Python Introduction Part 2

October 19, 2020

Week 2

1 Visualisation in Python

Showing plots that describe your data is a key part of any scientific analysis.

For example, here is one from Laura Hayes showing the occurrence of solar flares, and their power, against sunspot number:

Here are some tips to creating great figures: Ten simple rules for better figures

There are a number of options to create visualisations in Python - we will work with *Matplotlib*. As the name suggests, this provides plotting functionality very similar to Matlab. It is probably the most basic plotting package in Python, but still a good one.

There are a number of options for how the overall style of the plot looks, and as I plot different figures I will change the style to demonstrate different ones. Which style you end up choosing is down to personal taste!

I also note that I am only highlighting the basics of the plotting functionality here. There are a host of functions and methods to tailor the plots to look exactly as you desire.

You can check out the Matplotlib gallery to get ideas of what can be achieved: [https://matplotlib.org/gallery/index.html]

```
[1]: import numpy as np import matplotlib.pyplot as plt
```

Note The following instructions are tailored to working in Pycharm. If running python straight from the command line you have some additional flexibility with plotting.

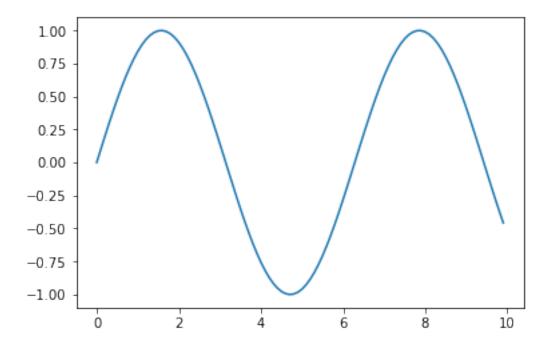
2 Line plots

We can now create a simple plot that will appear as a pop-up window in a separate tab within Pycharm.

Enter the following code in main.py

```
[2]: x = np.arange(0, 10, 0.1) # array from 0 to 10 in steps of 0.1
y = np.sin(x)

plt.plot(x, y)
plt.show() # This command is required to make the plot appear
```

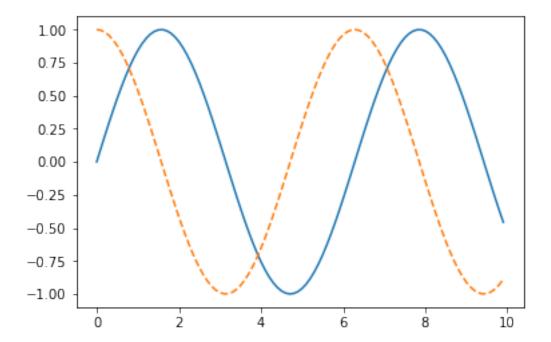


We can add another line to the plot. Replace the previous plotting code with:

```
[3]: x = np.arange(0, 10, 0.1) # array from 0 to 10 in steps of 0.1

y = np.sin(x)
y2 = np.cos(x)

plt.plot(x, y, '-')
plt.plot(x, y2, '--')
plt.show()
```



You can see that if we keep making calls to plt.plot(), then the results will be over-plotted on the open figure window. You should also notice that I selected the style of the line with the dashes between the quotation marks.

The colour of the plot lines is automatically chosen but can be adjusted manually.

We can save our figure by adding the following line of code above plot.show():

```
# plotting code
# .....
plt.savefig('myfigure.png')
plt.show()
```

If no filepath is specified, e.g., 'my_folder/pictures/myfigure.png' then the above command just saves to the directory in which you launched Python (the current working directory).

