A First Application: Classifying Iris Species

APT 3025: APPLIED MACHINE LEARNING

Notes taken from Introduction to Machine Learning with Python by Andreas C. Müller & Sarah Guido, O'Reilley Media, 2016

Lecture Overview

- Introduction to machine learning tools
- The iris classification problem
  - Load and inspect the data
  - Choose a learning algorithm
  - Train the classifier
  - Evaluate it

Why Python?

- Python has become the language of choice for many data science applications.
- It combines the power of general-purpose programming languages with the ease of use of domain-specific scripting languages like MATLAB or R.
- Python has libraries for data loading, visualization, statistics, natural language processing, image processing, and more.
- This vast toolbox provides data scientists with a large array of general- and special-purpose functionality.

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Why Python?

- One of the main advantages of using Python is the ability to interact directly with the code, using a terminal or other tools like the Jupyter Notebook, which we'll look at shortly.
- Machine learning and data analysis are fundamentally iterative processes.
- It is essential for these processes to have tools that allow quick iteration and easy interaction.

What is scikit-learn?

- scikit-learn is an open source project, meaning that it is free to use and distribute.
- The scikit-learn project is constantly being developed and improved, and it has a very active user community. It contains a number of state-of-the-art machine learning algorithms, as well as comprehensive documentation about each algorithm.
- scikit-learn is a very popular tool, and the most prominent Python library for machine learning. It is widely used in industry and academia, and a wealth of tutorials and code snippets are available online.

Other Libraries

- In addition to scikit-learn, we will need the following libraries:
  - numpy
  - scipy
  - matplotlib
  - jupyter
  - pandas
  - pillow
- The easiest way to get all these libraries (and many more) is to install Anaconda (www.anaconda.com), a fully featured scientific computing platform.

Jupyter Notebook

- The Jupyter Notebook is an interactive environment for running code in the browser.
- It is a great tool for exploratory data analysis and is widely used by data scientists.
- While the Jupyter Notebook supports many programming languages, we only need the Python support.
- The Jupyter Notebook makes it easy to incorporate code, text, and images

Jupyter Lab

- Jupyterlab is the next generation Jupyter Notebook platform. It adds many improvements and new features, including:
  - Ability to generate a table of contents for ease of navigating the notebook
  - A visual debugger
- To lauch jupyterlab, at the command prompt type
  - jupyter lab

Numpy

- NumPy is one of the fundamental packages for scientific computing in Python.
- It contains functionality for multidimensional arrays, high-level mathematical functions such as linear algebra operations and the Fourier transform, and pseudorandom number generators.

Numpy and scikit-learn

- In scikit-learn, the NumPy array is the fundamental data structure.
- scikit-learn takes in data in the form of NumPy arrays.
- Any data you’re using will have to be converted to a NumPy array.
- The core functionality of NumPy is the ndarray class, a multidimensional (n-dimensional) array.
- All elements of the array must be of the same type.

Creating a Numpy Array

In[1]:

```
import numpy as np

x = np.array([[1, 2, 3], [4, 5, 6]])
print("x:\n{}".format(x))
```

Out[1]:

```
x:
[[1 2 3]
 [4 5 6]]
```

SciPy

- SciPy is a collection of functions for scientific computing in Python. It provides, among other functionality, advanced linear algebra routines, mathematical function optimization, signal processing, special mathematical functions, and statistical distributions.
- scikit-learn draws from SciPy's collection of functions for implementing its algorithms.

Creating Sparse Matrices Using SciPy

- The most important part of SciPy for us is scipy.sparse: this provides sparse matrices, which are another representation that is used for data in scikit-learn.
- Sparse matrices are used whenever we want to store a 2D array that contains mostly zeros:

In[2]:

```
from scipy import sparse

# Create a 2D NumPy array with a diagonal of ones, and zeros everywhere else
eye = np.eye(4)
print("NumPy array:\n{}".format(eye))
```

The Compressed Sparse Row (CSR) Format

Out[2]:

```
NumPy array:
[[ 1.  0.  0.  0.]
 [ 0.  1.  0.  0.]
 [ 0.  0.  1.  0.]
 [ 0.  0.  0.  1.]]
```

