iris_lab

September 14, 2018

1 ML1 Lab

Welcome to ML1! This lab will use the famous Iris data set to introduce you to common python ML tools. You will explore, analyze, and then build and tune models to predict flower species. Click here for more about the Iris dataset.

1.1 About the tools

Scientific python uses a set of libraries that build on one another. Here's a one-line intro to each, from lowest level to highest.

- **NumPy**: fast vector and matrix math
- **pandas**: Tools to read/write/manipulate data with a structure called the DataFrame. A bit like Excel.
- **SciPy**: scientific computation code,like Linear Regression and sparse matrices
- **scikit-learn**: ML algorithms and helper routines, such as feature extraction
- **Matplotlib**: graphing stuff!
- **Jupyter notebooks**: the web-based UI you are using now that allows text, code, and output to be shared,edited, and viewed.

1.2 Getting Around

Not familar with notebooks? Think of it as a fancy word processor. Each section is a cell that can contain text or code. When code is run, output is shown below. A good introductory tutorial can be found here.

Now, let's get started!

```
In [45]: import pandas as pd
         import numpy as np
```

1.3 Loading data

To analyze data, we are going to need to import it from an external source first! Let's use the popular, high-level library `pandas` to load the Iris data csv as a `DataFrame`.

```
In [46]: iris_csv_path = './data/iris.data'
         iris_df = pd.read_csv(iris_csv_path)
```

`DataFrames` are tabular data structures; let's sample a few rows at random to get a preliminary sense of our table:

```
In [47]: iris_df.sample(n=5)
```

```
Out[47]:      sepal_length  sepal_width  petal_length  petal_width            class
         28            5.2          3.4           1.4          0.2      Iris-setosa
         38            4.4          3.0           1.3          0.2      Iris-setosa
         19            5.1          3.8           1.5          0.3      Iris-setosa
         88            5.6          3.0           4.1          1.3  Iris-versicolor
         137           6.4          3.1           5.5          1.8   Iris-virginica
```

Here are two observations:

1. The columns of a `DataFrame` need not be the same data-type (`petal_width` is a `float`, while `class` is a `string`); we can think of a `DataFrame` as being a dictionary that maps column labels to `pandas Series` objects, which are one-dimensional arrays of data. We'll explore the relationship between `DataFrames` and `Series` a little more deeply in a few steps!

2. All `pandas` Data Structures are "labeled", which we can see by values of the `index` (i.e. what looks to be the left-most column). This would come in handy when merging `Series` of end-of-day prices for various securities, for example, since `pandas` would line up the dates for us (see the **Appendix** for an example of this!)

1.4 Exploratory Data Analysis

The purpose of this lab is to use the features `sepal_length`, `sepal_width`, `petal_length` and `petal_width` to predict the correct class of Iris (e.g. `Iris-versicolor`) for each of the examples that we've been provided. Before we dive into visualizations and machine learning, however, let's spend a few minutes getting more familiar with the data.

```
In [48]: iris_df.describe(include='all')
```

```
Out[48]:         sepal_length  sepal_width  petal_length  petal_width        class
         count     150.000000   150.000000    150.000000   150.000000          150
         unique           NaN          NaN           NaN          NaN            3
         top              NaN          NaN           NaN          NaN  Iris-setosa
         freq             NaN          NaN           NaN          NaN           50
         mean        5.843333     3.054000      3.758667     1.198667          NaN
         std         0.828066     0.433594      1.764420     0.763161          NaN
```

```
min         4.300000     2.000000      1.000000     0.100000          NaN
25%         5.100000     2.800000      1.600000     0.300000          NaN
50%         5.800000     3.000000      4.350000     1.300000          NaN
75%         6.400000     3.300000      5.100000     1.800000          NaN
max         7.900000     4.400000      6.900000     2.500000          NaN
```

We can see the mean for each feature across all of the samples, but are these consistent across Iris classes?

```
In [49]: iris_df.groupby('class').mean()
```

```
Out[49]:                  sepal_length  sepal_width  petal_length  petal_width
         class
         Iris-setosa             5.006        3.418         1.464        0.244
         Iris-versicolor         5.936        2.770         4.260        1.326
         Iris-virginica          6.588        2.974         5.552        2.026
```

While 4 features is pretty manageable, suppose we were provided with hundreds of columns but only a few were of interest. We can sub-select columns as follows:

```
In [50]: iris_df[['sepal_length', 'sepal_width']].head()
```

```
Out[50]:    sepal_length  sepal_width
         0           5.1          3.5
         1           4.9          3.0
         2           4.7          3.2
         3           4.6          3.1
         4           5.0          3.6
```

And notice that if we select only one column, we get a `pandas Series` object back:

```
In [51]: sepal_length = iris_df['sepal_length']

         print(type(sepal_length))
         sepal_length.head()
```

```
<class 'pandas.core.series.Series'>


Out[51]: 0    5.1
         1    4.9
         2    4.7
         3    4.6
         4    5.0
         Name: sepal_length, dtype: float64
```

And this `Series` can easily converted back to a 1-column `DataFrame`:

```
In [52]: sepal_length.to_frame().head()
```

```
Out[52]:    sepal_length
         0           5.1
         1           4.9
         2           4.7
         3           4.6
         4           5.0
```

Now that we've been exposed to a few of these methods, let's combine them to check whether any Iris classes are more heavily represented than the others

```
In [53]: # .size() returns a Series
         iris_df.groupby('class').size().to_frame('counts')
```

```
Out[53]:                  counts
         class
         Iris-setosa          50
         Iris-versicolor      50
         Iris-virginica       50
```

Suppose we now want to examine a subset of *rows* in our `DataFrame`, and we want to select them based on their column values (similar to SQL):

```
In [54]: iris_df.query('sepal_length > 7')
```

```
Out[54]:      sepal_length  sepal_width  petal_length  petal_width           class
         102           7.1          3.0           5.9          2.1  Iris-virginica
         105           7.6          3.0           6.6          2.1  Iris-virginica
         107           7.3          2.9           6.3          1.8  Iris-virginica
         109           7.2          3.6           6.1          2.5  Iris-virginica
         117           7.7          3.8           6.7          2.2  Iris-virginica
         118           7.7          2.6           6.9          2.3  Iris-virginica
         122           7.7          2.8           6.7          2.0  Iris-virginica
         125           7.2          3.2           6.0          1.8  Iris-virginica
         129           7.2          3.0           5.8          1.6  Iris-virginica
         130           7.4          2.8           6.1          1.9  Iris-virginica
         131           7.9          3.8           6.4          2.0  Iris-virginica
         135           7.7          3.0           6.1          2.3  Iris-virginica
```

While pandas has become the tool of choice for most data science tasks, numpy is a lower-level (but also very popular) Python library that comes in handy when doing work with vectors and matrices, or implementing machine learning algorithms from scratch. Luckily, it plays very well with pandas and pure Python. For our purposes, let's just explore a few common use-cases.

Imagine we want to use a machine learning library that expects us to represent our observations as a 2-dimensional numpy array instead of a DataFrame. We can easily convert our DataFrame to this format as follows:

```
In [55]: # first drop the class labels, since **all values in a numpy array must have the same data-type**
         iris_features_df = iris_df.drop(['class'], axis=1)

         # The call to .values does the magic of converting our DataFrame to a numpy array. This works for Series objects, too!
         iris_features_ndarray = iris_features_df.values
         iris_features_ndarray[:5]
```

```
Out[55]: array([[5.1, 3.5, 1.4, 0.2],
                [4.9, 3. , 1.4, 0.2],
                [4.7, 3.2, 1.3, 0.2],
                [4.6, 3.1, 1.5, 0.2],
                [5. , 3.6, 1.4, 0.2]])
```

To go full circle, let's convert it back!

```
In [56]: pd.DataFrame(iris_features_ndarray, columns=['sepal_length', 'sepal_width', 'petal_length', 'petal_width']).head()
```

```
Out[56]:    sepal_length  sepal_width  petal_length  petal_width
         0           5.1          3.5           1.4          0.2
         1           4.9          3.0           1.4          0.2
         2           4.7          3.2           1.3          0.2
         3           4.6          3.1           1.5          0.2
         4           5.0          3.6           1.4          0.2
```

Here are some commonly-used numpy functions, which we'll use when tuning our model later in this lab

```
In [57]: # Create an evenly spaced array
         print(np.arange(5))

         # Convert a plain Python list to an array
         print(np.array([10**i for i in range(-1, 3)]))
```

```
[0 1 2 3 4]
[  0.1   1.   10.  100. ]
```

Please check out the **Appendix** at the bottom of this notebook for more advanced material on pandas and numpy

2 Data visualization

In this section we will use the module matplotlib.pyplot, a MATLAB-like plotting framework.

Overview of matplotlib, with links to documentation and tutorials

First of all, let's configure matplotlib so that it works fine in your environment.