2.1 Multi-panel plots

You can also create multiple subplots in a figure.

```
[5]: plt.style.use('seaborn-whitegrid') # Change plot theme

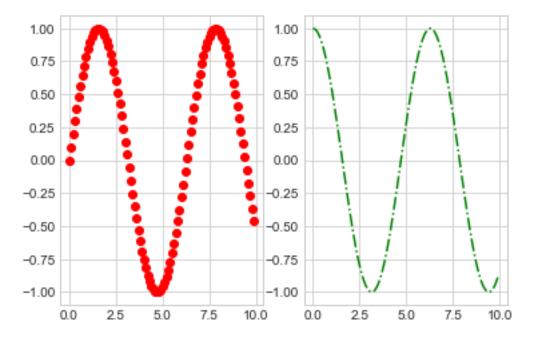
plt.figure() # Create a plot figure

# Create first panel of plot
```

```
plt.subplot(1, 2, 1) # (rows, columns, panel number)
plt.plot(x, y, 'ro') # 'ro' gives red dots

plt.subplot(1, 2, 2)
# alternative method for specifiying color and line-style
plt.plot(x, y2, linestyle='dashdot', color='g')

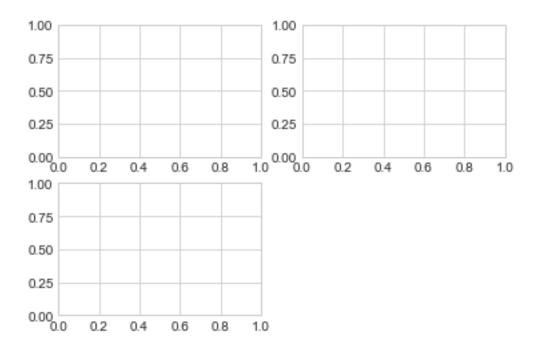
plt.show()
```



However, the best option might be to create a Figure object. First, we create the new figure and then add subplots to it.

```
[6]: fig = plt.figure() # create figure object

ax1 = fig.add_subplot(2, 2, 1)
ax2 = fig.add_subplot(2, 2, 2)
ax3 = fig.add_subplot(2, 2, 3)
```



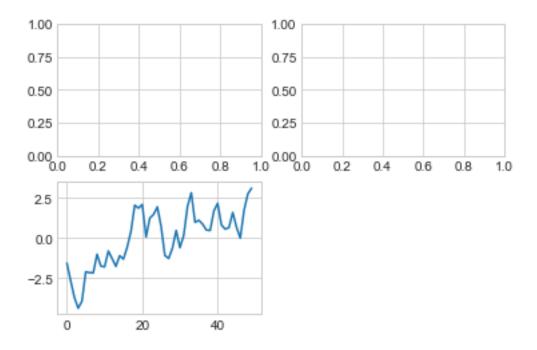
If we tried to add a plot now using plt.plot() then only the last plot is filled.

```
[7]: fig = plt.figure() # create figure object

ax1 = fig.add_subplot(2, 2, 1)
ax2 = fig.add_subplot(2, 2, 2)
ax3 = fig.add_subplot(2, 2, 3)

plt.plot(np.random.randn(50).cumsum())
```

[7]: [<matplotlib.lines.Line2D at 0x11c0d8860>]



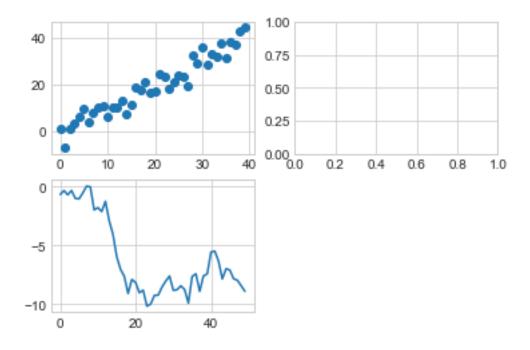
To plot to a specific subplot, you need to use each subplots instance method:

```
[8]: fig = plt.figure() # create figure object

ax1 = fig.add_subplot(2, 2, 1)
ax2 = fig.add_subplot(2, 2, 2)
ax3 = fig.add_subplot(2, 2, 3)

plt.plot(np.random.randn(50).cumsum())
ax1.scatter(np.arange(40), np.arange(40)+3*np.random.randn(40))
```

[8]: <matplotlib.collections.PathCollection at 0x1198f90f0>



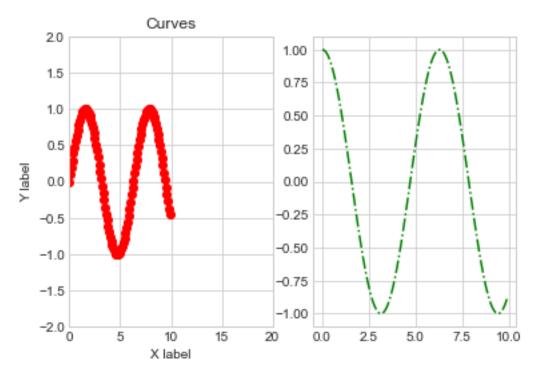
2.2 Adding information

You can customise any of the plots in an almost limitless number of ways. For example, you may want to change the axis ranges, or add titles to the axis and graph. We can achieve this with a variety of in-built plot methods.