In[3]:

```
# Convert the NumPy array to a SciPy sparse matrix in CSR format
# Only the nonzero entries are stored
sparse_matrix = sparse.csr_matrix(eye)
print("\nSciPy sparse CSR matrix:\n{}".format(sparse_matrix))
```

Out[3]:

```
SciPy sparse CSR matrix:
  (0, 0)    1.0
  (1, 1)    1.0
  (2, 2)    1.0
  (3, 3)    1.0
```

The Coordinate (COO) Format

- Usually it is not possible to create dense representations of sparse data (as they would not fit into memory), so we need to create sparse representations directly.
- Here is a way to create the same sparse matrix as before, using the COO format:

In[4]:

```
data = np.ones(4)
row_indices = np.arange(4)
col_indices = np.arange(4)
eye_coo = sparse.coo_matrix((data, (row_indices, col_indices)))
print("COO representation:\n{}".format(eye_coo))
```

Out[4]:

```
COO representation:
  (0, 0)    1.0
  (1, 1)    1.0
  (2, 2)    1.0
  (3, 3)    1.0
```

matplotlib

- matplotlib is the primary scientific plotting library in Python.
- It provides functions for making publication-quality visualizations such as line charts, histograms, scatter plots, and so on.
- Visualizing your data and different aspects of your analysis can give you important insights and provide guidance on needed adjustments

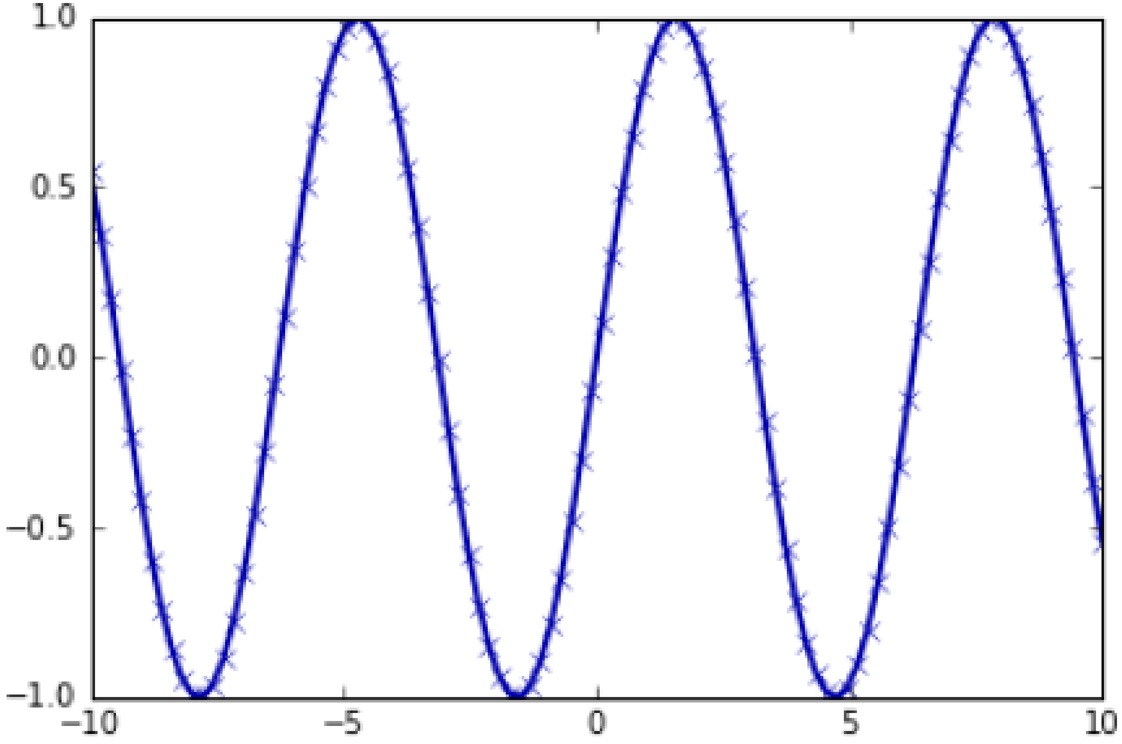
Using matplotlib

In[5]:

```
%matplotlib inline
import matplotlib.pyplot as plt

# Generate a sequence of numbers from -10 to 10 with 100 steps in between
x = np.linspace(-10, 10, 100)
# Create a second array using sine
y = np.sin(x)
# The plot function makes a line chart of one array against another
plt.plot(x, y, marker="x")
```