Important: Remember to set in_bqnt to True if you are in BQNT <GO>.

```
In [58]: import matplotlib.pyplot as plt

         # configure the notebook to display the figures inline
         %matplotlib inline

         # is this running in BQNT?
         in_bqnt = False

         # set up light coloring for BQNT's dark background
         if in_bqnt:
             rc_params = {
                 'xtick': {'color': 'white'},
                 'ytick': {'color': 'white'},
                 'axes': {'labelcolor': 'white'}
             }
             for group, args in rc_params.items():
                 plt.rc(group, **args)
```

2.1 Feature Histogram

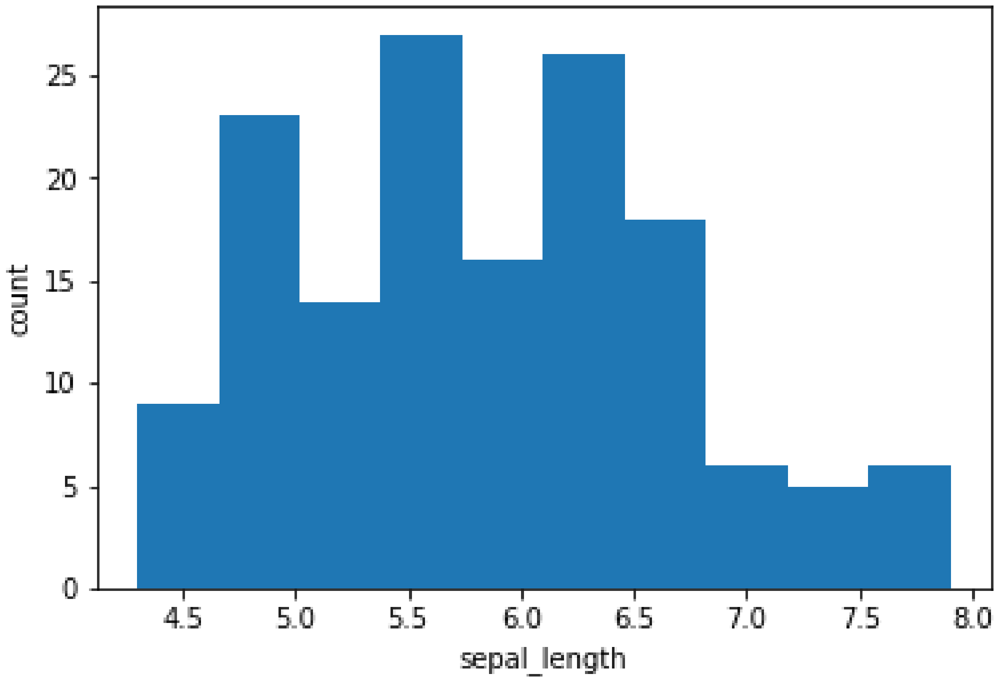
This section covers:

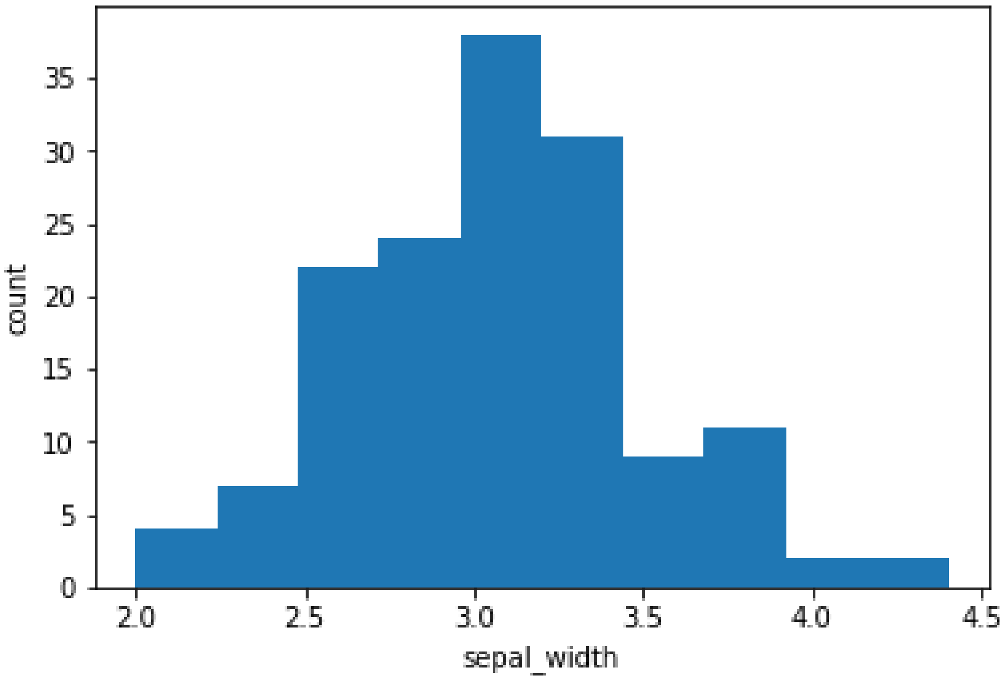
- Creating a histogram plot
- Adding axis labels
- Using a new figure for each plot

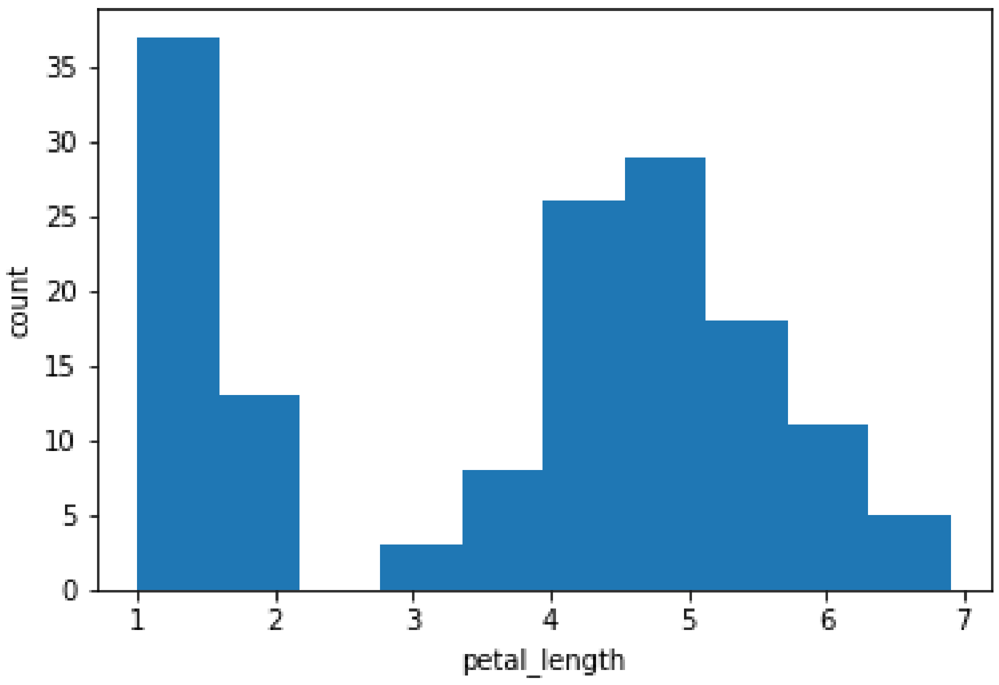
2.1.1 Histogram

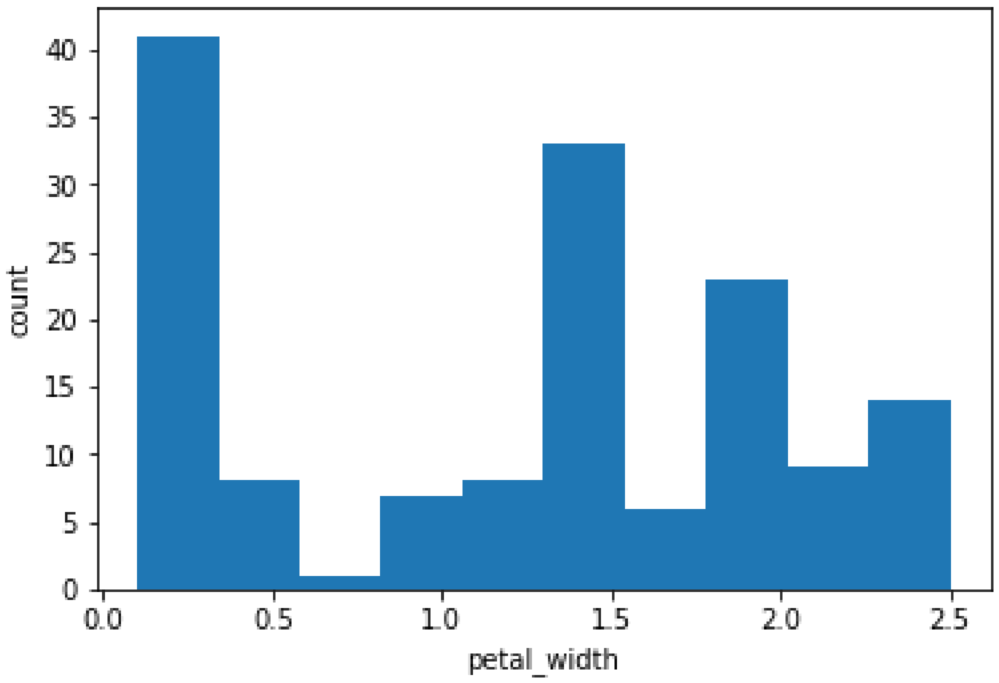
Just pass one-dimensional data (and optionally the number of bins) to the `plt.hist` function to draw a histogram.
To add a label to the *x* and *y* axes, you can use `plt.xlabel` and `plt.ylabel`.

```
In [59]: def draw_histogram(feature_values, feature_name):
             plt.hist(feature_values, bins=10) # draw a histogram of feature_values with 10 bins
             plt.xlabel(feature_name)  # set the x label to feature_name
             plt.ylabel('count')  # set the y label to 'count'

         feature_names = ['sepal_length', 'sepal_width', 'petal_length', 'petal_width']  # or iris_df.columns.values[:-1]
         for feature_name in feature_names:
             plt.figure()  # this line makes each histogram use a different figure, try removing it to see what happens!
             #feature_values = ...  # get the data for a given feature_name
             feature_values = iris_df[feature_name]
             draw_histogram(feature_values, feature_name)
```









2.2 Separating dataset by a value

In this classification problem, we want to find the species of a given flower given only the measurements.

When looking at the petal length and petal width histogram, we see that there seems to be two peaks (around 1.5 and around 5).

