

HPC Python Workshop: Matplotlib

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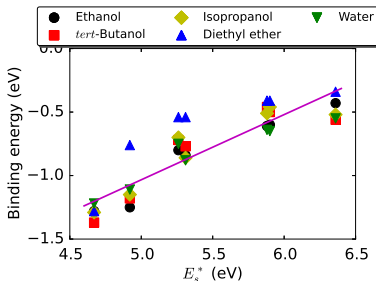
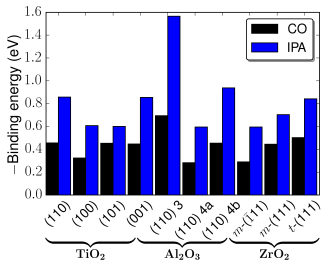
October 22, 2015

Introduction

What is Matplotlib?



- Python plotting environment that integrates directly with NumPy and SciPy
- Designed to be cross platform, flexible, and capable of producing publication ready figures



Why Matplotlib?

Advantages

- Cross platform
- Open Source (FREE!)
- High quality graphics production
- High reproducibility
- Interface with NumPy/SciPy allows for easy manipulation of data
- Variety of chart types supported (both 2D and 3D)

Disadvantages

- Intimidating interface
- Multiple ways to achieve a singular goal
- Not readily transparent

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Disadvantages

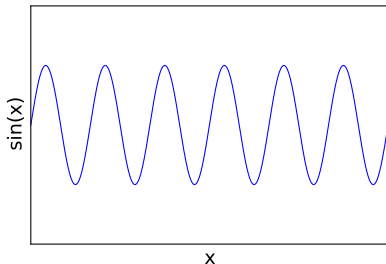
- Intimidating interface
- Multiple ways to achieve a singular goal
- Not readily transparent

If Matplotlib is so flexible, what sort of things can it do?

EXAMPLES

Example: Sine function

```
1 import numpy as np
2 import matplotlib
3 import matplotlib.pyplot as plt
4
5 font = {'size': 18}
6 matplotlib.rc('font', **font)
7
8 x = np.arange(0, 12 * np.pi, 0.001)
9 y = np.sin(x)
10
11 fig = plt.figure()
12 ax = fig.add_subplot(111)
13
14 line = ax.plot(x, y)
15
16 plt.ylim([-2.0, 2.0])
17 plt.xlim([0, 12 * np.pi])
18
19 ax.set_xticks([])
20 ax.set_yticks([])
21
22 ax.set_xlabel(r'X')
23 ax.set_ylabel('sin(x)')
24
25 for ext in ['png', 'pdf', 'eps']:
26     plt.savefig('sine_plot.%s' % ext, pad_inches=0.5,
27               bbox_inches='tight', dpi=500)
```

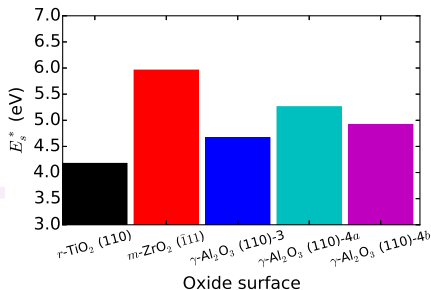


Example: Simple Bar Chart

```

8 import numpy as np
9 import matplotlib
10 import matplotlib.pyplot as plt
11
12 font = {'size': 16}
13 matplotlib.rc('font', **font)
14
15 sites = [r'$r$-TiO2$ (110)', r'$m$-ZrO2$ ( $\bar{1}$ 11)',
16         r'$\gamma$-Al2O3$ (110)-3', r'$\gamma$-Al2O3$ (110)-4a$',
17         r'$\gamma$-Al2O3$ (110)-4b$']
18
19 estars = [4.174374, 5.960088, 4.67, 5.26, 4.92]
20 colors = ['k', 'r', 'b', 'c', 'm', 'g', 'y']
21
22 index = np.arange(len(estars))
23 bar_width = 0.90
24
25 fig = plt.figure()
26 ax = fig.add_subplot(111)
27
28 bar1 = ax.bar(index, estars, width=bar_width)
29 for i in range(len(sites)):
30     bar1[i].set_color(colors[i])
31
32 ax.set_xticks(index + bar_width / 2)
33 ax.set_xticklabels(sites)
34 plt.xticks(rotation=15.)
35 for tick in ax.xaxis.get_major_ticks():
36     tick.label.set_fontsize(12)
37
38 plt.ylim([3, 7])
39 ax.set_xlabel('Oxide surface')
40 ax.set_ylabel('$E^*$ (eV)')
41
42 plt.subplots_adjust(bottom=0.22)
43 plt.savefig('oxide_band_energies.eps')

