Python's Scikit-learn

Nicolás García-Pedrajas

Computational Intelligence and Bioinformatics Research Group

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Table of contents

Scikit-learn

What is Scikit-Learn?

Extensions to SciPy (Scientific Python) are called SciKits. SciKit-Learn provides machine learning algorithms:

- Algorithms for supervised & unsupervised learning
- Built on SciPy and Numpy
- Standard Python API interface
- Sits on top of c libraries, LAPACK, LibSVM, and Cython
- Open Source: BSD License (part of Linux)

Probably the best general ML framework out there.

Scikit-learn

Where did it come from?

Started as a Google summer of code project in 2007 by David Cournapeau, then used as a thesis project by Matthieu Brucher.
In 2010, INRIA pushed the first public release, and sponsors the project, as do Google, Tinyclues, and the Python Software Foundation.

Scikit-learn

Primary features

- Generalized Linear Models
- SVMs, kNN, Bayes, Decision Trees, Ensembles
- Clustering and Density algorithms
- Cross Validation
- Grid Search
- Pipelining
- Model Evaluations
- Dataset Transformations
- Dataset Loading

Scikit-learn

API

Object-oriented interface centered around the concept of an Estimator:

> *An estimator is any object that learns from data; it may be a classification, regression or clustering algorithm or a transformer that extracts/filters useful features from raw data.*
>
> Scikit-Learn Tutorial

Scikit-learn

Estimator class

Class definition

```
class Estimator(object):

        def fit(self, X, y=None):
                """Fits estimator to data. """
                # set state of ``self``
                return self

        def predict(self, X):
                """Predict response of ``X``. """
                # compute predictions ``pred``
                return pred
```

Scikit-learn

Estimator

Estimators

- fit(X,y) sets the state of the estimator.
- X is usually a 2D numpy array of shape (num_samples, num_features).
- y is a 1D array with shape (n_samples,)
- predict(X) returns the class or value
- predict_proba() returns a 2D array of shape (n_samples, n_classes)

Example:

Estimator (SVM)

```
1 from sklearn import svm
2
3 estimator = svm.SVC(gamma=0.001)
4 estimator.fit(X, y)
5 estimator.predict(x)
```

Scikit-learn

Load and transform data

Load data using appropriate methods.
Transform data:

Transformers

```
class Transformer(Estimator):
        def transform(self, X):
                """Transforms the input data. """
                # transform ``X`` to ``X_prime``
                return X_prime

from sklearn import preprocessing

Xt = preprocessing.normalize(X) # Normalizer
Xt = preprocessing.scale(X)

# StandardScaler: Imputation of missing values
imputer = Imputer(missing_values='Nan', strategy='mean')

Xt = imputer.fit_transform(X)
```

Scikit-learn

Classification models

Scikit-learn includes the following models:

- Generalized linear models.
- Linear an quadratic discriminant analysis
- Support vector machines.
- Nearest neighbors.
- Decision trees.
- Naive Bayes.
- Ensemble methods.
- Neural networks (deep learning with Keras)
- Multi-class methods.

Decision trees

First step: import required libraries.

Libraries

```
# Load libraries
import pandas as pd
from sklearn.tree import DecisionTreeClassifier # Import Decision Tree Classifier
from sklearn.model_selection import train_test_split # Import train_test_split function
from sklearn import metrics #Import scikit-learn metrics module for accuracy calculation
```

Decision trees

Second step: load data.

Load data

```
# load dataset
col_names = ['pregnant', 'glucose', 'bp', 'skin', 'insulin', 'bmi',
↪  'pedigree', 'age', 'label']
pima = pd.read_csv("pima-indians-diabetes.csv", header=None,
↪  names=col_names)

# split dataset in features and target variable
feature_cols = ['pregnant', 'glucose', 'bp', 'skin', 'insulin', 'bmi',
↪  'pedigree', 'age']
X = pima[feature_cols] # Features
y = pima.label # Target variable
```

Decision trees

Data partitioning

We can split the data randomly (random partition, problem for reproduction):

Random partition

```
 # Split dataset into training set and test set
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
↪  random_state=1) # 70% training and 30% test
```

Or we can have two separate files:

Separate files

```
# Load dataset
col_names = ['pregnant', 'glucose', 'bp', 'skin', 'insulin', 'bmi',
↪  'pedigree', 'age', 'label']
pima_train = pd.read_csv("pima-indians-diabetes.train.csv", header=None,
↪  names=col_names)
pima_test = pd.read_csv("pima-indians-diabetes.test.csv", header=None,
↪  names=col_names)
```

Decision tree

Building model

The procedure is common for all classification models.

