tutorialspoint

SIMPLY EASY LEARNING

About the Tutorial

Scikit-learn (Sklearn) is the most useful and robust library for machine learning in Python. It provides a selection of efficient tools for machine learning and statistical modeling including classification, regression, clustering and dimensionality reduction via a consistence interface in Python. This library, which is largely written in Python, is built upon NumPy, SciPy and Matplotlib.

Audience

This tutorial will be useful for graduates, postgraduates, and research students who either have an interest in this Machine Learning subject or have this subject as a part of their curriculum. The reader can be a beginner or an advanced learner.

Prerequisites

The reader must have basic knowledge about Machine Learning. He/she should also be aware about Python, NumPy, Scipy, Matplotlib. If you are new to any of these concepts, we recommend you take up tutorials concerning these topics, before you dig further into this tutorial.

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Table of Contents

1. Scikit-Learn — Introduction

In this chapter, we will understand what is Scikit-Learn or Sklearn, origin of Scikit-Learn and some other related topics such as communities and contributors responsible for development and maintenance of Scikit-Learn, its prerequisites, installation and its features.

What is Scikit-Learn (Sklearn)?

Scikit-learn (Sklearn) is the most useful and robust library for machine learning in Python. It provides a selection of efficient tools for machine learning and statistical modeling including classification, regression, clustering and dimensionality reduction via a consistence interface in Python. This library, which is largely written in Python, is built upon **NumPy, SciPy** and **Matplotlib**.

Origin of Scikit-Learn

It was originally called ***scikits.learn*** and was initially developed by David Cournapeau as a Google summer of code project in 2007. Later, in 2010, Fabian Pedregosa, Gael Varoquaux, Alexandre Gramfort, and Vincent Michel, from FIRCA (French Institute for Research in Computer Science and Automation), took this project at another level and made the first public release (v0.1 beta) on 1st Feb. 2010.

Let's have a look at its version history:

- May 2019: scikit-learn 0.21.0
- March 2019: scikit-learn 0.20.3
- December 2018: scikit-learn 0.20.2
- November 2018: scikit-learn 0.20.1
- September 2018: scikit-learn 0.20.0
- July 2018: scikit-learn 0.19.2
- July 2017: scikit-learn 0.19.0
- September 2016. scikit-learn 0.18.0
- November 2015. scikit-learn 0.17.0
- March 2015. scikit-learn 0.16.0
- July 2014. scikit-learn 0.15.0
- August 2013. scikit-learn 0.14

Community & contributors

Scikit-learn is a community effort and anyone can contribute to it. This project is hosted on https://github.com/scikit-learn/scikit-learn. Following people are currently the core contributors to Sklearn's development and maintenance:

- Joris Van den Bossche (Data Scientist)
- Thomas J Fan (Software Developer)
- Alexandre Gramfort (Machine Learning Researcher)
- Olivier Grisel (Machine Learning Expert)
- Nicolas Hug (Associate Research Scientist)
- Andreas Mueller (Machine Learning Scientist)
- Hanmin Qin (Software Engineer)
- Adrin Jalali (Open Source Developer)
- Nelle Varoquaux (Data Science Researcher)
- Roman Yurchak (Data Scientist)

Various organisations like Booking.com, JP Morgan, Evernote, Inria, AWeber, Spotify and many more are using Sklearn.

Prerequisites

Before we start using scikit-learn latest release, we require the following:

- Python (>=3.5)
- NumPy (>= 1.11.0)
- Scipy (>= 0.17.0)
- Joblib (>= 0.11)
- Matplotlib (>= 1.5.1) is required for Sklearn plotting capabilities.
- Pandas (>= 0.18.0) is required for some of the scikit-learn examples using data structure and analysis.

Installation

If you already installed NumPy and Scipy, following are the two easiest ways to install scikit-learn:

Using pip

Following command can be used to install scikit-learn via pip:

```
pip install -U scikit-learn
```

Using conda

Following command can be used to install scikit-learn via conda:

```
conda install scikit-learn
```

On the other hand, if NumPy and Scipy is not yet installed on your Python workstation then, you can install them by using either **pip** or **conda**.

Another option to use scikit-learn is to use Python distributions like ***Canopy*** and ***Anaconda*** because they both ship the latest version of scikit-learn.

Features

Rather than focusing on loading, manipulating and summarising data, Scikit-learn library is focused on modeling the data. Some of the most popular groups of models provided by Sklearn are as follows:

Supervised Learning algorithms: Almost all the popular supervised learning algorithms, like Linear Regression, Support Vector Machine (SVM), Decision Tree etc., are the part of scikit-learn.

Unsupervised Learning algorithms: On the other hand, it also has all the popular unsupervised learning algorithms from clustering, factor analysis, PCA (Principal Component Analysis) to unsupervised neural networks.

Clustering: This model is used for grouping unlabeled data.

Cross Validation: It is used to check the accuracy of supervised models on unseen data.

Dimensionality Reduction: It is used for reducing the number of attributes in data which can be further used for summarisation, visualisation and feature selection.

Ensemble methods: As name suggest, it is used for combining the predictions of multiple supervised models.

Feature extraction: It is used to extract the features from data to define the attributes in image and text data.

Feature selection: It is used to identify useful attributes to create supervised models.
Open Source: It is open source library and also commercially usable under BSD license.

2. Scikit-Learn — Modelling Process

This chapter deals with the modelling process involved in Sklearn. Let us understand about the same in detail and begin with dataset loading.

Dataset Loading

A collection of data is called dataset. It is having the following two components:

Features: The variables of data are called its features. They are also known as predictors, inputs or attributes.

- **Feature matrix:** It is the collection of features, in case there are more than one.
- **Feature Names:** It is the list of all the names of the features.

Response: It is the output variable that basically depends upon the feature variables. They are also known as target, label or output.

- **Response Vector:** It is used to represent response column. Generally, we have just one response column.
- **Target Names:** It represent the possible values taken by a response vector.

Scikit-learn have few example datasets like **iris** and **digits** for classification and the **Boston house prices** for regression.

Following is an example to load **iris** dataset:

```
from sklearn.datasets import load_iris

iris = load_iris()

X = iris.data

y = iris.target

feature_names = iris.feature_names

target_names = iris.target_names



print("Feature names:", feature_names)
```

```
print("Target names:", target_names)


print("\nFirst 10 rows of X:\n", X[:10])
```

Output

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


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


First 10 rows of X:
 [[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]]
```

Splitting the dataset

To check the accuracy of our model, we can split the dataset into two pieces-**a training set** and **a testing set**. Use the training set to train the model and testing set to test the model. After that, we can evaluate how well our model did.

The following example will split the data into 70:30 ratio, i.e. 70% data will be used as training data and 30% will be used as testing data. The dataset is ***iris*** dataset as in above example.

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

X = iris.data
y = iris.target

from sklearn.model_selection import train_test_split

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

print(X_train.shape)
print(X_test.shape)

print(y_train.shape)
print(y_test.shape)
```

Output

```
(105, 4)
(45, 4)

(105,)
(45,)
```

As seen in the example above, it uses **train_test_split()** function of scikit-learn to split the dataset. This function has the following arguments:

- **X, y**: Here, **X** is the **feature matrix** and **y** is the **response vector**, which need to be split.
- **test_size**: This represents the ratio of test data to the total given data. As in the above example, we are setting **test_data = 0.3** for 150 rows of X. It will produce test data of 150*0.3 = 45 rows.
- **random_size**: It is used to guarantee that the split will always be the same. This is useful in the situations where you want reproducible results.

Train the Model

Next, we can use our dataset to train some prediction-model. As discussed, scikit-learn has wide range of **Machine Learning (ML) algorithms** which have a consistent interface for fitting, predicting accuracy, recall etc.

In the example below, we are going to use KNN (K nearest neighbors) classifier. Don't go into the details of KNN algorithms, as there will be a separate chapter for that. This example is used to make you understand the implementation part only.

```
from sklearn.datasets import load_iris

iris = load_iris()

X = iris.data

y = iris.target

from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.4,
random_state=1)

from sklearn.neighbors import KNeighborsClassifier

from sklearn import metrics

classifier_knn = KNeighborsClassifier(n_neighbors=3)
```

```
classifier_knn.fit(X_train, y_train)


y_pred = classifier_knn.predict(X_test)


# Finding accuracy by comparing actual response values(y_test)with predicted
response value(y_pred)


print("Accuracy:", metrics.accuracy_score(y_test, y_pred))


# Providing sample data and the model will make prediction out of that data


sample = [[5, 5, 3, 2], [2, 4, 3, 5]]

preds = classifier_knn.predict(sample)

pred_species = [iris.target_names[p] for p in preds] print("Predictions:",
pred_species)
```

Output

```
Accuracy: 0.9833333333333333


Predictions: ['versicolor', 'virginica']
```

Model Persistence

Once you train the model, it is desirable that the model should be persist for future use so that we do not need to retrain it again and again. It can be done with the help of **dump** and **load** features of ***joblib*** package.

Consider the example below in which we will be saving the above trained model (classifier_knn) for future use:

```
from sklearn.externals import joblib


joblib.dump(classifier_knn, 'iris_classifier_knn.joblib')
```

The above code will save the model into file named **iris_classifier_knn.joblib**. Now, the object can be reloaded from the file with the help of following code:

```
joblib.load('iris_classifier_knn.joblib')
```

Preprocessing the Data

As we are dealing with lots of data and that data is in raw form, before inputting that data to machine learning algorithms, we need to convert it into meaningful data. This process is called preprocessing the data. Scikit-learn has package named **preprocessing** for this purpose. The **preprocessing** package has the following techniques:

Binarisation

This preprocessing technique is used when we need to convert our numerical values into Boolean values.

Example

```
import numpy as np
from sklearn import preprocessing
Input_data = np.array([2.1, -1.9, 5.5],
                [-1.5, 2.4, 3.5],
                [0.5, -7.9, 5.6],
                [5.9, 2.3, -5.8]])

data_binarized = preprocessing.Binarizer(threshold=0.5).transform(input_data)
print("\nBinarized data:\n", data_binarized)
```

In the above example, we used **threshold value = 0.5** and that is why, all the values above 0.5 would be converted to 1, and all the values below 0.5 would be converted to 0.

Output

```
Binarized data:
 [[ 1.  0.  1.]
 [ 0.  1.  1.]
 [ 0.  0.  1.]
 [ 1.  1.  0.]]
```

Mean Removal

This technique is used to eliminate the mean from feature vector so that every feature centered on zero.

Example

```
import numpy as np
from sklearn import preprocessing
Input_data = np.array([2.1, -1.9, 5.5],
```

```
                [-1.5, 2.4, 3.5],
                [0.5, -7.9, 5.6],
                [5.9, 2.3, -5.8]])

#displaying the mean and the standard deviation of the input data
print("Mean =", input_data.mean(axis=0))
print("Stddeviation = ", input_data.std(axis=0))

#Removing the mean and the standard deviation of the input data

data_scaled = preprocessing.scale(input_data)
print("Mean_removed =", data_scaled.mean(axis=0))
print("Stddeviation_removed =", data_scaled.std(axis=0))
```

Output

```
Mean = [ 1.75  -1.275  2.2  ]
Stddeviation =  [ 2.71431391  4.20022321  4.69414529]

Mean_removed = [  1.11022302e-16   0.00000000e+00 0.00000000e+00]
Stddeviation_removed = [ 1.  1.  1.]
```

Scaling

We use this preprocessing technique for scaling the feature vectors. Scaling of feature vectors is important, because the features should not be synthetically large or small.

Example

```
import numpy as np
from sklearn import preprocessing

Input_data = np.array([2.1, -1.9, 5.5],

                      [-1.5, 2.4, 3.5],

                    [0.5, -7.9, 5.6],
                    [5.9, 2.3, -5.8]])
data_scaler_minmax = preprocessing.MinMaxScaler(feature_range=(0,1))
data_scaled_minmax = data_scaler_minmax.fit_transform(input_data)
```

```
print ("\nMin max scaled data:\n", data_scaled_minmax)
```

Output

```
Min max scaled data:
[[ 0.48648649  0.58252427  0.99122807]
[ 0.          1.          0.81578947]
[ 0.27027027  0.          1.        ]
[ 1.          0.99029126  0.        ]]
```

Normalisation

We use this preprocessing technique for modifying the feature vectors. Normalisation of feature vectors is necessary so that the feature vectors can be measured at common scale. There are two types of normalisation as follows:

L1 Normalisation

It is also called Least Absolute Deviations. It modifies the value in such a manner that the sum of the absolute values remains always up to 1 in each row. Following example shows the implementation of L1 normalisation on input data.

Example

```
import numpy as np
from sklearn import preprocessing
Input_data = np.array([2.1, -1.9, 5.5],
                [-1.5, 2.4, 3.5],
                [0.5, -7.9, 5.6],
                [5.9, 2.3, -5.8]])
data_normalized_l1 = preprocessing.normalize(input_data, norm='l1')
print("\nL1 normalized data:\n", data_normalized_l1)
```

Output

```
L1 normalized data:

[[ 0.22105263 -0.2         0.57894737]

[-0.2027027   0.32432432  0.47297297]
[ 0.03571429 -0.56428571  0.4       ]
[ 0.42142857  0.16428571 -0.41428571]]
```

L2 Normalisation

Also called Least Squares. It modifies the value in such a manner that the sum of the squares remains always up to 1 in each row. Following example shows the implementation of L2 normalisation on input data.

Example

```
import numpy as np
from sklearn import preprocessing
Input_data = np.array([2.1, -1.9, 5.5],
                [-1.5, 2.4, 3.5],
                [0.5, -7.9, 5.6],
                [5.9, 2.3, -5.8]])
data_normalized_l2 = preprocessing.normalize(input_data, norm='l2')
print("\nL1 normalized data:\n", data_normalized_l2)
```

Output

```
L2 normalized data:
[[ 0.33946114 -0.30713151  0.88906489]
[-0.33325106  0.53320169  0.7775858 ]
[ 0.05156558 -0.81473612  0.57753446]
[ 0.68706914  0.26784051 -0.6754239 ]]
```

3. Scikit-Learn — Data Representation

As we know that machine learning is about to create model from data. For this purpose, computer must understand the data first. Next, we are going to discuss various ways to represent the data in order to be understood by computer:

Data as table

The best way to represent data in Scikit-learn is in the form of tables. A table represents a 2-D grid of data where rows represent the individual elements of the dataset and the columns represents the quantities related to those individual elements.

Example

With the example given below, we can download ***iris dataset*** in the form of a Pandas DataFrame with the help of python ***seaborn*** library.

```
import seaborn as sns
iris = sns.load_dataset('iris')
iris.head()
```

Output

```
sepal_length  sepal_width  petal_length  petal_width      species
0       5.1          3.5             1.4          0.2    setosa
1       4.9          3.0             1.4          0.2    setosa
2       4.7          3.2             1.3          0.2    setosa
3       4.6          3.1           1.5          0.2      setosa
4       5.0          3.6           1.4          0.2      setosa
```

From above output, we can see that each row of the data represents a single observed flower and the number of rows represents the total number of flowers in the dataset. Generally, we refer the rows of the matrix as samples.

On the other hand, each column of the data represents a quantitative information describing each sample. Generally, we refer the columns of the matrix as features.

Data as Feature Matrix

Features matrix may be defined as the table layout where information can be thought of as a 2-D matrix. It is stored in a variable named **X** and assumed to be two dimensional

with shape [n_samples, n_features]. Mostly, it is contained in a NumPy array or a Pandas DataFrame. As told earlier, the samples always represent the individual objects described by the dataset and the features represents the distinct observations that describe each sample in a quantitative manner.

Data as Target array

Along with Features matrix, denoted by X, we also have target array. It is also called label. It is denoted by y. The label or target array is usually one-dimensional having length n_samples. It is generally contained in NumPy ***array*** or Pandas ***Series***. Target array may have both the values, continuous numerical values and discrete values.

How target array differs from feature columns?

We can distinguish both by one point that the target array is usually the quantity we want to predict from the data i.e. in statistical terms it is the dependent variable.

Example

In the example below, from *iris dataset* we predict the species of flower based on the other measurements. In this case, the *Species* column would be considered as the feature.

```
import seaborn as sns
iris = sns.load_dataset('iris')
%matplotlib inline
import seaborn as sns; sns.set()
sns.pairplot(iris, hue='species', height=3);
```

Output


```
X_iris = iris.drop('species', axis=1)
X_iris.shape
y_iris = iris['species']
y_iris.shape
```

Output

```
(150,4)
(150,)
```

4. Scikit-Learn — Estimator API

In this chapter, we will learn about **Estimator API** (application programming interface). Let us begin by understanding what is an Estimator API.

What is Estimator API?

It is one of the main APIs implemented by Scikit-learn. It provides a consistent interface for a wide range of ML applications that's why all machine learning algorithms in Scikit-Learn are implemented via Estimator API. The object that learns from the data (fitting the data) is an estimator. It can be used with any of the algorithms like classification, regression, clustering or even with a transformer, that extracts useful features from raw data.

For fitting the data, all estimator objects expose a fit method that takes a dataset shown as follows:

```
estimator.fit(data)
```

Next, all the parameters of an estimator can be set, as follows, when it is instantiated by the corresponding attribute.

```
estimator = Estimator (param1=1, param2=2)
estimator.param1
```

The output of the above would be 1.

Once data is fitted with an estimator, parameters are estimated from the data at hand. Now, all the estimated parameters will be the attributes of the estimator object ending by an underscore as follows:

```
estimator.estimated_param_
```

Use of Estimator API

Main uses of estimators are as follows:

Estimation and decoding of a model

Estimator object is used for estimation and decoding of a model. Furthermore, the model is estimated as a deterministic function of the following:

- The parameters which are provided in object construction.
- The global random state (numpy.random) if the estimator's random_state parameter is set to none.
- Any data passed to the most recent call to **fit, fit_transform**, or **fit_predict**.
- Any data passed in a sequence of calls to **partial_fit**.

Mapping non-rectangular data representation into rectangular data

It maps a non-rectangular data representation into rectangular data. In simple words, it takes input where each sample is not represented as an array-like object of fixed length, and producing an array-like object of features for each sample.

Distinction between core and outlying samples

It models the distinction between core and outlying samples by using following methods:

- fit
- fit_predict if transductive
- predict if inductive

Guiding Principles

While designing the Scikit-Learn API, following guiding principles kept in mind:

Consistency

This principle states that all the objects should share a common interface drawn from a limited set of methods. The documentation should also be consistent.

Limited object hierarchy

This guiding principle says:

- Algorithms should be represented by Python classes
- Datasets should be represented in standard format like NumPy arrays, Pandas DataFrames, SciPy sparse matrix.
- Parameters names should use standard Python strings.

Composition

As we know that, ML algorithms can be expressed as the sequence of many fundamental algorithms. Scikit-learn makes use of these fundamental algorithms whenever needed.

Sensible defaults

According to this principle, the Scikit-learn library defines an appropriate default value whenever ML models require user-specified parameters.

Inspection

As per this guiding principle, every specified parameter value is exposed as pubic attributes.

Steps in using Estimator API

Followings are the steps in using the Scikit-Learn estimator API:

Step 1: Choose a class of model

In this first step, we need to choose a class of model. It can be done by importing the appropriate Estimator class from Scikit-learn.

Step 2: Choose model hyperparameters

In this step, we need to choose class model hyperparameters. It can be done by instantiating the class with desired values.

Step 3: Arranging the data

Next**,** we need to arrange the data into features matrix (X) and target vector(y).

Step 4: Model Fitting

Now, we need to fit the model to your data. It can be done by calling **fit()** method of the model instance.

Step 5: Applying the model

After fitting the model, we can apply it to new data. For supervised learning, use **predict()** method to predict the labels for unknown data. While for unsupervised learning, use **predict()** or **transform()** to infer properties of the data.

Supervised Learning Example

Here, as an example of this process we are taking common case of fitting a line to (x,y) data i.e. ***simple linear regression***.

