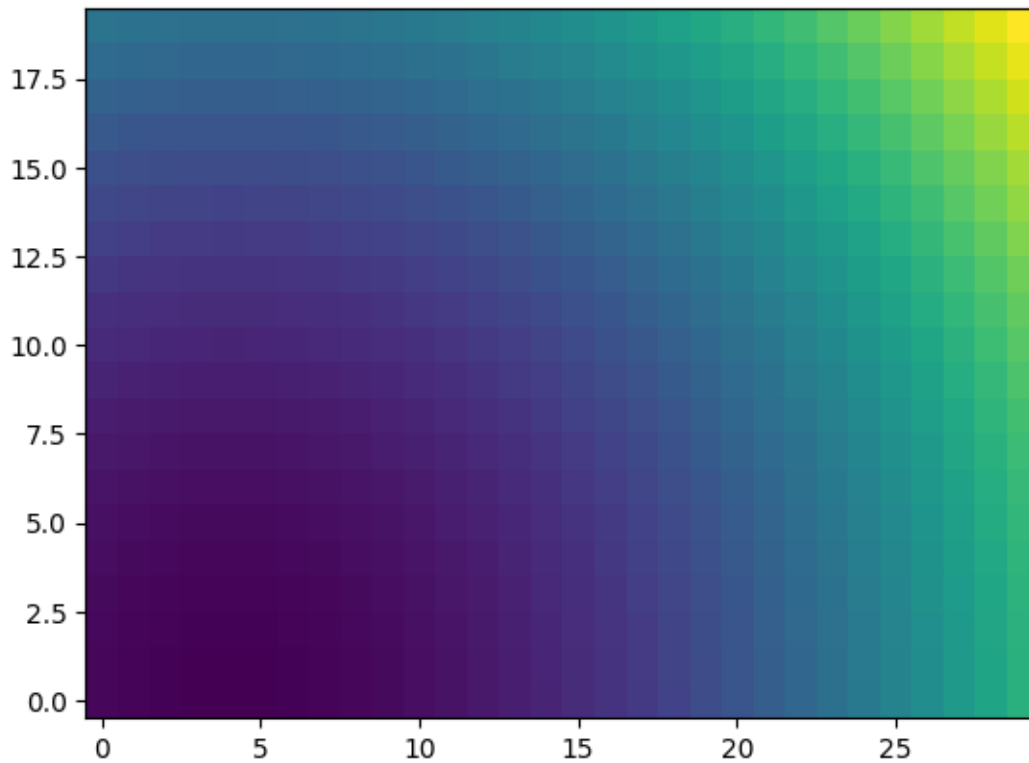




```
[76]: fig, ax = plt.subplots(2, sharex=True)
ax[0].plot(x, y)
ax[1].plot(x, y2)
ax[1].set_ylabel('y axis')
plt.show()
```



```
[77]: y, x = np.mgrid[0:20, 0:30]
      z = (x - 4)**2 + y**2
      plt.figure()
      plt.pcolormesh(x, y, z, shading='auto')
      plt.show()
```



## 4 SciPy: extra modules for scientific computation

<https://www.scipy.org/>

```
[78]: from scipy.optimize import curve_fit
import numpy as np
import matplotlib.pyplot as plt
```

