Scikit-Learn: Machine Learning in Python

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Machine Learning

Python Scientific Lecture Notes

- **Python**
  Widely used programming language for Machine Learning
- **NumPy**, **SciPy**, **Matplotlib**
  Scientific computing libraries in Python
- **Scikit-learn**
  Machine Learning library in Python (based on the above ones)

Basics of Python and scientific computing

- `http://scipy-lectures.github.io/`

Download and install Scikit-learn

Requires:

- Python ($\geq$2.6 or $\geq$3.3)
- NumPy ($\geq$ 1.6.1)
- SciPy ($\geq$ 0.9)

`http://scikit-learn.org/stable/install.html`

Documentation and Reference

Documentation

`http://scikit-learn.org/stable/documentation.html`

Reference Manual with class descriptions

`http://scikit-learn.org/stable/modules/classes.html`

Outline

Today's lecture will cover:

- Load and generate datasets
- Split a dataset for cross-validation
- Use some learning algorithms
  - Naive Bayes
  - SVM
  - Random forest
- Evalute the performance of the algorithms
  - Accuracy
  - F1-score
  - AUC ROC

Datasets

- Load and fetch popular reference datasets (e.g. Iris)

```
# load a default dataset
from sklearn import datasets
iris = datasets.load_iris()
```

http://scikit-learn.org/stable/modules/generated/sklearn.datasets.load_iris.html

- Artificial data generators (e.g. binary classification)

```
dataset = datasets.make_classification(n_samples=1000, n_features=10,
            n_informative=2, n_redundant=2, n_repeated=0, n_classes=2)
```

http://scikit-learn.org/stable/modules/generated/sklearn.datasets.make_classification.html

- Inspect the data structures

```
# dataset description
print iris.DESCR
# data examples (features)
print iris.data
# data target labels (classes)
print iris.target
```

Cross-validation

k-fold cross-validation

- Split the dataset D in k equally sized disjoint subsets D_i
- For $i \in [1, k]$
  - Train the predictor on $T_i = D \setminus D_i$
  - Compute the score of the predictor on the test set D_i
- Return the average score across the folds

Cross-validation

- We can use Scikit-learn for K-fold cross-validation:

```
from sklearn import cross_validation
kf = cross_validation.KFold(len(iris.data), n_folds=5, shuffle=True)
for train_index, test_index in kf:
    X_train, y_train = iris.data[train_index], iris.target[train_index]
    X_test, y_test   = iris.data[test_index],  iris.target[test_index]
```

http://scikit-learn.org/stable/modules/generated/sklearn.model_selection.KFold.html

- Inspect the structures:

```
print X_train
print y_train
print X_test
print y_test
```

Naive Bayes

Reminder

- Attribute values are assumed to be independent with each other

$$P(a_1, \ldots, a_m | y_i) = \prod_{j=1}^{m} P(a_j | y_i)$$

- Definition

$$y^* = \text{argmax}_{y_i} \prod_{j=1}^{m} P(a_j | y_i) P(y_i)$$

Naive Bayes

- Scikit-learn implements several naive Bayes algorithms
- e.g. Gaussian naive Bayes

```
# Naive Bayes
from sklearn.naive_bayes import GaussianNB
clf = GaussianNB()
clf.fit(X_train, y_train)
pred = clf.predict(X_test)
```