First, we need to load the dataset, we are using iris dataset:

```
import seaborn as sns
iris = sns.load_dataset('iris')

X_iris = iris.drop('species', axis = 1)
X_iris.shape
```

Output

```
(150, 4)
```

```
y_iris = iris['species']
y_iris.shape
```

Output

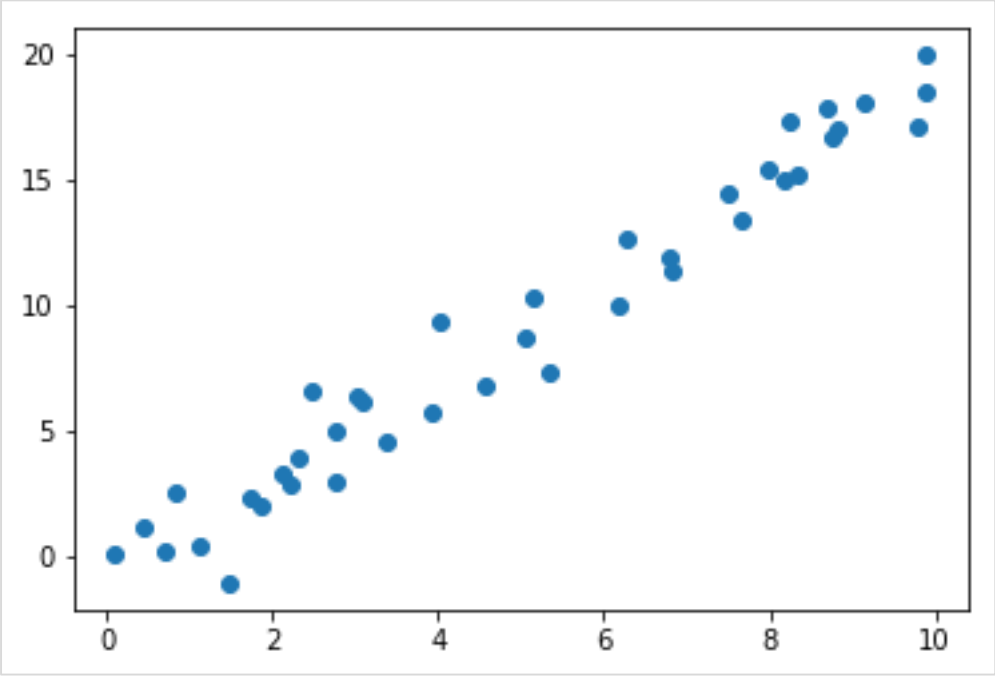
```
(150,)
```

Now, for this regression example, we are going to use the following sample data:

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

import numpy as np
rng = np.random.RandomState(35)
x = 10*rng.rand(40)
y = 2*x-1+rng.randn(40)
plt.scatter(x,y);
```

Output



So, we have the above data for our linear regression example.

Now, with this data, we can apply the above-mentioned steps.

Choose a class of model

Here, to compute a simple linear regression model, we need to import the linear regression class as follows:

```
from sklearn.linear_model import LinearRegression
```

Choose model hyperparameters

Once we choose a class of model, we need to make some important choices which are often represented as hyperparameters, or the parameters that must set before the model is fit to data. Here, for this example of linear regression, we would like to fit the intercept by using the **fit_intercept** hyperparameter as follows:

```
model = LinearRegression(fit_intercept=True)
model
```

Output

```
LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
         normalize=False)
```

Arranging the data

Now, as we know that our target variable **y** is in correct form i.e. a length **n_samples** array of 1-D. But, we need to reshape the feature matrix **X** to make it a matrix of size **[n_samples, n_features].** It can be done as follows:

```
X = x[:, np.newaxis]
X.shape
```

Output

```
(40, 1)
```

Model fitting

Once, we arrange the data, it is time to fit the model i.e. to apply our model to data. This can be done with the help of **fit()** method as follows:

```
model.fit(X, y)
```

Output

```
LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
```

```
        normalize=False)
```

In Scikit-learn, the **fit()** process have some trailing underscores.

For this example, the below parameter shows the slope of the simple linear fit of the data:

```
model.coef_
```

Output

```
array([1.99839352])
```

The below parameter represents the intercept of the simple linear fit to the data:

```
model.intercept_
```

Output

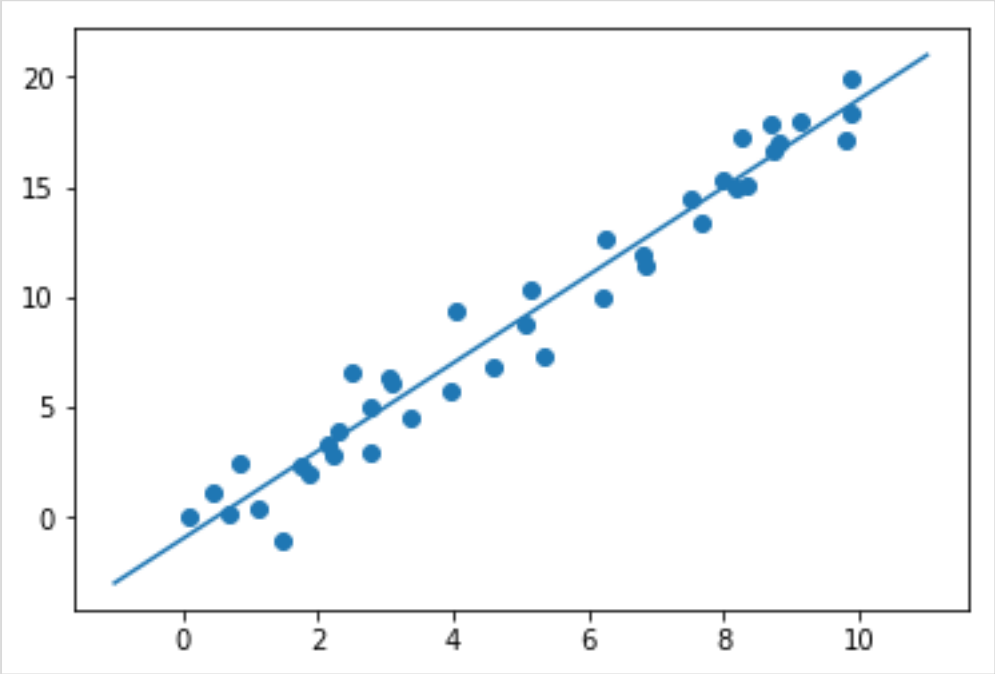
```
-0.9895459457775022
```

Applying the model to new data

After training the model, we can apply it to new data. As the main task of supervised machine learning is to evaluate the model based on new data that is not the part of the training set. It can be done with the help of **predict()** method as follows:

```
xfit = np.linspace(-1, 11)
Xfit = xfit[:, np.newaxis]
yfit = model.predict(Xfit)
plt.scatter(x, y)
plt.plot(xfit, yfit);
```

Output



Complete working/executable example

```
%matplotlib inline
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns

iris = sns.load_dataset('iris')
X_iris = iris.drop('species', axis = 1)
X_iris.shape
y_iris = iris['species']
y_iris.shape
rng = np.random.RandomState(35)
x = 10*rng.rand(40)

y = 2*x-1+rng.randn(40)
plt.scatter(x,y);
from sklearn.linear_model import LinearRegression
model = LinearRegression(fit_intercept=True)
model
X = x[:, np.newaxis]
X.shape
model.fit(X, y)
```

```
model.coef_
model.intercept_
xfit = np.linspace(-1, 11)
Xfit = xfit[:, np.newaxis]
yfit = model.predict(Xfit)
plt.scatter(x, y)
plt.plot(xfit, yfit);
```

Unsupervised Learning Example

Here, as an example of this process we are taking common case of reducing the dimensionality of the Iris dataset so that we can visualize it more easily. For this example, we are going to use principal component analysis (PCA), a fast-linear dimensionality reduction technique.

Like the above given example, we can load and plot the random data from iris dataset. After that we can follow the steps as below:

Choose a class of model

```
from sklearn.decomposition import PCA
```

Choose model hyperparameters

```
model = PCA(n_components=2)
model
```

Output

```
PCA(copy=True, iterated_power='auto', n_components=2, random_state=None,
  svd_solver='auto', tol=0.0, whiten=False)
```

Model fitting

```
model.fit(X_iris)
```

Output

```
PCA(copy=True, iterated_power='auto', n_components=2, random_state=None,
  svd_solver='auto', tol=0.0, whiten=False)
```

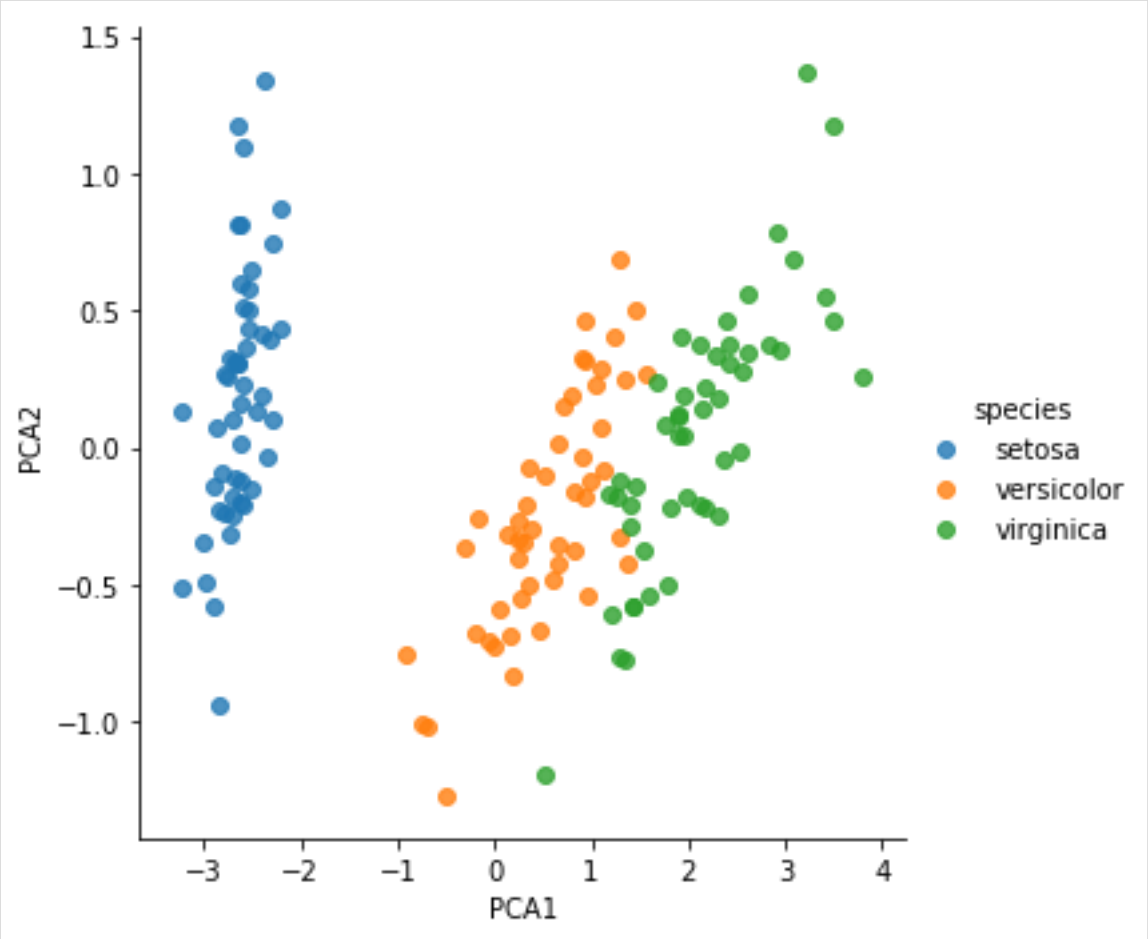
Transform the data to two-dimensional

```
X_2D = model.transform(X_iris)
```

Now, we can plot the result as follows:

```
iris['PCA1'] = X_2D[:, 0]
iris['PCA2'] = X_2D[:, 1]
sns.lmplot("PCA1", "PCA2", hue='species', data=iris, fit_reg=False);
```

Output



Complete working/executable example

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

import numpy as np
import seaborn as sns
iris = sns.load_dataset('iris')
```

```
X_iris = iris.drop('species', axis = 1)
X_iris.shape
y_iris = iris['species']
y_iris.shape
rng = np.random.RandomState(35)
x = 10*rng.rand(40)
y = 2*x-1+rng.randn(40)
plt.scatter(x,y);
from sklearn.decomposition import PCA
model = PCA(n_components=2)
model
model.fit(X_iris)
X_2D = model.transform(X_iris)
iris['PCA1'] = X_2D[:, 0]
iris['PCA2'] = X_2D[:, 1]
sns.lmplot("PCA1", "PCA2", hue='species', data=iris, fit_reg=False);
```

5. Scikit-Learn — Conventions

Scikit-learn's objects share a uniform basic API that consists of the following three complementary interfaces:

- **Estimator interface**: It is for building and fitting the models.
- **Predictor interface**: It is for making predictions.
- **Transformer interface**: It is for converting data.

The APIs adopt simple conventions and the design choices have been guided in a manner to avoid the proliferation of framework code.

Purpose of Conventions

The purpose of conventions is to make sure that the API stick to the following broad principles:

Consistency: All the objects whether they are basic, or composite must share a consistent interface which further composed of a limited set of methods.

Inspection: Constructor parameters and parameters values determined by learning algorithm should be stored and exposed as public attributes.

Non-proliferation of classes: Datasets should be represented as NumPy arrays or Scipy sparse matrix whereas hyper-parameters names and values should be represented as standard Python strings to avoid the proliferation of framework code.

Composition: The algorithms whether they are expressible as sequences or combinations of transformations to the data or naturally viewed as meta-algorithms parameterized on other algorithms, should be implemented and composed from existing building blocks.

Sensible defaults: In scikit-learn whenever an operation requires a user-defined parameter, an appropriate default value is defined. This default value should cause the operation to be performed in a sensible way, for example, giving a base-line solution for the task at hand.

Various Conventions

The conventions available in Sklearn are explained below:

Type casting

It states that the input should be cast to **float64**. In the following example, in which **sklearn.random_projection** module used to reduce the dimensionality of the data, will explain it:

```
import numpy as np
```

```
from sklearn import random_projection

rannge = np.random.RandomState(0)

X = range.rand(10,2000)

X = np.array(X, dtype = 'float32')

X.dtype



Transformer_data = random_projection.GaussianRandomProjection()

X_new = transformer.fit_transform(X)

X_new.dtype
```

Output

```
dtype('float32')
dtype('float64')
```

In the above example, we can see that X is **float32** which is cast to **float64** by **fit_transform(X).**

Refitting & Updating Parameters

Hyper-parameters of an estimator can be updated and refitted after it has been constructed via the **set_params()** method. Let's see the following example to understand it:

```
import numpy as np
from sklearn.datasets import load_iris
from sklearn.svm import SVC
X, y = load_iris(return_X_y=True)

clf = SVC()
clf.set_params(kernel='linear').fit(X, y)
clf.predict(X[:5])
```

Output

```
array([0, 0, 0, 0, 0])
```

Once the estimator has been constructed, above code will change the default kernel **rbf** to linear via **SVC.set_params().**

Now, the following code will change back the kernel to **rbf** to refit the estimator and to make a second prediction.

```
clf.set_params(kernel='rbf', gamma='scale').fit(X, y)


clf.predict(X[:5])
```

Output

```
array([0, 0, 0, 0, 0])
```

Complete code

The following is the complete executable program:

```
import numpy as np
from sklearn.datasets import load_iris
from sklearn.svm import SVC
X, y = load_iris(return_X_y=True)

clf = SVC()
clf.set_params(kernel='linear').fit(X, y)
clf.predict(X[:5])

clf.set_params(kernel='rbf', gamma='scale').fit(X, y)
clf.predict(X[:5])
```

Multiclass & Multilabel fitting

In case of multiclass fitting, both learning and the prediction tasks are dependent on the format of the target data fit upon. The module used is **sklearn.multiclass**. Check the example below, where multiclass classifier is fit on a 1d array.

```
from sklearn.svm import SVC
from sklearn.multiclass import OneVsRestClassifier
from sklearn.preprocessing import LabelBinarizer

X = [[1, 2], [3, 4], [4, 5], [5, 2], [1, 1]]
```

```
y = [0, 0, 1, 1, 2]

classif = OneVsRestClassifier(estimator=SVC(gamma='scale',random_state=0))
classif.fit(X, y).predict(X)
```

Output

```
array([0, 0, 1, 1, 2])
```

In the above example, classifier is fit on one dimensional array of multiclass labels and the **predict()** method hence provides corresponding multiclass prediction. But on the other hand, it is also possible to fit upon a two-dimensional array of binary label indicators as follows:

```
from sklearn.svm import SVC
from sklearn.multiclass import OneVsRestClassifier
from sklearn.preprocessing import LabelBinarizer

X = [[1, 2], [3, 4], [4, 5], [5, 2], [1, 1]]
y = LabelBinarizer().fit_transform(y)
classif.fit(X, y).predict(X)
```

Output

```
array([[0, 0, 0],
       [0, 0, 0],
       [0, 1, 0],
       [0, 1, 0],
       [0, 0, 0]])
```

Similarly, in case of multilabel fitting, an instance can be assigned multiple labels as follows:

```
from sklearn.preprocessing import MultiLabelBinarizer
y = [[0, 1], [0, 2], [1, 3], [0, 2, 3], [2, 4]]
y = MultiLabelBinarizer().fit_transform(y)
classif.fit(X, y).predict(X)
```

Output

```
array([[1, 0, 1, 0, 0],
       [1, 0, 1, 0, 0],
       [1, 0, 1, 1, 0],
```

```
        [1, 0, 1, 1, 0],
        [1, 0, 1, 0, 0]])
```

In the above example, **sklearn.MultiLabelBinarizer** is used to binarize the two dimensional array of multilabels to fit upon. That's why **predict()** function gives a 2d array as output with multiple labels for each instance.

6. Scikit-Learn — Linear Modeling

This chapter will help you in learning about the linear modeling in Scikit-Learn. Let us begin by understanding what is linear regression in Sklearn.

The following table lists out various linear models provided by Scikit-Learn:

Model	Description
Linear Regression	It is one of the best statistical models that studies the relationship between a dependent variable (Y) with a given set of independent variables (X).
Logistic Regression	Logistic regression, despite its name, is a classification algorithm rather than regression algorithm. Based on a given set of independent variables, it is used to estimate discrete value (0 or 1, yes/no, true/false).
Ridge Regression	Ridge regression or Tikhonov regularization is the regularization technique that performs L2 regularization. It modifies the loss function by adding the penalty (shrinkage quantity) equivalent to the square of the magnitude of coefficients.
Bayesian Ridge Regression	Bayesian regression allows a natural mechanism to survive insufficient data or poorly distributed data by formulating linear regression using probability distributors rather than point estimates.
LASSO	LASSO is the regularisation technique that performs L1 regularisation. It modifies the loss function by adding the penalty (shrinkage quantity) equivalent to the summation of the absolute value of coefficients.
Multi-task LASSO	It allows to fit multiple regression problems jointly enforcing the selected features to be same for all the regression problems, also called tasks. Sklearn provides a linear model named **MultiTaskLasso**, trained with a mixed L1, L2-norm for regularisation, which estimates sparse

	coefficients for multiple regression problems jointly.
Elastic-Net	The Elastic-Net is a regularized regression method that linearly combines both penalties i.e. L1 and L2 of the Lasso and Ridge regression methods. It is useful when there are multiple correlated features.
Multi-task Elastic-Net	It is an Elastic-Net model that allows to fit multiple regression problems jointly enforcing the selected features to be same for all the regression problems, also called tasks

Linear Regression

It is one of the best statistical models that studies the relationship between a dependent variable (Y) with a given set of independent variables (X). The relationship can be established with the help of fitting a best line.

sklearn.linear_model.LinearRegression is the module used to implement linear regression.

Parameters

Following table consists the parameters used by **Linear Regression** module:

Parameter	Description
fit_intercept*: Boolean, optional, default True*	Used to calculate the intercept for the model. No intercept will be used in the calculation if this set to false.
normalize*: Boolean, optional, default False*	If this parameter is set to True, the regressor X will be normalized before regression. The normalization will be done by subtracting the mean and dividing it by L2 norm. If *fit_intercept = False*, this parameter will be ignored.
copy_X*: Boolean, optional, default True*	By default, it is true which means X will be copied. But if it is set to false, X may be overwritten.
n_jobs*: int or None, optional(default=None)*	It represents the number of jobs to use for the computation.

Attributes

Following table consists the attributes used by **Linear Regression** module:

Attributes	Description

***coef_**: array, shape(n_features,) or (n_targets, n_features)*	It is used to estimate the coefficients for the linear regression problem. It would be a 2D array of shape (n_targets, n_features) if multiple targets are passed during fit. Ex. (y 2D). On the other hand, it would be a 1D array of length (n_features) if only one target is passed during fit.
***Intercept_**: array*	This is an independent term in this linear model.

Implementation Example

First, import the required packages:

```
import numpy as np
from sklearn.linear_model import LinearRegression
```

Now, provide the values for independent variable X:

```
X = np.array([[1,1],[1,2],[2,2],[2,3]])
```

Next, the value of dependent variable y can be calculated as follows:

```
y = np.dot(X, np.array([1,2])) + 3
```

Now, create a linear regression object as follows:

```
regr = LinearRegression(fit_intercept=True, normalize = True, copy_X=True,
n_jobs=2).fit(X,y)
```

Use predict() method to predict using this linear model as follows:

```
regr.predict(np.array([[3,5]]))
```

Output

```
array([16.])
```

To get the coefficient of determination of the prediction we can use Score() method as follows:

```
regr.score(X,y)
```

Output

```
1.0
```

We can estimate the coefficients by using attribute named 'coef' as follows:

```
regr.coef_
```

Output

```
array([1., 2.])
```

We can calculate the intercept i.e. the expected mean value of Y when all X = 0 by using attribute named 'intercept' as follows:

```
In [24]: regr.intercept_


Output
3.0000000000000018
```

Complete code of implementation example:

```
import numpy as np
from sklearn.linear_model import LinearRegression
X = np.array([[1,1],[1,2],[2,2],[2,3]])
y = np.dot(X, np.array([1,2])) + 3
regr = LinearRegression(fit_intercept=True, normalize = True, copy_X=True,
n_jobs=2).fit(X,y)
regr.predict(np.array([[3,5]]))
regr.score(X,y)
regr.coef_
regr.intercept_
```

Logistic Regression

Logistic regression, despite its name, is a classification algorithm rather than regression algorithm. Based on a given set of independent variables, it is used to estimate discrete value (0 or 1, yes/no, true/false). It is also called logit or MaxEnt Classifier.

Basically, it measures the relationship between the categorical dependent variable and one or more independent variables by estimating the probability of occurrence of an event using its logistics function.

sklearn.linear_model.LogisticRegression is the module used to implement logistic regression.

Parameters

Following table lists the parameters used by **Logistic Regression** module:

Parameter	Description
***penalty**: str, 'L1', 'L2', 'elasticnet' or none, optional, default = 'L2'*	This parameter is used to specify the norm (L1 or L2) used in penalization (regularization).

***dual**: Boolean, optional, default = False*	It is used for dual or primal formulation whereas dual formulation is only implemented for L2 penalty.
***tol**: float, optional, default=1e-4*	It represents the tolerance for stopping criteria.
***C**: float, optional, default=1.0*	It represents the inverse of regularization strength, which must always be a positive float.
***fit_intercept**: Boolean, optional, default = True*	This parameter specifies that a constant (bias or intercept) should be added to the decision function.
***intercept_scaling**: float, optional, default = 1*	This parameter is useful when • the **solver 'liblinear'** is used • ***fit_intercept*** is set to true
***class_weight**: dict or 'balanced' optional, default = none*	It represents the weights associated with classes. If we use the default option, it means all the classes are supposed to have weight one. On the other hand, if you choose *class_weight: balanced*, it will use the values of y to automatically adjust weights.
***random_state**: int, RandomState instance or None, optional, default = none*	This parameter represents the seed of the pseudo random number generated which is used while shuffling the data. Followings are the options: • **int**: in this case, *random_state* is the seed used by random number generator. • **RandomState instance**: in this case, *random_state* is the random number generator. • **None**: in this case, the random number generator is the RandonState instance used by np.random.
***solver**: str, {'newton-cg', 'lbfgs', 'liblinear', 'saag', 'saga'}, optional, default = 'liblinear'*	This parameter represents which algorithm to use in the optimization problem. Followings are the properties of options under this parameter: • **liblinear**: It is a good choice for small datasets. It also handles L1 penalty. For multiclass problems, it is limited to one-versus-rest schemes. • **newton-cg**: It handles only L2 penalty.

	• **lbfgs**: For multiclass problems, it handles multinomial loss. It also handles only L2 penalty. • **saga**: It is a good choice for large datasets. For multiclass problems, it also handles multinomial loss. Along with L1 penalty, it also supports 'elasticnet' penalty. • **sag**: It is also used for large datasets. For multiclass problems, it also handles multinomial loss.
***max_iter**: int, optional, default = 100*	As name suggest, it represents the maximum number of iterations taken for solvers to converge.
***multi_class**: str, {'ovr', 'multinomial', 'auto'}, optional, default = 'ovr'*	• **ovr**: For this option, a binary problem is fit for each label. • **multimonial**: For this option, the loss minimized is the multinomial loss fit across the entire probability distribution. We can't use this option if solver = 'liblinear'. • **auto**: This option will select 'ovr' if solver = 'liblinear' or data is binary, else it will choose 'multinomial'.
***verbose**: int, optional, default = 0*	By default, the value of this parameter is 0 but for liblinear and lbfgs solver we should set verbose to any positive number.
***warm_start**: bool, optional, default = false*	With this parameter set to True, we can reuse the solution of the previous call to fit as initialization. If we choose default i.e. false, it will erase the previous solution.
***n_jobs**: int or None, optional, default = None*	If multi_class = 'ovr', this parameter represents the number of CPU cores used when parallelizing over classes. It is ignored when solver = 'liblinear'.
***l1_ratio**: float or None, optional, default = None*	It is used in case when penalty = 'elasticnet'. It is basically the Elastic-Net mixing parameter with 0 < = l1_ratio < = 1.