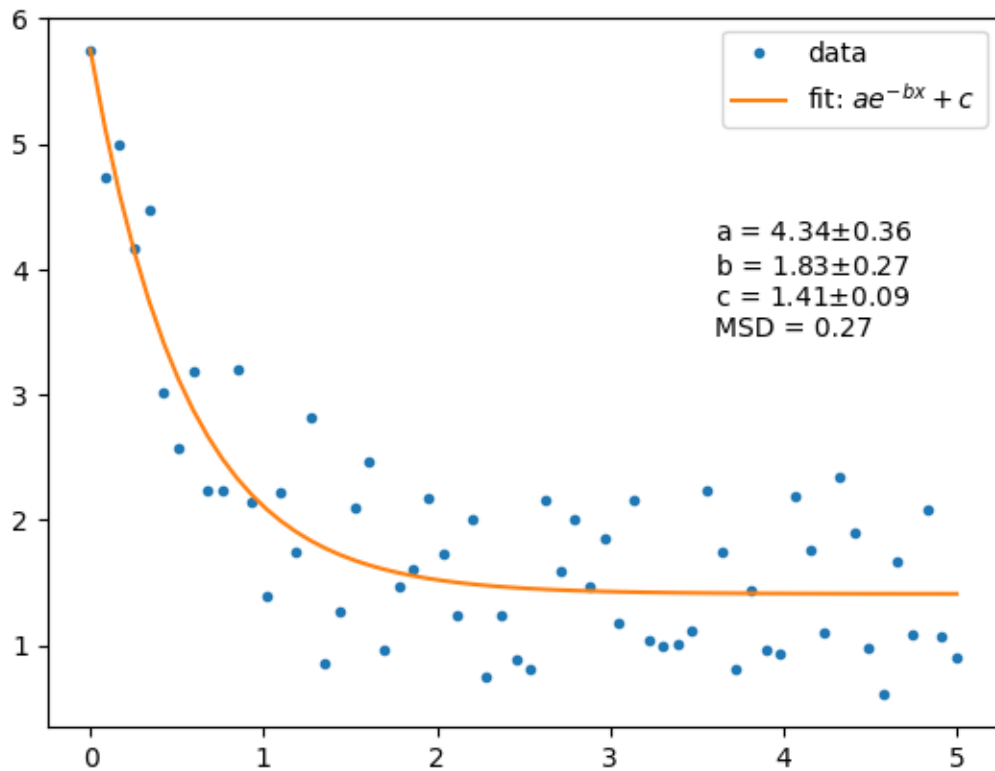
```
[79]: def f(x, a, b, c):
      return a * np.exp(-b * x) + c
```

```
[80]: n = 60
x = np.linspace(0, 5, n)
y = f(x, 5, 2, 0.5) + 2 * np.random.rand(n)
```

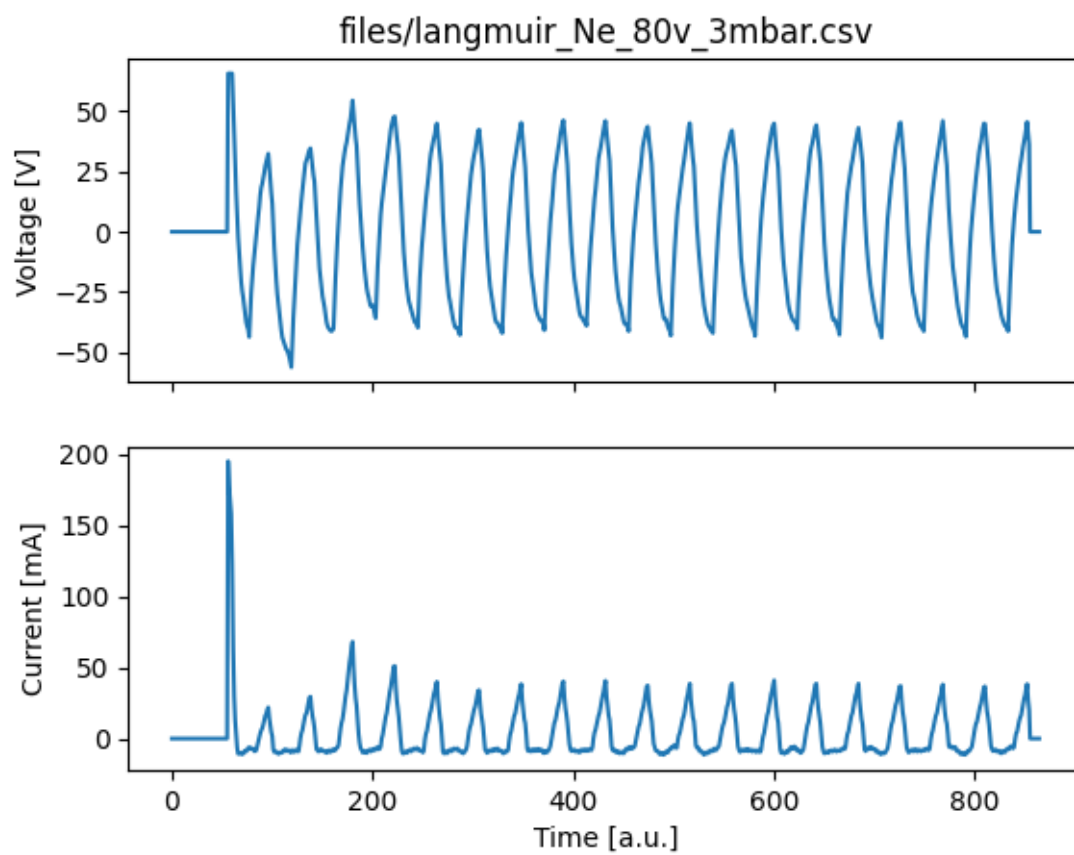
```
[81]: popt, pcov = curve_fit(f, x, y)
perr = np.sqrt(np.diag(pcov))
y_fit = f(x, *popt)
msd = np.sum((y - y_fit) ** 2) / n
```