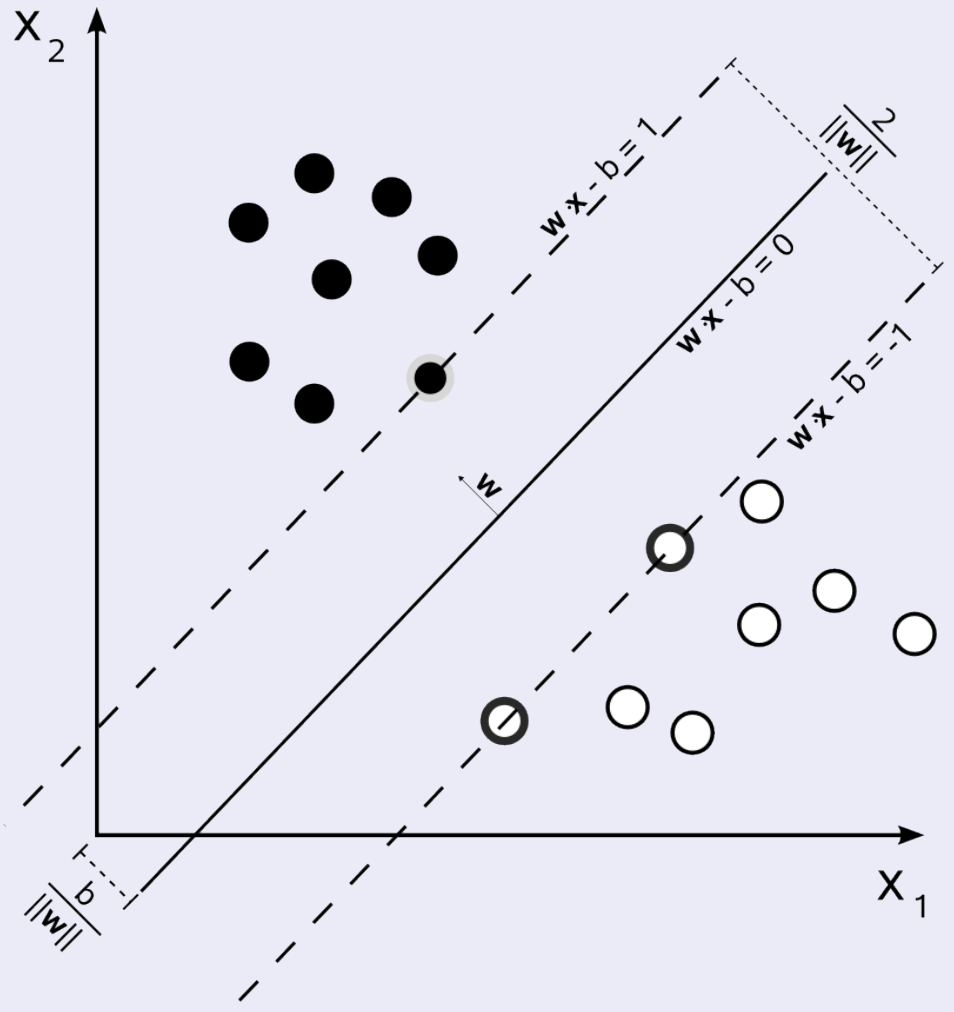
http://scikit-learn.org/stable/modules/generated/sklearn.naive_bayes.GaussianNB.html

- Inspect the data structures:

```
print pred
print y_test
```

SVM

Reminder



SVM

- Scikit-learn also includes Support Vector Machine algorithms
- e.g. Support-C Vector Classification

```
#SVM
from sklearn.svm import SVC
clf = SVC(C=1e-01, kernel='rbf', gamma=0.1)
clf.fit(X_train, y_train)
pred = clf.predict(X_test)
```