All matplotlib functions (e.g., plot, hist, scatter) can all be modified with the same methods.

```
[9]: plt.figure() # Create a plot figure
     # Create first panel of plot
     plt.subplot(1, 2, 1) # (rows, columns, panel number)
     plt.plot(x, y, 'ro') # 'ro' gives red dots
     plt.xlim(0, 20)
                         # changes x axis range
     plt.ylim(-2, 2)
                         # changes y axis range
     plt.xlabel('X label')
                              # Adds a label to the x axis
     plt.ylabel("Y label")
                             # Adds a label to the y axis
     plt.title('Curves')
                              # Adds a title to the plot
     plt.subplot(1, 2, 2)
     # alternative method for specifiying color and line-style
```

```
plt.plot(x, y2, linestyle='dashdot', color='g')
plt.show()
```

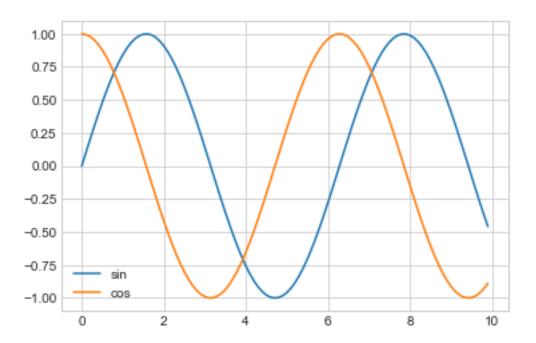


It is also possible to add a legend to the chart, but labels need to specified when calling plot.

```
[10]: fig = plt.figure() # Create figure object

plt.plot(x, y, label='sin') # Need to specify label here for legend
plt.plot(x, y2, label='cos')

plt.legend()
plt.show()
```



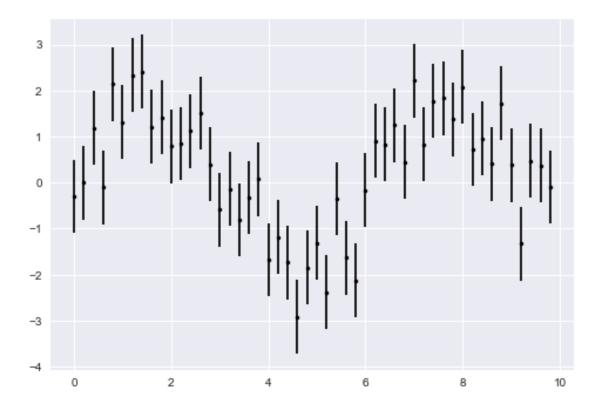
```
[11]: plt.style.use('seaborn') # Change plot theme
```

3 Plotting errors

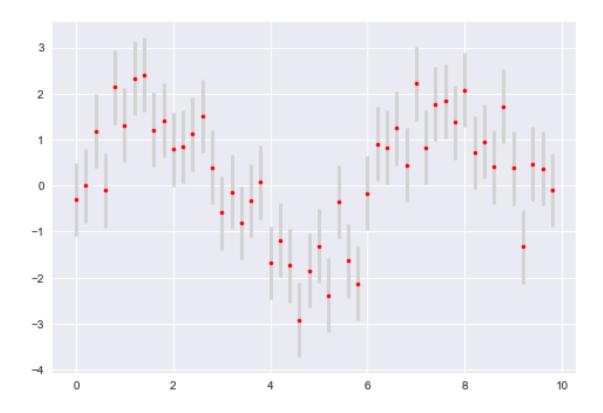
Any plot of scientific measurement data should also convey the uncertainties with each measurement. So we should know how to plot error bars on our data.

```
[12]: x = np.arange(0, 10, 0.2)
dy = 0.8
y = np.sin(x)+dy*np.random.randn(50) # Adds Guassian noise into the data

# fmt is a format code that controls
# appearence of lines & points
plt.errorbar(x, y, yerr=0.8, fmt='.k')
plt.show()
```



You can change the features of the error bars to make the plot more appealing.