Building decision tree

```
# Create Decision Tree classifer object
clf = DecisionTreeClassifier()

# Train Decision Tree Classifer
clf = clf.fit(X_train,y_train)

# Predict the response for test dataset
y_pred = clf.predict(X_test)
```

Visualizing decision trees

Decision trees can be visualize using `graphviz` and `pydotplus`:

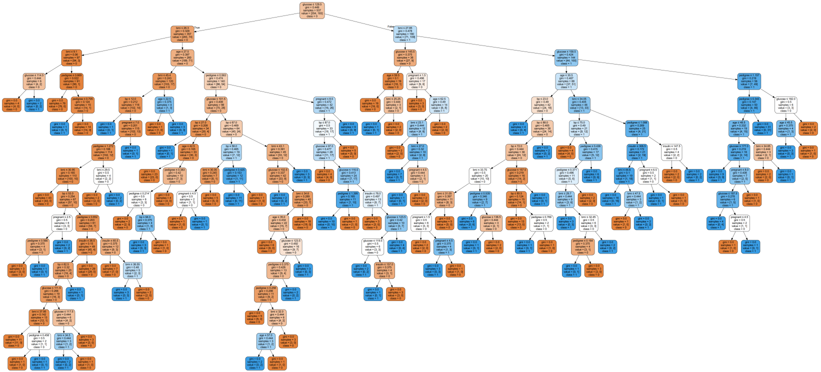
Building decision tree

```
from sklearn.tree import export_graphviz
from sklearn.externals.six import StringIO
from IPython.display import Image
import pydotplus

dot_data = StringIO()
export_graphviz(clf, out_file=dot_data,
                filled=True, rounded=True,
                special_characters=True,feature_names =
                ↪  feature_cols,class_names=['0','1'])
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
graph.write_png('diabetes.png')
Image(graph.create_png())
```

Visualizing decision trees

Decision tree:



Optimizing the decision tree

There are a few hyper-parameters:

- criterion: optional (default="gini") or Choose attribute selection measure: This parameter allows us to use the different-different attribute selection measure. Supported criteria are"gini" for the Gini index and "entropy" for the information gain.

- splitter: string, optional (default="best") or Split Strategy: This parameter allows us to choose the split strategy. Supported strategies are "best" to choose the best split and "random" to choose the best random split.

- max_depth: int or None, optional (default=None) or Maximum Depth of a Tree: The maximum depth of the tree. If None, then nodes are expanded until all the leaves contain less than min_samples_split samples. The higher value of maximum depth causes overfitting, and a lower value causes underfitting.

Decision trees

Probabilities output

The model can output categories and/or probabilities.

Models output

```
# Get predictions
preds = clf.predict(X_test)
np.savetxt("predictions", preds, fmt='%d')

# Get probabilities
probs = clf.predict_proba(X_test))
np.savetxt("probabilities", probs)
```

Metric module

The evaluation is common for all models.
Metric module implements many classification performance metrics:

```
metrics.accuracy_score(y_true, y_pred[, ...])
metrics.auc(x, y[, reorder])
metrics.average_precision_score(y_true, y_score)
metrics.balanced_accuracy_score(y_true, y_pred)
metrics.brier_score_loss(y_true, y_prob[, ...])
metrics.classification_report(y_true, y_pred)
metrics.cohen_kappa_score(y1, y2[, labels, ...])
metrics.confusion_matrix(y_true, y_pred[, ...])
metrics.f1_score(y_true, y_pred[, labels, ...])
metrics.fbeta_score(y_true, y_pred, beta[, ...])
metrics.hamming_loss(y_true, y_pred[, ...])
```

```
metrics.hinge_loss(y_true, pred_decision[, ...])
metrics.jaccard_score(y_true, y_pred[, ...])
metrics.log_loss(y_true, y_pred[, eps, ...])
metrics.matthews_corrcoef(y_true, y_pred[, ...])
metrics.multilabel_confusion_matrix(y_true, ...)
metrics.precision_recall_curve(y_true, ...)
metrics.precision_recall_fscore_support(...)
metrics.precision_score(y_true, y_pred[, ...])
metrics.recall_score(y_true, y_pred[, ...])
metrics.roc_auc_score(y_true, y_score[, ...])
metrics.roc_curve(y_true, y_score[, ...])
metrics.zero_one_loss(y_true, y_pred[, ...])
```

Example of evaluation

Once trained and tested the model can be evaluated:

Evaluating the decision tree

```
# Model Accuracy, how often is the classifier correct?
print("Accuracy:", metrics.accuracy_score(y_test, y_pred))

Accuracy: 0.6753246753246753
```

The confusion matrix can also be obtained from the predictions:

Confusion matrix for the decision tree

```
cm = confusion_matrix(y_test, y_pred)
```