Are these peaks a good way to distinguish species? Why do we have two peaks even though we have three possible species? A good way to answer these questions is to separate the dataset by classes, to see how each class is influencing the shape of the histogram.

This section covers:

- Separating the dataset by the value of a feature ('class' in this case)

- Adding multiple data series to the same plot
- Adding a legend to a plot

```
In [60]: classes = ['Iris-setosa', 'Iris-versicolor', 'Iris-virginica']  # or iris_df['class'].unique()
         feature_name = 'petal_length'

         true_if_setosa = iris_df['class'] == 'Iris-setosa'
         only_setosa_df = iris_df.loc[true_if_setosa]
         feature_values = only_setosa_df[feature_name]
         print('Iris-setosa {} average: {}'.format(feature_name, feature_values.mean()))
```

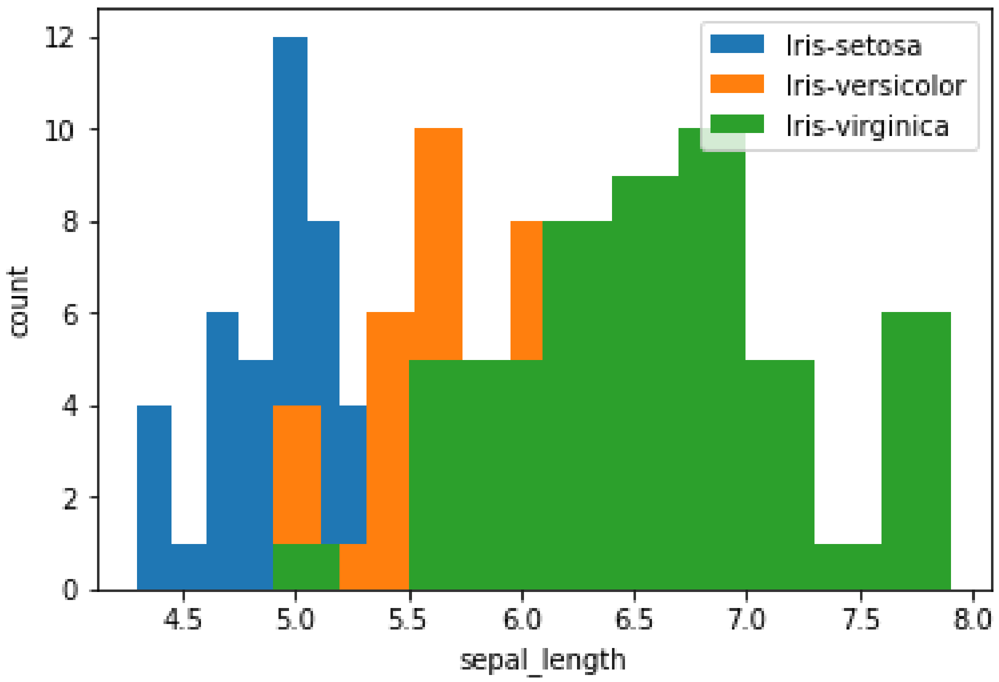
```
Iris-setosa petal_length average: 1.464
```

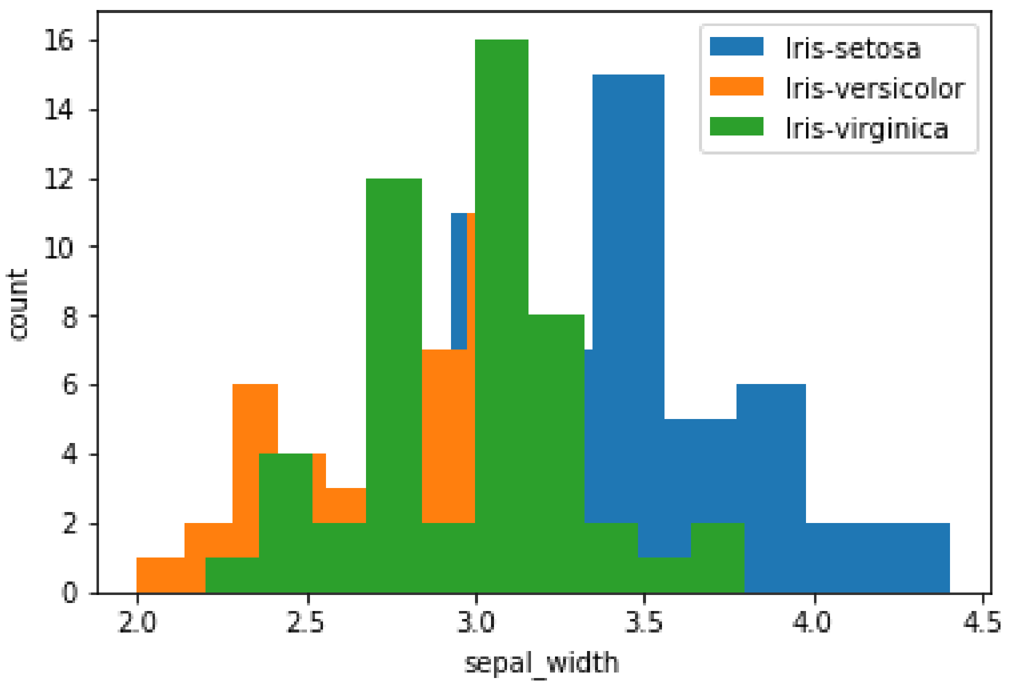
The `Iris-setosa` average is indeed around 1.5!
But what are the minimum and maximum values? And how about the other classes?

2.2.1 Exercise 1. Draw a separated feature histogram for each feature

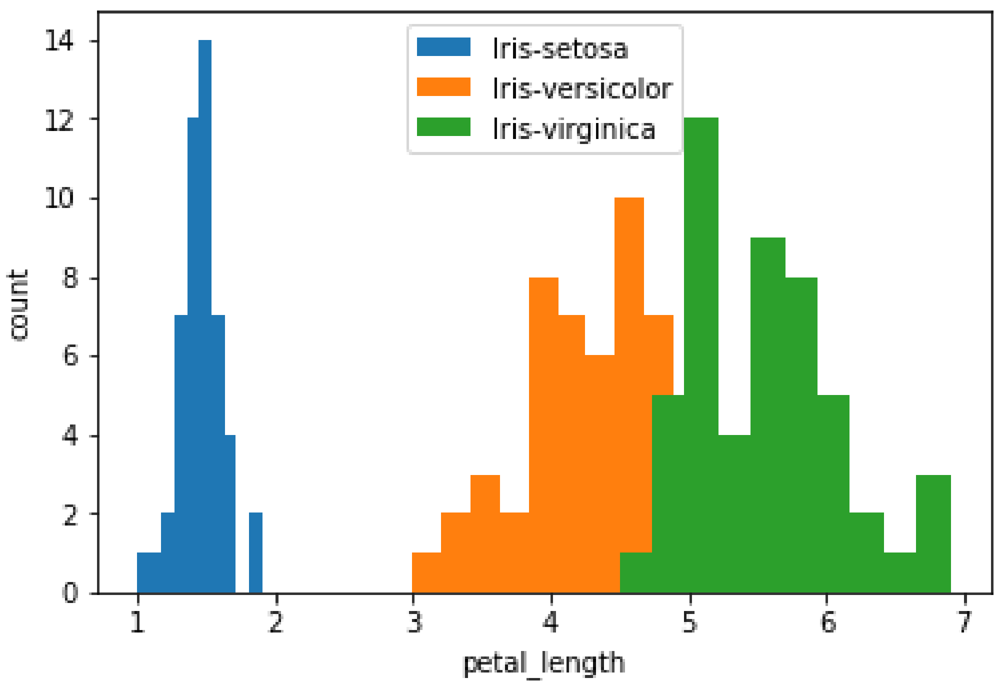
1. select **only** the feature values corresponding to `cls` in `feature_values`
2. look at the histogram with all three classes
3. Plot the separated histogram of each feature
4. Make sure that the x label and y label are set
5. Also make sure the legend is visible

```
In [61]: def only_cls_feature_values(input_df, cls, feature_name):
             return input_df.loc[input_df['class'] == cls][feature_name]

         for feature_name in feature_names:
             plt.figure()  # add plots to a new figure
             for cls in classes:
                 cls_fv = only_cls_feature_values(iris_df, cls, feature_name)
                 draw_histogram(cls_fv, feature_name)
             plt.legend(classes)
             #plt.title(feature_name)
```

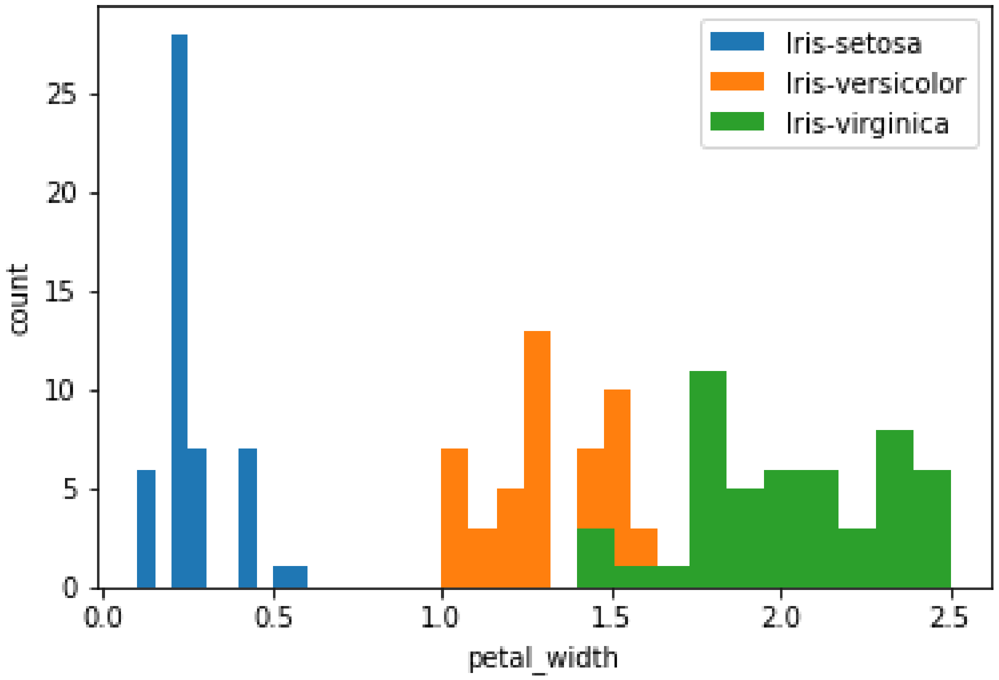




Iris-setosa
Iris-versicolor
Iris-virginica
count
sepal_width



Iris-setosa
Iris-versicolor
Iris-virginica
count
petal_length



2.3 Scatterplots of feature pairs

When analyzing multi dimensional data, it is sometimes interesting to see how some dimensions interact with each other. In order to do this, one possible tool is a scatter plot.