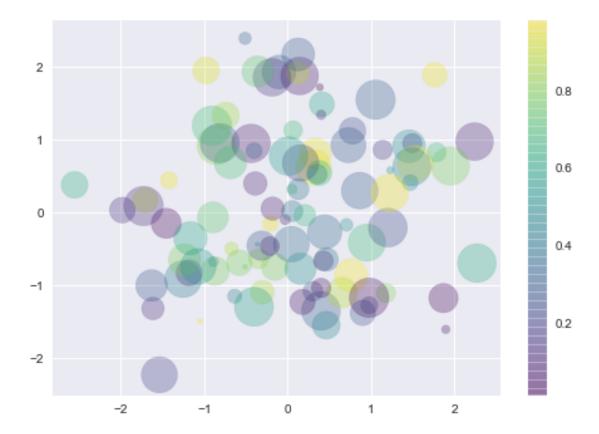


There is further flexibility for horizontal error bars, one sided errors, etc.

4 Scatter plots

While you can create scatter plots with the plot function, a more powerful option is plt.scatter .

This function enables you to control various aspects of each individual point, such as colour and size, to enable multi-dimensional information to be shown



Note that the color argument in *scatter* is automatically linked to the colourbar. Also, the size of the data point is given in pixels. Finally, to make all the overlapping data points visible we have changed the transparency of the plot using the *alpha* argument.

5 Contour plots

You may be working with three dimensional data (e.g. an image) and want to explore the data in two dimensions. One way to do this is with contour plots.

Let us first define some 3D function to work with, which is of the form z = f(x, y). We will use function in python to do the calculations for us. Functions will be discussed in detail next week for now don't worry too much about the details.

```
[15]: def f(x, y):
    return np.sin(x)**10+np.cos(10+y*x)*np.cos(x)
```

We will now plot the output of the function as a contour plot. To do this, we need to define a grid of values for x and y and z.

The easiest way to do this is to use a function called np.meshgrid (some of you may recognise the name from Matlab!).

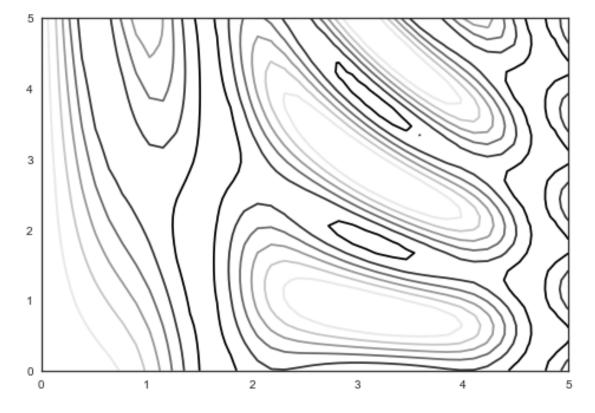
```
[16]: plt.style.use('seaborn-white')

x = np.linspace(0, 5, 40)  # Create 1 dimensional array
y = np.linspace(0, 5, 40)

X, Y = np.meshgrid(x, y)

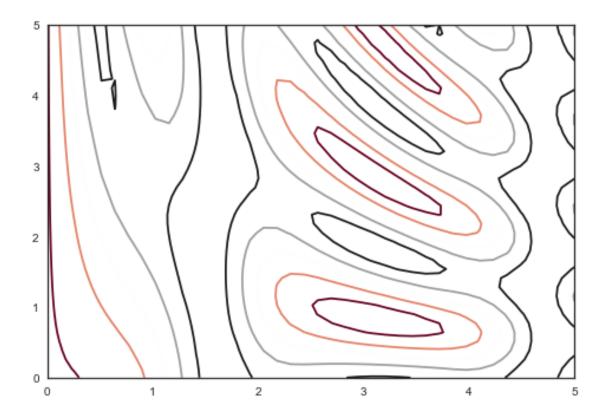
Z = f(X, Y)

plt.contour(X, Y, Z)
plt.show()
```