Output



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pandas

- pandas is a Python library for data wrangling and analysis.
- It is built around a data structure called the DataFrame, which a is a table, similar to an Excel spreadsheet.
- pandas provides methods to modify and operate on this table; in particular, it allows SQL-like queries and joins of tables.

pandas

- In contrast to NumPy, pandas allows each column to have a separate type (for example, integers, dates, floating-point numbers, and strings).
- pandas can ingest from a great variety of file formats and databases, like SQL, Excel files, and comma-separated values (CSV) files.

Using pandas

In[6]:

```
import pandas as pd
from IPython.display import display

# create a simple dataset of people
data = {'Name': ["John", "Anna", "Peter", "Linda"],
        'Location' : ["New York", "Paris", "Berlin", "London"],
        'Age' : [24, 13, 53, 33]
       }

data_pandas = pd.DataFrame(data)
# IPython.display allows "pretty printing" of dataframes
# in the Jupyter notebook
display(data_pandas)
```

	Age	Location	Name
0	24	New York	John
1	13	Paris	Anna
2	53	Berlin	Peter
3	33	London	Linda

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Querying the Table

- There are several possible ways to query the table, for example:

In[7]:

```
# Select all rows that have an age column greater than 30
display(data_pandas[data_pandas.Age > 30])
```

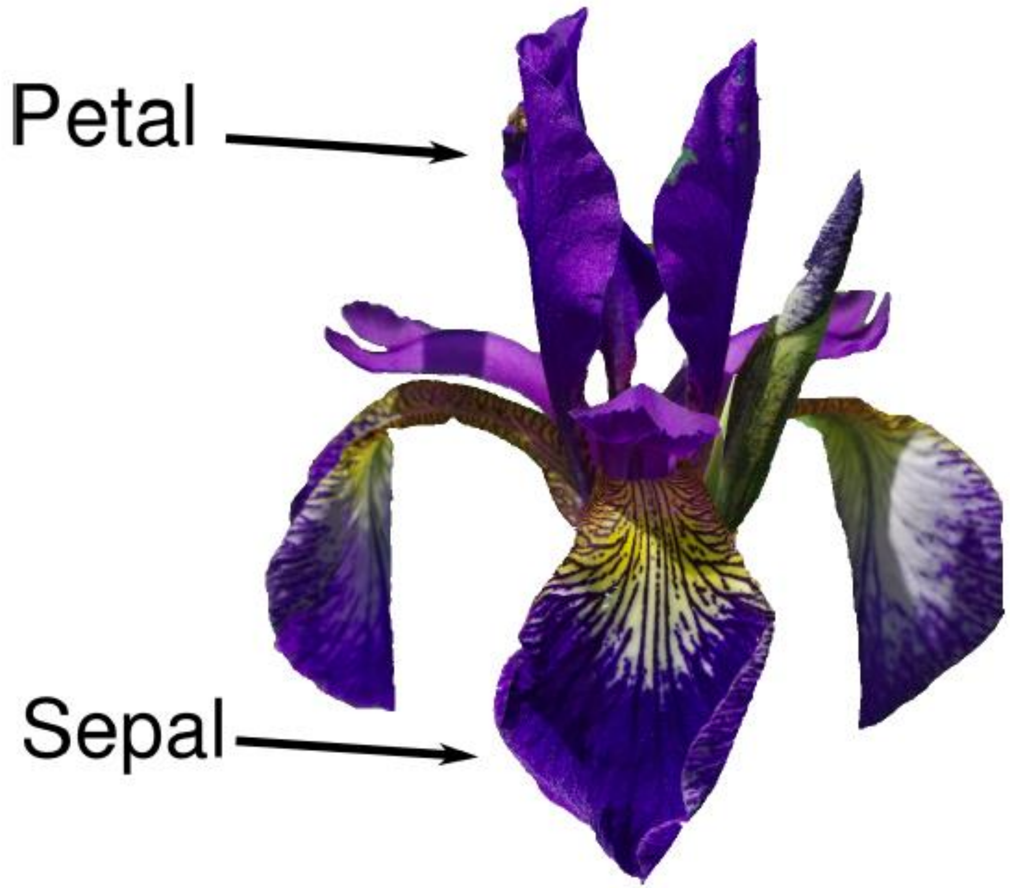
This produces the following result:

	Age	Location	Name
2	53	Berlin	Peter
3	33	London	Linda

The Iris Classification Problem

- We will go through a simple machine learning application and create our first model.
- Let's assume that a hobby botanist is interested in distinguishing the species of some iris flowers that she has found.
- She has collected some measurements associated with each iris: the length and width of the petals and the length and width of the sepals, all measured in centimeters

Parts of the Iris Flower



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A Supervised Learning Problem

- Because we have measurements for which we know the correct species of iris, this is a supervised learning problem.
- In this problem, we want to predict one of several options (the species of iris).
- This is an example of a classification problem.
- The possible outputs (different species of irises) are called classes.

Label

- Every iris in the dataset belongs to one of three classes, so this problem is a three-class classification problem.
- The desired output for a single data point (an iris) is the species of this flower.
- For a particular data point, the species it belongs to is called its label or its class.
- A data point is also called an instance or an example.

The Data

- The data we will use for this example is the Iris dataset, a well-known dataset in machine learning and statistics.
- It is included in scikit-learn in the datasets module.
- We can load it by calling the load_iris function:

In[9]:

```
from sklearn.datasets import load_iris
iris_dataset = load_iris()
```

The Bunch Object

- The iris object that is returned by load_iris is a Bunch object, which is very similar to a dictionary. It contains keys and values:

In[10]:

```
print("Keys of iris_dataset: \n{}".format(iris_dataset.keys()))
```

Out[10]:

```
Keys of iris_dataset:
dict_keys(['target_names', 'feature_names', 'DESCR', 'data', 'target'])
```

Description of the Dataset

- The value of the key DESCR is a short description of the dataset. We show the beginning of the description here:

In[11]:

```
print(iris_dataset['DESCR'][:193] + "\n...")
```

Out[11]:

```
Iris Plants Database
====================

Notes
----
Data Set Characteristics:
    :Number of Instances: 150 (50 in each of three classes)
    :Number of Attributes: 4 numeric, predictive att
...
----
```

Target Names

- The value of the key target_names is an array of strings, containing the species of flower that we want to predict:

In[12]:

```
print("Target names: {}".format(iris_dataset['target_names']))
```

Out[12]:

```
Target names: ['setosa' 'versicolor' 'virginica']
```

Feature Names

- The value of feature_names is a list of strings, giving the description of each feature:

In[13]:

```
print("Feature names: \n{}".format(iris_dataset['feature_names']))
```

Out[13]:

```
Feature names:
['sepal length (cm)', 'sepal width (cm)', 'petal length (cm)',
 'petal width (cm)']
```

Data and Target

- The data itself is contained in the target and data fields. data contains the numeric measurements of sepal length, sepal width, petal length, and petal width in a NumPy array:

In[14]:

```
print("Type of data: {}".format(type(iris_dataset['data'])))
```

Out[14]:

```
Type of data: <class 'numpy.ndarray'>
```

Rows and Columns

- The rows in the data array correspond to flowers, while the columns represent the four measurements that were taken for each flower.
- There are 150 samples (flowers) and each sample is described by four features (measurements).