This section covers:

- Creating a scatter plot of a pair of features
- Interpreting the plot

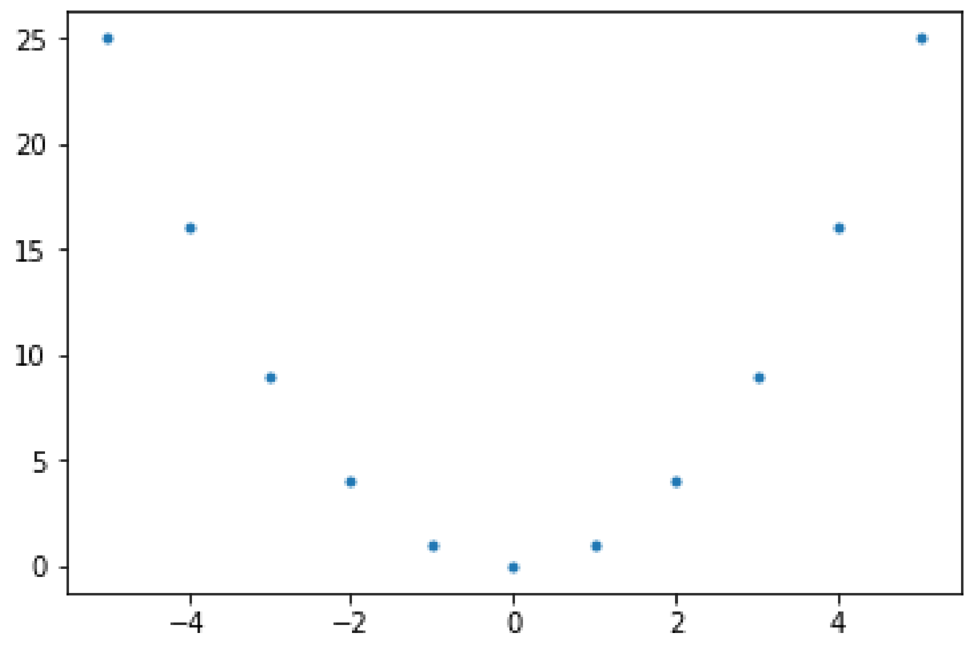
2.3.1 Scatterplots

The way to plot scatter plots with `matplotlib.pyplot` is the same as a line plot, except that we need to provide one more argument at the end, for the shape.

Here is a simple example, of the square function, using `'.'` instead of `'-'` (the default).

Other possible values include `'x'`, `'+'`, etc. (see https://matplotlib.org/api/pyplot_api.html#matplotlib.pyplot.plot for a full list).

```
In [62]: def square(x):
             return x ** 2

         x_values = np.linspace(-5, 5, num=11)
         plt.plot(x_values, square(x_values), '.');
```

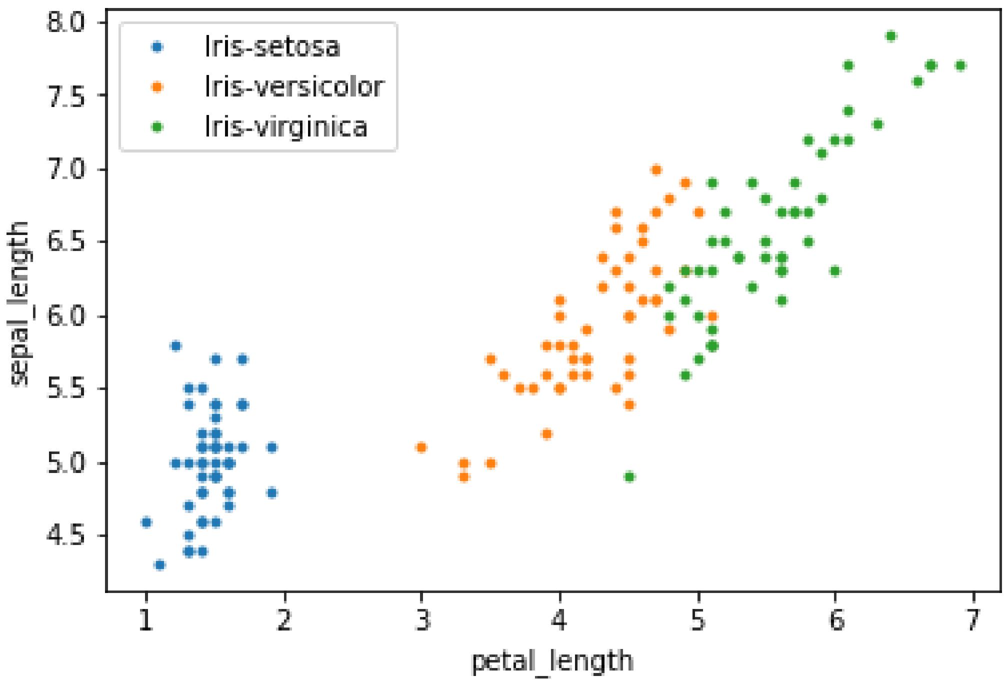


2.3.2 Exercise 2. Plot a pair of features

1. Get the `x_values` for a given class and the `x_feature` feature name
2. Same thing for `y_values`

(hint: use `only_cls_feature_values`) 3. Plot the `x_values` against `y_values` with a the `'.'` shape

```
In [63]: def scatter_plot_feature_pair(input_df, x_feature, y_feature, classes, plt=plt):
             handles = []  # used for plt.figlegend

             for cls in classes:
                 x_values = only_cls_feature_values(input_df, cls, x_feature)
                 y_values = only_cls_feature_values(input_df, cls, y_feature)
                 axis = plt.plot(x_values, y_values, '.')
                 handles.append(axis[0])

             return handles

         scatter_plot_feature_pair(iris_df, 'petal_length', 'sepal_length', classes)
         plt.xlabel('petal_length')
         plt.ylabel('sepal_length')
         plt.legend(classes);
```



2.4 Scatterplot matrix

In addition to the distribution of individual features, it is also useful to visualize the relationships between features. To do so, we can create scatterplots for each pair of features, arranged in a 'matrix' layout. Furthermore, by coloring the scatterplot according to 'class', we can gain further insight into the nature of the correlations.

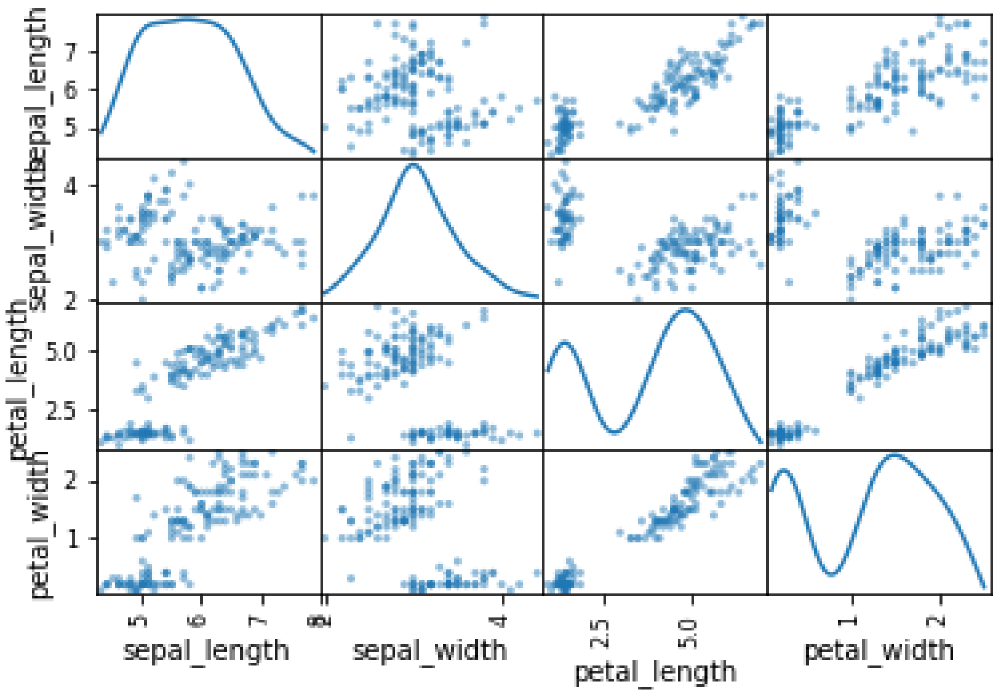
This section covers:

- Working with subplots

2.4.1 Cheating with pandas

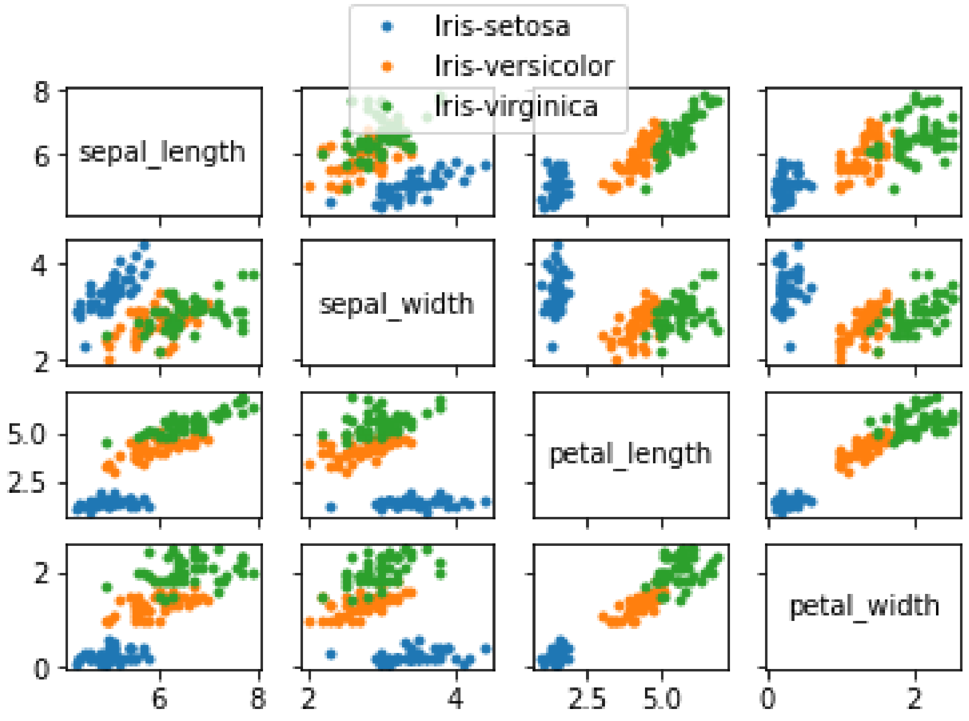
If you are willing to accept their default, pandas already have everything done for us (no need to use our previous functions).

```
In [64]: try:
             from pandas.plotting import scatter_matrix  # BQNT has an old version of pandas, without plotting
             scatter_matrix(iris_df, diagonal='kde')
             image = None
         except:
             from IPython.display import Image
             image = Image(filename='pandas_scatter_matrix.png')

         image
```



But this is not separated by class! No pretty colors!
The code below uses our functions to do a similar scatter matrix but separated by classes.

```
In [65]: from itertools import combinations

         def scatterplot_matrix(input_df, classes, kde_in_diagonal):
             # create the figure as a matrix of subplots, sharing x values in columns,
             # and y values in rows iff display_kde is False
             sharey = {'sharey': 'row'} if not kde_in_diagonal else {}
             _, axes_array = plt.subplots(len(feature_names), len(feature_names), sharex='col', **sharey)

             # loop over the diagonal
             # note: the enumerate(iterable) function returns tuples of (index, element) for all the elements in the iterable
             for i, feature in enumerate(feature_names):
                 # for the subplot at i,i:
                 # instead of plotting the feature against itself
                 if kde_in_diagonal:
                     # try implementing that function in the appendix
                     plot_kde(input_df, feature, classes, axes_array[i,i])
                 else:
                     # display name of the feature
                     plt.text(
                         0.5, 0.5, feature,
                         horizontalalignment='center',
                         verticalalignment='center',
                         transform=axes_array[i,i].transAxes
                     )

             # loop over the top right half of the matrix
             # note: combinations(iterable, 2) returns all pairs of features without considering order
             #       so in our case, we have [((0, 'sepal_length'), (1, 'sepal_width')), ...]
             for (i, feature1), (j, feature2) in combinations(enumerate(feature_names), 2):
                 # plot in the top right half (i, j)
                 scatter_plot_feature_pair(
                     input_df,
                     feature2,
                     feature1,
                     classes,
                     plt=axes_array[i,j]
                 )

                 # plot the mirror image in the bottom left half (j, i)
                 handles = scatter_plot_feature_pair(
                     input_df,
                     feature1,
            feature2,
            classes,
            plt=axes_array[j,i]
        )

    plt.figlegend(handles, classes, 'upper center')

scatterplot_matrix(iris_df, classes, kde_in_diagonal=False)

# you should also try this (see appendix 3 first):
# scatterplot_matrix(iris_df, classes, kde_in_diagonal=True)
```



We can easily see that setosa iris measurements form a separate cluster for any two sets of features! This is not obvious from the kernel densities for sepal measurements, though it can be seen in the bimodal petal measurement kernel densities. The strongest correlation is between petal width and petal length, as shown by the strong linearity in the scatter plot, and a similar linear relationship is shared between all classes of iris. This is not the case for e.g. petal length and sepal length, which also exhibit fairly strong correlation within a class but have different linear relationships between classes. These conclusions can be used to interpret the results of clustering and regression models.

Fitting A Model

Enough warming up, let's get to it!

To prep our data for building a model, we need to split it into three main categories:

1. Training set
2. Validation set
3. Test set

This is a critical best-practice in data science to guard against overfitting!

Notice that below we use the `sklearn` function `train_test_split` to partition the data randomly into the three categories described above. The default train/test proportions are 75%/25%, but they can be manually configured as desired. Here we'll use 80%/20%.

Additionally, if we had discovered that our data set contained relatively few of one of the classes, we could specify `stratify=y` to make sure that each split has equal representation from all classes. (This could be important so we don't end up with a split with 0 or very few examples from a particular class, just by random chance.)

```
In [66]: from sklearn.model_selection import train_test_split

         #Renaming the DataFrame to stick with popular convention
         X = iris_df.copy()

         # Similar to Python dictionaries, pop() removes the column from the DataFrame and returns the corresponding Series
         y = X.pop('class')

         X_train_all, X_test, y_train_all, y_test = train_test_split(X, y, test_size=0.2)
         X_train, X_val, y_train, y_val = train_test_split(X_train_all, y_train_all, test_size=0.2)
```

How would you get the counts of training examples across the Iris classes?

```
In [67]: # SOLUTION
         y_train.to_frame().groupby('class').size().to_frame('counts')

Out[67]:                   counts
         class
         Iris-setosa           33
         Iris-versicolor       33
         Iris-virginica        30
```

Logistic Regression

Once we've loaded, cleaned, split, and visualized the data, we're ready to try fitting some machine learning models! Logistic regression, despite its name, can be viewed as a machine learning model for doing classification. Logistic regression gives us prediction functions that produce "soft classifications", namely probability distributions over class labels. To get a hard classification, we will just choose the class with the highest probability.

Scikit-Learn contains a LogisticRegression class, which can train a model on your data and make predictions. There's a link to the full spec below, but the most important methods are:

1. fit(X, y): Fits the model to the provided training data.
2. predict(X): Predicts the classification for test data.

Full Spec: http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html

```
In [75]: #Train a logistic regression model and use it to predict the species for the validation data
         from sklearn.linear_model import LogisticRegression
         log_reg = LogisticRegression()
         log_reg.fit(X_train, y_train)
         y_pred = log_reg.predict(X_val)
         y_pred
         # SOLUTION

Out[75]: array(['Iris-setosa', 'Iris-virginica', 'Iris-versicolor', 'Iris-setosa',
                'Iris-versicolor', 'Iris-versicolor', 'Iris-virginica',
                'Iris-versicolor', 'Iris-versicolor', 'Iris-setosa',
                'Iris-virginica', 'Iris-setosa', 'Iris-virginica',
                'Iris-virginica', 'Iris-virginica', 'Iris-virginica',
                'Iris-virginica', 'Iris-setosa', 'Iris-setosa', 'Iris-virginica',
                'Iris-setosa', 'Iris-virginica', 'Iris-versicolor',
                'Iris-virginica'], dtype=object)
```

For any model, we need a way of assessing how good our predictions are. LogisticRegression has a method, score(X, y), which returns the mean accuracy, or the percent of samples correctly classified, on the given test data and provided labels. It first uses the trained model to predict the classes for the samples in X, then compares those to the true classes in y.

```
In [78]: #Output the score of your model on your validation set
         log_reg.score(X_val, y_val)
         # SOLUTION

Out[78]: 1.0
```

Confusion Matrix

Logistic regression appears to do a pretty good job of classifying the samples by species. We may want to look more carefully at where the classifier succeeded and where it failed. Doing so can illuminate similarities between classes or suggest the need for additional features to help the model differentiate between classes.

One tool for understanding the success of a classifier is a confusion matrix, which breaks down the predicted classifications by true class: for each true class, it shows how many samples were predicted to be in each possible class. Pandas contains a tool, crosstab, for creating them.

```
In [79]: # check if this logistic regression model has been fit
         if hasattr(log_reg, 'coef_') and log_reg.coef_ is not None:
             predictions = log_reg.predict(X_val)
             print(pd.crosstab(y_val, predictions, rownames = ['True Class'], colnames= ['Predicted Class'] ))

Predicted Class  Iris-setosa  Iris-versicolor  Iris-virginica
True Class
Iris-setosa                7                0               0
Iris-versicolor            0                6               0
Iris-virginica             0                0              11
```

Hyperparameters

Recall that hyperparameters are parameters of the machine learning model itself that can be adjusted to produce a better fitting model. One of the most important applications of hyperparameters is in regularization , a technique to help avoid overfitting. Regularization essentially sacrifices the "best" model for the training data in return for a model that can generalize better to test data.