Attributes

Followings table consist the attributes used by **Logistic Regression** module:

Attributes	Description

***coef_**: array, shape(n_features,) or (n_classes, n_features)*	It is used to estimate the coefficients of the features in the decision function. When the given problem is binary, it is of the shape (1, n_features).
***Intercept_**: array, shape(1) or (n_classes)*	It represents the constant, also known as bias, added to the decision function.
***classes_**: array, shape(n_classes)*	It will provide a list of class labels known to the classifier.
***n_iter_**: array, shape (n_classes) or (1)*	It returns the actual number of iterations for all the classes.

Implementation Example

Following Python script provides a simple example of implementing logistic regression on **iris** dataset of scikit-learn:

```
from sklearn import datasets

from sklearn import linear_model

from sklearn.datasets import load_iris

X, y = load_iris(return_X_y=True)

LRG = linear_model.LogisticRegression(random_state=0,solver='liblinear',multi
class='auto').fit(X, y)

LRG.score(X, y)
```

Output

```
0.96
```

The output shows that the above Logistic Regression model gave the accuracy of 96 percent.

Ridge Regression

Ridge regression or Tikhonov regularization is the regularization technique that performs L2 regularization. It modifies the loss function by adding the penalty (shrinkage quantity) equivalent to the square of the magnitude of coefficients.

$$\sum_{j=1}^{m}\left(Y_i - W_0 - \sum_{i=1}^{n} W_i X_{ji}\right)^2 + \alpha \sum_{i=1}^{n} W_i^2 = loss\_function + \alpha \sum_{i=1}^{n} W_i^2$$

- **sklearn.linear_model.Ridge** is the module used to solve a regression model where loss function is the linear least squares function and regularization is L2.

Parameters

Following table consists the parameters used by **Ridge** module:

Parameter	Description
alpha: {float, array-like}, shape(n_targets)	Alpha is the tuning parameter that decides how much we want to penalize the model.
fit_intercept: Boolean	This parameter specifies that a constant (bias or intercept) should be added to the decision function. No intercept will be used in calculation, if it will set to false.
tol: float, optional, default=1e-4	It represents the precision of the solution.
normalize: Boolean, optional, default = False	If this parameter is set to True, the regressor X will be normalized before regression. The normalization will be done by subtracting the mean and dividing it by L2 norm. If **fit_intercept = False**, this parameter will be ignored.
copy_X: Boolean, optional, default = True	By default, it is true which means X will be copied. But if it is set to false, X may be overwritten.
max_iter: int, optional	As name suggest, it represents the maximum number of iterations taken for conjugate gradient solvers.
solver: str, {'auto', 'svd', 'cholesky', 'lsqr', 'sparse_cg', 'sag', 'saga'}	This parameter represents which solver to use in the computational routines. Following are the properties of options under this parameter: • **auto:** It let choose the solver automatically based on the type of data**.** • **svd:** In order to calculate the Ridge coefficients, this parameter uses a Singular Value Decomposition of X. • **cholesky:** This parameter uses the standard **scipy.linalg.solve()** function to get a closed-form solution. • **Sparse_cg:** It uses the conjugate gradient solver which is more appropriate than 'cholesky' for large-scale data. • **lsqr:** It is the fastest and uses the dedicated regularized least-squares routine scipy.sparse.linalg.lsqr. • **sag:** It uses iterative process and a Stochastic Average Gradient descent.

	• **saga:** It also uses iterative process and an improved Stochastic Average Gradient descent.
random_state: int, RandomState instance or None, optional, default = none	This parameter represents the seed of the pseudo random number generated which is used while shuffling the data. Following are the options: • **int:** In this case, **random_state** is the seed used by random number generator. • **RandomState instance:** In this case, **random_state** is the random number generator. • **None:** In this case, the random number generator is the RandonState instance used by np.random.

Attributes

Followings table consist the attributes used by **Ridge** module:

Attributes	Description
***coef_**: array, shape(n_features,) or (n_target, n_features)*	This attribute provides the weight vectors.
***intercept_**: float | array, shape = (n_targets)*	It represents the independent term in decision function.
***n_iter_**: array or None, shape (n_targets)*	Available for only 'sag' and 'lsqr' solver, returns the actual number of iterations for each target.

Implementation Example

Following Python script provides a simple example of implementing Ridge Regression. We are using 15 samples and 10 features. The value of alpha is 0.5 in our case. There are two methods namely **fit()** and **score()** used to fit this model and calculate the score respectively.

```
from sklearn.linear_model import Ridge
import numpy as np
n_samples, n_features = 15, 10
rng = np.random.RandomState(0)
y = rng.randn(n_samples)
```

```
X = rng.randn(n_samples, n_features)
rdg = Ridge(alpha=0.5)
rdg.fit(X, y)
rdg.score(X,y)
```

Output

```
0.76294987
```

The output shows that the above Ridge Regression model gave the score of around 76 percent. For more accuracy, we can increase the number of samples and features.

For the above example, we can get the weight vector with the help of following python script:

```
rdg.coef_
```

Output

```
array([ 0.32720254, -0.34503436, -0.2913278 ,  0.2693125 , -0.22832508,
       -0.8635094 , -0.17079403, -0.36288055, -0.17241081, -0.43136046])
```

Similarly, we can get the value of intercept with the help of following python script:

```
rdg.intercept_
```

Output

```
0.527486
```

Bayesian Ridge Regression

Bayesian regression allows a natural mechanism to survive insufficient data or poorly distributed data by formulating linear regression using probability distributors rather than point estimates. The output or response 'y' is assumed to drawn from a probability distribution rather than estimated as a single value.

Mathematically, to obtain a fully probabilistic model the response y is assumed to be Gaussian distributed around X_w as follows:

$$p(y|X, w, \alpha) = N(y|X_w, \alpha)$$

One of the most useful type of Bayesian regression is Bayesian Ridge regression which estimates a probabilistic model of the regression problem. Here the prior for the coefficient w is given by spherical Gaussian as follows:

$$p(w|\lambda) = N(w|0, \lambda^{-1} I_p)$$

This resulting model is called Bayesian Ridge Regression and in scikit-learn **sklearn.linear_model.BeyesianRidge** module is used for Bayesian Ridge Regression.

Parameters

Followings table consist the parameters used by **BayesianRidge** module:

Parameter	Description
***n_iter**: int, optional*	It represents the maximum number of iterations. The default value is 300 but the user-defined value must be greater than or equal to 1.
***fit_intercept**: Boolean, optional, default True*	It decides whether to calculate the intercept for this model or not. No intercept will be used in calculation, if it will set to false.
***tol**: float, optional, default=1.e-3*	It represents the precision of the solution and will stop the algorithm if w has converged.
***alpha_1**: float, optional, default=1.e-6*	It is the 1st hyperparameter which is a shape parameter for the Gamma distribution prior over the alpha parameter.
***alpha_2**: float, optional, default=1.e-6*	It is the 2nd hyperparameter which is an inverse scale parameter for the Gamma distribution prior over the alpha parameter.
***lambda_1**: float, optional, default=1.e-6*	It is the 1st hyperparameter which is a shape parameter for the Gamma distribution prior over the lambda parameter.
***lambda_2**: float, optional, default=1.e-6*	It is the 2nd hyperparameter which is an inverse scale parameter for the Gamma distribution prior over the lambda parameter.
***copy_X**: Boolean, optional, default = True*	By default, it is true which means X will be copied. But if it is set to false, X may be overwritten.
***compute_score**: boolean, optional, default=False*	If set to true, it computes the log marginal likelihood at each iteration of the optimization.
***verbose**: Boolean, optional, default=False*	By default, it is false but if set true, verbose mode will be enabled while fitting the model.

Attributes

Followings table consist the attributes used by **BayesianRidge** module:

Attributes	Description
***coef_**: array, shape = n_features*	This attribute provides the weight vectors.
***intercept_**: float*	It represents the independent term in decision function.
***alpha_**: float*	This attribute provides the estimated precision of the noise.

***lambda_**: float*	This attribute provides the estimated precision of the weight.
***n_iter_**: int*	It provides the actual number of iterations taken by the algorithm to reach the stopping criterion.
***sigma_**: array, shape = (n_features, n_features)*	It provides the estimated variance-covariance matrix of the weights.
***scores_**: array, shape = (n_iter_+1)*	It provides the value of the log marginal likelihood at each iteration of the optimisation. In the resulting score, the array starts with the value of the log marginal likelihood obtained for the initial values of α and λ, and ends with the value obtained for estimated α and λ.

Implementation Example

Following Python script provides a simple example of fitting Bayesian Ridge Regression model using sklearn **BayesianRidge** module.

```
from sklearn import linear_model
X = [[0, 0], [1, 1], [2, 2], [3, 3]]
Y = [0, 1, 2, 3]
BayReg = linear_model.BayesianRidge()
BayReg.fit(X, Y)
```

Output

```
BayesianRidge(alpha_1=1e-06, alpha_2=1e-06, compute_score=False, copy_X=True,
       fit_intercept=True, lambda_1=1e-06, lambda_2=1e-06, n_iter=300,
       normalize=False, tol=0.001, verbose=False)
```

From the above output, we can check model's parameters used in the calculation.

Now, once fitted, the model can predict new values as follows:

```
BayReg.predict([[1,1]])
```

Output

```
array([1.00000007])
```

Similarly, we can access the coefficient w of the model as follows:

```
BayReg.coef_
```

Output

```
array([0.49999993, 0.49999993])
```

LASSO (Least Absolute Shrinkage and Selection Operator)

LASSO is the regularisation technique that performs L1 regularisation. It modifies the loss function by adding the penalty (shrinkage quantity) equivalent to the summation of the absolute value of coefficients.

$$\sum_{j=1}^{m}\left(Y_i - W_0 - \sum_{i=1}^{n} W_i X_{ji}\right)^2 + \alpha \sum_{i=1}^{n}|W_i| = loss\_function + \alpha \sum_{i=1}^{n}|W_i|$$

sklearn.linear_model. Lasso is a linear model, with an added regularisation term, used to estimate sparse coefficients.

Parameters

Followings table consist the parameters used by **Lasso** module:

Parameter	Description
***alpha**: float, optional, default = 1.0*	Alpha, the constant that multiplies the L1 term, is the tuning parameter that decides how much we want to penalize the model. The default value is 1.0.
***fit_intercept**: Boolean, optional. Default=True*	This parameter specifies that a constant (bias or intercept) should be added to the decision function. No intercept will be used in calculation, if it will set to false.
***tol**: float, optional*	This parameter represents the tolerance for the optimization. The ***tol*** value and updates would be compared and if found updates smaller than ***tol***, the optimization checks the dual gap for optimality and continues until it is smaller than ***tol***.
***normalize**: Boolean, optional, default = False*	If this parameter is set to True, the regressor X will be normalized before regression. The normalization will be done by subtracting the mean and dividing it by L2 norm. If ***fit_intercept = False***, this parameter will be ignored.
***copy_X**: Boolean, optional, default = True*	By default, it is true which means X will be copied. But if it is set to false, X may be overwritten.
***max_iter**: int, optional*	As name suggest, it represents the maximum number of iterations taken for conjugate gradient solvers.
***precompute**: True|False|array-like, default=False*	With this parameter we can decide whether to use a precomputed Gram matrix to speed up the calculation or not.

***warm_start**: bool, optional, default = false*	With this parameter set to True, we can reuse the solution of the previous call to fit as initialization. If we choose default i.e. false, it will erase the previous solution.
***random_state**: int, RandomState instance or None, optional, default = none*	This parameter represents the seed of the pseudo random number generated which is used while shuffling the data. Followings are the options: • **int**: In this case, *random_state* is the seed used by random number generator. • **RandomState instance**: In this case, ***random_state*** is the random number generator. • **None**: In this case, the random number generator is the RandonState instance used by np.random.
***selection**: str, default='cyclic'*	• **Cyclic**: The default value is cyclic which means the features will be looping over sequentially by default. • **Random**: If we set the selection to random, a random coefficient will be updated every iteration.

Attributes

Followings table consist the attributes used by **Lasso** module:

Attributes	Description
***coef_**: array, shape(n_features,) or (n_target, n_features)*	This attribute provides the weight vectors.
***intercept_**: float | array, shape = (n_targets)*	It represents the independent term in decision function.
***n_iter_**: int or array-like, shape (n_targets)*	It gives the number of iterations run by the coordinate descent solver to reach the specified tolerance.

Implementation Example

Following Python script uses Lasso model which further uses coordinate descent as the algorithm to fit the coefficients:

```
from sklearn import linear_model
Lreg = linear_model.Lasso(alpha=0.5)
Lreg.fit([[0,0], [1, 1], [2, 2]], [0, 1, 2])
```

Output

```
Lasso(alpha=0.5, copy_X=True, fit_intercept=True, max_iter=1000,
   normalize=False, positive=False, precompute=False, random_state=None,
   selection='cyclic', tol=0.0001, warm_start=False)
```

Now, once fitted, the model can predict new values as follows:

```
Lreg.predict([[0,1]])
```

Output

```
array([0.75])
```

For the above example, we can get the weight vector with the help of following python script:

```
Lreg.coef_
```

Output

```
array([0.25, 0.  ])
```

Similarly, we can get the value of intercept with the help of following python script:

```
Lreg.intercept_
```

Output

```
0.75
```

We can get the total number of iterations to get the specified tolerance with the help of following python script:

```
Lreg.n_iter_
```

Output

```
2
```

We can change the values of parameters to get the desired output from the model.

Multi-task LASSO

It allows to fit multiple regression problems jointly enforcing the selected features to be same for all the regression problems, also called tasks. Sklearn provides a linear model

named **MultiTaskLasso**, trained with a mixed L1, L2-norm for regularisation, which estimates sparse coefficients for multiple regression problems jointly. In this the response y is a 2D array of shape (n_samples, n_tasks).

The **parameters** and the **attributes** for **MultiTaskLasso** are like that of **Lasso**. The only difference is in the alpha parameter. In Lasso the alpha parameter is a constant that multiplies L1 norm, whereas in Multi-task Lasso it is a constant that multiplies the L1/L2 terms.

And, opposite to Lasso, MultiTaskLasso doesn't have **precompute** attribute.

Implementation Example

Following Python script uses **MultiTaskLasso** linear model which further uses coordinate descent as the algorithm to fit the coefficients:

```
from sklearn import linear_model
MTLReg = linear_model.MultiTaskLasso(alpha=0.5)
MTLReg.fit([[0,0], [1, 1], [2, 2]], [[0, 0],[1,1],[2,2]])
```

Output

```
MultiTaskLasso(alpha=0.5, copy_X=True, fit_intercept=True, max_iter=1000,
        normalize=False, random_state=None, selection='cyclic', tol=0.0001,
        warm_start=False)
```

Now, once fitted, the model can predict new values as follows:

```
MTLReg.predict([[0,1]])
```

Output

```
array([[0.53033009, 0.53033009]])
```

For the above example, we can get the weight vector with the help of following python script:

```
MTLReg.coef_
```

Output

```
array([[0.46966991, 0.        ],
       [0.46966991, 0.        ]])
```

Similarly, we can get the value of intercept with the help of following python script:

```
MTLReg.intercept_
```

Output

```
array([0.53033009, 0.53033009])
```

We can get the total number of iterations to get the specified tolerance with the help of following python script:

```
MTLReg.n_iter_
```

Output

```
2
```

We can change the values of parameters to get the desired output from the model.

Elastic-Net

The Elastic-Net is a regularised regression method that linearly combines both penalties i.e. L1 and L2 of the Lasso and Ridge regression methods. It is useful when there are multiple correlated features. The difference between Lass and Elastic-Net lies in the fact that Lasso is likely to pick one of these features at random while elastic-net is likely to pick both at once.

Sklearn provides a linear model named **ElasticNet** which is trained with both L1, L2-norm for regularisation of the coefficients. The advantage of such combination is that it allows for learning a sparse model where few of the weights are non-zero like Lasso regularisation method, while still maintaining the regularization properties of Ridge regularisation method.

Following is the objective function to minimise:

$$\min_{w} \frac{1}{2n_{samples}} ||X_w - y||_2^2 + \alpha\rho||w||_1 + \frac{\alpha(1-\rho)}{2}||w||_2^2$$

Parameters

Following table consist the parameters used by **ElasticNet** module:

Parameter	Description
***alpha**: float, optional, default = 1.0*	Alpha, the constant that multiplies the L1/L2 term, is the tuning parameter that decides how much we want to penalize the model. The default value is 1.0.
***l1_ratio**: float*	This is called the ElasticNet mixing parameter. Its range is 0 < = l1_ratio < = 1. If l1_ratio = 1, the penalty would be L1 penalty. If l1_ratio = 0, the penalty would be an L2 penalty. If the value of l1 ratio is between 0 and 1, the penalty would be the combination of L1 and L2.

***fit_intercept**: Boolean, optional. Default=True*	This parameter specifies that a constant (bias or intercept) should be added to the decision function. No intercept will be used in calculation, if it will set to false.
***tol**: float, optional*	This parameter represents the tolerance for the optimization. The *tol* value and updates would be compared and if found updates smaller than *tol*, the optimization checks the dual gap for optimality and continues until it is smaller than *tol.*
***normalise**: Boolean, optional, default = False*	If this parameter is set to True, the regressor X will be normalised before regression. The normalisation will be done by subtracting the mean and dividing it by L2 norm. If ***fit_intercept = False***, this parameter will be ignored.
***precompute**: True|False|array-like, default=False*	With this parameter we can decide whether to use a precomputed Gram matrix to speed up the calculation or not. To preserve sparsity, it would always be true for sparse input.
***copy_X**: Boolean, optional, default = True*	By default, it is true which means X will be copied. But if it is set to false, X may be overwritten.
***max_iter**: int, optional*	As name suggest, it represents the maximum number of iterations taken for conjugate gradient solvers.
***warm_start**: bool, optional, default = false*	With this parameter set to True, we can reuse the solution of the previous call to fit as initialisation. If we choose default i.e. false, it will erase the previous solution.

***random_state**: int, RandomState instance or None, optional, default = none*	This parameter represents the seed of the pseudo random number generated which is used while shuffling the data. Following are the options: • **int:** In this case, *random_state* is the seed used by random number generator. • **RandomState instance**: In this case, *random_state* is the random number generator. • **None:** In this case, the random number generator is the RandonState instance used by np.random.
***selection**: str, default='cyclic'*	• Cyclic: The default value is cyclic which means the features will be looping over sequentially by default. • Random: If we set the selection to random, a random coefficient will be updated every iteration.

Attributes

Followings table consist the attributes used by **ElasticNet** module:

Attributes	Description
***coef_**: array, shape (n_tasks, n_features)*	This attribute provides the weight vectors.
***intercept_**: array, shape (n_tasks)*	It represents the independent term in decision function.
***n_iter_**: int*	It gives the number of iterations run by the coordinate descent solver to reach the specified tolerance.

Implementation Example

Following Python script uses **ElasticNet** linear model which further uses coordinate descent as the algorithm to fit the coefficients:

```
from sklearn import linear_model
ENreg = linear_model.ElasticNet(alpha=0.5,random_state=0)
```

```
ENreg.fit([[0,0], [1, 1], [2, 2]], [0, 1, 2])
```

Output

```
ElasticNet(alpha=0.5, copy_X=True, fit_intercept=True, l1_ratio=0.5,
      max_iter=1000, normalize=False, positive=False, precompute=False,
      random_state=0, selection='cyclic', tol=0.0001, warm_start=False)
```

Now, once fitted, the model can predict new values as follows:

```
ENregReg.predict([[0,1]])
```

Output

```
array([0.73686077])
```

For the above example, we can get the weight vector with the help of following python script:

```
ENreg.coef_
```

Output

```
array([0.26318357, 0.26313923])
```

Similarly, we can get the value of intercept with the help of following python script:

```
ENreg.intercept_
```

Output

```
0.47367720941913904
```

We can get the total number of iterations to get the specified tolerance with the help of following python script:

```
ENreg.n_iter_
```

Output

```
15
```

We can change the values of alpha (towards 1) to get better results from the model.

Let us see same example with alpha = 1.

```
from sklearn import linear_model
ENreg = linear_model.ElasticNet(alpha=1,random_state=0)
ENreg.fit([[0,0], [1, 1], [2, 2]], [0, 1, 2])
```

```
Output
ElasticNet(alpha=1, copy_X=True, fit_intercept=True, l1_ratio=0.5,
      max_iter=1000, normalize=False, positive=False, precompute=False,
      random_state=0, selection='cyclic', tol=0.0001, warm_start=False)

#Predicting new values
ENreg.predict([[1,0]])

Output
array([0.90909216])

#weight vectors
ENreg.coef_

Output
array([0.09091128, 0.09090784])

#Calculating intercept
ENreg.intercept_

Output
0.818180878658411

#Calculating number of iterations

ENreg.n_iter_

Output
10
```

From the above examples, we can see the difference in the outputs.

MultiTaskElasticNet

It is an Elastic-Net model that allows to fit multiple regression problems jointly enforcing the selected features to be same for all the regression problems, also called tasks. Sklearn provides a linear model named **MultiTaskElasticNet**, trained with a mixed L1, L2-norm and L2 for regularisation, which estimates sparse coefficients for multiple regression problems jointly. In this, the response y is a 2D array of shape (n_samples, n_tasks).

Following is the objective function to minimize:

$$\min_{w} \frac{1}{2n_{samples}} ||X_w - y||_{Fro}^2 + \alpha\rho||w||_{21} + \frac{\alpha(1-\rho)}{2}||w||_{Fro}^2$$

As in MultiTaskLasso, here also, Fro indicates the Frobenius norm:

$$||A||_{Fro} = \sqrt{\sum_{ij} a_{ij}^2}$$

And L1L2 leads to the following:

$$||A||_{21} = \sum_{i} \sqrt{\sum_{j} a_{ij}^2}$$

The **parameters** and the **attributes** for **MultiTaskElasticNet** are like that of **ElasticNet**. The only difference is in li_ratio i.e. ElasticNet mixing parameter. In **MultiTaskElasticNet** its range is 0 < l1_ratio < = 1. If l1_ratio = 1, the penalty would be L1/L2 penalty. If l1_ratio = 0, the penalty would be an L2 penalty. If the value of l1 ratio is between 0 and 1, the penalty would be the combination of L1/L2 and L2.