In[15]:

```
print("Shape of data: {}".format(iris_dataset['data'].shape))
```

Out[15]:

```
Shape of data: (150, 4)
```

Displaying the Data

- Here are the feature values for the first five samples:

In[16]:

```
print("First five rows of data:\n{}".format(iris_dataset['data'][:5]))
```

Out[16]:

```
First five rows of data:
[[ 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]]
```

The Target Array

- The target array contains the species of each of the flowers that were measured, also as a NumPy array:

In[17]:

```
print("Type of target: {}".format(type(iris_dataset['target'])))
```

Out[17]:

```
Type of target: <class 'numpy.ndarray'>
```

Shape of Target Array

- target is a one-dimensional array with one entry per flower.

In[18]:

```
print("Shape of target: {}".format(iris_dataset['target'].shape))
```

Out[18]:

```
Shape of target: (150,)
```

Encoding of Classes

- The species (classes) are encoded as integers from 0 to 2.
- The meanings of the numbers are given by the iris['target_names'] array: 0 means setosa, 1 means versicolor, and 2 means virginica.

In[19]:

```
print("Target:\n{}".format(iris_dataset['target']))
```

Out[19]:

```
Target:
[0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 2 2]
```

Measuring Success

- We want to build a machine learning model from this data that can predict the species of iris for a new set of measurements.
- But before we can apply our model to new measurements, we need to know whether we should trust its predictions.

Generalising

- We cannot use the data we used to build the model to evaluate it.
- This is because our model can always simply remember the whole training set, and will therefore always predict the correct label for any point in the training set.
- This “remembering” does not indicate to us whether our model will generalize well (in other words, whether it will also perform well on new data)

Training and Testing Data

- To assess the model's performance, we show it new data (data that it hasn't seen before) for which we have labels.
- This is usually done by splitting the labeled data we have collected (here, our 150 flower measurements) into two parts.
- One part of the data is used to build our machine learning model, and is called the training data or training set.
- The rest of the data will be used to assess how well the model works; this is called the test data, test set, or hold-out set.

Splitting the Dataset

- scikit-learn contains a function that shuffles the dataset and splits it for you: the train_test_split function.
- This function extracts 75% of the rows in the data as the training set, together with the corresponding labels for this data.
- The remaining 25% of the data, together with the remaining labels, is declared as the test set.

Splitting the Dataset

- In scikit-learn, data is usually denoted with a capital X, while labels are denoted by a lowercase y.
- Setting the value of random_state makes it possible to repeat the experiment exactly.

