Tutorial SKlearn

Joaquin Vanschoren, Mykola Pechenizkiy, Anne Driemel

In [60]:
```
# Global imports and settings

# Matplotlib
%matplotlib inline
from matplotlib import pyplot as plt
plt.rcParams["figure.figsize"] = (8, 8)
plt.rcParams["figure.max_open_warning"] = -1

# Print options
import numpy as np
np.set_printoptions(precision=3)

# Slideshow
from notebook.services.config import ConfigManager
cm = ConfigManager()
cm.update('livereveal', {'width': 1440, 'height': 768, 'scroll': True, 'theme': 'simple'})

# Silence warnings
import warnings
warnings.simplefilter(action="ignore", category=FutureWarning)
warnings.simplefilter(action="ignore", category=UserWarning)
warnings.simplefilter(action="ignore", category=RuntimeWarning)

# Helper functions
def plot_surface(clf, X, y,
                 xlim=(-10, 10), ylim=(-10, 10), n_steps=250,
                 subplot=None, show=True):
    if subplot is None:
        fig = plt.figure()
    else:
        plt.subplot(*subplot)

    xx, yy = np.meshgrid(np.linspace(xlim[0], xlim[1], n_steps),
                         np.linspace(ylim[0], ylim[1], n_steps))

    if hasattr(clf, "decision_function"):
        z = clf.decision_function(np.c_[xx.ravel(), yy.ravel()])
    else:
        z = clf.predict_proba(np.c_[xx.ravel(), yy.ravel()])[:, 1]

    z = z.reshape(xx.shape)
    plt.contourf(xx, yy, z, alpha=0.8, cmap=plt.cm.RdBu_r)
    plt.scatter(X[:, 0], X[:, 1], c=y)
    plt.xlim(*xlim)
    plt.ylim(*ylim)
```

```
        if show:
            plt.show()
```

In [3]:
```
%%javascript
Reveal.addEventListener("slidechanged", function(event){ window.location.hash = "header"; });
```

```
<IPython.core.display.Javascript object>
```

1 Machine Learning with Scikit-Learn

1.1 Scikit-Learn

- Machine learning library written in **Python**
- **Simple and efficient**, for both experts and non-experts
- Classical, **well-established machine learning algorithms**
- Shipped with documentation and examples
- Community-driven

1.2 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, . . .)
- Matric Decomposition (PCA, . . .)
- Manifold Learning (Embeddings)
- Density estimation
- Outlier detection

Model selection and evaluation:

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

2 Classification

2.1 Data

- Input data = Numpy arrays or Scipy sparse matrices ;
- Algorithms are expressed using high-level operations defined on matrices or vectors (similar to MATLAB) ;
  - Leverage efficient low-leverage implementations ;

– Keep code short and readable.

```
In [42]: # Generate data
         from sklearn.datasets import make_blobs
         X, y = make_blobs(n_samples=1000, centers=20, random_state=123)
         labels = ["b", "r"]
         y = np.take(labels, (y < 10)) # Relabels numeric values to b,r
         print(X)
         print(y[:5])
```

```
[[-6.453 -8.764]
 [ 0.29   0.147]
 [-5.184 -1.253]
 ...,
 [-0.231 -1.608]
 [-0.603  6.873]
 [ 2.284  4.874]]
['r' 'r' 'b' 'r' 'b']
```