Evaluating the models

Cross-validation

Python implements cross-validation as an option for evaluating the models
The following example demonstrates how to estimate the accuracy of a linear kernel support vector machine on the iris dataset by splitting the data, fitting a model and computing the score 5 consecutive times (with different splits each time):

k-Fold cross-validation

```
>>> from sklearn.model_selection import cross_val_score
>>> clf = svm.SVC(kernel='linear', C=1)
>>> scores = cross_val_score(clf, iris.data, iris.target, cv=5, scoring='accuracy')
>>> scores
array([0.96..., 1.  ..., 0.96..., 0.96..., 1.        ])
```

Optimizing hyper-parameters

Hyper-parameters are critic for many classification models (e.g: Support vector machines)
A step of obtaining the best set of hyper-parameters is usually needed
Scikit provides a grid search using cross-validation

Optimizing hyper-parameters

Grid search

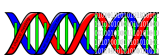
Grid search

```
# Grid Search
from sklearn.model_selection import GridSearchCV
clf = LogisticRegression()
grid_values = {'penalty': ['l1',
↪  'l2'],'C':[0.001,.009,0.01,.09,1,5,10,25]}
grid_clf_acc = GridSearchCV(clf, param_grid=grid_values,scoring='recall')
grid_clf_acc.fit(X_train, y_train)

# Predict values based on new parameters
y_pred_acc = grid_clf_acc.predict(X_test)

# New Model Evaluation metrics
print('Accuracy Score : ' + str(accuracy_score(y_test,y_pred_acc)))
print('Precision Score : ' + str(precision_score(y_test,y_pred_acc)))
print('Recall Score : ' + str(recall_score(y_test,y_pred_acc)))
print('F1 Score : ' + str(f1_score(y_test,y_pred_acc)))

#Logistic Regression (Grid Search) Confusion matrix
confusion_matrix(y_test,y_pred_acc)
```



Ensembles in Scikit-learn

Scitkit-learn provides many models for ensemble learning:

- Bagging
- Random forests
- Extremely randomized trees
- AdaBoost
- Gradient tree boosting
- Voting classifiers

Other methods can be easily implemented using the basic classification models

Bagging

Example of Bagging ensemble:

k-NN Bagging

```
16 # Split dataset into training set and test set
17 X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
   ↪  random_state=1)

18 bagging = BaggingClassifier(KNeighborsClassifier(),  max_samples=1.0,
   ↪  max_features=1.0)

19 # Then as in any other predictor
20 bagging = bagging.fit(X_train,y_train)

21 y_preds = bagging.predict(X_test)

22 probs = bagging.predict_proba(X_test)

23 cm = confusion_matrix(y_test, y_preds)
```

Random forest

Example of random forest:

Random forest

```
16 X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
   ↪  random_state=1)

17 rf = RandomForestClassifier(n_estimators=100, random_state=None)

18 # Then as in any other predictor
19 rf = rf.fit(X_train,y_train)

20 y_preds = rf.predict(X_test)

21 probs = rf.predict_proba(X_test)

22 cm = confusion_matrix(y_test, y_preds)
23 print(cm)
```

AdaBoost

AdaBoost is implemented using:

```
class sklearn.ensemble.AdaBoostClassifier(base_estimator=None,
    n_estimators=50, learning_rate=1.0, algorithm="SAMME.R",
    random_state=None)[source]
```

There are three major arguments to the constructor:

base_estimator: object, optional (default=None). The base estimator from which the boosted ensemble is built. Support for sample weighting is required, as well as proper `classes_` and `n_classes_` attributes. If None, then the base estimator is `DecisionTreeClassifier(max_depth=1)`

n_estimators: integer, optional (default=50). The maximum number of estimators at which boosting is terminated. In case of perfect fit, the learning procedure is stopped early.

algorithm: 'SAMME', 'SAMME.R', optional (default='SAMME.R'). If 'SAMME.R' then use the SAMME.R real boosting algorithm. `base_estimator` must support calculation of class probabilities. If 'SAMME' then use the SAMME discrete boosting algorithm. The SAMME.R algorithm typically converges faster than SAMME, achieving a lower test error with fewer boosting iterations.

Discrete AdaBoost

Discrete AdaBoost algorithm:

Data: $Z = \{\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N\}$, with $\mathbf{z}_i = (\mathbf{x}_i, y_i)$ as training set; M the maximum number of classifiers.