And, opposite to **ElasticNet, MultiTaskElasticNet** doesn't have **precompute** attribute.

Implementation Example

To show the difference, we are implementing the same example as we did in Multi-task Lasso:

```
from sklearn import linear_model
MTENReg = linear_model.MultiTaskElasticNet(alpha=0.5)
MTENReg.fit([[0,0], [1, 1], [2, 2]], [[0, 0],[1,1],[2,2]])

Output
MultiTaskElasticNet(alpha=0.5, copy_X=True, fit_intercept=True, l1_ratio=0.5,
          max_iter=1000, normalize=False, random_state=None,
          selection='cyclic', tol=0.0001, warm_start=False)

#Predicting new values
MTENReg.predict([[1,0]])

Output
array([[0.69056563, 0.69056563]])

#weight vectors
```

```
MTENReg.coef_
```

Output

```
array([[0.30943437, 0.30938224],
       [0.30943437, 0.30938224]])

#Calculating intercept
MTENReg.intercept_
```

Output

```
array([0.38118338, 0.38118338])

#Calculating number of iterations

MTENReg.n_iter_
```

Output

```
15
```

7. Scikit-Learn — Extended Linear Modeling

This chapter focusses on the polynomial features and pipelining tools in Sklearn.

Introduction to Polynomial Features

Linear models trained on non-linear functions of data generally maintains the fast performance of linear methods. It also allows them to fit a much wider range of data. That's the reason in machine learning such linear models, that are trained on nonlinear functions, are used.

One such example is that a simple linear regression can be extended by constructing polynomial features from the coefficients.

Mathematically, suppose we have standard linear regression model then for 2-D data it would look like this:

$$Y = w_0 + w_1 x_1 + w_2 x_2$$

Now, we can combine the features in second-order polynomials and our model will look like as follows:

$$Y = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1 x_2 + w_4 x_1^2 + w_5 x_2^2$$

The above is still a linear model. Here, we saw that the resulting polynomial regression is in the same class of linear models and can be solved similarly.

To do so, scikit-learn provides a module named **PolynomialFeatures**. This module transforms an input data matrix into a new data matrix of given degree.

Parameters

Followings table consist the parameters used by **PolynomialFeatures** module:

Parameter	Description
***degree**: integer, default = 2*	It represents the degree of the polynomial features.
***interaction_only**: Boolean, default = false*	By default, it is false but if set as true, the features that are products of most degree distinct input features, are produced. Such features are called interaction features.
***include_bias**: Boolean, default = true*	It includes a bias column i.e. the feature in which all polynomials powers are zero.

***order**: str in {'C', 'F'}, default = 'C'*	This parameter represents the order of output array in the dense case. 'F' order means faster to compute but on the other hand, it may slow down subsequent estimators.

Attributes

Followings table consist the attributes used by **PolynomialFeatures** module:

Attributes	Description
***powers_**: array, shape (n_output_features, n_input_features)*	It shows powers_ [i,j] is the exponent of the jth input in the ith output.
***n_input_features _:** int*	As name suggests, it gives the total number of input features.
***n_output_features _:** int*	As name suggests, it gives the total number of polynomial output features.

Implementation Example

Following Python script uses **PolynomialFeatures** transformer to transform array of 8 into shape (4,2):

```
from sklearn.preprocessing import PolynomialFeatures
import numpy as np
Y = np.arange(8).reshape(4, 2)
poly = PolynomialFeatures(degree=2)
poly.fit_transform(Y)
```

Output

```
array([[ 1.,  0.,  1.,  0.,  0.,  1.],
       [ 1.,  2.,  3.,  4.,  6.,  9.],
       [ 1.,  4.,  5., 16., 20., 25.],
       [ 1.,  6.,  7., 36., 42., 49.]])
```

Streamlining using Pipeline tools

The above sort of preprocessing i.e. transforming an input data matrix into a new data matrix of a given degree, can be streamlined with the **Pipeline** tools, which are basically used to chain multiple estimators into one.

Example

The below python scripts using Scikit-learn's Pipeline tools to streamline the preprocessing (will fit to an order-3 polynomial data).

```
#First, import the necessary packages.
```

```
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
from sklearn.pipeline import Pipeline
import numpy as np

#Next, create an object of Pipeline tool

Stream_model = Pipeline([('poly', PolynomialFeatures(degree=3)),
('linear', LinearRegression(fit_intercept=False))])

#Provide the size of array and order of polynomial data to fit the model.

x = np.arange(5)
y = 3 - 2 * x + x ** 2 - x ** 3
Stream_model = model.fit(x[:, np.newaxis], y)

#Calculate the input polynomial coefficients.

Stream_model.named_steps['linear'].coef_
```

Output

```
array([ 3., -2.,  1., -1.])
```

The above output shows that the linear model trained on polynomial features is able to recover the exact input polynomial coefficients.

8. Scikit-Learn — Stochastic Gradient Descent

Here, we will learn about an optimization algorithm in Sklearn, termed as Stochastic Gradient Descent (SGD).

Stochastic Gradient Descent (SGD) is a simple yet efficient optimization algorithm used to find the values of parameters/coefficients of functions that minimize a cost function. In other words, it is used for discriminative learning of linear classifiers under convex loss functions such as SVM and Logistic regression. It has been successfully applied to large-scale datasets because the update to the coefficients is performed for each training instance, rather than at the end of instances.

SGD Classifier

Stochastic Gradient Descent (SGD) classifier basically implements a plain SGD learning routine supporting various loss functions and penalties for classification. Scikit-learn provides **SGDClassifier** module to implement SGD classification.

Parameters

Followings table consist the parameters used by **SGDClassifier** module:

Parameter	Description
***loss**: str, default = 'hinge'*	It represents the loss function to be used while implementing. The default value is 'hinge' which will give us a linear SVM. The other options which can be used are: • **log**: This loss will give us logistic regression i.e. a probabilistic classifier. • **modified_huber**: a smooth loss that brings tolerance to outliers along with probability estimates. • **squared_hinge**: similar to 'hinge' loss but it is quadratically penalized. • **perceptron**: as the name suggests, it is a linear loss which is used by the perceptron algorithm.
***penalty**: str, 'none', 'l2', 'l1', 'elasticnet'*	It is the regularization term used in the model. By default, it is L2. We can use L1 or 'elasticnet; as well but both might bring sparsity to the model, hence not achievable with L2.
***alpha**: float, default = 0.0001*	Alpha, the constant that multiplies the regularization term, is the tuning parameter that decides how much we want to penalize the model. The default value is 0.0001.

***l1_ratio**: float, default = 0.15*	This is called the ElasticNet mixing parameter. Its range is 0 < = l1_ratio < = 1. If l1_ratio = 1, the penalty would be L1 penalty. If l1_ratio = 0, the penalty would be an L2 penalty.
***fit_intercept**: Boolean, Default=True*	This parameter specifies that a constant (bias or intercept) should be added to the decision function. No intercept will be used in calculation and data will be assumed already centered, if it will set to false.
***tol**: float or none, optional, default = 1.e-3*	This parameter represents the stopping criterion for iterations. Its default value is False but if set to None, the iterations will stop when $loss > best\_loss - tol$ **for** $n\_iter\_no\_change$ successive epochs.
***shuffle**: Boolean, optional, default = True*	This parameter represents that whether we want our training data to be shuffled after each epoch or not.
***verbose**: integer, default = 0*	It represents the verbosity level. Its default value is 0.
***epsilon**: float, default = 0.1*	This parameter specifies the width of the insensitive region. If loss = 'epsilon-insensitive', any difference, between current prediction and the correct label, less than the threshold would be ignored.
***max_iter**: int, optional, default = 1000*	As name suggest, it represents the maximum number of passes over the epochs i.e. training data.
***warm_start**: bool, optional, default = false*	With this parameter set to True, we can reuse the solution of the previous call to fit as initialization. If we choose default i.e. false, it will erase the previous solution.
***random_state**: int, RandomState instance or None, optional, default = none*	This parameter represents the seed of the pseudo random number generated which is used while shuffling the data. Followings are the options: • int: In this case, ***random_state*** is the seed used by random number generator. • RandomState instance: In this case, ***random_state*** is the random number generator. • None: In this case, the random number generator is the RandonState instance used by np.random.
***n_jobs**: int or none, optional, Default = None*	It represents the number of CPUs to be used in OVA (One Versus All) computation, for multi-class problems. The default value is none which means 1.

***learning_rate**: string, optional, default = 'optimal'*	• If learning rate is 'constant', eta = eta0; • If learning rate is 'optimal', eta = 1.0/(alpha*(t+t0)), where t0 is chosen by Leon Bottou; • If learning rate = 'invscalling', eta = eta0/pow(t, power_t). • If learning rate = 'adaptive', eta = eta0.
***eta0**: double, default = 0.0*	It represents the initial learning rate for above mentioned learning rate options i.e. 'constant', 'invscalling', or 'adaptive'.
***power_t** : double, default =0.5*	It is the exponent for 'incscalling' learning rate.
***early_stopping**: bool, default = False*	This parameter represents the use of early stopping to terminate training when validation score is not improving. Its default value is false but when set to true, it automatically set aside a stratified fraction of training data as validation and stop training when validation score is not improving.
***validation_fraction**: float, default = 0.1*	It is only used when early_stopping is true. It represents the proportion of training data to set asides as validation set for early termination of training data.
***n_iter_no_change** : int, default=5*	It represents the number of iteration with no improvement should algorithm run before early stopping.
***classs_weight**: dict, {class_label: weight} or "balanced", or None, optional*	This parameter represents the weights associated with classes. If not provided, the classes are supposed to have weight 1.
***warm_start**: bool, optional, default = false*	With this parameter set to True, we can reuse the solution of the previous call to fit as initialization. If we choose default i.e. false, it will erase the previous solution.
***average**: Boolean or int, optional, default = false*	Its default value is False but when set to True, it calculates the averaged Stochastic Gradient Descent weights and stores the result in the coef_ attribute. On the other hand, if its value set to an integer greater than 1, the averaging will begin once the total number of samples seen reaches.

Attributes

Following table consist the attributes used by **SGDClassifier** module:

Attributes	Description
***coef_**: array, shape (1, n_features) if n_classes==2, else (n_classes, n_features)*	This attribute provides the weight assigned to the features.
***intercept_**: array, shape (1,) if n_classes==2, else (n_classes,)*	It represents the independent term in decision function.
***n_iter_:** int*	It gives the number of iterations to reach the stopping criterion.

Implementation Example

Like other classifiers, Stochastic Gradient Descent (SGD) has to be fitted with following two arrays:

- An array X holding the training samples. It is of size [n_samples, n_features].
- An array Y holding the target values i.e. class labels for the training samples. It is of size [n_samples].

Following Python script uses SGDClassifier linear model:

```
import numpy as np
from sklearn import linear_model
X = np.array([[-1, -1], [-2, -1], [1, 1], [2, 1]])
Y = np.array([1, 1, 2, 2])
SGDClf = linear_model.SGDClassifier(max_iter=1000, tol=1e-
3,penalty="elasticnet")
SGDClf.fit(X, Y)
```

Output

```
SGDClassifier(alpha=0.0001, average=False, class_weight=None,
       early_stopping=False, epsilon=0.1, eta0=0.0, fit_intercept=True,
       l1_ratio=0.15, learning_rate='optimal', loss='hinge', max_iter=1000,
       n_iter=None, n_iter_no_change=5, n_jobs=None, penalty='elasticnet',
       power_t=0.5, random_state=None, shuffle=True, tol=0.001,
       validation_fraction=0.1, verbose=0, warm_start=False)
```

Now, once fitted, the model can predict new values as follows:

```
SGDClf.predict([[2.,2.]])
```

Output

```
array([2])
```

For the above example, we can get the weight vector with the help of following python script:

```
SGDClf.coef_
```

Output

```
array([[19.54811198,  9.77200712]])
```

Similarly, we can get the value of intercept with the help of following python script:

```
SGDClf.intercept_
```

Output

```
array([10.])
```

We can get the signed distance to the hyperplane by using **SGDClassifier.decision_function** as used in the following python script:

```
SGDClf.decision_function([[2., 2.]])
```

Output

```
array([68.6402382])
```

SGD Regressor

Stochastic Gradient Descent (SGD) regressor basically implements a plain SGD learning routine supporting various loss functions and penalties to fit linear regression models. Scikit-learn provides **SGDRegressor** module to implement SGD regression.

Parameters

Parameters used by **SGDRegressor** are almost same as that were used in **SGDClassifier** module. The difference lies in 'loss' parameter. For **SGDRegressor** modules' loss parameter the positives values are as follows:

- **squared_loss:** It refers to the ordinary least squares fit.
- **huber: SGDRegressor** correct the outliers by switching from squared to linear loss past a distance of epsilon. The work of 'huber' is to modify 'squared_loss' so that algorithm focus less on correcting outliers.
- **epsilon_insensitive:** Actually, it ignores the errors less than epsilon.
- **squared_epsilon_insensitive:** It is same as epsilon_insensitive. The only difference is that it becomes squared loss past a tolerance of epsilon.

Another difference is that the parameter named 'power_t' has the default value of 0.25 rather than 0.5 as in **SGDClassifier**. Furthermore, it doesn't have 'class_weight' and 'n_jobs' parameters.

Attributes

Attributes of **SGDRegressor** are also same as that were of **SGDClassifier** module. Rather it has three extra attributes as follows:

- **average_coef_**: array, shape(n_features,)

As name suggest, it provides the average weights assigned to the features.

- **average_intercept_**: array, shape(1,)

As name suggest, it provides the averaged intercept term.

- **t_**: int

It provides the number of weight updates performed during the training phase.

Note: the attributes average_coef_ and average_intercept_ will work after enabling parameter 'average' to True.

Implementation Example

Following Python script uses **SGDRegressor** linear model:

```
import numpy as np
from sklearn import linear_model
n_samples, n_features = 10, 5
rng = np.random.RandomState(0)
y = rng.randn(n_samples)

X = rng.randn(n_samples, n_features)
SGDReg
=linear_model.SGDRegressor(max_iter=1000,penalty="elasticnet",loss='huber',tol=
1e-3, average=True)
SGDReg.fit(X, y)
```

Output

```
SGDRegressor(alpha=0.0001, average=True, early_stopping=False, epsilon=0.1,
       eta0=0.01, fit_intercept=True, l1_ratio=0.15,
       learning_rate='invscaling', loss='huber', max_iter=1000,
       n_iter=None, n_iter_no_change=5, penalty='elasticnet', power_t=0.25,

       random_state=None, shuffle=True, tol=0.001, validation_fraction=0.1,
```

```
        verbose=0, warm_start=False)
```

Now, once fitted, we can get the weight vector with the help of following python script:

```
SGDReg.coef_
```

Output

```
array([-0.00423314,  0.00362922, -0.00380136,  0.00585455,  0.00396787])
```

Similarly, we can get the value of intercept with the help of following python script:

```
SGReg.intercept_
```

Output

```
array([0.00678258])
```

We can get the number of weight updates during training phase with the help of the following python script:

```
SGDReg.t_
```

Output

```
61.0
```

Pros and Cons of SGD

Following the pros of SGD:

- Stochastic Gradient Descent (SGD) is very efficient.
- It is very easy to implement as there are lots of opportunities for code tuning.

Following the cons of SGD:

- Stochastic Gradient Descent (SGD) requires several hyperparameters like regularization parameters.
- It is sensitive to feature scaling.

9. Scikit-Learn — Support Vector Machines (SVMs)

This chapter deals with a machine learning method termed as Support Vector Machines (SVMs).

Introduction

Support vector machines (SVMs) are powerful yet flexible supervised machine learning methods used for classification, regression, and, outliers' detection. SVMs are very efficient in high dimensional spaces and generally are used in classification problems. SVMs are popular and memory efficient because they use a subset of training points in the decision function.

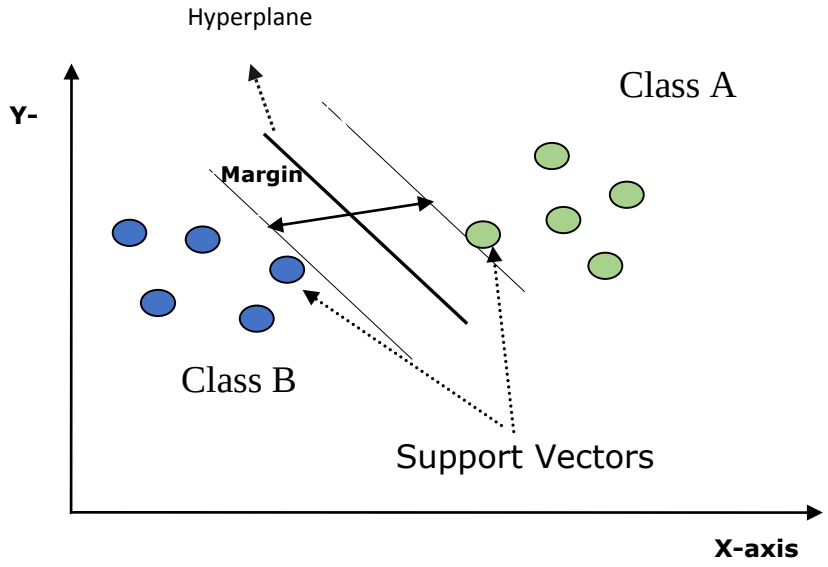
The main goal of SVMs is to divide the datasets into number of classes in order to find a **maximum marginal hyperplane (MMH)** which can be done in the following two steps:

- Support Vector Machines will first generate hyperplanes iteratively that separates the classes in the best way.
- After that it will choose the hyperplane that segregate the classes correctly.

Some important concepts in SVM are as follows:

- **Support Vectors:** They may be defined as the datapoints which are closest to the hyperplane. Support vectors help in deciding the separating line.
- **Hyperplane:** The decision plane or space that divides set of objects having different classes.
- **Margin:** The gap between two lines on the closet data points of different classes is called margin.

Following diagrams will give you an insight about these SVM concepts:



SVM in Scikit-learn supports both sparse and dense sample vectors as input.

Classification of SVM

Scikit-learn provides three classes namely **SVC, NuSVC** and **LinearSVC** which can perform multiclass-class classification.

SVC

It is C-support vector classification whose implementation is based on **libsvm**. The module used by scikit-learn is **sklearn.svm.SVC**. This class handles the multiclass support according to one-vs-one scheme.

Parameters

Followings table consist the parameters used by **sklearn.svm.SVC** class:

Parameter	Description
C: *float, optional, default = 1.0*	It is the penalty parameter of the error term.
kernel: *string, optional, default = 'rbf'*	This parameter specifies the type of kernel to be used in the algorithm. we can choose any one among, '**linear**', '**poly**', '**rbf**', '**sigmoid**', '**precomputed**'. The default value of kernel would be '**rbf**'.
degree: *int, optional, default = 3*	It represents the degree of the 'poly' kernel function and will be ignored by all other kernels.
gamma: *{'scale', 'auto'} or float,*	It is the kernel coefficient for kernels 'rbf', 'poly' and 'sigmoid'.

optinal default = *'scale'*	If you choose default i.e. gamma = 'scale' then the value of gamma to be used by SVC is $1/(n\_features * X.var())$. On the other hand, if gamma= 'auto', it uses $1/n\_features$.
coef0*: float, optional, Default=0.0*	An independent term in kernel function which is only significant in 'poly' and 'sigmoid'.
tol*: float, optional, default = 1.e-3*	This parameter represents the stopping criterion for iterations.
shrinking*: Boolean, optional, default = True*	This parameter represents that whether we want to use shrinking heuristic or not.
verbose*: Boolean, default: false*	It enables or disable verbose output. Its default value is false.
probability*: boolean, optional, default = true*	This parameter enables or disables probability estimates. The default value is false, but it must be enabled before we call `fit`.
max_iter*: int, optional, default = -1*	As name suggest, it represents the maximum number of iterations within the solver. Value -1 means there is no limit on the number of iterations.
cache_size*: float, optional*	This parameter will specify the size of the kernel cache. The value will be in MB(MegaBytes).
random_state*: int, RandomState instance or None, optional, default = none*	This parameter represents the seed of the pseudo random number generated which is used while shuffling the data. Followings are the options: • **int**: In this case, *random_state* is the seed used by random number generator. • **RandomState instance**: In this case, *random_state* is the random number generator. • **None**: In this case, the random number generator is the RandonState instance used by np.random.
class_weight*: {dict, 'balanced'}, optional*	This parameter will set the parameter C of class j to $class\_weight[j] * C$ for SVC. If we use the default option, it means all the classes are supposed to have weight one. On the other hand, if you choose ***class_weight: balanced***, it will use the values of y to automatically adjust weights.

***decision_function_shape**: 'ovo', 'ovr', default = 'ovr'*	This parameter will decide whether the algorithm will return '**ovr**' (one-vs-rest) decision function of shape as all other classifiers, or the original **ovo**(one-vs-one) decision function of libsvm.
***break_ties**: boolean, optional, default = false*	**True**: The predict will break ties according to the confidence values of decision_function **False**: The predict will return the first class among the tied classes.

Attributes

Followings table consist the attributes used by **sklearn.svm.SVC** class:

Attributes	Description
***support_**: array-like, shape = [n_SV]*	It returns the indices of support vectors.
***support_vectors_**: array-like, shape = [n_SV, n_features]*	It returns the support vectors.
***n_support_**: array-like, dtype=int32, shape = [n_class]*	It represents the number of support vectors for each class.
***dual_coef_**: array, shape = [n_class-1,n_SV]*	These are the coefficient of the support vectors in the decision function.
***coef_**: array, shape = [n_class * (n_class-1)/2, n_features]*	This attribute, only available in case of linear kernel, provides the weight assigned to the features.
***intercept_**: array, shape = [n_class * (n_class-1)/2]*	It represents the independent term (constant) in decision function.
***fit_status_**: int*	The output would be 0 if it is correctly fitted. The output would be 1 if it is incorrectly fitted.
***classes_**: array of shape = [n_classes]*	It gives the labels of the classes.

Implementation Example

Like other classifiers, SVC also has to be fitted with following two arrays:

- An array **X** holding the training samples. It is of size [n_samples, n_features].
- An array **Y** holding the target values i.e. class labels for the training samples. It is of size [n_samples].