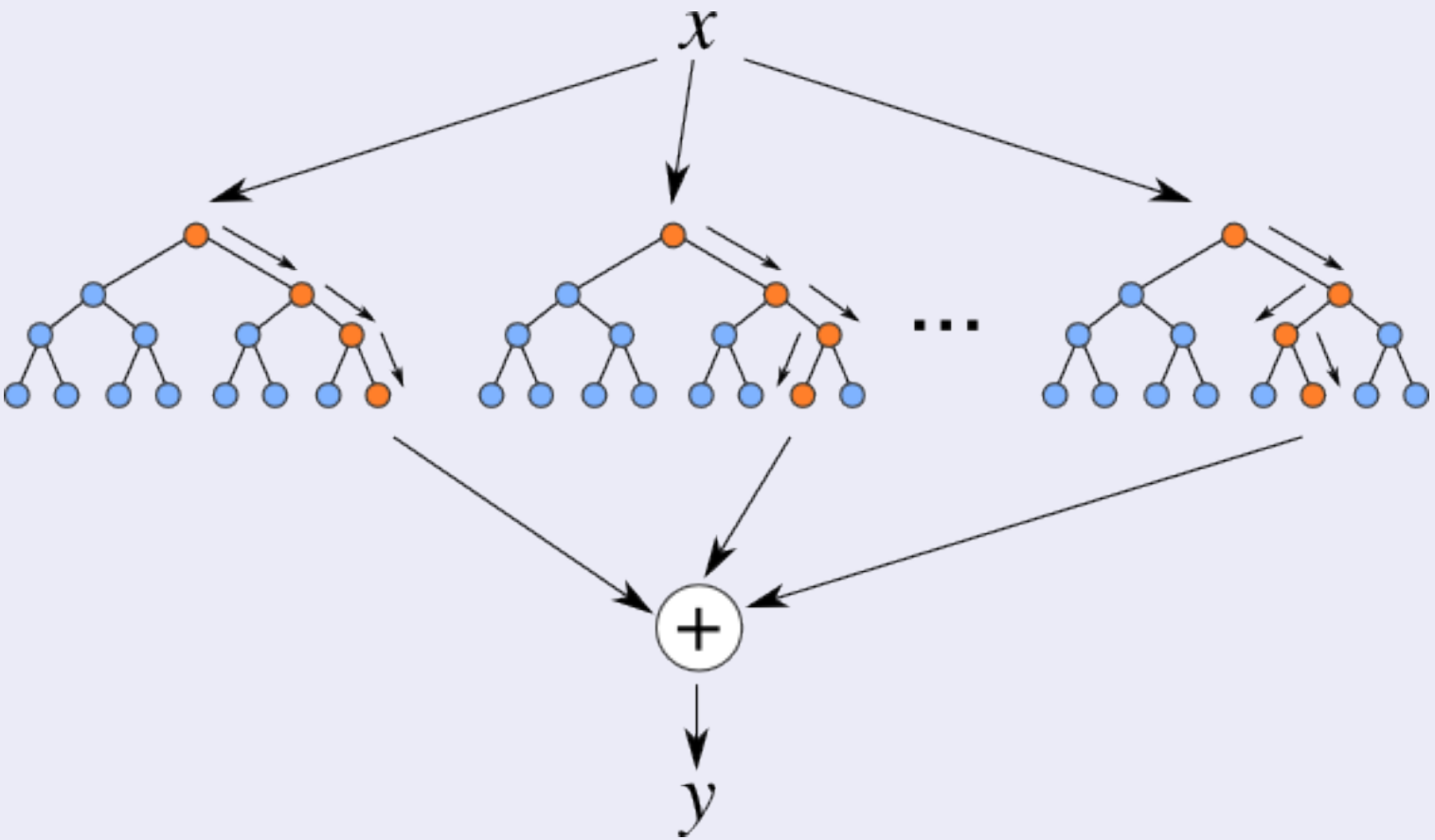
http://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html

- Inspect the data structures:

```
print pred
print y_test
```

Random Forest

Reminder



Random Forest

- Scikit-learn includes ensemble-based methods for classification
- e.g. Random Forest Classifier

```
# Random Forest
from sklearn.ensemble import RandomForestClassifier
clf = RandomForestClassifier(n_estimators=6)
clf.fit(X_train, y_train)
pred = clf.predict(X_test)
```

http://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html

- Inspect the data structures:

```
print pred
print y_test
```

Performance evaluation

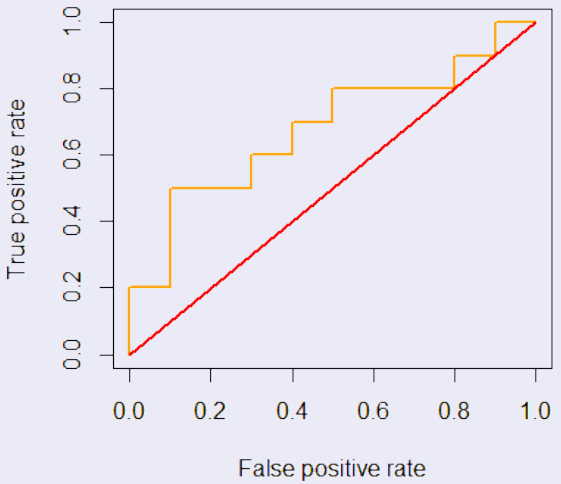
Reminder

$$Acc = \frac{TP + TN}{TP + TN + FP + FN}$$

$$Pre = \frac{TP}{TP + FP} \qquad Rec = \frac{TP}{TP + FN}$$

$$F_1 = \frac{2 \cdot Pre \cdot Rec}{Pre + Rec}$$

AUC ROC



Performance evaluation

- The `sklearn.metrics` module includes score functions, performance metrics, pairwise metrics and distance measures.
- e.g. Accuracy, F1-score, AUC ROC:

```
from sklearn import metrics
acc = metrics.accuracy_score(y_test, pred)
print acc
f1 = metrics.f1_score(y_test, pred)
print f1
auc = metrics.roc_auc_score(y_test, pred)
print auc
```

http://scikit-learn.org/stable/modules/generated/sklearn.metrics.accuracy_score.html
http://scikit-learn.org/stable/modules/generated/sklearn.metrics.f1_score.html
http://scikit-learn.org/stable/modules/generated/sklearn.metrics.auc.html