```

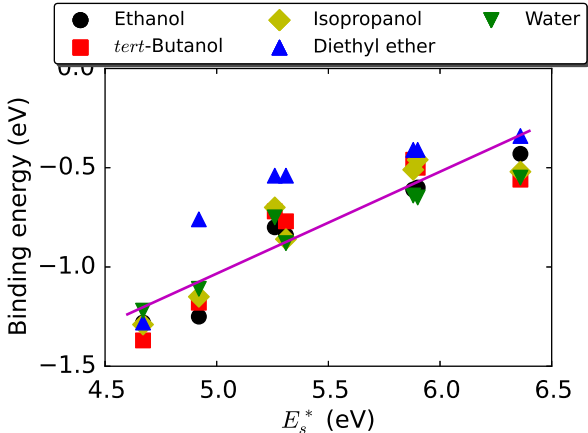


Example: Scatter with Best Fit

```

1 import numpy as np
2 from scipy.stats import linregress
3 import matplotlib
4 import matplotlib.pyplot as plt
5 import math
6
7 font = {'size': 18}
8 matplotlib.rc('font', **font)
9
10 sites = ['13', '450s', '450s', '1V5_05', '1V5_05', '1V5_05', '1V5_05']
11 etoh = np.array([-1.28, -0.88, -1.25, -0.84, -0.60, -0.43, -0.61])
12 tbutanol = np.array([-1.37, -0.72, -1.18, -0.77, -0.50, -0.56, -0.4]
13 ipa = np.array([-1.25, -0.70, -1.15, -0.86, -0.46, -0.51, -0.51])
14 deo = np.array([-1.28, -0.54, -0.76, -0.54, -0.41, -0.34, -0.41])
15 h2o = np.array([-1.22, -0.75, -1.11, -0.88, -0.65, -0.55, -0.64])
16
17 index = np.array([4.67, 5.26, 4.92, 5.31, 5.90, 6.36, 5.88])
18
19 fig = plt.figure()
20 ax = fig.add_subplot(111)
21
22 size = 120
23 scatplot = ax.scatter(index, etoh, color='k', marker='o', s=size,
24 label='Ethanol')
25 scatplot = ax.scatter(index, tbutanol, color='r', marker='s', s=size,
26 label='tert-Butanol')
27 scatplot = ax.scatter(index, ipa, color='y', marker='D', s=size,
28 label='Isopropanol')
29 scatplot = ax.scatter(index, deo, color='b', marker='^', s=size,
30 label='Diethyl ether')
31 scatplot = ax.scatter(index, h2o, color='g', marker='v', s=size, label='')
32
33 fits = [0.52, 0.52, 0.50]
34 fitb = [3.7, 3.6, 3.5]
35
36 a_ave = 0.0
37 b_ave = 0.0
38 for a in fits:
39     a_ave += a
40
41 for b in fitb:
42     b_ave += b
43
44 a_ave /= len(fits)
45 b_ave /= len(fitb)
46
47 print 'Ave. alpha = %f' % a_ave
48 print 'Ave. beta = %f' % b_ave
49
50 def linear(x):
51     return a_ave * x - b_ave
52
53 xlist = list()
54 ylist = list()
55 for i in np.arange(4.6, 6.4, 0.1):
56     xlist.append(i)
57     ylist.append(linear(i))
58
59 linplot = ax.plot(xlist, ylist, color='m', linewidth=2)
60
61 ax.set_xlabel('$E_s^*$ (eV)')
62 ax.set_ylabel('Binding energy (eV)')
63
64 ax.legend(loc='top center', prop={'size': 14}, scatterpoints=1,
65         frameon=True, shadow=True,
66         fancybox=True, ncol=3, bbox_to_anchor=(1.10, 1.25))