Following Python script uses **sklearn.svm.SVC** class:

```
import numpy as np
X = np.array([[-1, -1], [-2, -1], [1, 1], [2, 1]])
y = np.array([1, 1, 2, 2])
from sklearn.svm import SVC
SVCClf = SVC(kernel='linear',gamma='scale', shrinking=False,)
SVCClf.fit(X, y)
```

Output

```
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape='ovr', degree=3, gamma='scale', kernel='linear',
  max_iter=-1, probability=False, random_state=None, shrinking=False,
  tol=0.001, verbose=False)
```

Now, once fitted, we can get the weight vector with the help of following python script

```
SVCClf.coef_
```

Output

```
array([[0.5, 0.5]])
```

Similarly, we can get the value of other attributes as follows:

```
SVCClf.predict([[-0.5,-0.8]])
```

Output

```
array([1])
```

```
SVCClf.n_support_
```

Output

```
array([1, 1])
```

```
SVCClf.support_vectors_
```

Output

```
array([[-1., -1.],
       [ 1.,  1.]])
```

```
SVCClf.support_
```

Output

```
array([0, 2])
```

```
SVCClf.intercept_
```

Output

```
array([-0.])
```

```
SVCClf.fit_status_
```

Output

```
0
```

NuSVC

NuSVC is Nu Support Vector Classification. It is another class provided by scikit-learn which can perform multi-class classification. It is like SVC but NuSVC accepts slightly different sets of parameters. The parameter which is different from SVC is as follows:

- **nu:** float, optional, default = 0.5

It represents an upper bound on the fraction of training errors and a lower bound of the fraction of support vectors. Its value should be in the interval of (o,1].

Rest of the parameters and attributes are same as of SVC.

Implementation Example

We can implement the same example using **sklearn.svm.NuSVC** class also.

```
import numpy as np
X = np.array([[-1, -1], [-2, -1], [1, 1], [2, 1]])
y = np.array([1, 1, 2, 2])
from sklearn.svm import NuSVC
NuSVCClf = NuSVC(kernel='linear',gamma='scale', shrinking=False,)
NuSVCClf.fit(X, y)
```

Output

```
NuSVC(cache_size=200, class_weight=None, coef0=0.0,
```

```
decision_function_shape='ovr', degree=3, gamma='scale', kernel='linear',
max_iter=-1, nu=0.5, probability=False, random_state=None,
shrinking=False, tol=0.001, verbose=False)
```

We can get the outputs of rest of the attributes as did in the case of SVC.

LinearSVC

It is Linear Support Vector Classification. It is similar to SVC having kernel = 'linear'. The difference between them is that **LinearSVC** implemented in terms of **liblinear** while SVC is implemented in **libsvm**. That's the reason **LinearSVC** has more flexibility in the choice of penalties and loss functions. It also scales better to large number of samples.

If we talk about its parameters and attributes then it does not support **'kernel'** because it is assumed to be linear and it also lacks some of the attributes like **support_, support_vectors_, n_support_, fit_status_** and, **dual_coef_**.

However, it supports **penalty** and **loss** parameters as follows:

- **penalty**: **string, L1 or L2(default = 'L2')**
  This parameter is used to specify the norm (L1 or L2) used in penalization (regularization).
- **loss**: **string, hinge, squared_hinge (default = squared_hinge)**
  It represents the loss function where 'hinge' is the standard SVM loss and 'squared_hinge' is the square of hinge loss.

Implementation Example

Following Python script uses **sklearn.svm.LinearSVC** class:

```
from sklearn.svm import LinearSVC
from sklearn.datasets import make_classification
X, y = make_classification(n_features=4, random_state=0)
LSVCClf = LinearSVC(dual = False, random_state=0, penalty='l1',tol=1e-5)
LSVCClf.fit(X, y)
```

Output

```
LinearSVC(C=1.0, class_weight=None, dual=False, fit_intercept=True,
     intercept_scaling=1, loss='squared_hinge', max_iter=1000,
     multi_class='ovr', penalty='l1', random_state=0, tol=1e-05, verbose=0)
```

Now, once fitted, the model can predict new values as follows:

```
LSVCClf.predict([[0,0,0,0]])
```

Output

```
[1]
```

For the above example, we can get the weight vector with the help of following python script:

```
LSVCClf.coef_
```

Output

```
[[0.         0.         0.91214955 0.22630686]]
```

Similarly, we can get the value of intercept with the help of following python script:

```
LSVCClf.intercept_
```

Output

```
[0.26860518]
```

Regression with SVM

As discussed earlier, SVM is used for both classification and regression problems. Scikit-learn's method of Support Vector Classification (SVC) can be extended to solve regression problems as well. That extended method is called Support Vector Regression (SVR).

Basic similarity between SVM and SVR

The model created by SVC depends only on a subset of training data. Why? Because the cost function for building the model doesn't care about training data points that lie outside the margin.

Whereas, the model produced by SVR (Support Vector Regression) also only depends on a subset of the training data. Why? Because the cost function for building the model ignores any training data points close to the model prediction.

Scikit-learn provides three classes namely **SVR, NuSVR and LinearSVR** as three different implementations of SVR.

SVR

It is Epsilon-support vector regression whose implementation is based on **libsvm**. As opposite to **SVC** There are two free parameters in the model namely '**C**' and '**epsilon**'.

- **epsilon:** float, optional, default = 0.1

It represents the epsilon in the epsilon-SVR model, and specifies the epsilon-tube within which no penalty is associated in the training loss function with points predicted within a distance epsilon from the actual value.

Rest of the parameters and attributes are similar as we used in **SVC**.

Implementation Example

Following Python script uses **sklearn.svm.SVR** class:

```
from sklearn import svm
X = [[1, 1], [2, 2]]
y = [1, 2]
SVRReg = svm.SVR(kernel='linear', gamma='auto')
SVRReg.fit(X, y)
```

Output

```
SVR(C=1.0, cache_size=200, coef0=0.0, degree=3, epsilon=0.1, gamma='auto',
  kernel='linear', max_iter=-1, shrinking=True, tol=0.001, verbose=False)
```

Now, once fitted, we can get the weight vector with the help of following python script:

```
SVRReg.coef_
```

Output

```
array([[0.4, 0.4]])
```

Similarly, we can get the value of other attributes as follows:

```
SVRReg.predict([[1,1]])
```

Output

```
array([1.1])
```

Similarly, we can get the values of other attributes as well.

NuSVR

NuSVR is Nu Support Vector Regression. It is like NuSVC, but NuSVR uses a parameter **nu** to control the number of support vectors. And moreover, unlike NuSVC where **nu** replaced **C** parameter, here it replaces **epsilon.**

Implementation Example

Following Python script uses **sklearn.svm.SVR** class:

```
from sklearn.svm import NuSVR
import numpy as np
n_samples, n_features = 20, 15
np.random.seed(0)
y = np.random.randn(n_samples)
```

```
X = np.random.randn(n_samples, n_features)
NuSVRReg = NuSVR(kernel='linear', gamma='auto',C=1.0, nu=0.1)^M
NuSVRReg.fit(X, y)
```

Output

```
NuSVR(C=1.0, cache_size=200, coef0=0.0, degree=3, gamma='auto',
   kernel='linear', max_iter=-1, nu=0.1, shrinking=True, tol=0.001,
   verbose=False)
```

Now, once fitted, we can get the weight vector with the help of following python script:

```
NuSVRReg.coef_
```

Output

```
array([[-0.14904483,  0.04596145,  0.22605216, -0.08125403,  0.06564533,
         0.01104285,  0.04068767,  0.2918337 , -0.13473211,  0.36006765,
        -0.2185713 , -0.31836476, -0.03048429,  0.16102126, -0.29317051]])
```

Similarly, we can get the value of other attributes as well.

LinearSVR

It is Linear Support Vector Regression. It is similar to SVR having kernel = 'linear'. The difference between them is that **LinearSVR** implemented in terms of **liblinear,** while SVC implemented in **libsvm**. That's the reason **LinearSVR** has more flexibility in the choice of penalties and loss functions. It also scales better to large number of samples.

If we talk about its parameters and attributes then it does not support **'kernel'** because it is assumed to be linear and it also lacks some of the attributes like **support_, support_vectors_, n_support_, fit_status_** and, **dual_coef_**.

However, it supports 'loss' parameters as follows:

- **loss:** string, optional, default = 'epsilon_insensitive'

It represents the loss function where epsilon_insensitive loss is the L1 loss and the squared epsilon-insensitive loss is the L2 loss.

Implementation Example

Following Python script uses **sklearn.svm.LinearSVR** class:

```
from sklearn.svm import LinearSVR
from sklearn.datasets import make_regression
X, y = make_regression(n_features=4, random_state=0)
LSVRReg = LinearSVR(dual = False, random_state=0,
loss='squared_epsilon_insensitive',tol=1e-5)
```

```
LSVRReg.fit(X, y)
```

Output

```
LinearSVR(C=1.0, dual=False, epsilon=0.0, fit_intercept=True,
     intercept_scaling=1.0, loss='squared_epsilon_insensitive',
     max_iter=1000, random_state=0, tol=1e-05, verbose=0)
```

Now, once fitted, the model can predict new values as follows:

```
LSRReg.predict([[0,0,0,0]])
```

Output

```
array([-0.01041416])
```

For the above example, we can get the weight vector with the help of following python script:

```
LSRReg.coef_
```

Output

```
array([20.47354746, 34.08619401, 67.23189022, 87.47017787])
```

Similarly, we can get the value of intercept with the help of following python script:

```
LSRReg.intercept_
```

Output

```
array([-0.01041416])
```

10. Scikit-Learn — Anomaly Detection

Here, we will learn about what is anomaly detection in Sklearn and how it is used in identification of the data points.

Anomaly detection is a technique used to identify data points in dataset that does not fit well with the rest of the data. It has many applications in business such as fraud detection, intrusion detection, system health monitoring, surveillance, and predictive maintenance. Anomalies, which are also called outlier, can be divided into following three categories:

- **Point anomalies**: It occurs when an individual data instance is considered as anomalous w.r.t the rest of the data.
- **Contextual anomalies**: Such kind of anomaly is context specific. It occurs if a data instance is anomalous in a specific context.
- **Collective anomalies**: It occurs when a collection of related data instances is anomalous w.r.t entire dataset rather than individual values.

Methods

Two methods namely **outlier detection** and **novelty detection** can be used for anomaly detection. It's necessary to see the distinction between them.

Outlier detection

The training data contains outliers that are far from the rest of the data. Such outliers are defined as observations. That's the reason, outlier detection estimators always try to fit the region having most concentrated training data while ignoring the deviant observations. It is also known as unsupervised anomaly detection.

Novelty detection

It is concerned with detecting an unobserved pattern in new observations which is not included in training data. Here, the training data is not polluted by the outliers. It is also known as semi-supervised anomaly detection.

There are set of ML tools, provided by scikit-learn, which can be used for both outlier detection as well novelty detection. These tools first implementing object learning from the data in an unsupervised by using fit () method as follows:

```
estimator.fit(X_train)
```

Now, the new observations would be sorted as **inliers (labeled 1)** or **outliers (labeled -1)** by using predict() method as follows:

```
estimator.fit(X_test)
```

The estimator will first compute the raw scoring function and then predict method will make use of threshold on that raw scoring function. We can access this raw scoring

function with the help of **score_sample** method and can control the threshold by **contamination** parameter.

We can also define **decision_function** method that defines outliers as negative value and inliers as non-negative value.

```
estimator.decision_function(X_test)
```

Sklearn algorithms for Outlier Detection

Let us begin by understanding what an elliptic envelop is.

Fitting an elliptic envelop

This algorithm assume that regular data comes from a known distribution such as Gaussian distribution. For outlier detection, Scikit-learn provides an object named **covariance.EllipticEnvelop**.

This object fits a robust covariance estimate to the data, and thus, fits an ellipse to the central data points. It ignores the points outside the central mode.

Parameters

Following table consist the parameters used by **sklearn. covariance.EllipticEnvelop** method:

Parameter	Description
***store_precision**: Boolean, optional, default = True*	We can specify it if the estimated precision is stored.
***assume_centered** : Boolean, optional, default = False*	If we set it False, it will compute the robust location and covariance directly with the help of FastMCD algorithm. On the other hand, if set True, it will compute the support of robust location and covariance estimates and then recompute the covariance estimate.
***support_fraction**: float in (0., 1.), optional, default = None*	This parameter tells the method that how much proportion of points to be included in the support of the raw MCD estimates.
***contamination**: float in (0., 1.), optional, default = 0.1*	It provides the proportion of the outliers in the data set.

***random_state**: int, RandomState instance or None, optional, default = none*	This parameter represents the seed of the pseudo random number generated which is used while shuffling the data. Followings are the options: • **int**: In this case, ***random_state*** is the seed used by random number generator. • **RandomState instance**: In this case, *random_state* is the random number generator. • **None**: In this case, the random number generator is the RandonState instance used by np.random.

Attributes

Following table consist the attributes used by **sklearn. covariance.EllipticEnvelop** method:

Attributes	Description
***support_**: array-like, shape(n_samples,)*	It represents the mask of the observations used to compute robust estimates of location and shape.
***location_**: array-like, shape (n_features)*	It returns the estimated robust location.
***covariance_**: array-like, shape (n_features, n_features)*	It returns the estimated robust covariance matrix.
***precision_**: array-like, shape (n_features, n_features)*	It returns the estimated pseudo inverse matrix.
***offset_**: float*	It is used to define the decision function from the raw scores. **decision_function = score_samples -offset_**

Implementation Example

```
import numpy as np^M
from sklearn.covariance import EllipticEnvelope^M
true_cov = np.array([[.5, .6],[.6, .4]])
X = np.random.RandomState(0).multivariate_normal(mean=[0, 0],
cov=true_cov,size=500)
cov = EllipticEnvelope(random_state=0).fit(X)^M
```

```
# Now we can use predict method. It will return 1 for an inlier and -1 for an
outlier.

cov.predict([[0, 0],[2, 2]])
```

Output

```
array([ 1, -1])
```

Isolation Forest

In case of high-dimensional dataset, one efficient way for outlier detection is to use random forests. The scikit-learn provides **ensemble.IsolationForest** method that isolates the observations by randomly selecting a feature. Afterwards, it randomly selects a value between the maximum and minimum values of the selected features.

Here, the number of splitting needed to isolate a sample is equivalent to path length from the root node to the terminating node.

Parameters

Followings table consist the parameters used by **sklearn. ensemble.IsolationForest** method:

Parameter	Description
n_estimators*: int, optional, default = 100*	It represents the number of base estimators in the ensemble.
max_samples *: int or float, optional, default = "auto"*	It represents the number of samples to be drawn from X to train each base estimator. If we choose *int* as its value, it will draw $max\_samples$ samples. If we choose *float* as its value, it will draw $max\_samples * X.shape[0]$ samples. And, if we choose *auto* as its value, it will draw $max\_samples = min(256, n\_samples)$.
support_fraction*: float in (0., 1.), optional, default = None*	This parameter tells the method that how much proportion of points to be included in the support of the raw MCD estimates.
contamination*: auto or float, optional, default = auto*	It provides the proportion of the outliers in the data set. If we set it default i.e. auto, it will determine the threshold as in the original paper. If set to float, the range of contamination will be in the range of [0,0.5].

***random_state**: int, RandomState instance or None, optional, default = none*	This parameter represents the seed of the pseudo random number generated which is used while shuffling the data. Followings are the options: • **int**: In this case, *random_state* is the seed used by random number generator. • **RandomState instance**: In this case, *random_state* is the random number generator. • **None**: In this case, the random number generator is the RandonState instance used by np.random.
***max_features**: int or float, optional (default = 1.0)*	It represents the number of features to be drawn from X to train each base estimator. If we choose *int* as its value, it will draw $max\_features$ features. If we choose *float* as its value, it will draw $max\_features * X.shape[1]$ samples.
***bootstrap**: Boolean, optional (default = False)*	Its default option is False which means the sampling would be performed without replacement. And on the other hand, if set to True, means individual trees are fit on a random subset of the training data sampled with replacement.
***n_jobs**: int or None, optional (default = None)*	It represents the number of jobs to be run in parallel for **fit()** and **predict()** methods both.
***verbose**: int, optional (default = 0)*	This parameter controls the verbosity of the tree building process.
***warm_start**: Bool, optional (default=False)*	If warm_start = true, we can reuse previous call's solution to fit and can add more estimators to the ensemble. But if is set to false, we need to fit a whole new forest.

Attributes

Following table consist the attributes used by **sklearn. ensemble.IsolationForest** method:

Attributes	Description
***estimators_**: list of DecisionTreeClassifier*	Providing the collection of all fitted sub-estimators.

***max_samples_**: integer*	It provides the actual number of samples used.
***offset_**: float*	It is used to define the decision function from the raw scores. **decision_function = score_samples -offset_**

Implementation Example

The Python script below will use **sklearn. ensemble.IsolationForest** method to fit 10 trees on given data:

```
from sklearn.ensemble import IsolationForest
import numpy as np
X = np.array([[-1, -2], [-3, -3], [-3, -4], [0, 0], [-50, 60]])
OUTDClf = IsolationForest(n_estimators=10)
OUTDclf.fit(X)
```

Output

```
IsolationForest(behaviour='old', bootstrap=False, contamination='legacy',
        max_features=1.0, max_samples='auto', n_estimators=10, n_jobs=None,
        random_state=None, verbose=0)
```

Local Outlier Factor

Local Outlier Factor (LOF) algorithm is another efficient algorithm to perform outlier detection on high dimension data. The scikit-learn provides **neighbors.LocalOutlierFactor** method that computes a score, called local outlier factor, reflecting the degree of anomality of the observations. The main logic of this algorithm is to detect the samples that have a substantially lower density than its neighbors. That's why it measures the local density deviation of given data points w.r.t. their neighbors.

Parameters

Followings table consist the parameters used by **sklearn. neighbors.LocalOutlierFactor** method:

Parameter	Description
***n_neighbors:** int, optional, default = 20*	It represents the number of neighbors use by default for kneighbors query. All samples would be used if $n\_neighbors > given\ samples$.
***algorithm:** {'auto', 'ball_tree',*	Which algorithm to be used for computing nearest neighbors.

'kd_tree', 'brute'}, optional	• If you choose ball_tree, it will use BallTree algorithm. • If you choose kd_tree, it will use KDTree algorithm. • If you choose brute, it will use brute-force search algorithm. • If you choose auto, it will decide the most appropriate algorithm on the basis of the value we passed to fit() method.
leaf_size: *int, optional, default = 30*	The value of this parameter can affect the speed of the construction and query. It also affects the memory required to store the tree. This parameter is passed to BallTree or KdTree algorithms.
contamination: *auto or float, optional, default = auto*	It provides the proportion of the outliers in the data set. If we set it default i.e. auto, it will determine the threshold as in the original paper. If set to float, the range of contamination will be in the range of [0,0.5].
metric: *string or callable, default 'Minkowski'*	It represents the metric used for distance computation.
P: *int, optional (default = 2)*	It is the parameter for the Minkowski metric. P=1 is equivalent to using manhattan_distance i.e. L1, whereas P=2 is equivalent to using euclidean_distance i.e. L2.
novelty: *Boolean, (default = False)*	By default, LOF algorithm is used for outlier detection but it can be used for novelty detection if we set novelty = true.
n_jobs: *int or None, optional (default = None)*	It represents the number of jobs to be run in parallel for fit() and predict() methods both.

Attributes

Following table consist the attributes used by **sklearn.neighbors.LocalOutlierFactor** method:

Attributes	Description
negative_outlier_factor_: *numpy array, shape(n_samples,)*	Providing opposite LOF of the training samples.

n_neighbors_: *integer*	It provides the actual number of neighbors used for neighbors queries.
offset_: *float*	It is used to define the binary labels from the raw scores.

Implementation Example

The Python script given below will use **sklearn.neighbors.LocalOutlierFactor** method to construct NeighborsClassifier class from any array corresponding our data set:

```
from sklearn.neighbors import NearestNeighbors
samples = [[0., 0., 0.], [0., .5, 0.], [1., 1., .5]]
LOFneigh = NearestNeighbors(n_neighbors=1, algorithm="ball_tree",p=1)
LOFneigh.fit(samples)
```

Output

```
NearestNeighbors(algorithm='ball_tree', leaf_size=30, metric='minkowski',
         metric_params=None, n_jobs=None, n_neighbors=1, p=1, radius=1.0)
```

Now, we can ask from this constructed classifier who's is the closet point to [0.5, 1., 1.5] by using the following python script:

```
print(neigh.kneighbors([[.5, 1., 1.5]])
```

Output

```
(array([[1.7]]), array([[1]], dtype=int64))
```

One-Class SVM

The One-Class SVM, introduced by Schölkopf et al., is the unsupervised Outlier Detection. It is also very efficient in high-dimensional data and estimates the support of a high-dimensional distribution. It is implemented in the **Support Vector Machines** module in the **Sklearn.svm.OneClassSVM** object. For defining a frontier, it requires a kernel (mostly used is RBF) and a scalar parameter.

For better understanding let's fit our data with **svm.OneClassSVM** object:

```
from sklearn.svm import OneClassSVM
X = [[0], [0.89], [0.90], [0.91], [1]]
OSVMclf = OneClassSVM(gamma='scale').fit(X)
```

Now, we can get the score_samples for input data as follows:

```
OSVMclf.score_samples(X)
```

Output

```
array([1.12218594, 1.58645126, 1.58673086, 1.58645127, 1.55713767])
```

11. Scikit-Learn — K-Nearest Neighbors (KNN)

This chapter will help you in understanding the nearest neighbor methods in Sklearn.

Neighbor based learning method are of both types namely **supervised** and **unsupervised**. Supervised neighbors-based learning can be used for both classification as well as regression predictive problems but, it is mainly used for classification predictive problems in industry.

Neighbors based learning methods do not have a specialised training phase and uses all the data for training while classification. It also does not assume anything about the underlying data. That's the reason they are lazy and non-parametric in nature.

The main principle behind nearest neighbor methods is:

- To find a predefined number of training samples closet in distance to the new data point
- Predict the label from these number of training samples.

Here, the number of samples can be a user-defined constant like in K-nearest neighbor learning or vary based on the local density of point like in radius-based neighbor learning.

sklearn.neighbors Module

Scikit-learn have **sklearn.neighbors** module that provides functionality for both unsupervised and supervised neighbors-based learning methods. As input, the classes in this module can handle either NumPy arrays or **scipy.sparse** matrices.

Types of algorithms

Different types of algorithms which can be used in neighbor-based methods' implementation are as follows:

Brute Force

The brute-force computation of distances between all pairs of points in the dataset provides the most naïve neighbor search implementation. Mathematically, for N samples in D dimensions, brute-force approach scales as $O[DN^2]$.

For small data samples, this algorithm can be very useful, but it becomes infeasible as and when number of samples grows. Brute force neighbor search can be enabled by writing the keyword **algorithm='brute'**.

K-D Tree

One of the tree-based data structures that have been invented to address the computational inefficiencies of the brute-force approach, is KD tree data structure. Basically, the KD tree is a binary tree structure which is called K-dimensional tree. It recursively partitions the parameters space along the data axes by dividing it into nested orthographic regions into which the data points are filled.

Advantages

Following are some advantages of K-D tree algorithm:

Construction is fast: As the partitioning is performed only along the data axes, K-D tree's construction is very fast.

Less distance computations: This algorithm takes very less distance computations to determine the nearest neighbor of a query point. It only takes $O[\log(N)]$ distance computations.