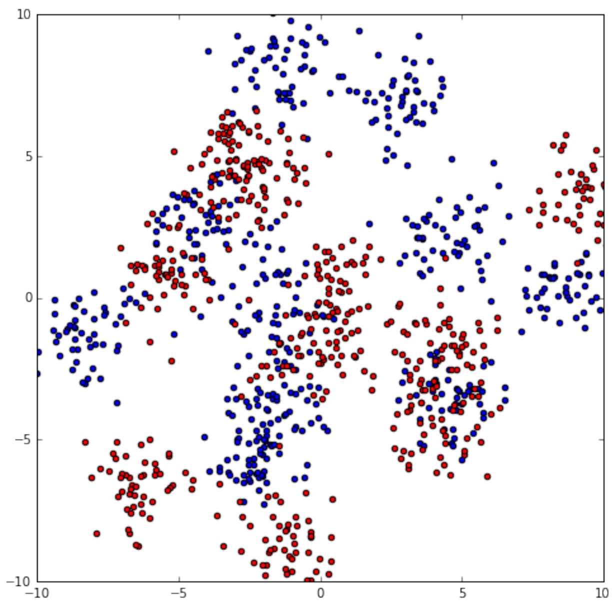
```
In [9]: # X is a 2 dimensional array, with 1000 rows and 2 columns
        print(X.shape)

        # y is a vector of 1000 elements
        print(y.shape)
```

```
(1000, 2)
(1000,)
```

```
In [10]: # Rows and columns can be accessed with lists, slices or masks
         print(X[[1, 2, 3]])     # rows 1, 2 and 3
         print(X[:5])            # 5 first rows
         print(X[500:510, 0])    # values from row 500 to row 510 at column 0
         print(X[y == "b"][:5])  # 5 first rows for which y is "b"
```

```
[[ 0.29   0.147]
 [-5.184 -1.253]
 [-4.714  3.674]]
[[-6.453 -8.764]
 [ 0.29   0.147]
 [-5.184 -1.253]
 [-4.714  3.674]
 [ 4.516 -2.881]]
[-4.438 -2.46   4.331 -7.921  1.57   0.565  4.996  4.758 -1.604  1.101]
[[-5.184 -1.253]
 [ 4.516 -2.881]
 [ 1.708  2.624]
 [-0.526  8.96 ]
 [-1.076  9.787]]
```

```
In [11]: # Plot
         plt.figure()
         for label in labels:
             mask = (y == label)
             plt.scatter(X[mask, 0], X[mask, 1], c=label)
         plt.xlim(-10, 10)
         plt.ylim(-10, 10)
         plt.show()
```



2.2 Loading external data

- Numpy provides some simple tools for loading data from files (CSV, binary, etc);
- For structured data, Pandas provides more advanced tools (CSV, JSON, Excel, HDF5, SQL, etc);
- For ROOT files, `root_numpy` provides loaders and converters to Numpy arrays.

2.3 Loading data from OpenML

- OpenML: An open machine learning collaboration platform with many datasets, models, experiments
- Register on openml.org, go to your profile to find API your key
  - Store it in a file (e.g. `.openml/apikey.txt`)
- Browse openml.org for interesting datasets, download by their ID

```
In [13]: from openml.apiconnector import APIConnector
         import pandas as pd
         import os

         home_dir = os.path.expanduser("~")
         openml_dir = os.path.join(home_dir, ".openml")
         cache_dir = os.path.join(openml_dir, "cache")
         with open(os.path.join(openml_dir, "apikey.txt"), 'r') as fh:
                 key = fh.readline().rstrip('\n')

         openml = APIConnector(cache_directory=cache_dir, apikey=key)
```

2.3.1 List ALL the datasets

```
In [15]: datasets = openml.get_dataset_list()

         data = pd.DataFrame(datasets)
```

```
print("First 10 of %s datasets..." % len(datasets))
print(data[:10][['did','name','NumberOfInstances','NumberOfFeatures']])
```

```
First 10 of 2422 datasets...
   did            name  NumberOfInstances  NumberOfFeatures
0    1          anneal                898                39
1    2          anneal                898                39
2    3        kr-vs-kp               3196                37
3    4           labor                 57                17
4    5      arrhythmia                452               280
5    6          letter              20000                17
6    7       audiology                226                70
7    8  liver-disorders                345                 7
8    9           autos                205                26
9   10           lymph                148                19
```