```

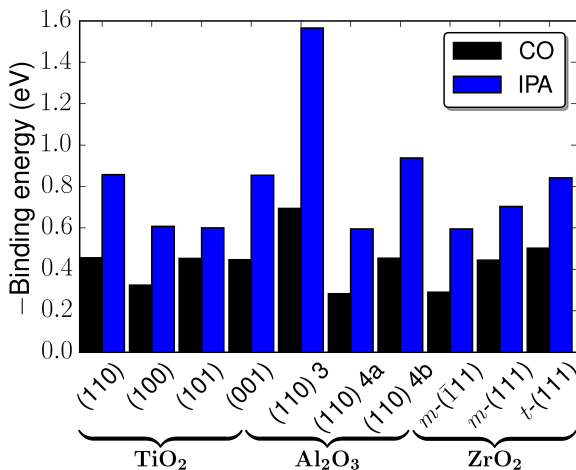


Example: \LaTeX + Matplotlib

```

1 import numpy as np
2 import matplotlib
3 import matplotlib.pyplot as plt
4
5 font = {'size': 18}
6 matplotlib.rc('font', **font)
7 matplotlib.rc('text', usetex=True)
8
9 latex = r'\usepackage{dvips}\graphicspath{graphics}\usepackage{xfrac}
10 matplotlib.rcParams["text.latex.preamble"].append(latex)
11
12 sites = ['(110)', '(100)', '(101)', '(001)',
13          '(110) 3', '(110) 4a', '(110) 4b',
14          r'$\sqrt{3}\times\sqrt{3}$', r'$\sqrt{3}\times\sqrt{3}$', r'$\sqrt{3}\times\sqrt{3}$']
15
16 co_be = [-0.456298, -0.323406, -0.453186, -0.446587,
17         -0.494235, -0.282424, -0.453259,
18         -0.289229, -0.444831, -0.582208]
19
20 ipa_be = [-0.857123, -0.607922, -0.600221, -0.854681,
21          -1.565287, -0.595685, -0.937462,
22          -0.595479, -0.789180, -0.841475]
23
24 co_be = np.array(co_be)
25 ipa_be = np.array(ipa_be)
26
27 index = np.arange(len(sites))
28 bar_width = 0.98
29
30 fig = plt.figure()
31 ax = fig.add_subplot(111)
32
33 barplot1 = ax.bar(index, -co_be, width=bar_width / 2, color='k', 1)
34 barplot2 = ax.bar(index+bar_width/2, -ipa_be, width=bar_width/2, 2)
35 label="IPA")
36
37 ax.set_xticks(index + bar_width / 2)
38 ax.set_xticklabels(sites, fontsize=16, rotation=45)
39
40 plt.ylim([0.0, 1.6])
41
42 brace = '-----'
43 down = -0.15
44 font = 22
45
46 text = r'$\underbrace{\text{\LaTeX}_{\text{\LaTeX}}}_{\text{\LaTeX}}$ % (brace, 'TiO_2')
47 plt.figtext(0.25, down, text, fontsize=font, ha='center')
48
49 text = r'$\underbrace{\text{\LaTeX}_{\text{\LaTeX}}}_{\text{\LaTeX}}$ % (brace, 'Al_2O_3')
50 plt.figtext(0.51, down, text, fontsize=font, ha='center')
51
52 text = r'$\underbrace{\text{\LaTeX}_{\text{\LaTeX}}}_{\text{\LaTeX}}$ % (brace, 'ZrO_2')
53 plt.figtext(0.771, down, text, fontsize=font, ha='center')
54
55 ax.set_ylabel(r'$-S$-binding energy (eV)')
56
57 location = 'upper right'
58 ax.legend(loc=location, prop={'size': 16},
59          frameon=True, shadow=True,
60          fancybox=True, bbox_to_anchor=(1.0, 1.0), ncol=1)
61
62 for ext in ['png', 'pdf']:
63     plt.savefig('results/oxides_co_ipa_ebind.%s' % ext, pad_inches=
64               bbox_inches='tight', dpi=500)

```

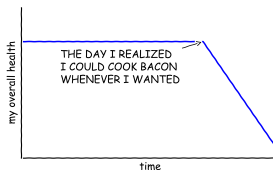


Example: XKCD

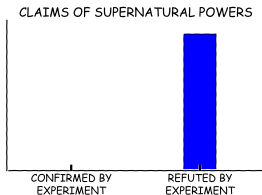
```

1 import matplotlib.pyplot as plt
2 import numpy as np
3
4 with plt.xkcd():
5     # Based on "Stove Ownership" from XKCD by Randall Monroe
6     # http://xkcd.com/418/
7
8     fig = plt.figure()
9     ax = fig.add_axes([0.1, 0.2, 0.8, 0.7])
10    ax.spines['right'].set_color('none')
11    ax.spines['top'].set_color('none')
12    plt.xticks([])
13    plt.yticks([])
14    ax.set_ylim([-30, 10])
15
16    data = np.ones(100)
17    data[70:] = np.arange(30)
18
19    plt.annotate(
20        "THE DAY I REALIZED I COULD COOK BACON WHENEVER I WANTED",
21        xy=(70, 1), arrowprops=dict(arrowstyle='->'), xytext=(15, -10))
22
23    plt.plot(data)
24
25    plt.xlabel('time')
26    plt.ylabel('my overall health')
27    fig.text(
28        0.5, 0.05,
29        "Stove Ownership" from xkcd by Randall Monroe',
30        ha='center')
31
32    for ext in ['png', 'pdf']:
33        plt.savefig('xkcd418.%s' % ext, pad_inches=0.5,
34                    bbox_inches='tight', dpi=500)
35    # Based on "The Data So Far" from XKCD by Randall Monroe
36    # http://xkcd.com/373/
37
38    fig = plt.figure()
39    ax = fig.add_axes([0.1, 0.2, 0.8, 0.7])
40    ax.bar([-0.125, 1.0-0.125], [0, 100], 0.25)
41    ax.spines['right'].set_color('none')
42    ax.spines['top'].set_color('none')
43    ax.xaxis.set_ticks_position('bottom')
44    ax.set_xticks([0, 1])
45    ax.set_xlim([-0.5, 1.5])
46    ax.set_ylim([0, 110])
47    ax.set_xticklabels(['CONFIRMED BY EXPERIMENT', 'REFUTED BY EXPERIMENT'])
48    plt.yticks([])
49
50    plt.title("CLAIMS OF SUPERNATURAL POWERS")
51
52    fig.text(
53        0.5, -0.05,
54        "The Data So Far" from xkcd by Randall Monroe',
55        ha='center')
56
57    for ext in ['png', 'pdf']:
58        plt.savefig('xkcd373.%s' % ext, pad_inches=0.5,
59                    bbox_inches='tight', dpi=500)
60