One form of regularization works by penalizing models that have coefficients that are "too big". For example, in a linear model $y = a_1 x + a_2$, we might want to avoid models that have very steep slopes or very large intercepts. Controlling a_1 and a_2 allows us to do so.

Two forms of regularization are commonly used for Logistic Regression: l1 and l2 (pronounced "ell 1" and "ell 2") 1. In l2 regularization, we control the size of the coefficients by penalizing the model for having a large sum of squared coefficients (eg, $a_1^2 + a_2^2$). This is the default regularization in Scikit-Learn's LogisticRegression. 3. In l1 regularization, we control the size of the coefficients by penalizing the model for having a large sum of the absolute value of the coefficients (eg, $|a_1| + |a_2|$). l1 regularization favors "sparse solutions". A sparse solution is when one or more of the feature weights is 0. The more l1 regularization we have, the sparser the solution we get. For this reason, l1 regularization can be used for feature selection.

To try different types of regularization in Scikit-Learn, you need to initialize LogisticRegression with two parameters:

1. penalty: Type of regularization; a string, either 'l1' or 'l2'
2. C: The inverse of regularization strength; a positive float that determines how much to penalize the model for large coefficients. Note that since it's the inverse, smaller values of C mean a more regularized model (i.e. smaller coefficients).

```
In [89]: # Try some different combinations of C and penalty and see how they affect the score on the validation set.
         log_reg = LogisticRegression(C=0.1, penalty='l2')
         log_reg.fit(X_train, y_train)
         if hasattr(log_reg, 'coef_') and log_reg.coef_ is not None:
             predictions = log_reg.predict(X_val)
             print(pd.crosstab(y_val, predictions, rownames = ['True Class'], colnames= ['Predicted Class'] ))
         # SOLUTION
```

```
Predicted Class  Iris-setosa  Iris-versicolor  Iris-virginica
True Class
Iris-setosa                7                0               0
Iris-versicolor            0                4               2
Iris-virginica             0                0              11
```

Using GridSearch for hyperparameter tuning

Scikit-Learn has a tool to make this kind of hyperparameter tuning easier.

Recall that cross validiation is another technique for assessing the quality of a model. Instead of splitting the training data once into a test set and a validation set, in cross validation, the data is divided into *n* subsets, called folds, and the model is trained *n* times, each time witholding a different fold to use as the validation set.

Cross validation can be helpful for small datasets, since every data point is used to assess the model performance, rather than just a fixed subset.

In Scikit-Learn, GridSearchCV is used to accomplish this kind of parameter tuning. Given a Scikit-Learn estimator object (eg, LogisticRegression), a dictionary listing all the parameters to try, and a scoring method, GridSearchCV will train a model for every parameter combination and show the score for every combination.

Once GridSearchCV has fit the model, you can access cv_results_, a matrix of results, as well as best_estimator_, best_score_, and others. See http://scikit-learn.org/stable/modules/generated/sklearn.model_selection.GridSearchCV.html for full details.

Since we are working on a classification problem, we will use accuracy as our scoring method, but GridSearchCV (and Scikit-Learn) supports many other types of scores, assuming they're supported by the estimator object. See http://scikit-learn.org/stable/modules/model_evaluation.html#scoring-parameter for a complete list.

```
In [90]: #Using GridSearchCV, train models on for a wide variety of hyperparameters

         from sklearn.model_selection import GridSearchCV
         param_grid = [{'C':[1e-5, 0.0001, 0.001, 0.01, 0.1, 1.0, 10.0, 100.0, 1000.0, 10000.0], 'penalty':['l1', 'l2']}]
         log_reg = LogisticRegression()
         grid_search = GridSearchCV(log_reg, param_grid, cv=5, scoring='accuracy', return_train_score=False)
         grid_search.fit(X_train_all, y_train_all)
         results = pd.DataFrame(grid_search.cv_results_)

         #There's lots of data in the results dataframe - we'll just look at a few columns here, but feel free to explore
         results[["param_C","param_penalty", "mean_test_score", "rank_test_score"]]
```

```
Out[90]:    param_C param_penalty  mean_test_score  rank_test_score
         0    1e-05            l1         0.333333               17
         1    1e-05            l2         0.341667               14
         2   0.0001            l1         0.333333               17
         3   0.0001            l2         0.341667               14
         4    0.001            l1         0.333333               17
         5    0.001            l2         0.341667               14
         6     0.01            l1         0.325000               20
         7     0.01            l2         0.675000               13
         8      0.1            l1         0.700000               12
         9      0.1            l2         0.816667               11
         10       1            l1         0.941667                9
         11       1            l2         0.941667                9
         12      10            l1         0.958333                7
         13      10            l2         0.966667                4
         14     100            l1         0.958333                7
         15     100            l2         0.975000                1
         16    1000            l1         0.966667                4
         17    1000            l2         0.975000                1
         18   10000            l1         0.966667                4
         19   10000            l2         0.975000                1
```

Trying other models

Logistic Regression is a very common basic classification algorithm, but there are others you can also try.

K Nearest Neighbors

In K Nearest Neighbors classification, the prediction function identifies the K "nearest neighbors" to an input feature vector, and predicts the most frequently occurring class among those neighbors. The nearest neighbors are typically found using the standard euclidean distance, though any other similarity score may be used instead.The K in K nearest neighbors is a hyperparameter: small values of K will provide a more flexible, granular fit, but will be sensitive to noise. Larger values of K will be more resilient to noise but less likely to pick up small variations in the boundaries.

To implement a K Nearest Neighbors model, use Scikit-Learn's KNeighborsClassifier. Initialize it with n_neighbors and then fit, predict, and score your model just like LogisticRegression. For more details, see http://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html

```
In [113]: # Try out K Nearest Neighbors
          from sklearn.neighbors import KNeighborsClassifier
          #Try out KNN with hp tuning
          from sklearn.model_selection import GridSearchCV
          param_grid = [{'n_neighbors':np.arange(1,10,1)}]
          KNN_model = KNeighborsClassifier()
          grid_search = GridSearchCV(KNN_model, param_grid, cv=5, scoring='accuracy', return_train_score=False)
          grid_search.fit(X_train_all, y_train_all)
          results = pd.DataFrame(grid_search.cv_results_)
          #There's lots of data in the results dataframe - we'll just look at a few columns here, but feel free to explore
          results[["param_n_neighbors", "mean_test_score", "rank_test_score"]]

          KNN_model_opt = KNeighborsClassifier(n_neighbors = 3)
          KNN_model_opt.fit(X_train, y_train)
          predictions = KNN_model_opt.predict(X_val)
          print(pd.crosstab(y_val, predictions, rownames = ['True Class'], colnames= ['Predicted Class'] ))
          # SOLUTION
```

```
Predicted Class  Iris-setosa  Iris-versicolor  Iris-virginica
True Class
Iris-setosa                7                0               0
Iris-versicolor            0                6               0
Iris-virginica             0                0              11
```

Random Forest Classifier

Random forest is an aggregation of another type of model, decision trees. A decision tree uses a series of decisions to try to classify a sample. For example, possible decision tree logic could be:

If sepal length is less than 4.5, classify as versicolor. If sepal length is greater than 4.5, then look at petal length; if petal length is greater than 1.5, classify as setosa, otherwise classify as virginica.

In Random Forest classification, many decision trees are built on the data, and each will be different because of some randomness introduced in the tree-building process. These trees then all "vote" on the classification of an input. One benefit of random forest models is insight into feature selection, since the multiple trees can generate data about which features are most relevant to each decision.

In Scikit-Learn, use RandomForestClassifier to implement a Random Forest model. Initialize it with n_estimators, the number of trees in the forest. It is also helpful to initialize the random_state so you can reproduce your model. Fit, predict, and score work as they do for the other estimators, but you can also take a look at feature_importances_ to see which features are most important in your model. See the docs at http://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html

```
In [114]: # Try out Random Forest Classifier
          from sklearn.ensemble import RandomForestClassifier
          random_forest = RandomForestClassifier(random_state=42, n_estimators=20)
          random_forest.fit(X_train, y_train)
          predictions = random_forest.predict(X_val)
          print(pd.crosstab(y_val, predictions, rownames = ['True Class'], colnames= ['Predicted Class'] ))
          # SOLUTION
```

```
Predicted Class  Iris-setosa  Iris-versicolor  Iris-virginica
True Class
Iris-setosa                7                0               0
Iris-versicolor            0                5               1
Iris-virginica             0                1              10


/usr/local/lib/python2.7/dist-packages/sklearn/ensemble/weight_boosting.py:29: DeprecationWarning: numpy.core.umath_tests is an internal NumP
  from numpy.core.umath_tests import inner1d
```

Comparing Between Models

With three different models, all with pretty good performance, we need some way to choose the best. Because the dataset is so small, looking at the score on the validation set is very sensitive to variations in how the data was split. Cross validation will be helpful here; training and scoring the different models on different folds of the data will give us a better sense of overall performance.