Subset based on any property

```
In [17]: bin_data = data.loc[data['NumberOfClasses'] == 2]
         print("First 10 of %s datasets..." % len(bin_data))
         print(bin_data[:10][['did','name', 'NumberOfInstances','NumberOfFeatures']])
```

```
First 10 of 591 datasets...
    did           name  NumberOfInstances  NumberOfFeatures
2     3       kr-vs-kp               3196                37
3     4          labor                 57                17
12   13  breast-cancer                286                10
14   15       breast-w                699                10
21   24       mushroom               8124                23
22   25          colic                368                28
24   27          colic                368                23
26   29       credit-a                690                16
28   31       credit-g               1000                21
33   37       diabetes                768                 9
```

```
In [21]: big_data = data.loc[data['NumberOfInstances'] > 60000]
         big_data = big_data.sort_values(by='NumberOfInstances', ascending=True)
         print("First 10 of %s datasets..." % len(big_data))
         print(big_data[:10][['did','name', 'NumberOfInstances']])
```

```
First 10 of 219 datasets...
       did                          name  NumberOfInstances
1289  1588                           w8a              64700
2402  4533  KEGGMetabolicReactionNetwork              65554
1292  1591                     connect-4              67557
413    554                     mnist_784              70000
1280  1578                      real-sim              72309
1050  1213                       BNG(mv)              78732
2401  4532                         higgs              98050
1067  1242                   vehicleNorm              98528
1294  1593        SensIT-Vehicle-Combined              98528
240    357                  vehicle_sensIT              98528
```

Download a specific dataset. This is done based on the dataset ID (called 'did' in the table above).

```
In [22]: dataset = openml.download_dataset(61)

         print("This is dataset '%s', the target feature is called '%s'" % (dataset.name, dataset.defaul
         print("URL: %s" % dataset.url)
         print(dataset.description[:500])
```

```
This is dataset 'iris', the target feature is called 'class'
URL: http://www.openml.org/data/download/61/dataset_61_iris.arff
**Author**: R.A. Fisher
**Source**: [UCI](https://archive.ics.uci.edu/ml/datasets/Iris) - 1936 - Donated by Michael Marshall
**Please cite**:

**Iris Plants Database**
This is perhaps the best known database to be found in the pattern recognition literature.  Fisher's pa
```

Get the actual data

```
In [27]: X, y = dataset.get_dataset(target=dataset.default_target_attribute)
         print(X[:10])
         print(y[:10])
```

```
[[ 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]
 [ 5.4  3.9  1.7  0.4]
 [ 4.6  3.4  1.4  0.3]
 [ 5.   3.4  1.5  0.2]
 [ 4.4  2.9  1.4  0.2]
 [ 4.9  3.1  1.5  0.1]]
[0 0 0 0 0 0 0 0 0 0]
```

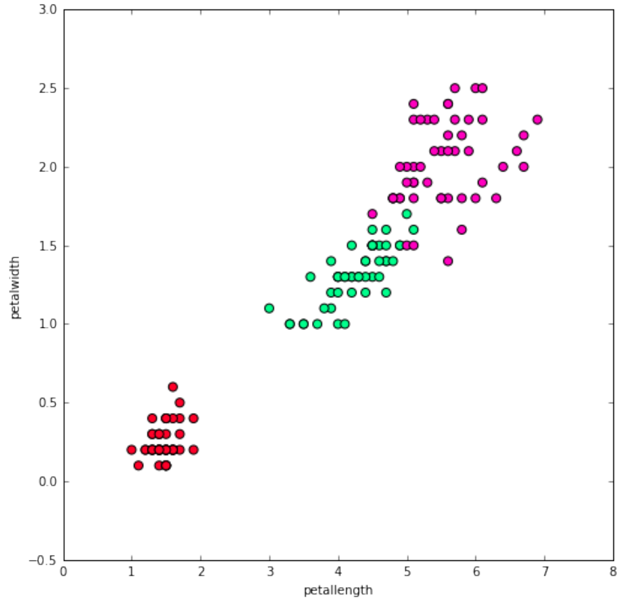
Or in a pandas dataframe:

```
In [23]: X, y, attribute_names = dataset.get_dataset(target=dataset.default_target_attribute, return_at
         iris = pd.DataFrame(X, columns=attribute_names)
         iris['class'] = y
         print(iris[:10])
```

```
sepallength  sepalwidth  petallength  petalwidth  class
0          5.1         3.5          1.4         0.2      0
1          4.9         3.0          1.4         0.2      0
2          4.7         3.2          1.3         0.2      0
3          4.6         3.1          1.5         0.2      0
4          5.0         3.6          1.4         0.2      0
5          5.4         3.9          1.7         0.4      0
6          4.6         3.4          1.4         0.3      0
7          5.0         3.4          1.5         0.2      0
8          4.4         2.9          1.4         0.2      0
9          4.9         3.1          1.5         0.1      0
```