```



"Stove Ownership" from xkcd by Randall Monroe



"The Data So Far" from xkcd by Randall Monroe

How to get Matplotlib

Those graphs look great! Where do I get Matplotlib?

- ▶ Source code: <http://matplotlib.org>
- ▶ Linux Package installer (look for the SciPy stack!)
- ▶ Enthought Canopy (<https://enthought.com/>)
- ▶ Anaconda Python (<https://www.continuum.io/downloads>)
- ▶ If on Farber, load the following (`vpkg_require`):
 - ★ `python-numpy python-scipy python-matplotlib`

USING MATPLOTLIB

Plotting a Sine function

```
1 import numpy as np
```

```
1 Import numpy
```

Plotting a Sine function

```
1 import numpy as np
2 import matplotlib
3 import matplotlib.pyplot as plt
```

- 1 Import numpy
- 2-3 Import Matplotlib
 - ▶ pylab vs. pyplot
 - ▶ pylab: used for interactive plotting, MatLab like
 - ▶ pyplot: used more for scripting

Plotting a Sine function

```
1 import numpy as np
2 import matplotlib
3 import matplotlib.pyplot as plt
4 font = {'size': 16}
5 matplotlib.rc('font', **font)
```

- 1 Import numpy
- 2-3 Import Matplotlib
- 4-5 Change the graph font size to 16
 - ▶ matplotlib.rc is used to change many of the behaviors of Matplotlib!
 - ▶ Can even use rc parameters to utilize \LaTeX

Plotting a Sine function

```
1 import numpy as np
2 import matplotlib
3 import matplotlib.pyplot as plt
4 font = {'size': 16}
5 matplotlib.rc('font', **font)
6 x = np.arange(0, 12 * np.pi, 0.001)
7 y = np.sin(x)
```

- 1 Import numpy
- 2-3 Import Matplotlib
- 4-5 Change the graph font size to 16
- 6-7 Generate some (x, y) data

Plotting a Sine function

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1 import numpy as np
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4 font = {'size': 16}
5 matplotlib.rc('font', **font)
6 x = np.arange(0, 12 * np.pi, 0.001)
7 y = np.sin(x)
8 fig = plt.figure()
9 ax = fig.add_subplot(111)
```

- 1 Import numpy
- 2-3 Import Matplotlib
- 4-5 Change the graph font size to 16
- 6-7 Generate some (x, y) data
- 8-9 Generate the plotting environment
 - ▶ figure is the top level graphics object
 - ▶ add_subplot adds a plot to the figure object
 - ▶ 111 does mean something, but ignore it for now

Plotting a Sine function

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5 matplotlib.rc('font', **font)
6 x = np.arange(0, 12 * np.pi, 0.001)
7 y = np.sin(x)
8 fig = plt.figure()
9 ax = fig.add_subplot(111)
10 line = ax.plot(x, y)
```

- 1 Import numpy
- 2-3 Import Matplotlib
- 4-5 Change the graph font size to 16
- 6-7 Generate some (x, y) data
- 8-9 Generate the plotting environment
- 10 Add the (x, y) data to the plot!

Plotting a Sine function

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1 import numpy as np
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5 matplotlib.rc('font', **font)
6 x = np.arange(0, 12 * np.pi, 0.001)
7 y = np.sin(x)
8 fig = plt.figure()
9 ax = fig.add_subplot(111)
10 line = ax.plot(x, y)
11 plt.ylim([-2.0, 2.0])
12 plt.xlim([0, 12 * np.pi])
13 ax.set_xticks([])
14 ax.set_yticks([])
```

- 1 Import numpy
- 2-3 Import Matplotlib
- 4-5 Change the graph font size to 16
- 6-7 Generate some (x, y) data
- 8-9 Generate the plotting environment
- 10 Add the (x, y) data to the plot!
- 11-14 Change some behavior of the axes

Plotting a Sine function

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6 x = np.arange(0, 12 * np.pi, 0.001)
7 y = np.sin(x)
8 fig = plt.figure()
9 ax = fig.add_subplot(111)
10 line = ax.plot(x, y)
11 plt.ylim([-2.0, 2.0])
12 plt.xlim([0, 12 * np.pi])
13 ax.set_xticks([])
14 ax.set_yticks([])
15 ax.set_xlabel('x')
16 ax.set_ylabel('sin(x)')
```