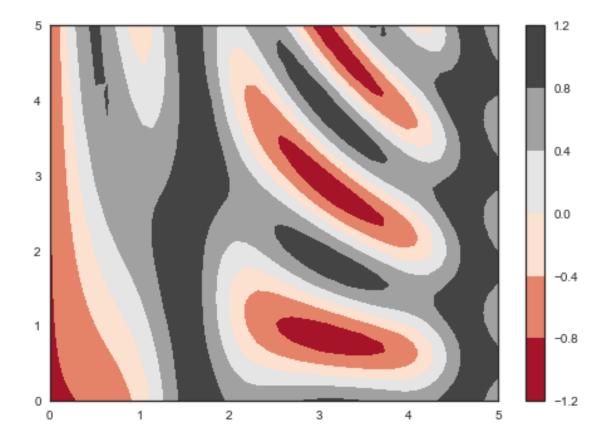
Of course, there is flexibility to play with various features of the plot, e.g. change the contour spacing, change the colour.

```
[17]: plt.contour(X, Y, Z, 5, cmap='RdGy')
plt.show()
```



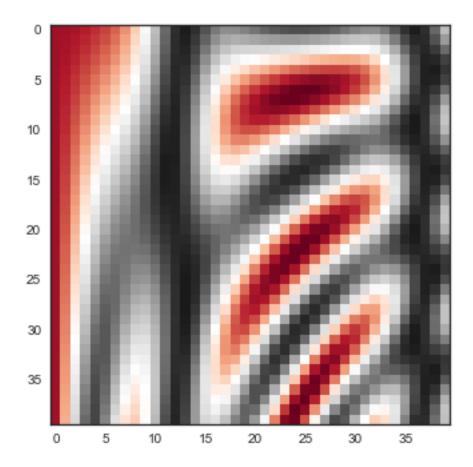
You may want to fill the contours instead:

```
[18]: plt.contourf(X, Y, Z, 5, cmap='RdGy')
   plt.colorbar()
   plt.show()
```



Another way to show such data is to use the imshow function, which interprets a 2D grid of data as an image.

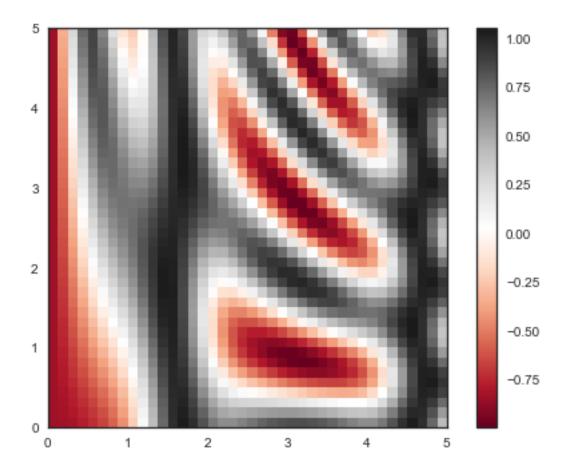
```
[19]: plt.imshow(Z, cmap='RdGy')
plt.show()
```



You can see this image is plotted upside down! When using imshow, the origin is placed in the top left corner. To show the figure in the standard orientation, you should use the origin keyword.

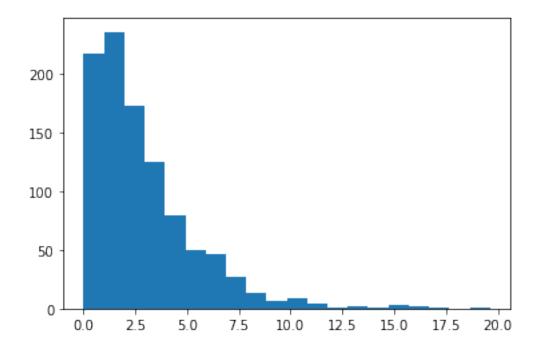
Also, imshow doesn't accept the x and y grid. Hence, you have to give instructions about the extent of the image.

```
[20]: plt.imshow(Z, cmap='RdGy', origin='lower', extent=[0, 5, 0, 5])
plt.colorbar()
plt.show()
```



6 Histograms

Histograms are a vital tool in probing data-sets. They show us the distribution of the quantity of interest and often inform how further analysis should proceed.



The histogram function has a very basic when it comes to binning the data. The default value is 10 bins.

The bin size of histograms is important as it can hide or reveal details. If the bin size is too coarse, then distinct features (peaks or troughs) can be obscured. If the bin size if too sparse, then we don't have enough information in each bin.

Fortunately, the bin size can be adjusted. The size can be specified 'by hand' by changing the number of bins. However, there is likely an optimal choice of bin size that balances to much versus to little detail. The optimal choice is not straightforward to calculate, however a few formulae have been derived that try to give a guide. For example there is Sturge's Rule, Scott's Rule, Square root. You are able to implement some of these with the latest versions of matplotlib and numpy.