GridSearchCV is written for only one model. We can get around that by writing a wrapper class that takes the model we want to use as a hyperparameter. GridSearchCV will be able to use our wrapper as long as we provide the standard API.

```
In [115]: from sklearn.base import BaseEstimator, RegressorMixin, ClassifierMixin

          class CrossValidationModelWrapper(BaseEstimator, RegressorMixin):
              """sklearn wrapper for our classifiers"""

              def __init__(self, model='LogisticRegression', n_neighbors=20, n_estimators=20, C=1, penalty='l2'):
                  self.model = model
                  self.n_neighbors = n_neighbors
                  self.n_estimators = n_estimators
                  self.C = C
                  self.penalty = penalty

              def fit(self, X, y=None):
```

```
        if (self.model == "LogisticRegression"):
            self.classifier = LogisticRegression(C=self.C, penalty=self.penalty)
        elif (self.model == "KNeighborsClassifier"):
            self.classifier = KNeighborsClassifier(n_neighbors = self.n_neighbors)
        elif (self.model == "RandomForestClassifier"):
            self.classifier = RandomForestClassifier(random_state=42, n_estimators=self.n_estimators)
        else:
            raise ValueError('Unrecognized Classifier')

        self.classifier.fit(X, y)

        return self

    def predict(self, X, y=None):
        try:
            getattr(self, "classifier")
        except AttributeError:
            raise RuntimeError("You must train classifer before predicting data!")

        return(self.classifier.predict(X))

    def score(self, X, y=None):
        return(self.classifier.score(X, y))
```

We can now use this wrapper to perform GridSearch. Customize the parameters in the parameter grid below to find the optimal sets of hyperparameters.

```
In [120]: param_grid = [{'model': ['LogisticRegression'], 'C': [0.1, 1.0, 10.0], 'penalty':['l1', 'l2'] },
                        {'model': ['KNeighborsClassifier'], 'n_neighbors': [1, 3, 5, 6, 8, 10]},
                        {'model': ['RandomForestClassifier'], 'n_estimators':[5, 10, 15, 20, 25]}]
          cv_wrapper = CrossValidationModelWrapper()
          grid_search = GridSearchCV(cv_wrapper, param_grid, cv=5, scoring='accuracy', return_train_score=False)
          grid_search.fit(X_train_all, y_train_all)
          results = pd.DataFrame(grid_search.cv_results_)
          results[["param_model", "param_n_neighbors", "param_n_estimators",
                   "param_C","param_penalty", "mean_test_score", "rank_test_score"]].fillna('-')
```

```
Out[120]:                param_model param_n_neighbors param_n_estimators param_C  \
          0       LogisticRegression                 -                  -     0.1
          1       LogisticRegression                 -                  -     0.1
          2       LogisticRegression                 -                  -       1
          3       LogisticRegression                 -                  -       1
          4       LogisticRegression                 -                  -      10
          5       LogisticRegression                 -                  -      10
          6     KNeighborsClassifier                 1                  -       -
          7     KNeighborsClassifier                 3                  -       -
          8     KNeighborsClassifier                 5                  -       -
          9     KNeighborsClassifier                 6                  -       -
          10    KNeighborsClassifier                 8                  -       -
          11    KNeighborsClassifier                10                  -       -
          12  RandomForestClassifier                 -                  5       -
          13  RandomForestClassifier                 -                 10       -
          14  RandomForestClassifier                 -                 15       -
          15  RandomForestClassifier                 -                 20       -
          16  RandomForestClassifier                 -                 25       -

             param_penalty  mean_test_score  rank_test_score
          0             l1         0.691667               17
          1             l2         0.791667               16
          2             l1         0.950000               14
          3             l2         0.950000               14
          4             l1         0.958333               10
          5             l2         0.975000                4
          6              -         0.975000                4
          7              -         0.983333                1
          8              -         0.983333                1
          9              -         0.983333                1
          10             -         0.958333               10
          11             -         0.975000                4
          12             -         0.966667                7
          13             -         0.958333               10
          14             -         0.958333               10
          15             -         0.966667                7
          16             -         0.966667                7
```

Train and test your final model!
Choose your best performing model from above and use it to predict the species of your test data.

```
In [121]: # SOLUTION
          KNN_model_opt = KNeighborsClassifier(n_neighbors = 3)
          KNN_model_opt.fit(X_train, y_train)
          predictions = KNN_model_opt.predict(X_val)
          print(pd.crosstab(y_val, predictions, rownames = ['True Class'], colnames= ['Predicted Class'] ))
```

```
Predicted Class  Iris-setosa  Iris-versicolor  Iris-virginica
True Class
Iris-setosa                7                0               0
Iris-versicolor            0                6               0
Iris-virginica             0                0              11
```

2.5 Appendix 1: Numpy

```
In [122]: def load_csv(path, loader=lambda x: open(x).read(), **kwargs):
              return loader(path, **kwargs)

          iris_text = load_csv(iris_csv_path)
```

```
In [123]: iris_text[:200]
```

```
Out[123]: 'sepal_length,sepal_width,petal_length,petal_width,class\n5.1,3.5,1.4,0.2,Iris-setosa\n4.9,3.0,1.4,0.2,Iris-setosa\n4.7,3.2,1.3,0.2
```

Obviously, this format is not going to be very easy to work with!

Our next thought might be to parse the csv into a list of lists, but using the popular library `numpy`, we can do even better. The following code loads the csv into an n-dimensional array, called an `ndarray` in numpy parlance.

This data structure is similar in principal to python's native lists, but are faster, more memory efficient, and have some handy additional features.

```
In [124]: def array_loader(path, **kwargs):
              return np.genfromtxt(path, delimiter=',', autostrip=True, **kwargs)

          iris_ndarray = load_csv(iris_csv_path, loader=array_loader, names=True, dtype=None)
```

```
/usr/local/lib/python2.7/dist-packages/ipykernel_launcher.py:2: VisibleDeprecationWarning: Reading unicode strings without specifying the enc
```

```
In [125]: iris_ndarray[:10]
```

```
Out[125]: array([(5.1, 3.5, 1.4, 0.2, 'Iris-setosa'),
                 (4.9, 3. , 1.4, 0.2, 'Iris-setosa'),
                 (4.7, 3.2, 1.3, 0.2, 'Iris-setosa'),
                 (4.6, 3.1, 1.5, 0.2, 'Iris-setosa'),
                 (5. , 3.6, 1.4, 0.2, 'Iris-setosa'),
                 (5.4, 3.9, 1.7, 0.4, 'Iris-setosa'),
                 (4.6, 3.4, 1.4, 0.3, 'Iris-setosa'),
                 (5. , 3.4, 1.5, 0.2, 'Iris-setosa'),
                 (4.4, 2.9, 1.4, 0.2, 'Iris-setosa'),
                 (4.9, 3.1, 1.5, 0.1, 'Iris-setosa')],
                dtype=[('sepal_length', '<f8'), ('sepal_width', '<f8'), ('petal_length', '<f8'), ('petal_width', '<f8'), ('class', 'S15')])
```

```
In [126]: iris_ndarray.shape
```

```
Out[126]: (150,)
```

An important point to note is that the `ndarray` is a homogenous data-structure. Since our CSV has both floats and strings, `numpy` gives us a one-dimensional array where each row is a tuple!

One solution is to encode the the classes as floats:

```
In [127]: def class_converter(flower_class):
              classes = [b'Iris-setosa', b'Iris-versicolor', b'Iris-virginica']
              return float(classes.index(flower_class))

          iris_ndarray = load_csv(iris_csv_path, loader=array_loader, skip_header=1, converters={4: class_converter})
```

```
In [128]: iris_ndarray[:10]
```

```
Out[128]: array([[5.1, 3.5, 1.4, 0.2, 0. ],
                 [4.9, 3. , 1.4, 0.2, 0. ],
                 [4.7, 3.2, 1.3, 0.2, 0. ],
                 [4.6, 3.1, 1.5, 0.2, 0. ],
                 [5. , 3.6, 1.4, 0.2, 0. ],
                 [5.4, 3.9, 1.7, 0.4, 0. ],
                 [4.6, 3.4, 1.4, 0.3, 0. ],
                 [5. , 3.4, 1.5, 0.2, 0. ],
                 [4.4, 2.9, 1.4, 0.2, 0. ],
                 [4.9, 3.1, 1.5, 0.1, 0. ]])
```

```
In [129]: iris_ndarray.shape

Out[129]: (150, 5)
```

When doing matrix operations, it is often to transpose some of the inputs. `numpy` makes this easy (compare these values to those from the first column above):

```
In [130]: iris_ndarray.transpose()[0]

Out[130]: array([5.1, 4.9, 4.7, 4.6, 5. , 5.4, 4.6, 5. , 4.4, 4.9, 5.4, 4.8, 4.8,
                 4.3, 5.8, 5.7, 5.4, 5.1, 5.7, 5.1, 5.4, 5.1, 4.6, 5.1, 4.8, 5. ,
                 5. , 5.2, 5.2, 4.7, 4.8, 5.4, 5.2, 5.5, 4.9, 5. , 5.5, 4.9, 4.4,
                 5.1, 5. , 4.5, 4.4, 5. , 5.1, 4.8, 5.1, 4.6, 5.3, 5. , 7. , 6.4,
                 6.9, 5.5, 6.5, 5.7, 6.3, 4.9, 6.6, 5.2, 5. , 5.9, 6. , 6.1, 5.6,
                 6.7, 5.6, 5.8, 6.2, 5.6, 5.9, 6.1, 6.3, 6.1, 6.4, 6.6, 6.8, 6.7,
                 6. , 5.7, 5.5, 5.5, 5.8, 6. , 5.4, 6. , 6.7, 6.3, 5.6, 5.5, 5.5,
                 6.1, 5.8, 5. , 5.6, 5.7, 5.7, 6.2, 5.1, 5.7, 6.3, 5.8, 7.1, 6.3,
                 6.5, 7.6, 4.9, 7.3, 6.7, 7.2, 6.5, 6.4, 6.8, 5.7, 5.8, 6.4, 6.5,
                 7.7, 7.7, 6. , 6.9, 5.6, 7.7, 6.3, 6.7, 7.2, 6.2, 6.1, 6.4, 7.2,
                 7.4, 7.9, 6.4, 6.3, 6.1, 7.7, 6.3, 6.4, 6. , 6.9, 6.7, 6.9, 5.8,
                 6.8, 6.7, 6.7, 6.3, 6.5, 6.2, 5.9])
```