- 1 Import numpy
- 2-3 Import Matplotlib
- 4-5 Change the graph font size to 16
- 6-7 Generate some (x, y) data
- 8-9 Generate the plotting environment
- 10 Add the (x, y) data to the plot!
- 11-14 Change some behavior of the axes
- 15-16 Label the axes

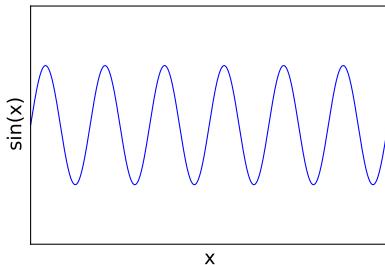
Plotting a Sine function

```
6 x = np.arange(0, 12 * np.pi, 0.001)
7 y = np.sin(x)
8 fig = plt.figure()
9 ax = fig.add_subplot(111)
10 line = ax.plot(x, y)
11 plt.ylim([-2.0, 2.0])
12 plt.xlim([0, 12 * np.pi])
13 ax.set_xticks([])
14 ax.set_yticks([])
15 ax.set_xlabel('x')
16 ax.set_ylabel('sin(x)')
17 plt.savefig('sine_plot.png')
    or
17 plt.show()
```

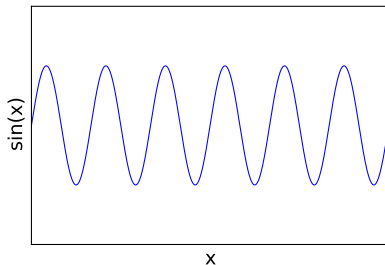
- 1 Import numpy
- 2-3 Import Matplotlib
- 4-5 Change the graph font size to 16
- 6-7 Generate some (x, y) data
- 8-9 Generate the plotting environment
- 10 Add the (x, y) data to the plot!
- 11-14 Change some behavior of the axes
- 15-16 Label the axes
- 17 Visualize and/or save the plot

Plotting a Sine function

```
6 x = np.arange(0, 12 * np.pi, 0.001)
7 y = np.sin(x)
8 fig = plt.figure()
9 ax = fig.add_subplot(111)
10 line = ax.plot(x, y)
11 plt.ylim([-2.0, 2.0])
12 plt.xlim([0, 12 * np.pi])
13 ax.set_xticks([])
14 ax.set_yticks([])
15 ax.set_xlabel('x')
16 ax.set_ylabel('sin(x)')
17 plt.savefig('sine_plot.png')
    or
17 plt.show()
```

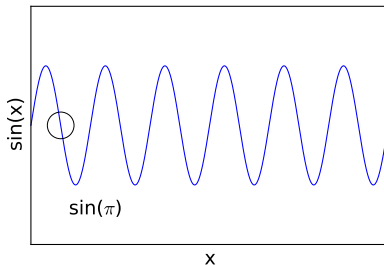


Plotting a Sine function — Modifications



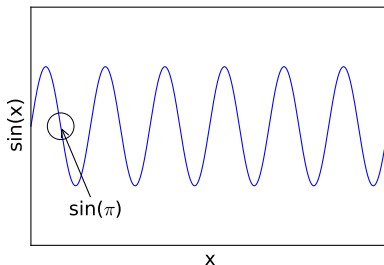
Plotting a Sine function — Modifications

- `circle = ax.plot(np.pi, 0.0, 'bo', fillstyle='none', markersize=25, color='k')`



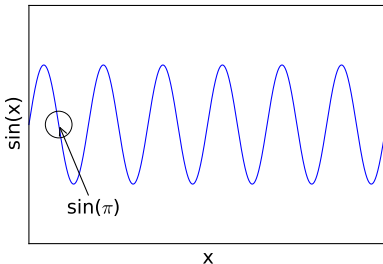
Plotting a Sine function — Modifications

- `circle = ax.plot(np.pi, 0.0, 'bo', fillstyle='none', markersize=25, color='k')`
- `ax.annotate(r'sin(π)', xy=(np.pi, 0.0), xycoords='data', xytext=(4.0, -1.5), textcoords='data')`



Plotting a Sine function — Modifications

- `circle = ax.plot(np.pi, 0.0, 'bo', fillstyle='none', markersize=25, color='k')`
- `arrow = {'arrowstyle': '->'}`
`ax.annotate(r'sin(π)', xy=(np.pi, 0.0), xycoords='data', xytext=(4.0, -1.5), textcoords='data', arrowprops=arrow)`