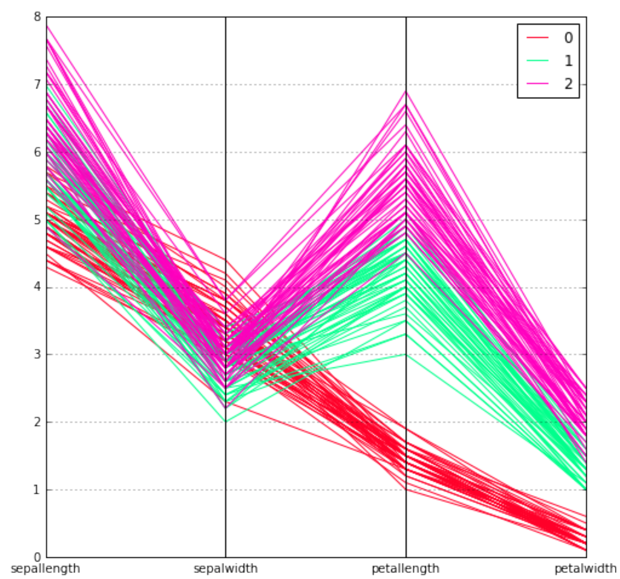
```
In [41]: iris.plot(kind='scatter', x='petallength', y='petalwidth', c='class', colormap='gist_rainbow',
```

```
Out[41]: <matplotlib.axes._subplots.AxesSubplot at 0x11bac1860>
```




```
In [40]: from pandas.tools.plotting import parallel_coordinates
         plt.figure()
         parallel_coordinates(iris, 'class', colormap='gist_rainbow')
```

```
Out[40]: <matplotlib.axes._subplots.AxesSubplot at 0x11b6be470>
```



2.4 A simple and unified API

All learning algorithms in scikit-learn share a uniform and limited API consisting of complementary interfaces:

- an `estimator` interface for building and fitting models;
- a `predictor` interface for making predictions;
- a `transformer` interface for converting data.

You can **swap or plug algorithms**

2.4.1 Estimators

```
In [ ]: class Estimator(object):
            def fit(self, X, y=None):
                """Fits estimator to data."""
                # set state of ``self``
                return self
```

```
In [52]: # Import the nearest neighbor class
         from sklearn.tree import DecisionTreeClassifier  # Change this to try
                                                          # something else

         # Set hyper-parameters, for controlling algorithm
         clf = DecisionTreeClassifier()


         # Learn a model from training data
         clf.fit(X, y)
```

```
Out[52]: DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=None,
                     max_features=None, max_leaf_nodes=None, min_samples_leaf=1,
                     min_samples_split=2, min_weight_fraction_leaf=0.0,
                     presort=False, random_state=None, splitter='best')
```