2.6 Appendix 2: Pandas

Here's an example of leveraging data labels in order to merge two `Series` into a `DataFrame`

```
In [131]: ibm_eod_prices = [159.55, 155.88, 153.50, 153.60, 154.36, 154.06]
          ibm_dates = pd.DatetimeIndex(['2017-10-23', '2017-10-24', '2017-10-25', '2017-10-26', '2017-10-30', '2017-10-31'])
          ibm_series = pd.Series(ibm_eod_prices, index=ibm_dates)

In [132]: # mix up the dates a little
          aapl_eod_prices = [156.17, 157.10, 156.41, 163.05, 166.72, 169.04]
          aapl_dates = pd.DatetimeIndex(['2017-10-23', '2017-10-24', '2017-10-25', '2017-10-27', '2017-10-30', '2017-10-31'])
          aapl_series = pd.Series(aapl_eod_prices, index=aapl_dates)

In [133]: pd.DataFrame({'IBM': ibm_series, 'AAPL': aapl_series})

Out[133]:               AAPL     IBM
          2017-10-23  156.17  159.55
          2017-10-24  157.10  155.88
          2017-10-25  156.41  153.50
          2017-10-26     NaN  153.60
          2017-10-27  163.05     NaN
          2017-10-30  166.72  154.36
          2017-10-31  169.04  154.06
```

Often the dataframe requires some preprocessing before it's suitable in a model

```
In [134]: iris_features_copy = iris_df.drop('class', axis=1)

In [135]: iris_features_copy['sepal_interaction'] = iris_features_copy. \
              apply(lambda sample: sample['sepal_length'] * sample['sepal_width'], axis=1)

In [136]: iris_features_copy.head()

Out[136]:    sepal_length  sepal_width  petal_length  petal_width  sepal_interaction
          0           5.1          3.5           1.4          0.2              17.85
          1           4.9          3.0           1.4          0.2              14.70
          2           4.7          3.2           1.3          0.2              15.04
          3           4.6          3.1           1.5          0.2              14.26
          4           5.0          3.6           1.4          0.2              18.00
```

2.7 Appendix 3: Kernel density plot

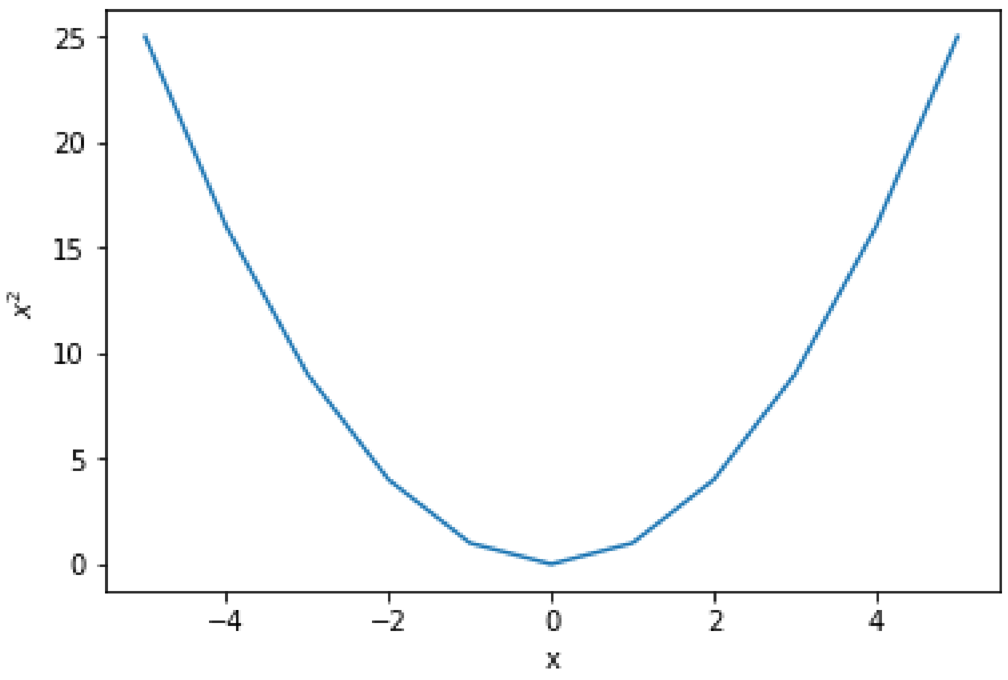
The histogram produced in the previous section was a good start. However, the shape of the histogram can be sensitive to the number of bins, so it is hard to say if this distribution is really multi-modal (i.e. multiple peaks), or if we have simply chosen an inconvenient bin size. Furthermore, for some features (like sepal length and width) the histograms overlap, so it's hard to read. An alternative way to visualize the distribution of a feature is to use a kernel density estimate, which estimates the probability density function of the feature values (using a Gaussian kernel in this case). This section covers:

- Creating a kernel density estimate of the distribution of a feature
- Creating a line plot
- Interpreting the plot

2.7.1 Line plots

Simply pass an array of x values and its corresponding y values to `plt.plot` to draw a line plot.

```
In [137]: x_values = np.linspace(-5, 5, num=11)  # array of 11 numbers, from -5 to 5, evenly spaced
          x_values

Out[137]: array([-5., -4., -3., -2., -1.,  0.,  1.,  2.,  3.,  4.,  5.])

In [138]: def square(x):
              return x ** 2

          y_values = square(x_values)
          y_values

Out[138]: array([25., 16.,  9.,  4.,  1.,  0.,  1.,  4.,  9., 16., 25.])

In [139]: plt.plot(x_values, y_values)
          plt.xlabel('x')
          plt.ylabel('$x^2$');
```



2.7.2 Kernel density

In order to plot a kernel density estimate instead of a histogram, we need to use `scipy.stats.gaussian_kde`.
This function needs:

1. the one-dimensional data whose density we want to estimate
2. the kernel width of the gaussian to apply

It returns a function that returns the estimated probability density for a given value.

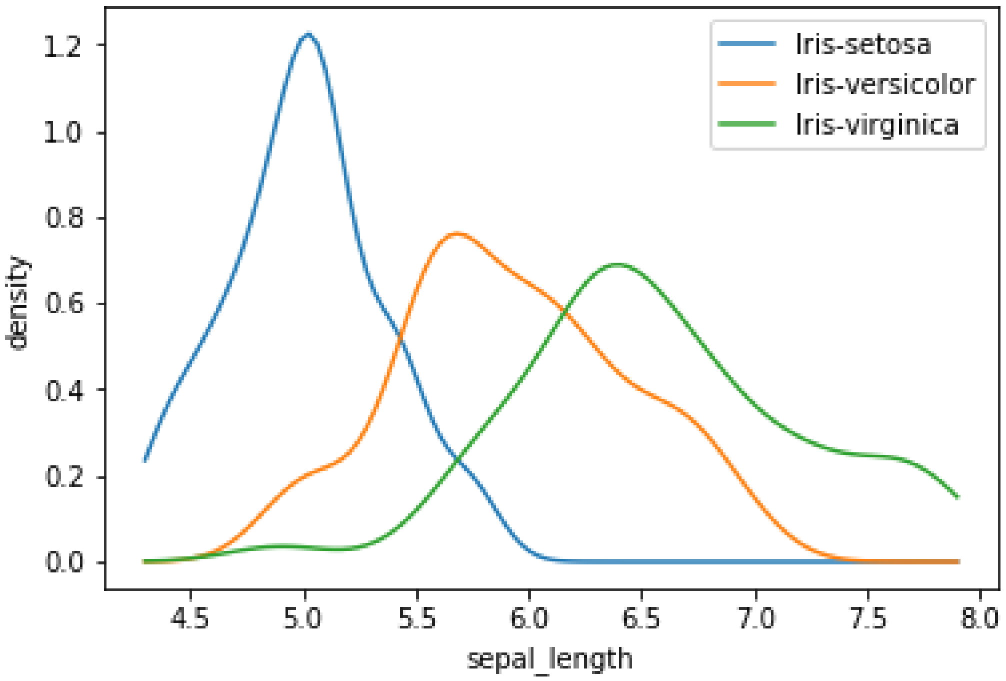
2.7.3 Exercise: Kernel density estimates separated by classes

1. Replace the `...` with code to plot the KDE (kernel density estimate) of the given `feature_name`.
2. Create a new cell to see what the density is for each feature (looping over `feature_names`):

which feature seems to be the best for discriminating species? Which is the worst?

```
In [155]: import scipy.stats as stats

          def plot_kde(input_df, feature_name, classes, plt=plt):
              # prepare the kernel density estimate parameters
              min_val = input_df[feature_name].min()
              max_val = input_df[feature_name].max()
              # perform a rough estimate for an appropriate kernel width (alternatively, accept the default)
              kernel_width = (max_val - min_val) / 10
```

```
    # generate the feature values at which to estimate the density
    x_values = np.linspace(min_val, max_val, num=100)
    plt.figure()

    # extract the data by class
    for cls in classes:
        # get the feature values corresponding to the current class
        feature_values = only_cls_feature_values(input_df, cls, feature_name)
        # perform the kernel density estimate
        kernel = stats.gaussian_kde(feature_values, bw_method=kernel_width)
        # evaluate the density at our pre-selected feature values
        density = kernel(x_values)
        # add a line plot of the density estimate to the current figure
        plt.plot(x_values, density)  # plot the density of x_values

feature_name = 'sepal_length'
plot_kde(iris_df, feature_name, classes)

# format the plot
plt.xlabel(feature_name)
plt.ylabel('density')
plt.legend(classes);
```



From these kernel density estimate plots, it seems that each class may have a different `sepal_length` distribution. Perhaps we can use `sepal_length` to help predict the correct class. At the very least, it seems like it could be used to help distinguish iris-setosa from iris-virginica: in most cases, if `sepal_length > 5.6` then the class is more likely to be iris-virginica than iris-setosa.