01c - Introduction - scikit-learn

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1 scikit-learn

scikit-learn is the most prominent Python library for machine learning:

- Contains many state-of-the-art machine learning algorithms
- Offers comprehensive documentation about each algorithm
- Widely used, and a wealth of tutorials and code snippets are available
- scikit-learn works well with numpy, scipy, pandas, matplotlib,...

1.1 Algorithms

See the Reference

Supervised learning:

- Linear models (Ridge, Lasso, Elastic Net, ...)
- Support Vector Machines
- Tree-based methods (Classification/Regression Trees, Random Forests,...)
- Nearest neighbors
- Neural networks
- Gaussian Processes
- Feature selection

Unsupervised learning:

- Clustering (KMeans, ...)
- Matrix Decomposition (PCA, ...)
- Manifold Learning (Embeddings)
- Density estimation
- Outlier detection

Model selection and evaluation:

- Cross-validation
- Grid-search
- Lots of metrics

1.1.1 Data import

Multiple options:

- A few toy datasets are included in `sklearn.datasets`
- You can import data files (CSV) with `pandas` or `numpy`
- You can import 1000s of machine learning datasets from OpenML

1.2 Example: classification

Classify types of Iris flowers (setosa, versicolor, or virginica) based on the flower sepals and petal leave sizes. Iris image

```
In [1]: from preamble import * # Imports to make code nicer
        %matplotlib inline
        InteractiveShell.ast_node_interactivity = "all"
        HTML('''<style>html, body{overflow-y: visible !important} .CodeMirror{min-width:105% !im
```

```
Out[1]: <IPython.core.display.HTML object>
```

Note: scikitlearn will return a `Bunch` object (similar to a `dict`)

```
In [2]: from sklearn.datasets import load_iris
        iris_dataset = load_iris()

        print("Keys of iris_dataset: {}".format(iris_dataset.keys()))
        print(iris_dataset['DESCR'][:193] + "\n...")
```

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

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

The targets (classes) and features are stored as `lists`, the data as an `ndarray`

```
In [3]: print("Targets: {}".format(iris_dataset['target_names']))
        print("Features: {}".format(iris_dataset['feature_names']))
        print("Shape of data: {}".format(iris_dataset['data'].shape))
        print("First 5 rows:\n{}".format(iris_dataset['data'][:5]))
```

```
Targets: ['setosa' 'versicolor' 'virginica']
Features: ['sepal length (cm)', 'sepal width (cm)', 'petal length (cm)', 'petal width (cm)']
Shape of data: (150, 4)
```

```
First 5 rows:
[[ 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 targets are stored separately as an `ndarray`, with indices pointing to the features

```
In [4]: print("Target names: {}".format(iris_dataset['target_names']))
        print("Targets:\n{}".format(iris_dataset['target']))
```

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

1.2.1 Measuring Success: Training and testing data

To test our classifier, we need to test it on unseen data.
`train_test_split`: splits data randomly in 75% training and 25% test data.

```
In [5]: 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)
        print("X_train shape: {}".format(X_train.shape))
        print("y_train shape: {}".format(y_train.shape))
        print("X_test shape: {}".format(X_test.shape))
        print("y_test shape: {}".format(y_test.shape))
```

```
X_train shape: (112, 4)
y_train shape: (112,)
X_test shape: (38, 4)
y_test shape: (38,)
```

Note: there are several problems with this approach that we will discuss later:

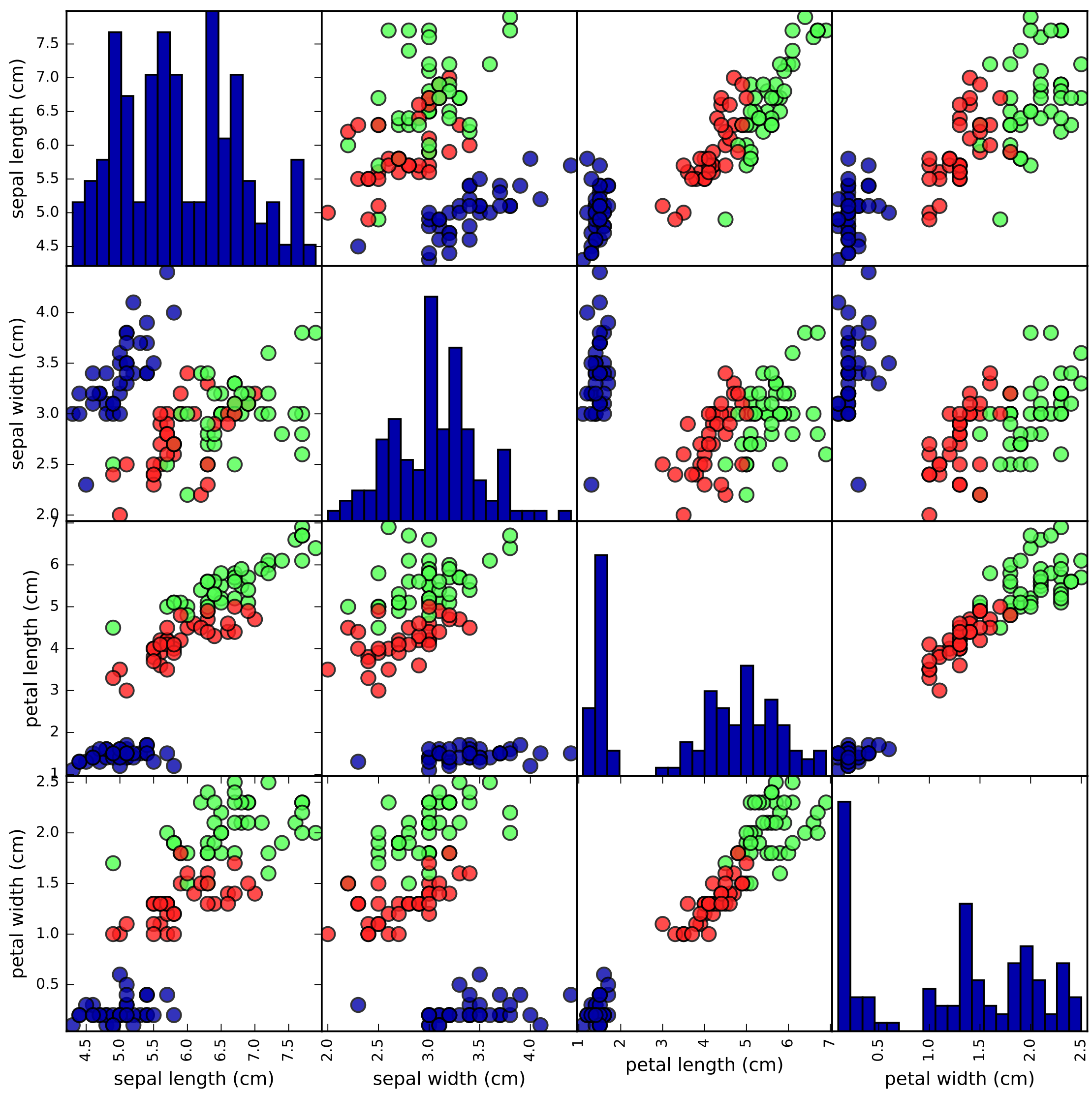
- Why 75%? Are there better ways to split?
- What if one random split yields different models than another?
- What if all examples of one class all end up in the training/test set?

1.2.2 First things first: Look at your data

Let's use pandas to visualize our data.