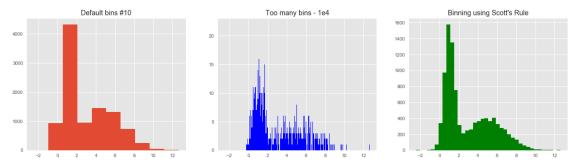
```
[23]: # Draw 10000 values from a normal distriburtion
    peak1 = np.random.randn(5000)*2.+5
    peak2 = np.random.randn(5000)*0.5+1

    combined_data = np.concatenate([peak1, peak2])

    plt.figure(figsize=(20, 5))
    plt.subplot(1, 3, 1)
    plt.hist(combined_data) # default bin value
    plt.title('Default bins #10')

    plt.subplot(1, 3, 2)
    plt.hist(combined_data, color='b', bins=5000)
    plt.title('Too many bins - 1e4')
```

```
plt.subplot(1, 3, 3)
plt.hist(combined_data, bins='scott', color='g')
plt.title("Binning using Scott's Rule")
plt.show()
```



6.1 Over-plotting multiple histograms

It is also possible to over-plot multiple histograms. Here we use the density keyword to show the probablity density function instead of the counts.

```
[24]: # Draw random samples from a normal distribution
    x1 = np.random.normal(0, 0.8, 1000)+4

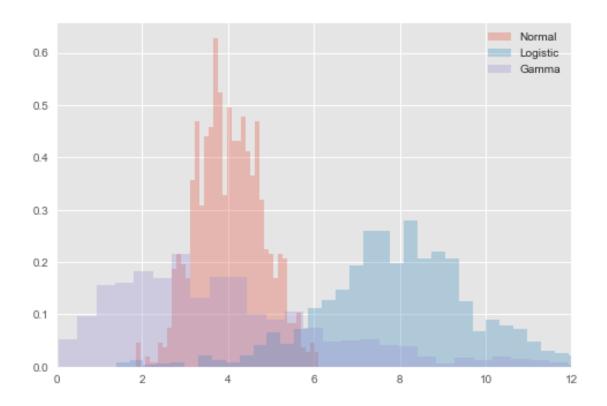
# Draw random samples from a logistic distribution
    x2 = np.random.logistic(8, 1, 1000)

# Draw random samples from a gamma distribution
    x3 = np.random.gamma(2, 2, size=1000)

# provide keywords as a dictionary
    kwargs = dict(alpha=0.3, density=True, bins=40)
    plt.hist(x1, **kwargs, label='Normal')
    plt.hist(x2, **kwargs, label='Logistic')
    plt.hist(x3, **kwargs, label='Gamma')

plt.xlim(0, 12)
    plt.legend()

plt.show()
```



6.2 Changing tick values

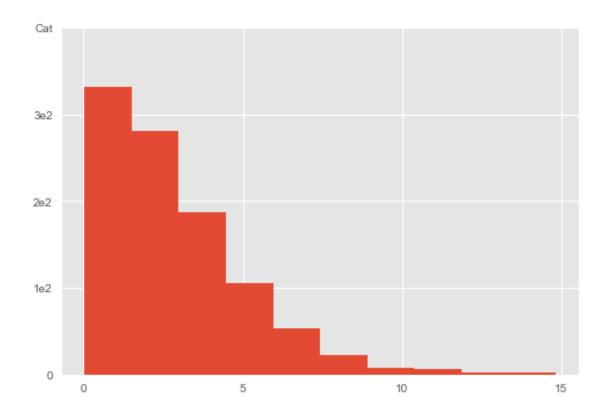
The histogram for the χ_3^2 (chi-squared with 3 degrees of freedom) data has a rather ugly set of tick labels. Of course, it s possible to change these to your taste.

```
[26]: plt.hist(data_chisq)

x_tick_vals = [0, 5, 10, 15]
plt.xticks(x_tick_vals)

y_tick_vals = [0, 100, 200, 300, 400]
y_tick_labels = ['0', '1e2', '2e2', '3e2', 'Cat']
plt.yticks(y_tick_vals, y_tick_labels)

plt.show()
```