In[20]:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(
    iris_dataset['data'], iris_dataset['target'], random_state=0)
```

The Shapes of the Resulting Datasets

- The output of the train_test_split function is X_train, X_test, y_train, and y_test, which are all NumPy arrays.
- X_train contains 75% of the rows of the dataset, and X_test contains the remaining 25%.
- The shape of X_train is (112, 4)
- The shape of y_train is (112,)
- The shape of X_test is (38, 4)
- The shape of y_test is (38,)

Inspecting the Data

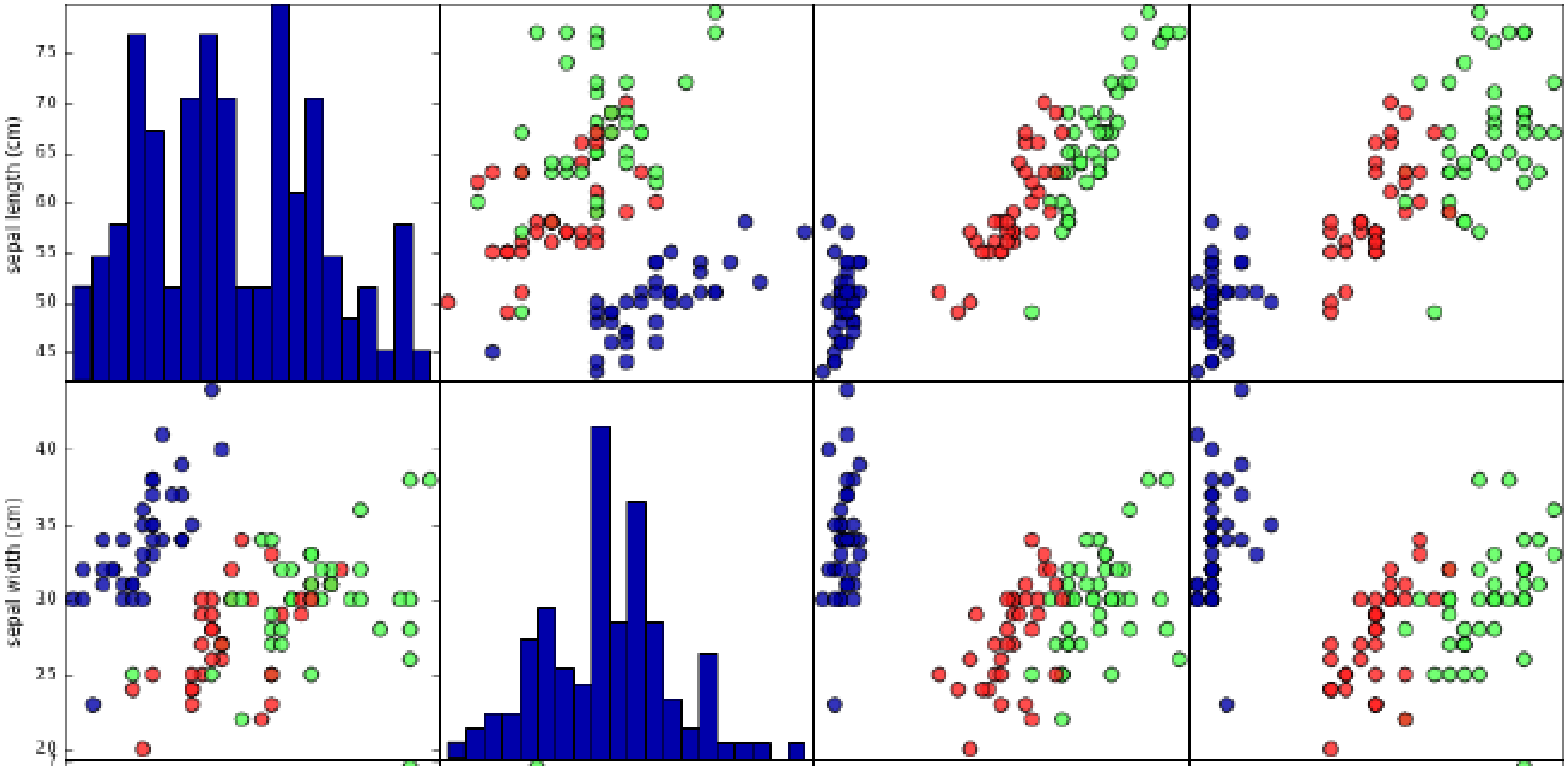
- Before building a machine learning model it is often a good idea to inspect the data, to see if the task is easily solvable without machine learning, or if the desired information might not be contained in the data.
- We can inspect the data by visualizing it.
- One form of visualization is a scatter plot.
- Since a scatter plot is only possible for two variables, we will generate several pair plots.

Using pandas to Create Visualizations

- To create the plot, we first convert the NumPy array into a pandas DataFrame. pandas has a function to create pair plots called scatter_matrix. The diagonal of this matrix is filled with histograms of each feature:

In[23]:

```
# create dataframe from data in X_train
# label the columns using the strings in iris_dataset.feature_names
iris_dataframe = pd.DataFrame(X_train, columns=iris_dataset.feature_names)
# create a scatter matrix from the dataframe, color by y_train
pd.plotting.scatter_matrix(iris_dataframe, c=y_train, figsize=(15, 15),
                           marker='o', hist_kwds={'bins': 20}, s=60,
                           alpha=.8, cmap=mglearn.cm3)
```



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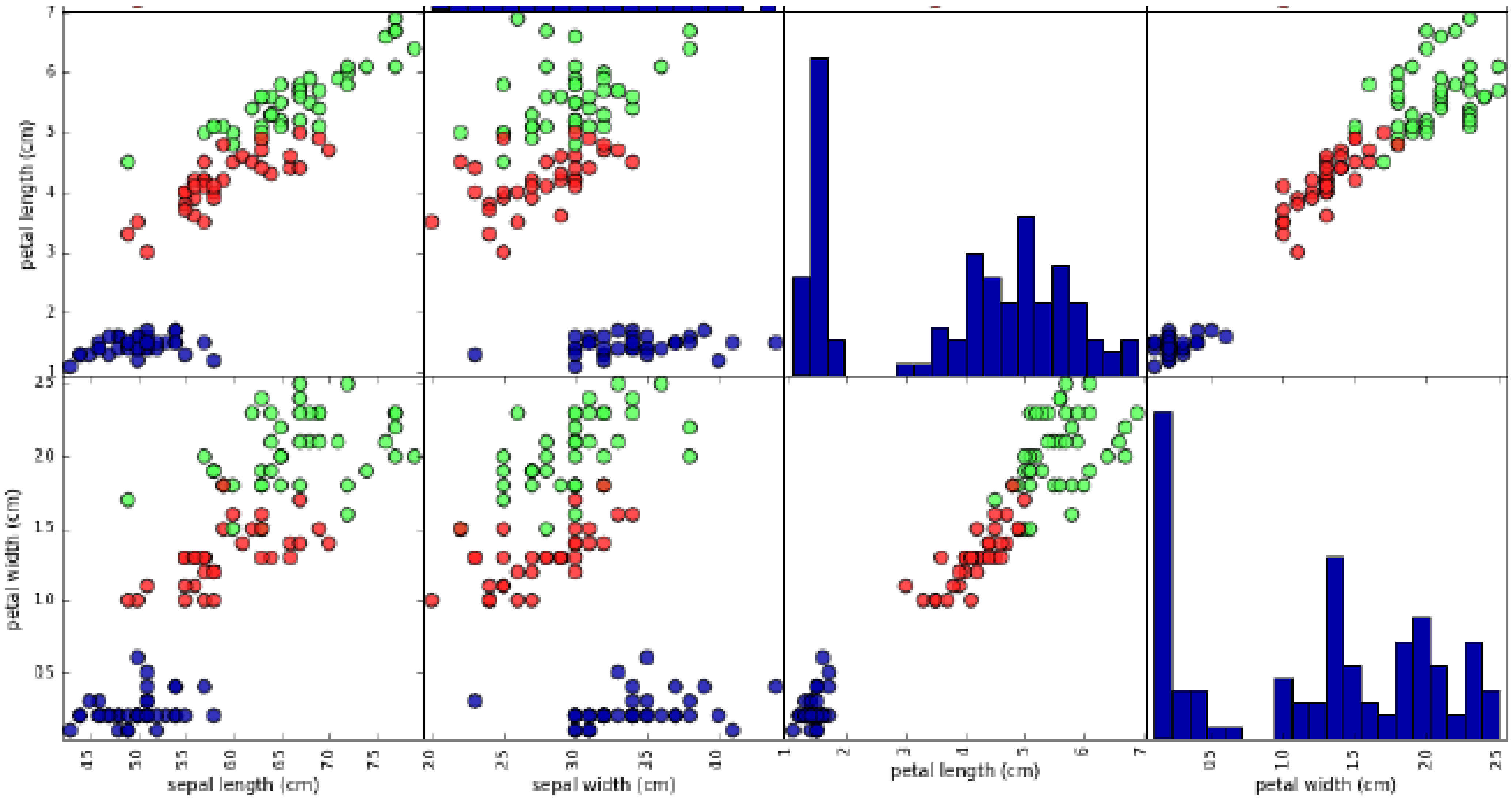

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Interpreting the Plots

- The above figure is a pair plot of the features in the training set.
- The data points are colored according to the species the iris belongs to (i.e., the class).
- To create the plot, we first convert the NumPy array into a pandas DataFrame. pandas has a function to create pair plots called scatter_matrix.
- The diagonal of this matrix is filled with histograms of each feature.
- We can see that the three classes seem to be relatively well separated using the sepal and petal measurements. This means that a machine learning model will likely be able to learn to separate them.

Building a k-Nearest Neighbors (kNN) Model

- There are many classification algorithms in scikit-learn that we could use.
- Here we will use a k-nearest neighbors classifier, which is easy to understand.
- Building this model only consists of storing the training set.
- To make a prediction for a new data point, the algorithm finds the point in the training set that is closes to the new point.
- Then it assigns the label of this training point to the new data point.

The k in kNN

- The k in k-nearest neighbors signifies that instead of using only the closest neighbor to the new data point, we can consider any fixed number k of neighbors in the training (for example, the closest three or five neighbors).
- Then, we can make a prediction using the majority class among these neighbors.
- For now we will use a single neighbour.

Implementing kNN with scikit-learn

- All machine learning models in scikit-learn are implemented in their own classes which are called Estimator classes.
- The k-nearest neighbors classification algorithm is implemented in the kNeighborsClassifier class in the neighbors module.

Implementing kNN with scikit-learn

- Before we can use the model, we need to instantiate the class into an object.
- This is when we will set any parameters of the model. The most important parameter of KNeighborsClassifier is the number of neighbors, which we will set to 1.

In[24]:

```
from sklearn.neighbors import KNeighborsClassifier
knn = KNeighborsClassifier(n_neighbors=1)
```

The Classifier Object

- The knn object encapsulates the algorithm that will be used to build the model from the training data, as well as the algorithm to make predictions on new data points.
- It will also hold the information that the algorithm has extracted from the training data.
- In the case of kNeighborsClassifier, it will just store the training set.

Building the Model

- To build the model on the training set, we call the fit method of the knn object, which takes as arguments the NumPy array X_train containing the training data and the NumPy array y_train of the corresponding training labels:

In[25]:

```
knn.fit(X_train, y_train)
```

Out[25]:

```
KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
           metric_params=None, n_jobs=1, n_neighbors=1, p=2,
           weights='uniform')
```

Parameters used in building the model

- The fit method returns the knn object itself (and modifies it in place), so we get a string representation of our classifier.
- The representation shows us which parameters were used in creating the model, including the one we set, n_neighbors=1.

Making Predictions

- We can now make predictions using this model on new data for which we might not know the correct labels.
- Imagine we found an iris in the wild with a sepal length of 5 cm, a sepal width of 2.9 cm, a petal length of 1 cm, and a petal width of 0.2 cm.
- What species of iris would this be?
- We can put this data into a NumPy array, again by calculating the shape--that is, the number of samples (1) by the number of features (4).

New Sample for Prediction

- Note that we made the measurements of this single flower into a row in a two dimensional NumPy array, as scikit-learn always expects two-dimensional arrays for the data.

In[26]:

```
X_new = np.array([[5, 2.9, 1, 0.2]])
print("X_new.shape: {}".format(X_new.shape))
```

Out[26]:

```
X_new.shape: (1, 4)
```

Making a Prediction

- To make a prediction, we can call the predict method of the knn object:

In[27]:

```
prediction = knn.predict(X_new)
print("Prediction: {}".format(prediction))
print("Predicted target name: {}".format(
       iris_dataset['target_names'][prediction]))
```

Out[27]:

```
Prediction: [0]
Predicted target name: ['setosa']
```

Evaluating the Model

- This is where the test set that we created earlier comes in.
- This data was not used to build the model, but we know what the correct species is for each iris in the test set.
- Therefore, we can make a prediction for each iris in the test data and compare it against its label (the known species).
- We can measure how well the model works by computing the accuracy, which is the fraction of flowers for which the right species was predicted.

Evaluating the Model

In[28]:

```
y_pred = knn.predict(X_test)
print("Test set predictions:\n {}".format(y_pred))
```

Out[28]:

```
Test set predictions:
 [2 1 0 2 0 2 0 1 1 1 2 1 1 1 1 0 1 1 0 0 2 1 0 0 2 0 0 1 1 0 2 1 0 2 2 1 0 2]
```

In[29]:

```
print("Test set score: {:.2f}".format(np.mean(y_pred == y_test)))
```

Out[29]:

```
Test set score: 0.97
```

Evaluating the Model

- We can also use the score method of the knn object, which will compute the test set accuracy for us:

In[30]:

```
print("Test set score: {:.2f}".format(knn.score(X_test, y_test)))
```

Out[30]:

```
Test set score: 0.97
```