Disadvantages

Fast for only low-dimensional neighbor searches: It is very fast for low-dimensional (D < 20) neighbor searches but as and when D grow it becomes inefficient. As the partitioning is performed only along the data axes,

K-D tree neighbor searches can be enabled by writing the keyword **algorithm='kd_tree'**.

Ball Tree

As we know that KD Tree is inefficient in higher dimensions, hence, to address this inefficiency of KD Tree, Ball tree data structure was developed. Mathematically, it recursively divides the data, into nodes defined by a centroid C and radius r, in such a way that each point in the node lies within the hyper-sphere defined by centroid **C** and radius **r**. It uses triangle inequality, given below, which reduces the number of candidate points for a neighbor search:

$$|X + Y| \leq |X| + |Y|$$

Advantages

Following are some advantages of Ball Tree algorithm:

Efficient on highly structured data: As ball tree partition the data in a series of nesting hyper-spheres, it is efficient on highly structured data.

Out-performs KD-tree: Ball tree out-performs KD tree in high dimensions because it has spherical geometry of the ball tree nodes.

Disadvantages

Costly: Partition the data in a series of nesting hyper-spheres makes its construction very costly

Ball tree neighbor searches can be enabled by writing the keyword **algorithm='ball_tree'**.

Choosing Nearest Neighbors Algorithm

The choice of an optimal algorithm for a given dataset depends upon the following factors:

Number of samples (N) and Dimensionality (D)

These are the most important factors to be considered while choosing Nearest Neighbor algorithm. It is because of the reasons given below:

- The query time of Brute Force algorithm grows as O[DN].
- The query time of Ball tree algorithm grows as O[D log(N)].
- The query time of KD tree algorithm changes with D in a strange manner that is very difficult to characterize. When D < 20, the cost is O[D log(N)] and this algorithm is very efficient. On the other hand, it is inefficient in case when D > 20 because the cost increases to nearly O[DN].

Data Structure

Another factor that affect the performance of these algorithms is intrinsic dimensionality of the data or sparsity of the data. It is because the query times of Ball tree and KD tree algorithms can be greatly influenced by it. Whereas, the query time of Brute Force algorithm is unchanged by data structure. Generally, Ball tree and KD tree algorithms produces faster query time when implanted on sparser data with smaller intrinsic dimensionality.

Number of Neighbors (k)

The number of neighbors (k) requested for a query point affects the query time of Ball tree and KD tree algorithms. Their query time becomes slower as number of neighbors (k) increases. Whereas the query time of Brute Force will remain unaffected by the value of k.

Number of query points

Because, they need construction phase, both KD tree and Ball tree algorithms will be effective if there are large number of query points. On the other hand, if there are a smaller number of query points, Brute Force algorithm performs better than KD tree and Ball tree algorithms.

12. Scikit-Learn — KNN Learning

k-NN (k-Nearest Neighbor), one of the simplest machine learning algorithms, is non-parametric and lazy in nature. Non-parametric means that there is no assumption for the underlying data distribution i.e. the model structure is determined from the dataset. Lazy or instance-based learning means that for the purpose of model generation, it does not require any training data points and whole training data is used in the testing phase.

The k-NN algorithm consist of the following two steps:

Step 1

In this step, it computes and stores the k nearest neighbors for each sample in the training set.

Step 2

In this step, for an unlabeled sample, it retrieves the k nearest neighbors from dataset. Then among these k-nearest neighbors, it predicts the class through voting (class with majority votes wins).

The module, **sklearn.neighbors** that implements the k-nearest neighbors algorithm, provides the functionality for **unsupervised** as well as **supervised** neighbors-based learning methods.

The unsupervised nearest neighbors implement different algorithms (BallTree, KDTree or Brute Force) to find the nearest neighbor(s) for each sample. This unsupervised version is basically only step 1, which is discussed above, and the foundation of many algorithms (KNN and K-means being the famous one) which require the neighbor search. In simple words, it is Unsupervised learner for implementing neighbor searches.

On the other hand, the supervised neighbors-based learning is used for classification as well as regression.

Unsupervised KNN Learning

As discussed, there exist many algorithms like KNN and K-Means that requires nearest neighbor searches. That is why Scikit-learn decided to implement the neighbor search part as its own "learner". The reason behind making neighbor search as a separate learner is that computing all pairwise distance for finding a nearest neighbor is obviously not very efficient. Let's see the module used by Sklearn to implement unsupervised nearest neighbor learning along with example.

Scikit-learn module

sklearn.neighbors.NearestNeighbors is the module used to implement unsupervised nearest neighbor learning. It uses specific nearest neighbor algorithms named BallTree, KDTree or Brute Force. In other words, it acts as a uniform interface to these three algorithms.

Parameters

Followings table consist the parameters used by **NearestNeighbors** module:

Parameter	Description
***n_neighbors**: int, optional*	The number of neighbors to get. The default value is 5.
***radius**: float, optional*	It limits the distance of neighbors to returns. The default value is 1.0.
***algorithm**: {'auto', 'ball_tree', 'kd_tree', 'brute'}, optional*	This parameter will take the algorithm (BallTree, KDTree or Brute-force) you want to use to compute the nearest neighbors. If you will provide 'auto', it will attempt to decide the most appropriate algorithm based on the values passed to fit method.
***leaf_size**: int, optional*	It can affect the speed of the construction & query as well as the memory required to store the tree. It is passed to BallTree or KDTree. Although the optimal value depends on the nature of the problem, its default value is 30.
***metric**: string or callable*	It is the metric to use for distance computation between points. We can pass it as a string or callable function. In case of callable function, the metric is called on each pair of rows and the resulting value is recorded. It is less efficient than passing the metric name as a string. We can choose from metric from scikit-learn or scipy.spatial.distance. the valid values are as follows: Scikit-learn: ['cosine','manhattan','Euclidean', 'l1','l2', 'cityblock'] Scipy.spatial.distance: ['braycurtis','canberra','chebyshev','dice','hamming','jaccard', 'correlation','kulsinski','mahalanobis','minkowski','rogerstanimoto','russellrao', 'sokalmicheme','sokalsneath', 'seuclidean', 'sqeuclidean', 'yule']. The default metric is 'Minkowski'.
***p**: integer, optional*	It is the parameter for the Minkowski metric. The default value is 2 which is equivalent to using Euclidean_distance(l2).
***metric_params**: dict, optional*	This is the additional keyword arguments for the metric function. The default value is None.

***N_jobs**: int or None, optional*	It reprsetst the numer of parallel jobs to run for neighbor search. The default value is None.

Implementation Example

The example below will find the nearest neighbors between two sets of data by using the **sklearn.neighbors.NearestNeighbors** module.

First, we need to import the required module and packages:

```
from sklearn.neighbors import NearestNeighbors
import numpy as np
```

Now, after importing the packages, define the sets of data in between we want to find the nearest neighbors:

```
Input_data = np.array([[-1, 1], [-2, 2], [-3, 3], [1, 2], [2, 3], [3, 4],[4,
5]])
```

Next, apply the unsupervised learning algorithm, as follows:

```
nrst_neigh = NearestNeighbors(n_neighbors = 3, algorithm='ball_tree')
```

Next, fit the model with input data set.

```
nrst_neigh.fit(Input_data)
```

Now, find the K-neighbors of data set. It will return the indices and distances of the neighbors of each point.

```
distances, indices = nbrs.kneighbors(Input_data)
indices
```

Output

```
array([[0, 1, 3],
       [1, 2, 0],
       [2, 1, 0],
       [3, 4, 0],
       [4, 5, 3],
       [5, 6, 4],
       [6, 5, 4]], dtype=int64)


distances
```

Output

```
array([[0.        , 1.41421356, 2.23606798],
```

```
       [0.        , 1.41421356, 1.41421356],
       [0.        , 1.41421356, 2.82842712],
       [0.        , 1.41421356, 2.23606798],
       [0.        , 1.41421356, 1.41421356],
       [0.        , 1.41421356, 1.41421356],
       [0.        , 1.41421356, 2.82842712]])
```

The above output shows that the nearest neighbor of each point is the point itself i.e. at zero. It is because the query set matches the training set.

We can also show a connection between neighboring points by producing a sparse graph as follows:

```
nrst_neigh.kneighbors_graph(Input_data).toarray()
```

Output

```
array([[1., 1., 0., 1., 0., 0., 0.],
       [1., 1., 1., 0., 0., 0., 0.],
       [1., 1., 1., 0., 0., 0., 0.],
       [1., 0., 0., 1., 1., 0., 0.],
       [0., 0., 0., 1., 1., 1., 0.],
       [0., 0., 0., 0., 1., 1., 1.],
       [0., 0., 0., 0., 1., 1., 1.]])
```

Once we fit the unsupervised **NearestNeighbors** model, the data will be stored in a data structure based on the value set for the argument **'algorithm'**. After that we can use this unsupervised learner's **kneighbors** in a model which requires neighbor searches.

Complete working/executable program

```
from sklearn.neighbors import NearestNeighbors
 import numpy as np
Input_data = np.array([[-1, 1], [-2, 2], [-3, 3], [1, 2], [2, 3], [3, 4],[4,
5]])
nrst_neigh = NearestNeighbors(n_neighbors = 3, algorithm='ball_tree')
nrst_neigh.fit(Input_data)
distances, indices = nbrs.kneighbors(Input_data)
indices
distances
nrst_neigh.kneighbors_graph(Input_data).toarray()
```

Supervised KNN Learning

The supervised neighbors-based learning is used for following:

- Classification, for the data with discrete labels
- Regression, for the data with continuous labels.

Nearest Neighbor Classifier

We can understand Neighbors-based classification with the help of following two characteristics:

- It is computed from a simple majority vote of the nearest neighbors of each point.
- It simply stores instances of the training data, that's why it is a type of non-generalizing learning.

Scikit-learn modules

Followings are the two different types of nearest neighbor classifiers used by scikit-learn:

KNeighborsClassifier

The K in the name of this classifier represents the k nearest neighbors, where k is an integer value specified by the user. Hence as the name suggests, this classifier implements learning based on the k nearest neighbors. The choice of the value of k is dependent on data. Let's understand it more with the help if an implementation example:

Implementation Example

In this example, we will be implementing KNN on data set named Iris Flower data set by using scikit-learn **KneighborsClassifer**.

- This data set has 50 samples for each different species (setosa, versicolor, virginica) of iris flower i.e. total of 150 samples.
- For each sample, we have 4 features named sepal length, sepal width, petal length, petal width)

First, import the dataset and print the features names as follows:

```
from sklearn.datasets import load_iris
iris = load_iris()
print(iris.feature_names)
```

Output

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

Now we can print target i.e the integers representing the different species. Here **0 = setos**, **1 = versicolor** and **2 = virginica**.

```
print(iris.target)
```

Output

```
[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 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]
```

Following line of code will show the names of the target:

```
print(iris.target_names)
```

Output

```
['setosa' 'versicolor' 'virginica']
```

We can check the number of observations and features with the help of following line of code (iris data set has 150 observations and 4 features)

```
print(iris.data.shape)
```

Output

```
(150, 4)
```

Now, we need to split the data into training and testing data. We will be using Sklearn **train_test_split** function to split the data into the ratio of 70 (training data) and 30 (testing data):

```
X = iris.data[:, :4]
y = iris.target
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.30)
```

Next, we will be doing data scaling with the help of Sklearn preprocessing module as follows:

```
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(X_train)
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)
```

Following line of codes will give you the shape of train and test objects:

```
print(X_train.shape)
print(X_test.shape)
```

Output

```
(105, 4)
(45, 4)
```

Following line of codes will give you the shape of new **y** object:

```
print(y_train.shape)
print(y_test.shape)
```

Output

```
(105,)
(45,)
```

Next, import the **KneighborsClassifier** class from Sklearn as follows:

```
from sklearn.neighbors import KNeighborsClassifier
```

To check accuracy, we need to import Metrics model as follows;

```
from sklearn import metrics
We are going to run it for k = 1 to 15 and will be recording testing accuracy,
plotting it, showing confusion matrix and classification report:
Range_k = range(1,15)
scores = {}
scores_list = []
for k in range_k:
    classifier = KNeighborsClassifier(n_neighbors=k)
    classifier.fit(X_train, y_train)
    y_pred = classifier.predict(X_test)
    scores[k] = metrics.accuracy_score(y_test,y_pred)
    scores_list.append(metrics.accuracy_score(y_test,y_pred))

result = metrics.confusion_matrix(y_test, y_pred)
print("Confusion Matrix:")
print(result)
result1 = metrics.classification_report(y_test, y_pred)
print("Classification Report:",)
print (result1)
```

Now, we will be plotting the relationship between the values of K and the corresponding testing accuracy. It will be done using matplotlib library.

```
%matplotlib inline
import matplotlib.pyplot as plt
plt.plot(k_range,scores_list)
plt.xlabel("Value of K")
plt.ylabel("Accuracy")
```

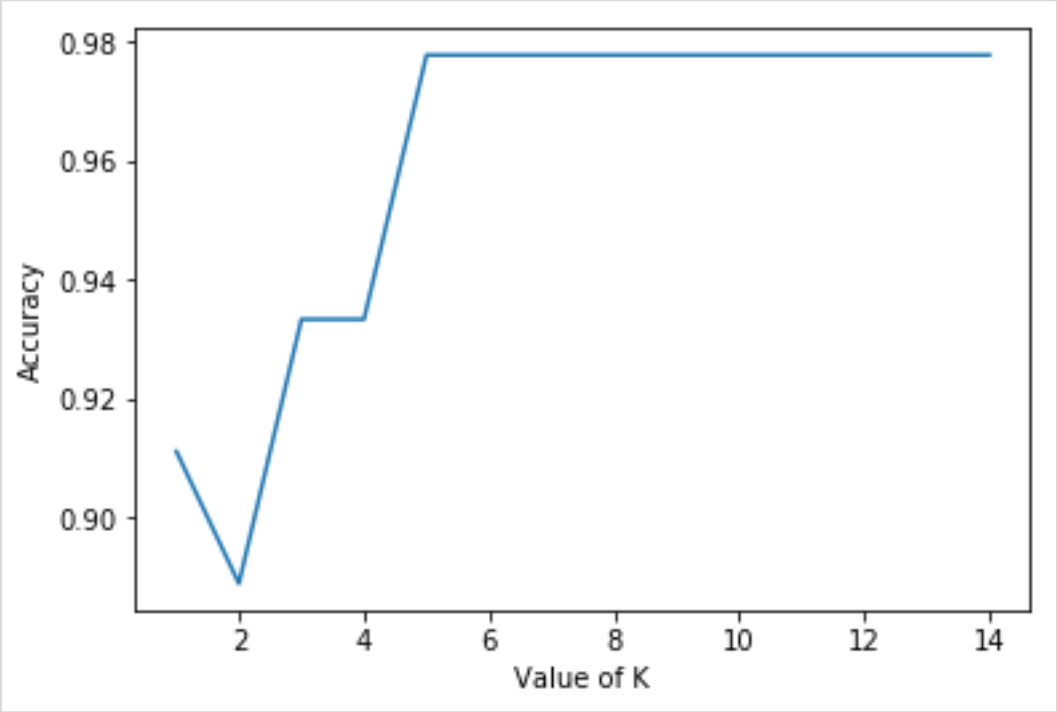
Output

```
Confusion Matrix:
[[15  0  0]
 [ 0 15  0]
 [ 0  1 14]]
Classification Report:
              precision    recall  f1-score   support

           0       1.00      1.00      1.00        15
           1       0.94      1.00      0.97        15
           2       1.00      0.93      0.97        15

   micro avg       0.98      0.98      0.98        45
   macro avg       0.98      0.98      0.98        45
weighted avg       0.98      0.98      0.98        45

Text(0, 0.5, 'Accuracy')
```



For the above model, we can choose the optimal value of K (any value between 6 to 14, as the accuracy is highest for this range) as 8 and retrain the model as follows:

```
classifier = KNeighborsClassifier(n_neighbors=8)
classifier.fit(X_train, y_train)
```

Output

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


classes = {0:'setosa',1:'versicolor',2:'virginicia'}
x_new = [[1,1,1,1],[4,3,1.3,0.2]]
y_predict = rnc.predict(x_new)
print(classes[y_predict[0]])
print(classes[y_predict[1]])
```

Output

```
virginicia
virginicia
```

Complete working/executable program

```
from sklearn.datasets import load_iris
iris = load_iris()
print(iris.target_names)
print(iris.data.shape)
X = iris.data[:, :4]
y = iris.target
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.30)
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(X_train)
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)



print(X_train.shape)
print(X_test.shape)

from sklearn.neighbors import KNeighborsClassifier

from sklearn import metrics

Range_k = range(1,15)
scores = {}
scores_list = []
for k in range_k:
    classifier = KNeighborsClassifier(n_neighbors=k)
    classifier.fit(X_train, y_train)
    y_pred = classifier.predict(X_test)
    scores[k] = metrics.accuracy_score(y_test,y_pred)
    scores_list.append(metrics.accuracy_score(y_test,y_pred))

result = metrics.confusion_matrix(y_test, y_pred)
print("Confusion Matrix:")
print(result)
```

```
result1 = metrics.classification_report(y_test, y_pred)
print("Classification Report:",)
print (result1)
%matplotlib inline
import matplotlib.pyplot as plt
plt.plot(k_range,scores_list)
plt.xlabel("Value of K")
plt.ylabel("Accuracy")

classifier = KNeighborsClassifier(n_neighbors=8)
classifier.fit(X_train, y_train)

classes = {0:'setosa',1:'versicolor',2:'virginicia'}
x_new = [[1,1,1,1],[4,3,1.3,0.2]]
y_predict = rnc.predict(x_new)
print(classes[y_predict[0]])
print(classes[y_predict[1]])
```

RadiusNeighborsClassifier

The Radius in the name of this classifier represents the nearest neighbors within a specified radius r, where r is a floating-point value specified by the user. Hence as the name suggests, this classifier implements learning based on the number neighbors within a fixed radius r of each training point. Let's understand it more with the help if an implementation example:

Implementation Example

In this example, we will be implementing KNN on data set named Iris Flower data set by using scikit-learn **RadiusNeighborsClassifer**:

First, import the iris dataset as follows:

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

Now, we need to split the data into training and testing data. We will be using Sklearn **train_test_split** function to split the data into the ratio of 70 (training data) and 20 (testing data):

```
X = iris.data[:, :4]
y = iris.target
from sklearn.model_selection import train_test_split
```

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20)
```

Next, we will be doing data scaling with the help of Sklearn preprocessing module as follows:

```
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(X_train)
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)
```

Next, import the **RadiusneighborsClassifier** class from Sklearn and provide the value of radius as follows:

```
from sklearn.neighbors import RadiusNeighborsClassifier
rnc = RadiusNeighborsClassifier(radius=5)
rnc.fit(X_train, y_train)
```

Now, create and predict the class of two observations as follows:

```
classes = {0:'setosa',1:'versicolor',2:'virginicia'}

x_new = [[1,1,1,1]]
y_predict = rnc.predict(x_new)
print(classes[y_predict[0]])
```

Output

```
versicolor
```

Complete working/executable program

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

X = iris.data[:, :4]
y = iris.target
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20)

from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(X_train)
```

```
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)



from sklearn.neighbors import RadiusNeighborsClassifier
rnc = RadiusNeighborsClassifier(radius=5)
rnc.fit(X_train, y_train)



classes = {0:'setosa',1:'versicolor',2:'virginicia'}
x_new = [[1,1,1,1]]
y_predict = rnc.predict(x_new)
print(classes[y_predict[0]])
```

Nearest Neighbor Regressor

It is used in the cases where data labels are continuous in nature. The assigned data labels are computed on the basis on the mean of the labels of its nearest neighbors.

Followings are the two different types of nearest neighbor regressors used by scikit-learn:

KNeighborsRegressor

The K in the name of this regressor represents the k nearest neighbors, where **k** is an **integer value** specified by the user. Hence, as the name suggests, this regressor implements learning based on the k nearest neighbors. The choice of the value of k is dependent on data. Let's understand it more with the help of an implementation example:

Implementation Example

In this example, we will be implementing KNN on data set named Iris Flower data set by using scikit-learn **KNeighborsRegressor**.

First, import the iris dataset as follows:

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

Now, we need to split the data into training and testing data. We will be using Sklearn **train_test_split** function to split the data into the ratio of 70 (training data) and 20 (testing data):

```
X = iris.data[:, :4]
y = iris.target
from sklearn.model_selection import train_test_split
```

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20)
```

Next, we will be doing data scaling with the help of Sklearn preprocessing module as follows:

```
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(X_train)
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)
```

Next, import the **KNeighborsRegressor** class from Sklearn and provide the value of neighbors as follows:

```
import numpy as np
from sklearn.neighbors import KNeighborsRegressor
knnr = KNeighborsRegressor(n_neighbors=8)
knnr.fit(X_train, y_train)
```

Output

```
KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='minkowski',
          metric_params=None, n_jobs=None, n_neighbors=8, p=2,
          weights='uniform')
```

Now, we can find the MSE (Mean Squared Error) as follows:

```
print ("The MSE is:",format(np.power(y-knnr.predict(X),4).mean()))
```

Output

```
The MSE is: 4.4333349609375
```

Now, use it to predict the value as follows:

```
X = [[0], [1], [2], [3]]
y = [0, 0, 1, 1]
from sklearn.neighbors import KNeighborsRegressor
knnr = KNeighborsRegressor(n_neighbors=3)
knnr.fit(X, y)
print(knnr.predict([[2.5]]))
```

Output

```
[0.66666667]
```

Complete working/executable program

```
from sklearn.datasets import load_iris
iris = load_iris()
X = iris.data[:, :4]
y = iris.target
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20)
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()

scaler.fit(X_train)
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)

import numpy as np
from sklearn.neighbors import KNeighborsRegressor
knnr = KNeighborsRegressor(n_neighbors=8)
knnr.fit(X_train, y_train)

print ("The MSE is:",format(np.power(y-knnr.predict(X),4).mean()))

X = [[0], [1], [2], [3]]
y = [0, 0, 1, 1]
from sklearn.neighbors import KNeighborsRegressor
knnr = KNeighborsRegressor(n_neighbors=3)
knnr.fit(X, y)
print(knnr.predict([[2.5]]))
```

RadiusNeighborsRegressor

The Radius in the name of this regressor represents the nearest neighbors within a specified radius r, where r is a floating-point value specified by the user. Hence as the name suggests, this regressor implements learning based on the number neighbors within a fixed radius r of each training point. Let's understand it more with the help if an implementation example:

Implementation Example

In this example, we will be implementing KNN on data set named Iris Flower data set by using scikit-learn **RadiusNeighborsRegressor**:

First, import the iris dataset as follows:

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

Now, we need to split the data into training and testing data. We will be using Sklearn **train_test_split** function to split the data into the ratio of 70 (training data) and 20 (testing data):

```
X = iris.data[:, :4]
y = iris.target
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20)
```

Next, we will be doing data scaling with the help of Sklearn preprocessing module as follows:

```
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(X_train)
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)
```

Next, import the **RadiusneighborsRegressor** class from Sklearn and provide the value of radius as follows:

```
import numpy as np
from sklearn.neighbors import RadiusNeighborsRegressor
knnr_r = RadiusNeighborsRegressor(radius=1)
knnr_r.fit(X_train, y_train)
```

Now, we can find the MSE (Mean Squared Error) as follows:

```
print ("The MSE is:",format(np.power(y-knnr_r.predict(X),4).mean()))
```

Output

```
The MSE is: The MSE is: 5.666666666666667
```

Now, use it to predict the value as follows:

```
X = [[0], [1], [2], [3]]
y = [0, 0, 1, 1]
```

```
from sklearn.neighbors import RadiusNeighborsRegressor
knnr_r = RadiusNeighborsRegressor(radius=1)
knnr_r.fit(X, y)
print(knnr_r.predict([[2.5]]))
```

Output

```
[1.]
```

Complete working/executable program

```
from sklearn.datasets import load_iris

iris = load_iris()

X = iris.data[:, :4]
y = iris.target
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20)
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(X_train)
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)
import numpy as np
from sklearn.neighbors import RadiusNeighborsRegressor
knnr_r = RadiusNeighborsRegressor(radius=1)
knnr_r.fit(X_train, y_train)
print ("The MSE is:",format(np.power(y-knnr_r.predict(X),4).mean()))
X = [[0], [1], [2], [3]]
y = [0, 0, 1, 1]
from sklearn.neighbors import RadiusNeighborsRegressor
knnr_r = RadiusNeighborsRegressor(radius=1)
knnr_r.fit(X, y)
print(knnr_r.predict([[2.5]]))
```

13. Scikit-Learn — Classification with Naïve Bayes

Naïve Bayes methods are a set of supervised learning algorithms based on applying Bayes' theorem with a strong assumption that all the predictors are independent to each other i.e. the presence of a feature in a class is independent to the presence of any other feature in the same class. This is naïve assumption that is why these methods are called Naïve Bayes methods.