2.4.2 Predictors

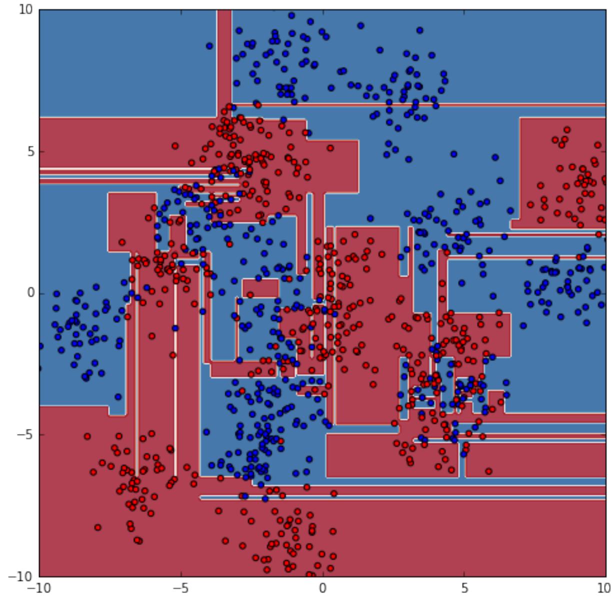
```
In [55]: # Make predictions
         print(clf.predict(X[:5]))
```

```
['r' 'r' 'b' 'r' 'b']
```

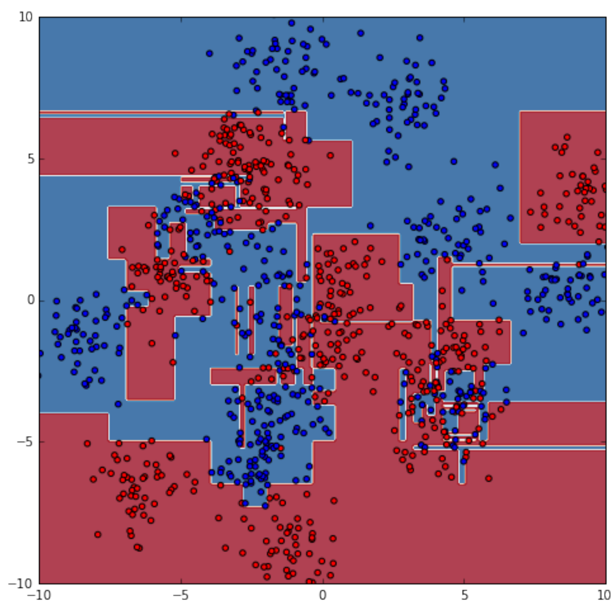
```
In [56]: # Compute (approximate) class probabilities
         print(clf.predict_proba(X[:5]))
```

```
[[ 0.  1.]
 [ 0.  1.]
 [ 1.  0.]
 [ 0.  1.]
 [ 1.  0.]]
```

```
In [57]: plot_surface(clf, X, y)
```




```
In [74]: clf = DecisionTreeClassifier(criterion='entropy', max_depth=None) # information gain
         clf.fit(X, y)
         plot_surface(clf, X, y)
```

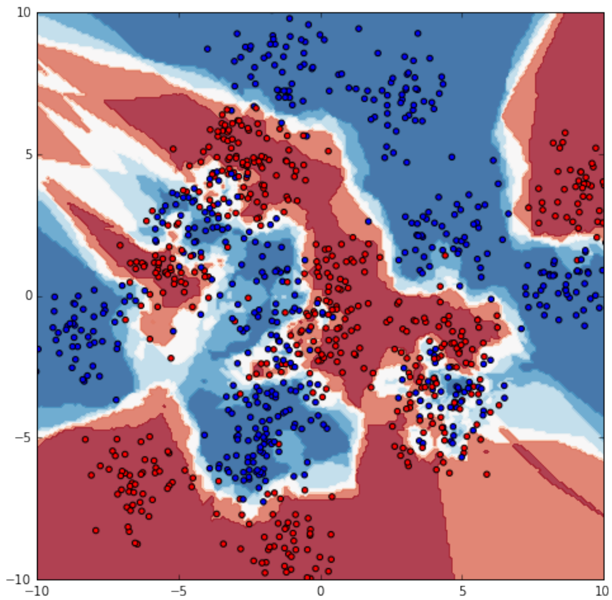


2.5 Classifier zoo

2.5.1 K-nearest neighbours

Idea: Make prediction based on target class of k nearest neighbors (vote)

