Matplotlib Introduction

Molecular Statistics

2014

1 Introduction

Matplotlib (MPL) is a module for Python used for plotting. It is very useful for visualizing all kinds of data types and extremely customizable. For plot examples see matplotlib.org/gallery.html and weblo-ria.loria.fr/~rougier/teaching/matplotlib.

This short introduction will go through small plots with code examples. For advanced examples (like 3D plots), see the examples above or use "Google".

To utilize the power of matplotlib in a simple way we use a wrapper function called **pyplot** (PLT), which basically means we can use matplotlib without any crazy coding (involving class and instances etc). This is simply done by importing the pyplot module in the head of your `.py` file.

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

There are several ways to show the results of MPL, open a windows show the results or saving the plot as an image or other formats.

```
1 plt.show()                    # Show the result in a new window
2 plt.savefig('my_plot.png')    # Save the result in a file
```

The `savefig()` function can save to `.png`, `.eps`, `.svg`, as well as `.pdf` formats. The last formats are very useful for LaTeX work.

When working with multiple plots in the same script, remember to clear the PLT data, or you will see a mess of data in the plot. This is done using the `clf()` function from PLT.

```
1 plt.clf()
```

If you want to make you graphs to look good, with different colors, fonts and spacings, then I would recommend you to look at github.com/charnley/matplotlib-header and matplotlib.org/users/customizing.html.

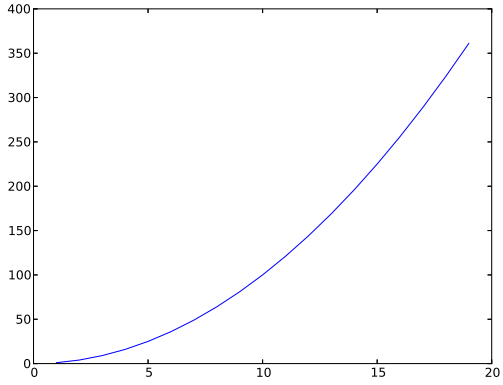
Happy Pyplot'ing!

2 Examples

2.1 XY

A simple example is to plot x and y coordinates based on two simple python lists. For $y(x) = x^2$.

```
1 import matplotlib.pyplot as plt
2
3 x = range(1, 20)
4 y = [i**2 for i in x]
5
6 plt.plot(x, y)
7 plt.savefig('figure_xy.eps')
```

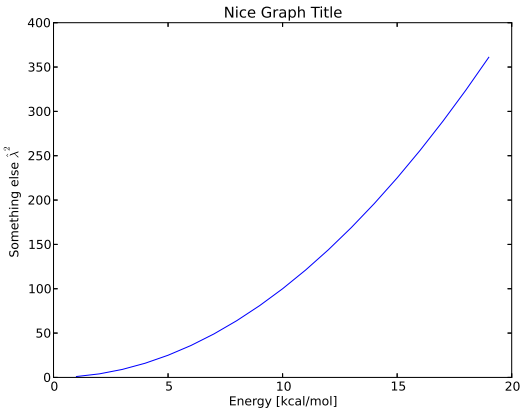


2.2 Titles and labels

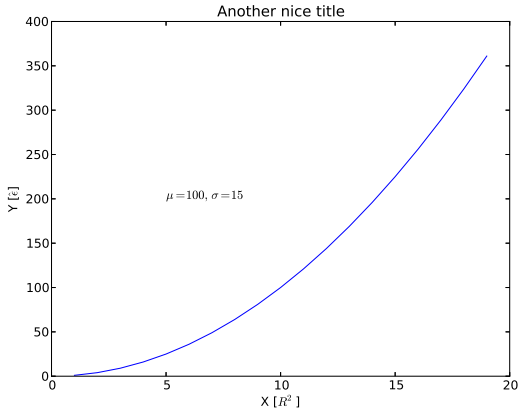
However a graph is worth nothing without title and axis-labels, which can be included by the following syntax. It is also possible to include latex code in the strings.

```
import matplotlib.pyplot as plt

# Data
x = range(1, 20)
y = [i**2 for i in x]


# First graph
plt.title('Nice Graph Title')
plt.xlabel('Energy [kcal/mol]')
plt.ylabel('Something else $\hat \
    lambda^2$')

plt.plot(x, y)
plt.savefig('figure_title.eps')


# Clear data
plt.clf()


# Second graph
plt.title('Another nice title')
plt.xlabel('X [$R^2$]')
plt.ylabel('Y [$\hat \epsilon$]')

# Place some text
plt.text(5, 200, r'$\mu=100,\ \sigma=15
    $')

plt.plot(x, y)
plt.savefig('figure_title_text.eps')
```