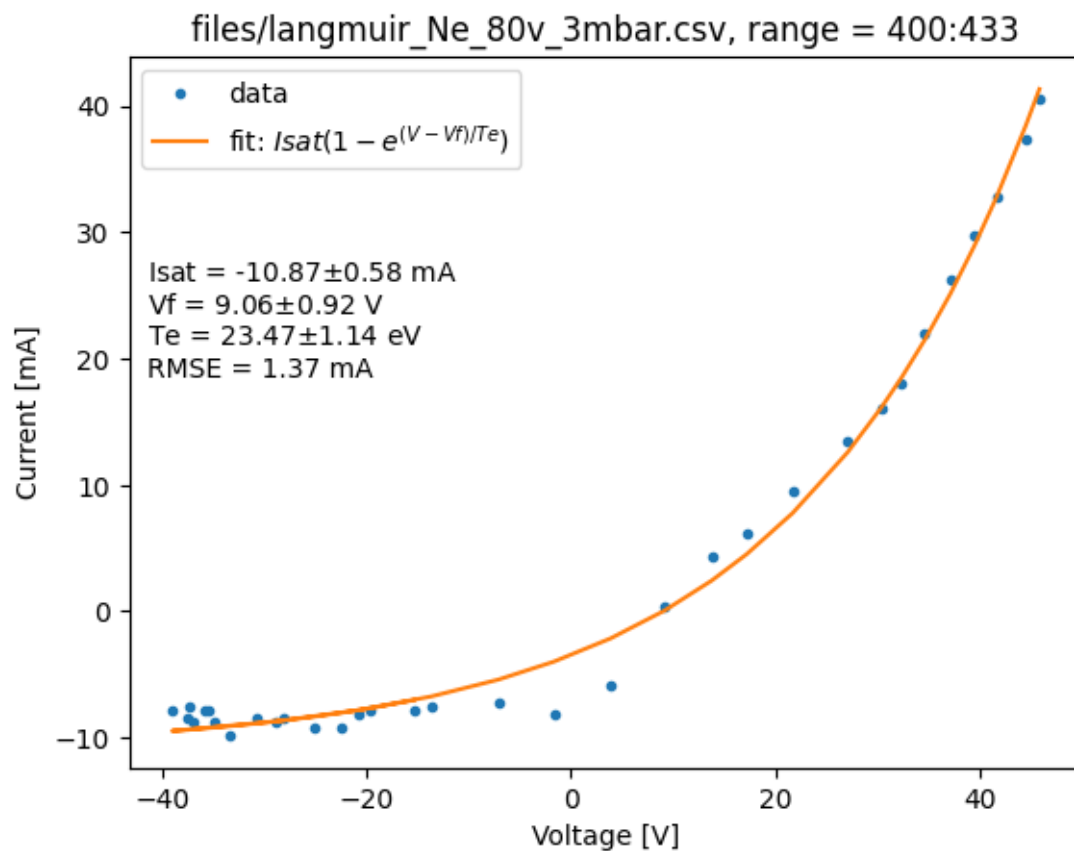
```
[82]: pnames = ['a', 'b', 'c']
      results = ''
      for name, value, error in zip(pnames, popt, perr):
          results += '{} = {:.2f}$\pm${:.2f}\n'.format(name, value, error)
      results += 'MSD = {:.2f}'.format(msd)

      plt.plot(x, y, '.', label='data')
      plt.plot(x, y_fit, label='fit: $ae^{-bx} + c$')
      plt.annotate(results, xy=(0.7, 0.55), xycoords='axes fraction')
      plt.legend()
      plt.show()
```



```
[84]: %run langmuir_fit.py
```





<Figure size 640x480 with 0 Axes>

```
[ ]:
```

```
[ ]:
```