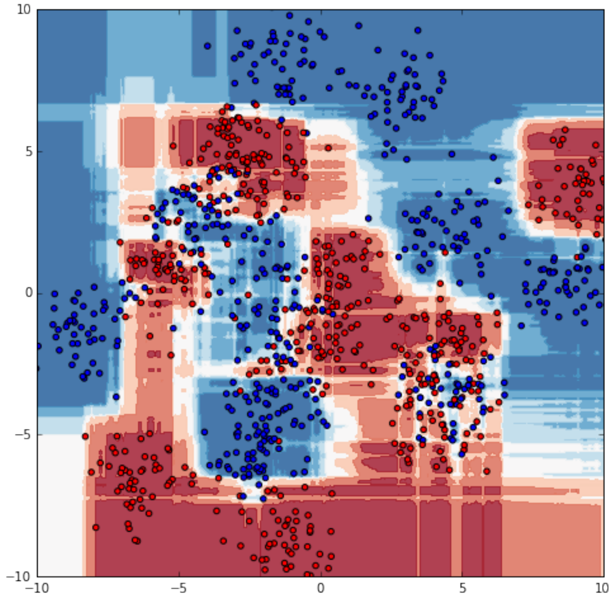
```
In [59]: from sklearn.neighbors import KNeighborsClassifier
         # Set hyper-parameters, for controlling algorithm
         clf = KNeighborsClassifier(n_neighbors=5)
         clf.fit(X, y)
         plot_surface(clf, X, y)
```



2.5.2 Random Forests

Idea: Build several decision trees with controlled randomness and average their decisions.

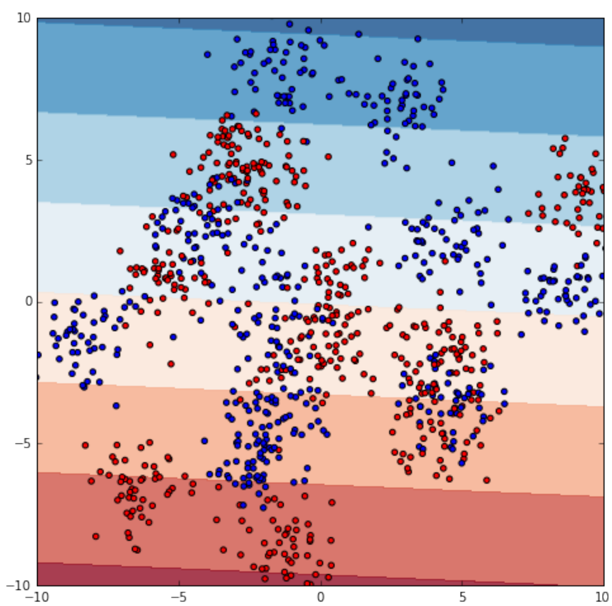
```
In [115]: from sklearn.ensemble import RandomForestClassifier
          clf = RandomForestClassifier(n_estimators=500)
          clf.fit(X, y)
          plot_surface(clf, X, y)
```



2.5.3 Support vector machines

Idea: Find the hyperplane which has the largest distance to the nearest training points of any class.

```
In [65]: from sklearn.svm import SVC
         clf = SVC(kernel="linear")  # try kernel="rbf" instead
         clf.fit(X, y)
         plot_surface(clf, X, y)
```



3 Model evaluation and selection

Meant as demonstration. Theory given in next lecture.

3.1 Training error

In [79]:
```
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import zero_one_loss
clf = DecisionTreeClassifier()
clf.fit(X, y)
print("Training error =", zero_one_loss(y, clf.predict(X)))
```

```
Training error = 0.0
```

3.2 Test error

Issue: the training error is a **biased** estimate of the generalization error.