6.3 Two-dimensional histograms

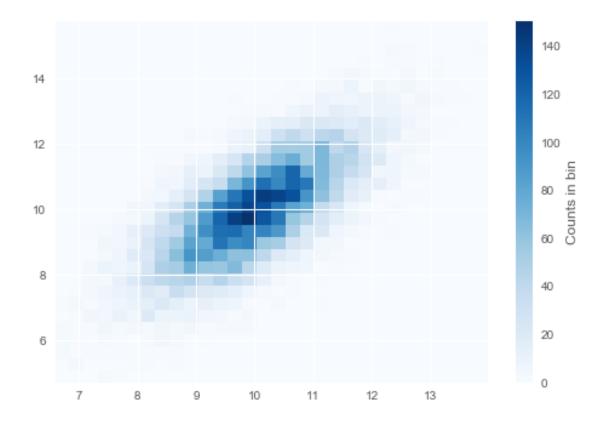
It is also possible to create histograms in two dimensions, dividing points in two dimensional bins. This shows the joint probability distribution.

Here is an example of how to do this. We create data from a multivariate Gaussian distribution.

```
[27]: mean = [10, 10]  # means
    cov = [[1, 1], [1, 2]]  # covariances

x, y = np.random.multivariate_normal(mean, cov, 10000).T

plt.hist2d(x, y, bins=30, cmap='Blues')
    cb = plt.colorbar()
    cb.set_label('Counts in bin')
    plt.show()
```



7 Fitting data

One key part of almost any analysis is fitting a model to your data. The simplest form of this is fitting a function using a least-squares method.

Note that the least-squares method makes the implicit assumption that your data has normally distributed errors.

With this in mind, we will create some fake data and use one of the optimisation routines in *scipy* to fit a model to our data.

There are a number of other modules that can also perform model fitting (e.g. astropy).

```
[]: # a least-squares curve fitting tool

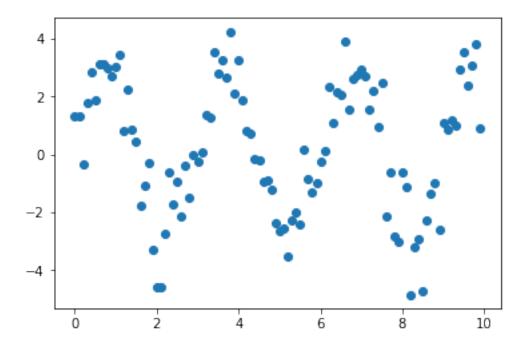
from scipy.optimize import curve_fit
```

Our data will be a sin curve with noise drawn from a normal distribution.

```
[9]: # Create a sin surve with noise
x = np.arange(0, 10, 0.1)
```

```
data = 3.*np.sin(x*2.*np.pi/3)
noise = np.random.RandomState(10).normal(size=100)
y = data+noise
plt.scatter(x, y)
```

[9]: <matplotlib.collections.PathCollection at 0x151895c8d0>



Now, we have to set up a function which defines our model we want to fit. (We will discuss functions further in the next lecture.)

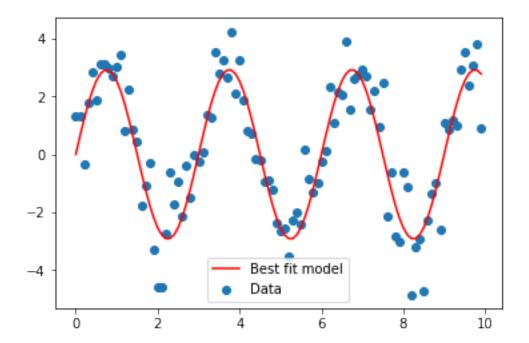
```
[27]: # define model to fit with parameters a and b
def sin_func(x, a, b):
    return a*np.sin(x*2.*np.pi/b)
```

Then, we pass the model function, the x and y values for our data and an initial guess for the model parameters to $curve_fit$.

```
[30]: popt, pcov = curve_fit(sin_func, x, y, p0=[4, 3.5])
# popt - best guess for model parameters
# pcov - error on model parameters
# p0 - initial guess for parameters
print('Best model parameters', popt)
```

```
plt.scatter(x, y, label='Data')
plt.plot(x, sin_func(x, *popt), 'r', label='Best fit model')
plt.legend()
plt.show()
```

[2.92169545 2.99925415]



There are many tools out there for fitting models/curves to data. Each one finds its use in specific situations. As you explore Python you will come across many packages that offer interesting and exciting tools for analysing your data.