Bayes theorem states the following relationship in order to find the posterior probability of class i.e. the probability of a label and some observed features, $\boldsymbol{P(Y \mid features)}$.

$$P(Y \mid features) = \frac{P(Y)P(features \mid Y)}{P(features)}$$

Here, $\boldsymbol{P(Y \mid features)}$ is the posterior probability of class.

$\boldsymbol{P(Y)}$ is the prior probability of class.

$\boldsymbol{P(features \mid Y)}$ is the likelihood which is the probability of predictor given class.

$\boldsymbol{P(features)}$ is the prior probability of predictor.

The Scikit-learn provides different naïve Bayes classifiers models namely Gaussian, Multinomial, Complement and Bernoulli. All of them differ mainly by the assumption they make regarding the distribution of $\boldsymbol{P(features \mid Y)}$ i.e. the probability of predictor given class.

Model	Description
Gaussian Naïve Bayes	Gaussian Naïve Bayes classifier assumes that the data from each label is drawn from a simple Gaussian distribution.
Multinomial Naïve Bayes	It assumes that the features are drawn from a simple Multinomial distribution.
Bernoulli Naïve Bayes	The assumption in this model is that the features binary (0s and 1s) in nature. An application of Bernoulli Naïve Bayes classification is Text classification with 'bag of words' model
Complement Naïve Bayes	It was designed to correct the severe assumptions made by Multinomial Bayes classifier. This kind of NB classifier is suitable for imbalanced data sets

Gaussian Naïve Bayes

As the name suggest, Gaussian Naïve Bayes classifier assumes that the data from each label is drawn from a simple Gaussian distribution. The Scikit-learn provides **sklearn.naive_bayes.GaussianNB** to implement the Gaussian Naïve Bayes algorithm for classification.

Parameters: Following table consist the parameters used by **sklearn.naive_bayes.GaussianNB** method:

Parameter	Description
***priors**: arrray-like, shape(n_classes)*	It represents the prior probabilities of the classes. If we specify this parameter while fitting the data, then the prior probabilities will not be justified according to the data.
***Var_smoothing**: float, optional, default = 1e-9*	This parameter gives the portion of the largest variance of the features that is added to variance in order to stabilize calculation.

Attributes

Following table consist the attributes used by **sklearn.naive_bayes.GaussianNB** method:

Attributes	Description
***class_prior_:** array, shape(n_classes,)*	It provides the probability of every class.
***class_count_:** array, shape(n_classes,)*	It provides the actual number of training samples observed in every class.
***theta_:** array, shape (n_classes, n_features)*	It gives the mean of each feature per class.
***sigma_:** array, shape (n_classes, n_features)*	It gives the variance of each feature per class.
***epsilon_:** float*	These are the absolute additive value to variance.

Methods

Following table consist the methods used by **sklearn.naive_bayes.GaussianNB** method:

Method	Description

fit (self, X, y[, sample_weight])	This method will Fit Gaussian Naive Bayes classifier according to X and y.
get_params (self[, deep])	With the help of this method we can get the parameters for this estimator.
partial_fit (self, X, y[,classes, sample_weight])	This method allows the incremental fit on a batch of samples.
predict (self, X)	This method will perform classification on an array of test vectors X.
predict_log_proba(self, X)	This method will return the log-probability estimates for the test vector X.
predict_proba(self, X)	This method will return the probability estimates for the test vector X.
score(self, X, y[, sample_weight])	With this method we can get the mean accuracy on the given test data and labels.
set_params(self, **params)	This method allows us to set the parameters of this estimator.

Implementation Example

The Python script below will use **sklearn.naive_bayes.GaussianNB** method to construct Gaussian Naïve Bayes Classifier from our data set:

```
import numpy as np
X = np.array([[-1, -1], [-2, -4], [-4, -6], [1, 2]])
Y = np.array([1, 1, 2, 2])
from sklearn.naive_bayes import GaussianNB
GNBclf = GaussianNB()
GNBclf.fit(X, Y)
```

Output

```
GaussianNB(priors=None, var_smoothing=1e-09)
```

Now, once fitted we can predict the new value by using predict() method as follows:

```
print((GNBclf.predict([[-0.5, 2]])))
```

Output

```
[2]
```

Multinomial Naïve Bayes

It is another useful Naïve Bayes classifier. It assumes that the features are drawn from a simple Multinomial distribution. The Scikit-learn provides **sklearn.naive_bayes.MultinomialNB** to implement the Multinomial Naïve Bayes algorithm for classification.

Parameters

Following table consist the parameters used by **sklearn.naive_bayes.MultinomialNB** method:

Parameter	Description
alpha: *float, optional, default = 1.0*	It represents the additive smoothing parameter. If you choose 0 as its value, then there will be no smoothing.
fit_prior: *Boolean, optional, default = true*	It tells the model that whether to learn class prior probabilities or not. The default value is True but if set to False, the algorithms will use a uniform prior.
class_prior: *array-like, size(n_classes,), optional, Default = None*	This parameter represents the prior probabilities of each class.

Attributes

Following table consist the attributes used by **sklearn.naive_bayes.MultinomialNB** method:

Attributes	Description
class_log_prior_: *array, shape(n_classes,)*	It provides the smoothed log probability for every class.
class_count_: *array, shape(n_classes,)*	It provides the actual number of training samples encountered for each class.
intercept_: *array, shape (n_classes,)*	These are the Mirrors *class_log_prior_* for interpreting MultinomilaNB model as a linear model.
feature_log_prob_: *array, shape (n_classes, n_features)*	It gives the empirical log probability of features given a class $P(features \mid Y)$.

coef_: *array, shape (n_classes, n_features)*	These are the Mirrors *feature_log_prior_* for interpreting MultinomilaNB model as a linear model.
feature_count_: *array, shape (n_classes, n_features)*	It provides the actual number of training samples encountered for each (class,feature).

The methods of sklearn.naive_bayes. MultinomialNB are same as we have used in sklearn.naive_bayes.GaussianNB.

Implementation Example

The Python script below will use **sklearn.naive_bayes.GaussianNB** method to construct Gaussian Naïve Bayes Classifier from our data set:

```
import numpy as np
X = np.random.randint(8, size=(8, 100))
y = np.array([1, 2, 3, 4, 5, 6, 7, 8])

from sklearn.naive_bayes import MultinomialNB
MNBclf = MultinomialNB()
MNBclf.fit(X, y)
```

Output

```
MultinomialNB(alpha=1.0, class_prior=None, fit_prior=True)
```

Now, once fitted we can predict the new value aby using predict() method as follows:

```
print((MNBclf.predict(X[4:5]))
```

Output

```
[5]
```

Bernoulli Naïve Bayes

Bernoulli Naïve Bayes is another useful naïve Bayes model. The assumption in this model is that the features binary (0s and 1s) in nature. An application of Bernoulli Naïve Bayes classification is Text classification with 'bag of words' model. The Scikit-learn provides **sklearn.naive_bayes.BernoulliNB** to implement the Gaussian Naïve Bayes algorithm for classification.

Parameters

Following table consist the parameters used by **sklearn.naive_bayes.BernoulliNB** method:

Parameter	Description
alpha: *float, optional, default = 1.0*	It represents the additive smoothing parameter. If you choose 0 as its value, then there will be no smoothing.
binarize: *float or None, optional, default = 0.0*	With this parameter we can set the threshold for binarizing of sample features. Binarization here means mapping to the Booleans. If you choose its value to be None it means input consists of binary vectors.
fit_prior: *Boolean, optional, default = true*	It tells the model that whether to learn class prior probabilities or not. The default value is True but if set to False, the algorithms will use a uniform prior.
class_prior: *array-like, size(n_classes,), optional, Default = None*	This parameter represents the prior probabilities of each class.

Attributes

Following table consist the attributes used by **sklearn.naive_bayes.BernoulliNB** method:

Attributes	Description
class_log_prior_: *array, shape(n_classes,)*	It provides the smoothed log probability for every class.
class_count_: *array, shape(n_classes,)*	It provides the actual number of training samples encountered for each class.
feature_log_prob_: *array, shape (n_classes, n_features)*	It gives the empirical log probability of features given a class $P(features \mid Y)$.
feature_count_: *array, shape (n_classes, n_features)*	It provides the actual number of training samples encountered for each (class,feature).

The methods of **sklearn.naive_bayes.BernoulliNB** are same as we have used in **sklearn.naive_bayes.GaussianNB.**

Implementation Example

The Python script below will use **sklearn.naive_bayes.BernoulliNB** method to construct Bernoulli Naïve Bayes Classifier from our data set:

```
import numpy as np
X = np.random.randint(10, size=(10, 1000))
y = np.array([1, 2, 3, 4, 5, 6, 7, 8, 9, 10])
from sklearn.naive_bayes import BernoulliNB
BNBclf = BernoulliNB()
BNBclf.fit(X, y)
```

Output

```
BernoulliNB(alpha=1.0, binarize=0.0, class_prior=None, fit_prior=True)
```

Now, once fitted we can predict the new value by using predict() method as follows:

```
print((BNBclf.predict(X[0:5]))
```

Output

```
[1 2 3 4 5]
```

Complement Naïve Bayes

Another useful naïve Bayes model which was designed to correct the severe assumptions made by Multinomial Bayes classifier. This kind of NB classifier is suitable for imbalanced data sets. The Scikit-learn provides **sklearn.naive_bayes.ComplementNB** to implement the Gaussian Naïve Bayes algorithm for classification.

Parameters

Followings table consist the parameters used by **sklearn.naive_bayes.ComplementNB** method:

Parameter	Description
alpha: *float, optional, default = 1.0*	It represents the additive smoothing parameter. If you choose 0 as its value, then there will be no smoothing.
fit_prior: *Boolean, optional, default = true*	It tells the model that whether to learn class prior probabilities or not. The default value is True but if set to False, the algorithms will use a uniform prior. This parameter is only used in edge case with a single class in the training data set.
class_prior: *array-like,*	This parameter represents the prior probabilities of each class.

size(n_classes,), optional, Default = None	
norm: *Boolean, optional, default = False*	It tells the model that whether to perform second normalization of the weights or not.

Attributes

Following table consist the attributes used by **sklearn.naive_bayes.ComplementNB** method:

Attributes	Description
class_log_prior_: *array, shape(n_classes,)*	It provides the smoothed empirical log probability for every class. This attribute is only used in edge case with a single class in the training data set.
class_count_: *array, shape(n_classes,)*	It provides the actual number of training samples encountered for each class.
feature_log_prob_: *array, shape (n_classes, n_features)*	It gives the empirical weights for class components.
feature_count_: *array, shape (n_classes, n_features)*	It provides the actual number of training samples encountered for each (class,feature).
feature_all_: *array, shape(n_features,)*	It provides the actual number of training samples encountered for each feature.

The methods of **sklearn.naive_bayes.ComplementNB** are same as we have used in **sklearn.naive_bayes.GaussianNB**.

Implementation Example

The Python script below will use **sklearn.naive_bayes.BernoulliNB** method to construct Bernoulli Naïve Bayes Classifier from our data set:

```
import numpy as np
X = np.random.randint(15, size=(15, 1000))
y = np.array([1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15])
from sklearn.naive_bayes import ComplementNB
CNBclf = ComplementNB()
CNBclf.fit(X, y)
```

Output

```
ComplementNB(alpha=1.0, class_prior=None, fit_prior=True, norm=False)
```

Now, once fitted we can predict the new value aby using predict() method as follows:

```
print((CNBclf.predict(X[10:15]))
```

Output

```
[11 12 13 14 15]
```

Building Naïve Bayes Classifier

We can also apply Naïve Bayes classifier on Scikit-learn dataset. In the example below, we are applying GaussianNB and fitting the breast_cancer dataset of Scikit-leran.

```
Import Sklearn
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
data = load_breast_cancer()
label_names = data['target_names']
labels = data['target']
feature_names = data['feature_names']
features = data['data']
     print(label_names)
     print(labels[0])
     print(feature_names[0])
     print(features[0])
train, test, train_labels, test_labels =
train_test_split(features,labels,test_size = 0.40, random_state = 42)
from sklearn.naive_bayes import GaussianNB
GNBclf = GaussianNB()
model = GNBclf.fit(train, train_labels)
preds = GNBclf.predict(test)
print(preds)
```

Output

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

The above output consists of a series of **0s** and **1s** which are basically the predicted values from tumor classes namely malignant and benign.

14. Scikit-Learn — Decision Trees

In this chapter, we will learn about learning method in Sklearn which is termed as decision trees.

Decisions tress (DTs) are the most powerful non-parametric supervised learning method. They can be used for the classification and regression tasks. The main goal of DTs is to create a model predicting target variable value by learning simple decision rules deduced from the data features. Decision trees have two main entities; one is root node, where the data splits, and other is decision nodes or leaves, where we got final output.

Decision Tree Algorithms

Different Decision Tree algorithms are explained below:

ID3

It was developed by Ross Quinlan in 1986. It is also called Iterative Dichotomiser 3. The main goal of this algorithm is to find those categorical features, for every node, that will yield the largest information gain for categorical targets.

It lets the tree to be grown to their maximum size and then to improve the tree's ability on unseen data, applies a pruning step. The output of this algorithm would be a multiway tree.

C4.5

It is the successor to ID3 and dynamically defines a discrete attribute that partition the continuous attribute value into a discrete set of intervals. That's the reason it removed the restriction of categorical features. It converts the ID3 trained tree into sets of 'IF-THEN' rules.

In order to determine the sequence in which these rules should applied, the accuracy of each rule will be evaluated first.

C5.0

It works similar as C4.5 but it uses less memory and build smaller rulesets. It is more accurate than C4.5.

CART

It is called Classification and Regression Trees alsgorithm. It basically generates binary splits by using the features and threshold yielding the largest information gain at each node (called the Gini index).

Homogeneity depends upon Gini index, higher the value of Gini index, higher would be the homogeneity. It is like C4.5 algorithm, but, the difference is that it does not compute rule sets and does not support numerical target variables (regression) as well.

Classification with decision trees

In this case, the decision variables are categorical.

Sklearn Module: The Scikit-learn library provides the module name **DecisionTreeClassifier** for performing multiclass classification on dataset.

Parameters

Following table consist the parameters used by **sklearn.tree.DecisionTreeClassifier** module:

Parameter	Description
criterion: *string, optional default= "gini"*	It represents the function to measure the quality of a split. Supported criteria are "gini" and "entropy". The default is gini which is for Gini impurity while entropy is for the information gain.
splitter: *string, optional default= "best"*	It tells the model, which strategy from "best" or "random" to choose the split at each node.
max_depth : *int or None, optional default=None*	This parameter decides the maximum depth of the tree. The default value is None which means the nodes will expand until all leaves are pure or until all leaves contain less than min_smaples_split samples.
min_samples_split: *int , float, optional default=2*	This parameter provides the minimum number of samples required to split an internal node.
min_samples_leaf: *int, float, optional default=1*	This parameter provides the minimum number of samples required to be at a leaf node.
min_weight_fraction_leaf: *float, optional default=0.*	With this parameter, the model will get the minimum weighted fraction of the sum of weights required to be at a leaf node.
max_features: *int, float, string or None, optional default=None*	It gives the model the number of features to be considered when looking for the best split.
***random_state**: int, RandomState instance or None, optional, default = none*	This parameter represents the seed of the pseudo random number generated which is used while shuffling the data. Followings are the options: • **int**: In this case, *random_state* is the seed used by random number generator. • **RandomState instance**: In this case, *random_state* is the random number generator. • **None**: In this case, the random number generator is the RandonState instance used by np.random.

max_leaf_nodes: *int or None, optional default=None*	This parameter will let grow a tree with *max_leaf_nodes* in best-first fashion. The default is none which means there would be unlimited number of leaf nodes.
min_impurity_decrease: *float, optional default=0.*	This value works as a criterion for a node to split because the model will split a node if this split induces a decrease of the impurity greater than or equal to **min_impurity_decrease value.**
min_impurity_split: *float, default=1e-7*	It represents the threshold for early stopping in tree growth.
class_weight: *dict, list of dicts, "balanced" or None, default=None*	It represents the weights associated with classes. The form is {class_label: weight}. If we use the default option, it means all the classes are supposed to have weight one. On the other hand, if you choose ***class_weight: balanced***, it will use the values of y to automatically adjust weights.
presort: *bool, optional default=False*	It tells the model whether to presort the data to speed up the finding of best splits in fitting. The default is false but of set to true, it may slow down the training process.

Attributes

Following table consist the attributes used by **sklearn.tree.DecisionTreeClassifier** module:

Attributes	Description
feature_importances_: *array of shape =[n_features]*	This attribute will return the feature importance.
classes_: *array of shape = [n_classes] or a list of such arrays*	It represents the classes labels i.e. the single output problem, or a list of arrays of class labels i.e. multi-output problem.
max_features_: *int*	It represents the deduced value of ***max_features*** parameter.
n_classes_: *int or list*	It represents the number of classes i.e. the single output problem, or a list of number of classes for every output i.e. multi-output problem.
n_features_: *int*	It gives the number of **features** when fit() method is performed.
n_outputs_: *int*	It gives the number of **outputs** when fit() method is performed.

Methods

Following table consist the methods used by **sklearn.tree.DecisionTreeClassifier** module:

Method	Description
apply(self, X[, check_input])	This method will return the index of the leaf.
decision_path(self, X[, check_input])	As name suggests, this method will return the decision path in the tree
fit(self, X, y[, sample_weight, …])	fit() method will build a decision tree classifier from given training set (X, y).
get_depth(self)	As name suggests, this method will return the depth of the decision tree
get_n_leaves(self)	As name suggests, this method will return the number of leaves of the decision tree.
get_params(self[, deep])	We can use this method to get the parameters for estimator.
predict(self, X[, check_input])	It will predict class value for X.
predict_log_proba(self, X)	It will predict class log-probabilities of the input samples provided by us, X.
predict_proba(self, X[, check_input])	It will predict class probabilities of the input samples provided by us, X.
score(self, X, y[, sample_weight])	As the name implies, the score() method will return the mean accuracy on the given test data and labels.
set_params(self, **params)	We can set the parameters of estimator with this method.

Implementation Example

The Python script below will use **sklearn.tree.DecisionTreeClassifier** module to construct a classifier for predicting male or female from our data set having 25 samples and two features namely 'height' and 'length of hair':

```
from sklearn import tree

from sklearn.model_selection import train_test_split

X=[[165,19],[175,32],[136,35],[174,65],[141,28],[176,15],[131,32],[166,6],[128,
32],[179,10],[136,34],[186,2],[126,25],[176,28],[112,38],[169,9],[171,36],[116,
25],[196,25], [196,38], [126,40], [197,20], [150,25], [140,32],[136,35]]
```

```
Y=['Man','Woman','Woman','Man','Woman','Man','Woman','Man','Woman','Man','Woman
','Man','Woman','Woman','Woman','Man','Woman','Woman','Man', 'Woman', 'Woman',
'Man', 'Man', 'Woman', 'Woman']

data_feature_names = ['height','length of hair']

X_train, X_test, y_train, y_test = train_test_split(X, Y, test_size=0.3,
random_state=1)

DTclf = tree.DecisionTreeClassifier()

DTclf = clf.fit(X,Y)

prediction = DTclf.predict([[135,29]])

print(prediction)
```

Output

```
['Woman']
```

We can also predict the probability of each class by using following python predict_proba() method as follows:

```
prediction = DTclf.predict_proba([[135,29]])

print(prediction)
```

Output

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

Regression with decision trees

In this case the decision variables are continuous.

Sklearn Module: The Scikit-learn library provides the module name **DecisionTreeRegressor** for applying decision trees on regression problems.

Parameters

Parameters used by **DecisionTreeRegressor** are almost same as that were used in **DecisionTreeClassifier** module. The difference lies in 'criterion' parameter. For **DecisionTreeRegressor** modules '**criterion:** *string, optional default= "mse"*' parameter have the following values:

- **mse:** It stands for the mean squared error. It is equal to variance reduction as feature selectin criterion. It minimises the L2 loss using the mean of each terminal node.
- **freidman_mse:** It also uses mean squared error but with Friedman's improvement score.
- **mae:** It stands for the mean absolute error. It minimizes the L1 loss using the median of each terminal node.

Another difference is that it does not have ***'class_weight'*** parameter.

Attributes

Attributes of **DecisionTreeRegressor** are also same as that were of **DecisionTreeClassifier** module. The difference is that it does not have **'classes_'** and '***n_classes_***' attributes.

Methods

Methods of **DecisionTreeRegressor** are also same as that were of **DecisionTreeClassifier** module. The difference is that it does not have **'predict_log_proba()'** and '**predict_proba()**' methods.