Solution: Divide data into two disjoint parts called training and test sets (usually using 70% for training and 30% for test). - Use the training set for fitting the model; - Use the test set for evaluation only, thereby yielding an unbiased estimate. - **The same data should not be used both for training and evaluation.**

In [85]:
```
from sklearn.cross_validation import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y)
clf = DecisionTreeClassifier()
clf.fit(X_train, y_train)
print("Training error =", zero_one_loss(y_train, clf.predict(X_train)))
print("Test error =", zero_one_loss(y_test, clf.predict(X_test)))
```

```
Training error = 0.0
Test error = 0.164
```

3.3 Cross-validation

Issue: - When data is small, training on 70% of the data may lead to a model that is significantly different from a model that would have been learned on the entire set. - Yet, increasing the size of the training set (resp. decreasing the size of the test set), might lead to an inaccurate estimate of the generalization error.

Solution: K-Fold cross-validation. - Split data into K small disjoint folds. - Train on K-1 folds, evaluate the test error one the held-out fold. - Repeat for all combinations and average the K estimates of the generalization error.

In [108]:
```
from sklearn.cross_validation import KFold

scores = []

for train, test in KFold(n=len(X), n_folds=5, random_state=42):
    X_train, y_train = X[train], y[train]
    X_test, y_test = X[test], y[test]
    clf = DecisionTreeClassifier().fit(X_train, y_train)
    scores.append(zero_one_loss(y_test, clf.predict(X_test)))

print("CV error = %f +-%f" % (np.mean(scores), np.std(scores)))
```

```
CV error = 0.187000 +-0.022935
```

```
In [100]: # Shortcut
          from sklearn.cross_validation import cross_val_score
          scores = cross_val_score(DecisionTreeClassifier(), X, y,
                                   cv=KFold(n=len(X), n_folds=5, random_state=42),
                                   scoring="accuracy")
          print("CV error = %f +-%f" % (1. - np.mean(scores), np.std(scores)))
```

```
CV error = 0.185000 +-0.020000
```

3.4 Metrics

3.4.1 Default score

Estimators come with a built-in default evaluation score * Accuracy for classification * R2 score for regression

```
In [101]: y_train = (y_train == "r")
          y_test = (y_test == "r")
          clf = KNeighborsClassifier(n_neighbors=5)
          clf.fit(X_train, y_train)
          print("Default score =", clf.score(X_test, y_test))
```

```
Default score = 0.84
```

3.4.2 Accuracy

Definition: The accuracy is the proportion of correct predictions.

```
In [102]: from sklearn.metrics import accuracy_score
          print("Accuracy =", accuracy_score(y_test, clf.predict(X_test)))
```

```
Accuracy = 0.84
```

3.4.3 Precision, recall and F-measure

$$Precision = \frac{TP}{TP + FP}$$

$$Recall = \frac{TP}{TP + FN}$$

$$F = \frac{2 * Precision * Recall}{Precision + Recall}$$

```
In [103]: from sklearn.metrics import precision_score
          from sklearn.metrics import recall_score
          from sklearn.metrics import fbeta_score
          print("Precision =", precision_score(y_test, clf.predict(X_test)))
          print("Recall =", recall_score(y_test, clf.predict(X_test)))
          print("F =", fbeta_score(y_test, clf.predict(X_test), beta=1))
```

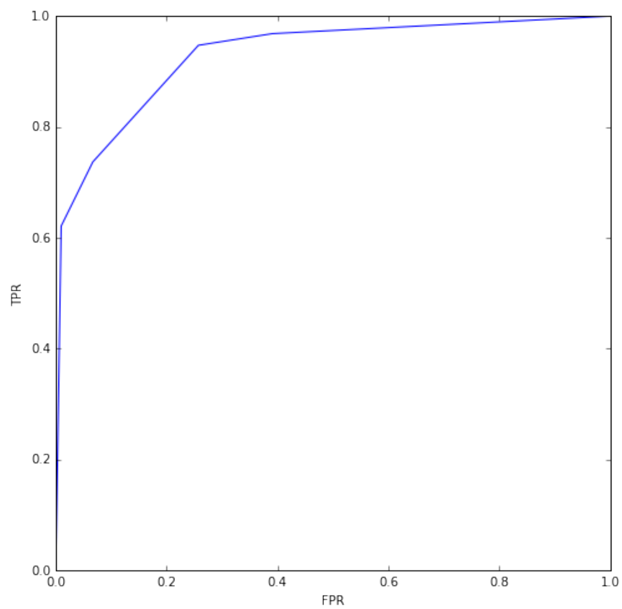
```
Precision = 0.811881188119
Recall = 0.863157894737
F = 0.836734693878
```