Choosing parameters

- Some algorithms have parameters
- e.g. parameter C for SVM, number of trees for Random Forest
- Performance can vary according to the chosen parameters
- It is important to choose wisely
- You have to separate the sets for selecting the parameters and the ones for testing the model!

Choosing parameters e.g. SVM

`np.argmax` requires: `import numpy as np`

```
# SVM with rbf kernel
# 10-fold cross validation
kf = cross_validation.KFold(n, n_folds=10, shuffle=True, random_state=1234)
accuracy = []
f1 = []
auc_roc = []
for train_index, test_index in kf:
    X_train, X_test = dataset[0][train_index], dataset[0][test_index]
    y_train, y_test = dataset[1][train_index], dataset[1][test_index]
    nn = len(X_train)
    bestC = None
    Cvalues = [1e-2,1e-1,1e0,1e1,1e2]
    innerscore = []
    for C in Cvalues:
        # inner 5-fold cross validation on the original training set for parameter selection (C)
        ikf = cross_validation.KFold(nn, n_folds=5, shuffle=True, random_state=5678)
        innerf1 = []
        for t_index, v_index in ikf:
            X_t, X_v = X_train[t_index], X_train[v_index]
            y_t, y_v = y_train[t_index], y_train[v_index]

            ipred = rbf_svm(X_t,y_t,X_v,C)
            # save the F1-score of the inner cross validation
            innerf1.append(metrics.f1_score(y_v,ipred))
        # compute the average
        innerscore.append(sum(innerf1)/len(innerf1))
    # pick the C that gives best F1-score
    # Note: the test set is never involved in the decision of the parameter
    bestC = Cvalues[np.argmax(innerscore)]
    # predict the labels for the test set usign the best C parameter
    pred = rbf_svm(X_train,y_train,X_test,bestC)
    accuracy.append(metrics.accuracy_score(y_test,pred))
    f1.append(metrics.f1_score(y_test, pred))
    auc_roc.append(metrics.roc_auc_score(y_test,pred))
```

```
# SVM with RBF kernel
def rbf_svm(X_train, y_train, X_test, C):
    clf = SVC(C=C, kernel='rbf', class_weight='auto')
    clf.fit(X_train,y_train)
    return clf.predict(X_test)
```

Summary

Scikit-learn allows to:

- Load and generate datasets
- Split them to perform cross-validation
- Easily apply learning algorithms
- Evaluate the performace of such algorithms

Assignment

In the second ML assignment you have to compare the performance of three different classification algorithms, namely Naive Bayes, SVM, and Random Forest.
For this assignment you need to generate a random binary classification problem, and then train and test (using 10-fold cross validation) the three algorithms. For some algorithms inner cross validation (5-fold) for choosing the parameters is needed. Then, show the classification performace (per-fold and averaged) in the report, and briefly discussing the results.

Note

The report has to contain also a short description of the methodology used to obtain the results.

Assignment

Steps

1. Create a classification dataset (n_samples $\geq$ 1000, n_features $\geq$ 10)
2. Split the dataset using 10-fold cross validation
3. Train the algorithms
   - GaussianNB
   - SVC (possible C values [1e-02, 1e-01, 1e00, 1e01, 1e02], RBF kernel)
   - RandomForestClassifier (possible n_estimators values [10, 100, 1000])
4. Evaluate the cross-validated performance
   - Accuracy
   - F1-score
   - AUC ROC
5. Write a short report summarizing the methodology and the results

Assignment

- After completing the assignment submit it via email
- Send an email to paolo.dragone@unitn.it (cc: passerini@disi.unitn.it)
- Subject: sklearnSubmit2016
- Attachment: id_name_surname.zip containing:
  - The Python code
  - The report (PDF format)

NOTE

- No group work
- This assignment is mandatory in order to enroll to the oral exam