Reading from external file

First, write the (x, y) data to a file to have something to work with:

```
with open('data.txt', 'w') as dfile:  
    for i in range(len(x)):  
        dfile.write('%16.6f%16.6f\n' % (x[i], y[i]))
```

Now read this data in using numpy:

```
x, y = np.loadtxt('data.txt', unpack=True)
```

Fitting data

```
1 import numpy as np
2 import matplotlib
3 import matplotlib.pyplot as plt
4 from scipy.optimize import curve_fit
```

1-4 Load the requisite namespaces

Fitting data

```
4 def func(x, a, b, c):
5     return a * np.exp(-b * x) + c
6 xdata = np.linspace(0, 4, 100)
7 y = func(xdata, 2.5, 1.3, 0.5)
8 ydata = y + 0.2 *
    np.random.normal(size=len(xdata))
```

- 4-5 Define a function to create data
- 6-8 Generate some data. The y data is generated via a normal Gaussian distribution for some extra randomness

Fitting data

```
4 def func(x, a, b, c):  
5     return a * np.exp(-b * x) + c  
6 xdata = np.linspace(0, 4, 100)  
7 y = func(xdata, 2.5, 1.3, 0.5)  
8 ydata = y + 0.2 *  
    np.random.normal(size=len(xdata))  
9 popt, pcov = curve_fit(func, xdata, ydata)
```

9 Use `scipy`'s `curve_fit` to fit the data. The parameters are in `popt`, and error information is in `pcov`

Fitting data

```
4 def func(x, a, b, c):
5     return a * np.exp(-b * x) + c
6 xdata = np.linspace(0, 4, 100)
7 y = func(xdata, 2.5, 1.3, 0.5)
8 ydata = y + 0.2 *
    np.random.normal(size=len(xdata))
9 popt, pcov = curve_fit(func, xdata, ydata)
10 ydata2 = func(xdata, popt[0], popt[1], popt[2])
```

- 9 Use `scipy`'s `curve_fit` to fit the data. The parameters are in `popt`, and error information is in `pcov`
- 10 `popt` is then used to generate a 2nd set of `y`-data

Fitting data

```
4 def func(x, a, b, c):
5     return a * np.exp(-b * x) + c
6 xdata = np.linspace(0, 4, 100)
7 y = func(xdata, 2.5, 1.3, 0.5)
8 ydata = y + 0.2 *
    np.random.normal(size=len(xdata))
9 popt, pcov = curve_fit(func, xdata, ydata)
10 ydata2 = func(xdata, popt[0], popt[1], popt[2])
11 fig = plt.figure()
12 ax = fig.add_subplot(111)
```

9 Use `scipy`'s `curve_fit` to fit the data. The parameters are in `popt`, and error information is in `pcov`

10 `popt` is then used to generate a 2nd set of `y`-data

11-12 Create the plotting environment

Fitting data

- ```
4 def func(x, a, b, c):
5 return a * np.exp(-b * x) + c
6 xdata = np.linspace(0, 4, 100)
7 y = func(xdata, 2.5, 1.3, 0.5)
8 ydata = y + 0.2 *
 np.random.normal(size=len(xdata))
9 popt, pcov = curve_fit(func, xdata, ydata)
10 ydata2 = func(xdata, popt[0], popt[1], popt[2])
11 fig = plt.figure()
12 ax = fig.add_subplot(111)
13 ax.scatter(xdata, ydata,)
14 ax.plot(xdata, ydata2, linewidth=2, color='r')
```
- 9 Use `scipy`'s `curve_fit` to fit the data. The parameters are in `popt`, and error information is in `pcov`
- 10 `popt` is then used to generate a 2<sup>nd</sup> set of `y`-data
- 11-12 Create the plotting environment
- 13-14 Plot the data. The random data is plotted as a scatter plot.

# Fitting data

```
4 def func(x, a, b, c):
5 return a * np.exp(-b * x) + c
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11 fig = plt.figure()
12 ax = fig.add_subplot(111)
13 ax.scatter(xdata, ydata,)
14 ax.plot(xdata, ydata2, linewidth=2, color='r')
15 plt.xlim([0, 4])
16 plt.ylim([0, 3.0])
17 plt.savefig('fit_test.eps')
```

9 Use `scipy`'s `curve_fit` to fit the data. The parameters are in `popt`, and error information is in `pcov`

10 `popt` is then used to generate a 2<sup>nd</sup> set of `y`-data

11-12 Create the plotting environment

13-14 Plot the data. The random data is plotted as a scatter plot.