Result: $H(\mathbf{x})$

[2] Initialize the weights $w_i = 1/N$

[3] **for** $m = 1$ *to* M **do**

[5] Fit a classifier $H_m(\mathbf{x})$ to the training set using weights w_i

[7] Let $\epsilon = \sum_{i=1}^{N} w_i I(y_i \neq H_m(\mathbf{x}_i))$

[9] Compute $\alpha_m = 0.5 \log\left(\frac{1-\epsilon_m}{\epsilon_m}\right)$

[11] Set $w_i = w_i \exp\left(-\alpha_m I(y_i \neq H_m(\mathbf{x}_i))\right)$ and renormalize $\sum_i w_i = 1$

[12] **end**

[14] Output $H(x) = \text{sign}\left(\sum_{m=1}^{M} \alpha_m H_m(\mathbf{x})\right)$

Real AdaBoost

The *Real* AdaBoost algorithm refers to the fact that the classifiers produces a real value:

Data: $Z = \{\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N\}$, with $\mathbf{z}_i = (\mathbf{x}_i, y_i)$ as training set; M the maximum number of classifiers.

Result: $H(\mathbf{x})$

[2] Initialize the weights $w_i = 1/N$

[3] **for** $m = 1$ *to* M **do**

[5] Fit a the class probability estimate $p_m(\mathbf{x}) = \hat{P}_w(y = 1/x) \in [0, 1]$ on the training set using weights w_i

[7] Set $H_m(\mathbf{x}) = 0.5 \log\left(\frac{1-p_m(\mathbf{x})}{p_m(\mathbf{x})}\right) \in R$

[9] Set $w_i = w_i \exp\left(-y_i H_m(\mathbf{x}_i)\right))$ and renormalize $\sum_i w_i = 1$

[10] **end**

[12] Output $H(x) = \text{sign}\left(\sum_{m=1}^{M} \alpha_m H_m(\mathbf{x})\right)$

One-vs.-one

Multi-class methodsGarcía-Pedrajas and Ortiz-Boyer [2011] follow the same structure than the rest of classifiers.
No `predict_proba()` method.

OVO method

```
8  col_names = ['RI', 'Na', 'Mg', 'Al', 'Si', 'K', 'Ca', 'Ba', 'Fe', 'label']
9  glass = pd.read_csv("glass.csv", header=None, names=col_names)

10 # split dataset in features and target variable
11 feature_cols = ['RI', 'Na', 'Mg', 'Al', 'Si', 'K', 'Ca', 'Ba', 'Fe']
12 X = glass[feature_cols] # Features
13 y = glass.label # Target variable

14 # Split dataset into training set and test set
15 X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=1)

16 ovo = OneVsOneClassifier(LogisticRegression(random_state=0, solver='liblinear'))

17 # Then as in any other predictor
18 ovo = ovo.fit(X_train,y_train)

19 y_preds = ovo.predict(X_test)

20 cm = confusion_matrix(y_test, y_preds)
```

One-vs.-all

One-vs.-all example:

OVA method

```
8  col_names = ['RI', 'Na', 'Mg', 'Al', 'Si', 'K', 'Ca', 'Ba', 'Fe', 'label']
9  glass = pd.read_csv("glass.csv", header=None, names=col_names)

10 # split dataset in features and target variable
11 feature_cols = ['RI', 'Na', 'Mg', 'Al', 'Si', 'K', 'Ca', 'Ba', 'Fe']
12 X = glass[feature_cols] # Features
13 y = glass.label # Target variable

14 # Split dataset into training set and test set
15 X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=1)

16 ova = OneVsRestClassifier(LogisticRegression(random_state=0, solver='liblinear'))

17 # Then as in any other predictor
18 ova = ova.fit(X_train,y_train)

19 y_preds = ova.predict(X_test)
20 probs = ova.predict_proba(X_test)

21 cm = confusion_matrix(y_test, y_preds)
```

ECOC

No `predict_proba()` method.

Error correcting output codeDietterich and Bakiri [1995] example:

ECOC

```
8  col_names = ['RI', 'Na', 'Mg', 'Al', 'Si', 'K', 'Ca', 'Ba', 'Fe', 'label']
9  glass = pd.read_csv("glass.csv", header=None, names=col_names)

10 # split dataset in features and target variable
11 feature_cols = ['RI', 'Na', 'Mg', 'Al', 'Si', 'K', 'Ca', 'Ba', 'Fe']
12 X = glass[feature_cols] # Features
13 y = glass.label # Target variable

14 # Split dataset into training set and test set
15 X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=1)

16 ecoc = OutputCodeClassifier(LogisticRegression(random_state=0, solver='liblinear'), code_size=3)

17 # Then as in any other predictor
18 ecoc = ecoc.fit(X_train,y_train)

19 y_preds = ecoc.predict(X_test)

20 cm = confusion_matrix(y_test, y_preds)
```

References 1

Dietterich, T. G. and G. Bakiri (1995). Solving multiclass learning problems via error-correcting output codes. *Journal of Artificial Intelligence Research 2*, 263–286.

García-Pedrajas, N. and D. Ortiz-Boyer (2011). An empirical study of binary classifier fusion methods for multiclass classification. *Information Fusion 12*(2), 111–130.