3.4.4 ROC AUC

Definition: Area under the curve of the false positive rate (FPR) against the true positive rate (TPR) as the decision threshold of the classifier is varied.

```
In [104]: from sklearn.metrics import get_scorer
          roc_auc_scorer = get_scorer("roc_auc")
          print("ROC AUC =", roc_auc_scorer(clf, X_test, y_test))

          from sklearn.metrics import roc_curve
          fpr, tpr, thresholds = roc_curve(y_test, clf.predict_proba(X_test)[:, 1])
          plt.plot(fpr, tpr)
          plt.xlabel("FPR")
          plt.ylabel("TPR")
          plt.show()
```

```
ROC AUC = 0.92977443609
```



3.4.5 Confusion matrix

Definition: number of samples of class i predicted as class j.

```
In [105]: from sklearn.metrics import confusion_matrix
          confusion_matrix(y_test, clf.predict(X_test))
```

```
Out[105]: array([[86, 19],
                 [13, 82]])
```

4 Transformers, pipelines and feature unions

4.1 Transformers

- Classification (or regression) is often only one or the last step of a long and complicated process;

- In most cases, input data needs to be cleaned, massaged or extended before being fed to a learning algorithm;
- For this purpose, Scikit-Learn provides the `transformer` API.

```
In [ ]: class Transformer(object):
            def fit(self, X, y=None):
                """Fits estimator to data."""
                # set state of ``self``
                return self

            def transform(self, X):
                """Transform X into Xt."""
                # transform X in some way to produce Xt
                return Xt

            # Shortcut
            def fit_transform(self, X, y=None):
                self.fit(X, y)
                Xt = self.transform(X)
                return Xt
```

4.2 Pipelines

Transformers can be chained in sequence to form a pipeline.

```
In [130]: from sklearn.pipeline import make_pipeline
          from sklearn.feature_selection import SelectKBest, f_classif

          # Get more complex data
          dataset = openml.download_dataset(337)
          X, y = dataset.get_dataset(target=dataset.default_target_attribute)
          X_train, X_test, y_train, y_test = train_test_split(X, y)

          # Chain transformers + a classifier to build a new classifier
          clf = make_pipeline(SelectKBest(score_func=f_classif, k=44),
                              RandomForestClassifier())
          clf.fit(X_train, y_train)
          print(clf.predict_proba(X_test)[:5])
```

```
[[ 0.5  0.5]
 [ 0.   1. ]
 [ 0.6  0.4]
 [ 0.4  0.6]
 [ 0.2  0.8]]
```

4.3 Optimizing parameters

Search for the best hyperparameter settings

```
In [131]: # Hyper-parameters can be accessed using step names
          print("K =", clf.get_params()["selectkbest__k"])
```

```
K = 44
```

```
In [134]: from sklearn.grid_search import GridSearchCV
          grid = GridSearchCV(clf,
```

```
                            param_grid={"selectkbest__k": [1, 10, 20, 30, 40],
                                        "randomforestclassifier__max_features": [0.1, 0.25, 0.5]})
        grid.fit(X_train, y_train)

        print("Best params =", grid.best_params_)
```

```
Best params = {'selectkbest__k': 30, 'randomforestclassifier__max_features': 0.25}
```

5 Summary

- Scikit-Learn provides essential tools for machine learning.
- It is more than training classifiers!
- It integrates within a larger Python scientific ecosystem.
- Try it for yourself!

```
In [ ]: questions?
```

5.1 Acknowledgements

Based on a tutorial by Gilles Loupe

```
In [ ]:
```