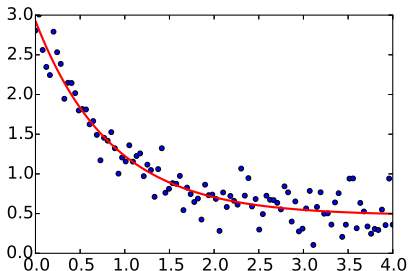
15-16 Set axes limits

17 Save the plot

# Fitting data

```
4 def func(x, a, b, c):
5 return a * np.exp(-b * x) + c
6 xdata = np.linspace(0, 4, 100)
7 y = func(xdata, 2.5, 1.3, 0.5)
8 ydata = y + 0.2 *
 np.random.normal(size=len(xdata))
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12 ax = fig.add_subplot(111)
13 ax.scatter(xdata, ydata,)
14 ax.plot(xdata, ydata2, linewidth=2, color='r')
15 plt.xlim([0, 4])
16 plt.ylim([0, 3.0])
17 plt.savefig('fit_test.eps')
```



# Bar Plot

```
1 import numpy as np
2 import matplotlib
3 import matplotlib.pyplot as plt
4 font = {'size': 16}
5 matplotlib.rc('font', **font)
6 colors = ['k', 'r', 'b', 'c', 'm']
```

1-6 Load up the requisite namespace, set font, and pick some colors

# Bar Plot

```
7 sites = [r'r-TiO$_2$ (110)',
8 r'm-ZrO$_2$ ($\bar{1}11$)',
9 r'γ-Al$_2$O$_3$ (110)-3',
10 r'γ-Al$_2$O$_3$
(110)-4a',
11 r'γ-Al$_2$O$_3$
(110)-4b']
10 index = np.arange(len(estars))
11 estars = [4.174374, 5.960088, 4.67, 5.26, 4.92]
12 bar_width = 0.90
```

7-12 Define some data. Here, we define two datasets for the x-coordinate. Also define a “width” of each bar.

# Bar Plot

```
13 fig = plt.figure()
```

```
14 ax = fig.add_subplot(111)
```

13-14 Define a figure and axes objects

# Bar Plot

```
13 fig = plt.figure()
14 ax = fig.add_subplot(111)
15 bar1 = ax.bar(index, estars, width=bar_width)
16 for i in range(len(sites)):
17 bar1[i].set_color(colors[i])
```

15-17 Add bars to the plot. Want each bar to be a different color, so iterate through them.

# Bar Plot

```
13 fig = plt.figure()
14 ax = fig.add_subplot(111)
15 bar1 = ax.bar(index, estars, width=bar_width)
16 for i in range(len(sites)):
17 bar1[i].set_color(colors[i])
18 ax.set_xticks(index + bar_width / 2)
19 ax.set_xticklabels(sites)
20 plt.xticks(rotation=15.)
21 for tick in ax.xaxis.get_major_ticks():
22 tick.label.set_fontsize(12)
23 plt.ylim([3, 7])
24 ax.set_xlabel('Oxide surface')
25 ax.set_ylabel('E^*_s (eV)')
```

18-19 Default is that each bar is labeled via a number. Want a text label, and these lines enable this.

20-22 Rotate the labels by 15°, and change the font size on the labels.

23-25 Set a limit to y axis, and label both axes



# Bar Plot

```
13 fig = plt.figure()
14 ax = fig.add_subplot(111)
15 bar1 = ax.bar(index, estars, width=bar_width)
16 for i in range(len(sites)):
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19 ax.set_xticklabels(sites)
20 plt.xticks(rotation=15.)
21 for tick in ax.xaxis.get_major_ticks():
22 tick.label.set_fontsize(12)
23 plt.ylim([3, 7])
24 ax.set_xlabel('Oxide surface')
25 ax.set_ylabel('E^*_s (eV)')
26 plt.subplots_adjust(bottom=0.22)
27 plt.savefig('oxide_band_energies.eps')
```

18-19 Default is that each bar is labeled via a number. Want a text label, and these lines enable this.

20-22 Rotate the labels by 15°, and change the font size on the labels.

23-25 Set a limit to y axis, and label both axes

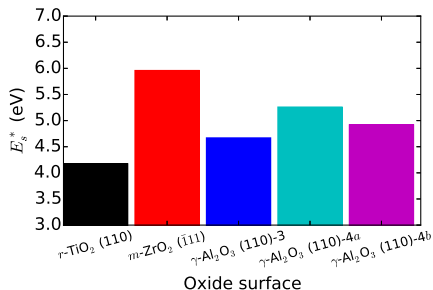
26 Pad out the bottom

27 Save the figure

- ▶ The following can be added to the `savefig` function to avoid the padding:  
`pad_inches=0.5,`  
`bbox_inches='tight'`