figure_title.eps



figure_title_text.eps



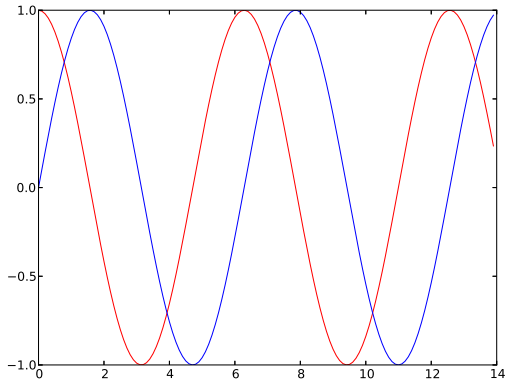
2.3 Multiple lines

Usually you will need to plot multiple datasets in the same figure. This is practically just adding more `plot()` functions. For customization you can add labels and choose color and line-type for the specific data sets. See appendix A for a full list of colors and line styles. If you do not choose a color, a color will be chosen by default.

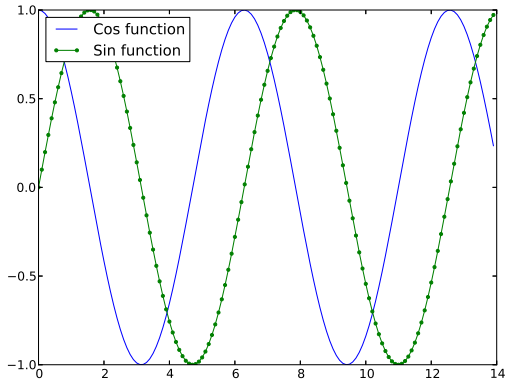
Note that the location of the legend box can be set by changing the string location.

```
1  import matplotlib.pyplot as plt
2  import numpy as np
3
4  # Data
5  x = np.arange(0, 14, 0.1)
6  y_cos = [np.cos(i) for i in x]
7  y_sin = [np.sin(i) for i in x]
8
9  # First plot
10 plt.plot(x, y_cos, 'r-')
11 plt.plot(x, y_sin, 'b-')
12
13 plt.savefig('figure_sincos1.eps')
14
15 # Clear MPL data
16 plt.clf()
17
18 # Second figure
19 plt.plot(x, y_cos, '-', label="Cos
       function")
20 plt.plot(x, y_sin, '.-', label="Sin
       function")
21
22 # Location of legend
23 plt.legend(loc='upper left')
24
25 plt.savefig('figure_sincos2.eps')
```

figure_sincos2.eps



figure_sincos2.eps



A Plot styling

A.1 Colors

b	blue
g	green
r	red
c	cyan
m	magenta
y	yellow
k	black
w	white

A.2 Line styles

0	tickleft
1	tickright
2	tickup
3	tickdown
4	caretleft
D	diamond
6	caretup
7	caretdown
s	square
—	vline
x	x
5	caretright
_	hline
^	triangle up
d	thin diamond
h	hexagon1
+	plus
*	star
,	pixel
o	circle
.	point
’1’	tri down
p	pentagon
’3’	tri left
’2’	tri up
’4’	tri right
H	hexagon2
v	triangle down
’8’	octagon
<	triangle left
>	triangle right