```
In [6]: # Build a DataFrame with training examples and feature names
        iris_df = pd.DataFrame(X_train,
                               columns=iris_dataset.feature_names)

        # scatter matrix from the dataframe, color by class
        sm = pd.scatter_matrix(iris_df, c=y_train, figsize=(10, 10),
                          marker='o', hist_kwds={'bins': 20}, s=60,
                          alpha=.8, cmap=mglearn.cm3)
```



1.2.3 Building your first model

All scikitlearn classifiers follow the same interface

```
In [ ]: class SupervisedEstimator(...):
            def __init__(self, hyperparam, ...):

            def fit(self, X, y):   # Fit/model the training data
                ...                # given data X and targets y
                return self

            def predict(self, X):  # Make predictions
                ...                # on unseen data X
                return y_pred

            def score(self, X, y): # Predict and compare to true
                ...                # labels y
                return score
```

1.2.4 K nearest nearest neighbors

- Simplest learning algorithm
- Just stores the training set (in a special data structure)
- To make a prediction for a new data point, find the k points in the training set that are closest to the new point.
- Return the class that is most prevalent among the k training points
  - Can also return a probability per class

kNN image
kNN is included in `sklearn.neighbors`, so let's build our first model

```
In [8]: from sklearn.neighbors import KNeighborsClassifier
        knn = KNeighborsClassifier(n_neighbors=1)
        knn.fit(X_train, y_train)
```

```
Out[8]: KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
                   metric_params=None, n_jobs=1, n_neighbors=1, p=2,
                   weights='uniform')
```

1.2.5 Making predictions

Let's create a new example and ask the kNN model to classify it

```
In [9]: X_new = np.array([[5, 2.9, 1, 0.2]])
        prediction = knn.predict(X_new)
        print("Prediction: {}".format(prediction))
        print("Predicted target name: {}".format(
               iris_dataset['target_names'][prediction]))
```

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

1.2.6 Evaluating the model

Feeding all test examples to the model yields all predictions

```
In [10]: y_pred = knn.predict(X_test)
         print("Test set predictions:\n {}".format(y_pred))
```

```
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]
```

We can now just count what percentage was correct

```
In [11]: print("Score: {:.2f}".format(np.mean(y_pred == y_test)))
```

```
Score: 0.97
```

The `score` function does the same thing (by default)

```
In [12]: print("Score: {:.2f}".format(knn.score(X_test, y_test)))
```

```
Score: 0.97
```

1.3 Summary

This is all you need to train and evaluate a model

```
In [13]: X_train, X_test, y_train, y_test = train_test_split(
             iris_dataset['data'], iris_dataset['target'],
             random_state=0)

         knn = KNeighborsClassifier(n_neighbors=1)
         knn.fit(X_train, y_train)

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

```
Out[13]: KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
                    metric_params=None, n_jobs=1, n_neighbors=1, p=2,
                    weights='uniform')
```

```
Score: 0.97
```

1.4 The road ahead

This is NOT how we *actually* build and evaluate machine learning models There are many more things to take into account:

- How to build optimal train/test splits?
- Is the percentage of correct predictions actually a good evaluator?
- Which other algorithms can I try to build models?
- How do we tune the hyperparameters (e.g. the k of kNN)?
- What if the data has missing values, outliers, noise,...?
- Which features can we actually use to build models?
- Will future examples be anything like our current data?

```
In [ ]:
```