## Bar Plot

```
13 fig = plt.figure()
14 ax = fig.add_subplot(111)
15 bar1 = ax.bar(index, estars, width=bar_width)
16 for i in range(len(sites)):
17 bar1[i].set_color(colors[i])
18 ax.set_xticks(index + bar_width / 2)
19 ax.set_xticklabels(sites)
20 plt.xticks(rotation=15.)
21 for tick in ax.xaxis.get_major_ticks():
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24 ax.set_xlabel('Oxide surface')
25 ax.set_ylabel('E_s^* (eV)')
26 plt.subplots_adjust(bottom=0.22)
27 plt.savefig('oxide_band_energies.eps')
```



# Subplots

## 11-12 Create the plotting environment

```
11 fig = plt.figure()
12 ax = fig.add_subplot(221)
```

# Subplots

```
11 fig = plt.figure()
12 ax = fig.add_subplot(221)
13 ax.scatter(xdata, ydata,)
14 ax.plot(xdata, ydata2, linewidth=2, color='r')
```

11-12 Create the plotting environment

13-14 Plot the data. The random data is plotted as a scatter plot.

- ▶ subplot now takes something besides (111)
- ▶ (ncols, nrows, number)

# Subplots

- 11 `fig = plt.figure()`
  - 12 `ax = fig.add_subplot(221)`
  - 13 `ax.scatter(xdata, ydata,)`
  - 14 `ax.plot(xdata, ydata2, linewidth=2, color='r')`
  - 15 `plt.xlim([0, 4])`
  - 16 `plt.ylim([0, 3.0])`
  - 17 `ax.set_xticks([])`
  - 18 `ax.set_yticks(np.arange(0, 4, 1))`
- 11-12 Create the plotting environment
  - 13-14 Plot the data. The random data is plotted as a scatter plot.
  - 15-16 Set axes limits
  - 17 Clear the x, set the y

# Subplots

- 19 `ax2 = fig.add_subplot(222)`
  - 20 `ax2.scatter(xdata, ydata,)`
  - 21 `ax2.plot(xdata, ydata2, linewidth=2, color='k')`
  - 22 `ax2.tick_params(labelcolor='w', top='on', bottom='on', left='off', right='off')`
- 15-16 Set axes limits
  - 17 Clear the x, set the y
  - 19 Second plot
  - 20-21 Add the same data (being lazy!)
  - 22 Clear axes labels

# Subplots

- 19 ax2 = fig.add\_subplot(222)
  - 20 ax2.scatter(xdata, ydata,)
  - 21 ax2.plot(xdata, ydata2, linewidth=2, color='k')
  - 22 ax2.tick\_params(labelcolor='w', top='on', bottom='on', left='off', right='off')
  - 23 ax3 = fig.add\_subplot(223)
  - 24 ax3.scatter(xdata, ydata,)
  - 25 ax3.plot(xdata, ydata2, linewidth=2, color='m')
  - 26 plt.xlim([0, 4])
  - 27 plt.ylim([0, 3.0])
  - 29 ax3.set\_xticks(np.arange(0, 5, 1))
  - 30 ax3.set\_yticks(np.arange(0, 4, 1))
- 15-16 Set axes limits
  - 17 Clear the x, set the y
  - 19 Second plot
  - 20-21 Add the same data (being lazy!)
  - 22 Clear axes labels
  - 23 Third plot
  - 24-25 Add the same data (being lazy!)
  - 26-30 Set axes labels

# Subplots

```
31 ax4 = fig.add_subplot(224)
```

```
32 ax4.scatter(xdata, ydata,)
```

```
33 ax4.plot(xdata, ydata2, linewidth=2, color='g')
```

```
35 plt.xlim([0, 4])
```

```
36 plt.ylim([0, 3.0])
```

```
37 ax4.set_xticks(np.arange(0, 5, 1))
```

```
38 ax4.set_yticks([])
```

15-16 Set axes limits

17 Clear the x, set the y

19 Second plot

20-21 Add the same data (being lazy!)

22 Clear axes labels

23 Third plot

24-25 Add the same data (being lazy!)

26-30 Set axes labels

31 Fourth plot

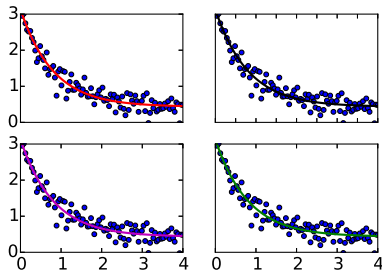
32-33 Add the same data (being lazy!)

34-38 Set axes labels



# Subplots

```
31 ax4 = fig.add_subplot(224)
32 ax4.scatter(xdata, ydata,)
33 ax4.plot(xdata, ydata2, linewidth=2, color='g')
35 plt.xlim([0, 4])
36 plt.ylim([0, 3.0])
37 ax4.set_xticks(np.arange(0, 5, 1))
38 ax4.set_yticks([])
```



# QUESTIONS?