Implementation Example

The fit() method in Decision tree regression model will take floating point values of y. let's see a simple implementation example by using **Sklearn.tree.DecisionTreeRegressor**:

```
from sklearn import tree
X = [[1, 1], [5, 5]]
y = [0.1, 1.5]
DTreg = tree.DecisionTreeRegressor()
DTreg = clf.fit(X, y)
```

Once fitted, we can use this regression model to make prediction as follows:

```
DTreg.predict([[4, 5]])
```

Output

```
array([1.5])
```

15. Scikit-Learn — Randomized Decision Trees

This chapter will help you in understanding randomized decision trees in Sklearn.

Randomized Decision Tree algorithms

As we know that a DT is usually trained by recursively splitting the data, but being prone to overfit, they have been transformed to random forests by training many trees over various subsamples of the data. The **sklearn.ensemble** module is having following two algorithms based on randomized decision trees:

The Random Forest algorithm

For each feature under consideration, it computes the locally optimal feature/split combination. In Random forest, each decision tree in the ensemble is built from a sample drawn with replacement from the training set and then gets the prediction from each of them and finally selects the best solution by means of voting. It can be used for both classification as well as regression tasks.

Classification with Random Forest

For creating a random forest classifier, the Scikit-learn module provides **sklearn.ensemble.RandomForestClassifier**. While building random forest classifier, the main parameters this module uses are '**max_features'** and **'n_estimators'**.

Here, **'max_features'** is the size of the random subsets of features to consider when splitting a node. If we choose this parameter's value to none then it will consider all the features rather than a random subset. On the other hand, **n_estimators** are the number of trees in the forest. The higher the number of trees, the better the result will be. But it will take longer to compute also.

Implementation example

In the following example, we are building a random forest classifier by using **sklearn.ensemble.RandomForestClassifier** and also checking its accuracy also by using **cross_val_score** module.

```
from sklearn.model_selection import cross_val_score

from sklearn.datasets import make_blobs

from sklearn.ensemble import RandomForestClassifier

X, y = make_blobs(n_samples=10000, n_features=10, centers=100,random_state=0)
RFclf =
RandomForestClassifier(n_estimators=10,max_depth=None,min_samples_split=2,
random_state=0)

scores = cross_val_score(RFclf, X, y, cv=5)

scores.mean()
```

Output

```
0.9997
```

We can also use the sklearn dataset to build Random Forest classifier. As in the following example we are using iris dataset. We will also find its accuracy score and confusion matrix.

```
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import classification_report, confusion_matrix,
accuracy_score


path = "https://archive.ics.uci.edu/ml/machine-learning-
databases/iris/iris.data"
headernames = ['sepal-length', 'sepal-width', 'petal-length', 'petal-width',
'Class']
dataset = pd.read_csv(path, names=headernames)
X = dataset.iloc[:, :-1].values
y = dataset.iloc[:, 4].values
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.30)
RFclf = RandomForestClassifier(n_estimators=50)
RFclf.fit(X_train, y_train)
y_pred = RFclf.predict(X_test)
result = confusion_matrix(y_test, y_pred)
print("Confusion Matrix:")
print(result)
result1 = classification_report(y_test, y_pred)
print("Classification Report:",)
print (result1)
result2 = accuracy_score(y_test,y_pred)
print("Accuracy:",result2)
```

Output

```
Confusion Matrix:
[[14  0  0]
 [ 0 18  1]
 [ 0  0 12]]
```

```
Classification Report:
                 precision    recall  f1-score   support

    Iris-setosa       1.00      1.00      1.00        14
Iris-versicolor       1.00      0.95      0.97        19
 Iris-virginica       0.92      1.00      0.96        12

      micro avg       0.98      0.98      0.98        45
      macro avg       0.97      0.98      0.98        45
   weighted avg       0.98      0.98      0.98        45

Accuracy: 0.9777777777777777
```

Regression with Random Forest

For creating a random forest regression, the Scikit-learn module provides **sklearn.ensemble.RandomForestRegressor.** While building random forest regressor, it will use the same parameters as used by **sklearn.ensemble.RandomForestClassifier.**

Implementation example

In the following example, we are building a random forest regressor by using **sklearn.ensemble.RandomForestregressor** and also predicting for new values by using predict() method.

```
from sklearn.ensemble import RandomForestRegressor
from sklearn.datasets import make_regression
X, y = make_regression(n_features=10, n_informative=2,random_state=0,
shuffle=False)
RFregr = RandomForestRegressor(max_depth=10,random_state=0,n_estimators=100)
RFregr.fit(X, y)
```

Output

```
RandomForestRegressor(bootstrap=True, criterion='mse', max_depth=10,
           max_features='auto', max_leaf_nodes=None,
           min_impurity_decrease=0.0, min_impurity_split=None,
           min_samples_leaf=1, min_samples_split=2,

           min_weight_fraction_leaf=0.0, n_estimators=100, n_jobs=None,
           oob_score=False, random_state=0, verbose=0, warm_start=False)
```

```
```

Once fitted we can predict from regression model as follows:

```
print(RFregr.predict([[0, 2, 3, 0, 1, 1, 1, 1, 2, 2]]))
```

Output

```
[98.47729198]
```

Extra-Tree Methods

For each feature under consideration, it selects a random value for the split. The benefit of using extra tree methods is that it allows to reduce the variance of the model a bit more. The disadvantage of using these methods is that it slightly increases the bias.

Classification with Extra-Tree Method

For creating a classifier using Extra-tree method, the Scikit-learn module provides **sklearn.ensemble.ExtraTreesClassifier**. It uses the same parameters as used by **sklearn.ensemble.RandomForestClassifier**. The only difference is in the way, discussed above, they build trees.

Implementation example

In the following example, we are building a random forest classifier by using **sklearn.ensemble.ExtraTreeClassifier** and also checking its accuracy by using **cross_val_score** module.

```
from sklearn.model_selection import cross_val_score

from sklearn.datasets import make_blobs

from sklearn.ensemble import ExtraTreesClassifier

X, y = make_blobs(n_samples=10000, n_features=10, centers=100,random_state=0)

ETclf =
ExtraTreesClassifier(n_estimators=10,max_depth=None,min_samples_split=10,
random_state=0)

scores = cross_val_score(ETclf, X, y, cv=5)

scores.mean()
```

Output

```
1.0
```

We can also use the sklearn dataset to build classifier using Extra-Tree method. As in the following example we are using Pima-Indian dataset.

```
from pandas import read_csv
```

```
from sklearn.model_selection import KFold
from sklearn.model_selection import cross_val_score
from sklearn.ensemble import ExtraTreesClassifier
path = r"C:\pima-indians-diabetes.csv"
headernames = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age',
'class']
data = read_csv(path, names=headernames)
array = data.values
X = array[:,0:8]
Y = array[:,8]
seed = 7
kfold = KFold(n_splits=10, random_state=seed)
num_trees = 150
max_features = 5
ETclf = ExtraTreesClassifier(n_estimators=num_trees, max_features=max_features)
results = cross_val_score(ETclf, X, Y, cv=kfold)
print(results.mean())
```

Output

```
    0.7551435406698566
```

Regression with Extra-Tree Method

For creating a **Extra-Tree** regression, the Scikit-learn module provides **sklearn.ensemble.ExtraTreesRegressor.** While building random forest regressor, it will use the same parameters as used by **sklearn.ensemble.ExtraTreesClassifier.**

Implementation example

In the following example, we are applying **sklearn.ensemble.ExtraTreesregressor** and on the same data as we used while creating random forest regressor. Let's see the difference in the Output

```
from sklearn.ensemble import ExtraTreesRegressor
from sklearn.datasets import make_regression
X, y = make_regression(n_features=10, n_informative=2,random_state=0,
shuffle=False)
ETregr = ExtraTreesRegressor(max_depth=10,random_state=0,n_estimators=100)
ETregr.fit(X, y)
```

Output

```
ExtraTreesRegressor(bootstrap=False, criterion='mse', max_depth=10,
```

```
            max_features='auto', max_leaf_nodes=None,
            min_impurity_decrease=0.0, min_impurity_split=None,
            min_samples_leaf=1, min_samples_split=2,
            min_weight_fraction_leaf=0.0, n_estimators=100, n_jobs=None,
            oob_score=False, random_state=0, verbose=0, warm_start=False)
```

Once fitted we can predict from regression model as follows:

```
print(ETregr.predict([[0, 2, 3, 0, 1, 1, 1, 1, 2, 2]]))
```

Output

```
[85.50955817]
```

16. Scikit-Learn — Boosting Methods

In this chapter, we will learn about the boosting methods in Sklearn, which enables building an ensemble model.

Boosting methods build ensemble model in an increment way. The main principle is to build the model incrementally by training each base model estimator sequentially. In order to build powerful ensemble, these methods basically combine several week learners which are sequentially trained over multiple iterations of training data. The **sklearn.ensemble** module is having following two boosting methods.

AdaBoost

It is one of the most successful boosting ensemble method whose main key is in the way they give weights to the instances in dataset. That's why the algorithm needs to pay less attention to the instances while constructing subsequent models.

Classification with AdaBoost

For creating a AdaBoost classifier, the Scikit-learn module provides **sklearn.ensemble.AdaBoostClassifier.** While building this classifier, the main parameter this module use is **base_estimator.** Here, **base_estimator** is the value of the base estimator from which the boosted ensemble is built. If we choose this parameter's value to none then, the base estimator would be **DecisionTreeClassifier(max_depth=1).**

Implementation example

In the following example, we are building a AdaBoost classifier by using **sklearn.ensemble.AdaBoostClassifier** and also predicting and checking its score.

```
from sklearn.ensemble import AdaBoostClassifier
from sklearn.datasets import make_classification
X, y = make_classification(n_samples=1000, n_features=10,n_informative=2,
n_redundant=0,random_state=0, shuffle=False)
ADBclf = AdaBoostClassifier(n_estimators=100, random_state=0)
ADBclf.fit(X, y)
```

Output

```
AdaBoostClassifier(algorithm='SAMME.R', base_estimator=None,
          learning_rate=1.0, n_estimators=100, random_state=0)
```

Once fitted, we can predict for new values as follows:

```
print(ADBclf.predict([[0, 2, 3, 0, 1, 1, 1, 1, 2, 2]]))
```

Output

```
[1]
```

Now we can check the score as follows:

```
ADBclf.score(X, y)
```

Output

```
0.995
```

We can also use the sklearn dataset to build classifier using Extra-Tree method. For example, in an example given below, we are using Pima-Indian dataset.

```
from pandas import read_csv
from sklearn.model_selection import KFold
from sklearn.model_selection import cross_val_score
from sklearn.ensemble import AdaBoostClassifier
path = r"C:\pima-indians-diabetes.csv"
headernames = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age',
'class']
data = read_csv(path, names=headernames)
array = data.values
X = array[:,0:8]
Y = array[:,8]
seed = 5
kfold = KFold(n_splits=10, random_state=seed)
num_trees = 100
max_features = 5
ADBclf = AdaBoostClassifier(n_estimators=num_trees, max_features=max_features)
results = cross_val_score(ADBclf, X, Y, cv=kfold)
print(results.mean())
```

Output

```
    0.7851435406698566
```

Regression with AdaBoost

For creating a regressor with Ada Boost method, the Scikit-learn library provides **sklearn.ensemble.AdaBoostRegressor**. While building regressor, it will use the same parameters as used by **sklearn.ensemble.AdaBoostClassifier**.

Implementation example

In the following example, we are building a AdaBoost regressor by using **sklearn.ensemble.AdaBoostregressor** and also predicting for new values by using predict() method.

```
from sklearn.ensemble import AdaBoostRegressor

from sklearn.datasets import make_regression

X, y = make_regression(n_features=10, n_informative=2,random_state=0,
shuffle=False)

ADBregr = RandomForestRegressor(random_state=0,n_estimators=100)

ADBregr.fit(X, y)
```

Output

```
AdaBoostRegressor(base_estimator=None, learning_rate=1.0, loss='linear',

         n_estimators=100, random_state=0)
```

Once fitted we can predict from regression model as follows:

```
print(ADBregr.predict([[0, 2, 3, 0, 1, 1, 1, 1, 2, 2]]))
```

Output

```
[85.50955817]
```

Gradient Tree Boosting

It is also called **Gradient Boosted Regression Trees** (GRBT). It is basically a generalization of boosting to arbitrary differentiable loss functions. It produces a prediction model in the form of an ensemble of week prediction models. It can be used for the regression and classification problems. Their main advantage lies in the fact that they naturally handle the mixed type data.

Classification with Gradient Tree Boost

For creating a Gradient Tree Boost classifier, the Scikit-learn module provides **sklearn.ensemble.GradientBoostingClassifier**. While building this classifier, the main parameter this module use is '**loss**'. Here, '**loss**' is the value of loss function to be optimized. If we choose loss = deviance, it refers to deviance for classification with probabilistic outputs.

On the other hand, if we choose this parameter's value to exponential then it recovers the AdaBoost algorithm. The parameter **n_estimators** will control the number of week learners. A hyper-parameter named **learning_rate** (in the range of (0.0, 1.0]) will control overfitting via shrinkage.

Implementation example

In the following example, we are building a Gradient Boosting classifier by using **sklearn.ensemble.GradientBoostingClassifier**. We are fitting this classifier with 50 week learners.

```
from sklearn.datasets import make_hastie_10_2
from sklearn.ensemble import GradientBoostingClassifier
X, y = make_hastie_10_2(random_state=0)
X_train, X_test = X[:5000], X[5000:]
y_train, y_test = y[:5000], y[5000:]

GDBclf = GradientBoostingClassifier(n_estimators=50,
learning_rate=1.0,max_depth=1, random_state=0).fit(X_train, y_train)
GDBclf.score(X_test, y_test)
```

Output

```
from pandas import read_csv
from sklearn.model_selection import KFold
from sklearn.model_selection import cross_val_score
from sklearn.ensemble import GradientBoostingClassifier
path = r"C:\pima-indians-diabetes.csv"
headernames = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age',
'class']
data = read_csv(path, names=headernames)
array = data.values
X = array[:,0:8]
Y = array[:,8]
seed = 5
kfold = KFold(n_splits=10, random_state=seed)
num_trees = 100
max_features = 5
ADBclf = GradientBoostingClassifier(n_estimators=num_trees,
max_features=max_features)
results = cross_val_score(ADBclf, X, Y, cv=kfold)
print(results.mean())
```

```
0.8724285714285714
```

We can also use the sklearn dataset to build classifier using Gradient Boosting Classifier. As in the following example we are using Pima-Indian dataset.

Output

```
0.7946582356674234
```

Regression with Gradient Tree Boost

For creating a regressor with Gradient Tree Boost method, the Scikit-learn library provides **sklearn.ensemble.GradientBoostingRegressor**. It can specify the loss function for regression via the parameter name **loss**. The default value for loss is 'ls'.

Implementation example

In the following example, we are building a Gradient Boosting regressor by using **sklearn.ensemble.GradientBoostingregressor** and also finding the mean squared error by using mean_squared_error() method.

```
import numpy as np
from sklearn.metrics import mean_squared_error
from sklearn.datasets import make_friedman1
from sklearn.ensemble import GradientBoostingRegressor
X, y = make_friedman1(n_samples=2000, random_state=0, noise=1.0)
X_train, X_test = X[:1000], X[1000:]
y_train, y_test = y[:1000], y[1000:]
GDBreg = GradientBoostingRegressor(n_estimators=80, learning_rate=0.1,
max_depth=1, random_state=0, loss='ls').fit(X_train, y_train)
```

Once fitted we can find the mean squared error as follows:

```
mean_squared_error(y_test, GDBreg.predict(X_test))
```

Output

```
5.391246106657164
```

17. Scikit-Learn — Clustering Methods

Here, we will study about the clustering methods in Sklearn which will help in identification of any similarity in the data samples.

Clustering methods, one of the most useful unsupervised ML methods, used to find similarity & relationship patterns among data samples. After that, they cluster those samples into groups having similarity based on features. Clustering determines the intrinsic grouping among the present unlabeled data, that's why it is important.

The Scikit-learn library have **sklearn.cluster** to perform clustering of unlabeled data. Under this module scikit-leran have the following clustering methods:

KMeans

This algorithm computes the centroids and iterates until it finds optimal centroid. It requires the number of clusters to be specified that's why it assumes that they are already known. The main logic of this algorithm is to cluster the data separating samples in n number of groups of equal variances by minimizing the criteria known as the inertia. The number of clusters identified by algorithm is represented by 'K.

Scikit-learn have **sklearn.cluster.KMeans** module to perform K-Means clustering. While computing cluster centers and value of inertia, the parameter named **sample_weight** allows **sklearn.cluster.KMeans** module to assign more weight to some samples.

Affinity Propagation

This algorithm is based on the concept of 'message passing' between different pairs of samples until convergence. It does not require the number of clusters to be specified before running the algorithm. The algorithm has a time complexity of the order $O(N^2T)$, which is the biggest disadvantage of it.

Scikit-learn have **sklearn.cluster.AffinityPropagation** module to perform Affinity Propagation clustering.

Mean Shift

This algorithm mainly discovers ***blobs*** in a smooth density of samples. It assigns the datapoints to the clusters iteratively by shifting points towards the highest density of datapoints. Instead of relying on a parameter named **bandwidth** dictating the size of the region to search through, it automatically sets the number of clusters.

Scikit-learn have **sklearn.cluster.MeanShift** module to perform Mean Shift clustering.

Spectral Clustering

Before clustering, this algorithm basically uses the eigenvalues i.e. spectrum of the similarity matrix of the data to perform dimensionality reduction in fewer dimensions. The use of this algorithm is not advisable when there are large number of clusters.

Scikit-learn have **sklearn.cluster.SpectralClustering** module to perform Spectral clustering.

Hierarchical Clustering

This algorithm builds nested clusters by merging or splitting the clusters successively. This cluster hierarchy is represented as dendrogram i.e. tree. It falls into following two categories:

Agglomerative hierarchical algorithms: In this kind of hierarchical algorithm, every data point is treated like a single cluster. It then successively agglomerates the pairs of clusters. This uses the bottom-up approach.

Divisive hierarchical algorithms: In this hierarchical algorithm, all data points are treated as one big cluster. In this the process of clustering involves dividing, by using top-down approach, the one big cluster into various small clusters.

Scikit-learn have **sklearn.cluster.AgglomerativeClustering** module to perform Agglomerative Hierarchical clustering.

DBSCAN

It stands for "**Density-based spatial clustering of applications with noise**". This algorithm is based on the intuitive notion of "clusters" & "noise" that clusters are dense regions of the lower density in the data space, separated by lower density regions of data points.

Scikit-learn have **sklearn.cluster.DBSCAN** module to perform DBSCAN clustering. There are two important parameters namely **min_samples** and **eps** used by this algorithm to define ***dense.***

Higher value of parameter **min_samples** or lower value of the parameter **eps** will give an indication about the higher density of data points which is necessary to form a cluster.

OPTICS

It stands for "**Ordering points to identify the clustering structure**". This algorithm also finds density-based clusters in spatial data. It's basic working logic is like DBSCAN.

It addresses a major weakness of DBSCAN algorithm-the problem of detecting meaningful clusters in data of varying density-by ordering the points of the database in such a way that spatially closest points become neighbors in the ordering.

Scikit-learn have **sklearn.cluster.OPTICS** module to perform OPTICS clustering.

BIRCH

It stands for Balanced iterative reducing and clustering using hierarchies. It is used to perform hierarchical clustering over large data sets. It builds a tree named **CFT** i.e. **Characteristics Feature Tree**, for the given data.

The advantage of CFT is that the data nodes called CF (Characteristics Feature) nodes holds the necessary information for clustering which further prevents the need to hold the entire input data in memory.

Scikit-learn have **sklearn.cluster.Birch** module to perform BIRCH clustering.

Comparing Clustering Algorithms

Following table will give a comparison (based on parameters, scalability and metric) of the clustering algorithms in scikit-learn.

Sr. No.	Algorithm Name	Parameters	Scalability	Metric Used
1.	K-Means	No. of clusters	Very large n_samples	The distance between points.
2.	Affinity Propagation	Damping	It's not scalable with n_samples	Graph Distance
3.	Mean-Shift	Bandwidth	It's not scalable with n_samples.	The distance between points.
4.	Spectral Clustering	No. of clusters	Medium level of scalability with n_samples. Small level of scalability with n_clusters.	Graph Distance
5.	Hierarchical Clustering	Distance threshold or No. of clusters	Large n_samples Large n_clusters	The distance between points.
6.	DBSCAN	Size of neighborhood	Very large n_samples and medium n_clusters.	Nearest point distance
7.	OPTICS	Minimum cluster membership	Very large n_samples and large n_clusters.	The distance between points.
8.	BIRCH	Threshold, Branching factor	Large n_samples Large n_clusters	The Euclidean distance between points.

K-Means Clustering on Scikit-learn Digit dataset

In this example, we will apply K-means clustering on digits dataset. This algorithm will identify similar digits without using the original label information. Implementation is done on Jupyter notebook.

```
%matplotlib inline

import matplotlib.pyplot as plt
```

```
import seaborn as sns; sns.set()
import numpy as np
from sklearn.cluster import KMeans
from sklearn.datasets import load_digits
digits = load_digits()
digits.data.shape
```

Output

```
1797, 64)
```

This output shows that digit dataset is having 1797 samples with 64 features.

Now, perform the K-Means clustering as follows:

```
kmeans = KMeans(n_clusters=10, random_state=0)
clusters = kmeans.fit_predict(digits.data)
kmeans.cluster_centers_.shape
```

Output

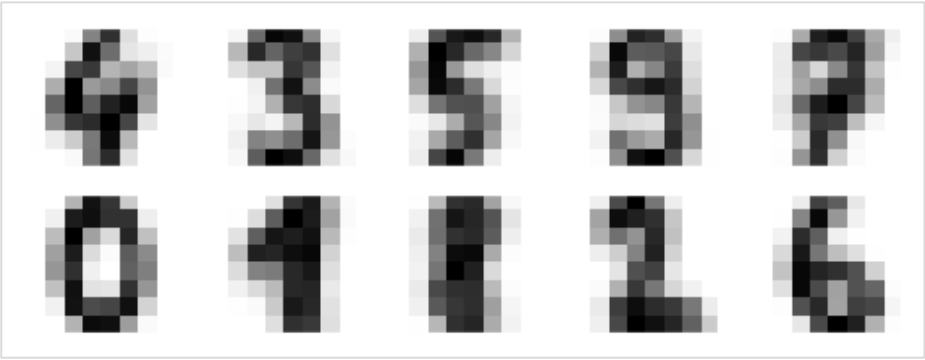
```
(10, 64)
```

This output shows that K-means clustering created 10 clusters with 64 features.

```
fig, ax = plt.subplots(2, 5, figsize=(8, 3))
centers = kmeans.cluster_centers_.reshape(10, 8, 8)
for axi, center in zip(ax.flat, centers):
    axi.set(xticks=[], yticks=[])
    axi.imshow(center, interpolation='nearest', cmap=plt.cm.binary)
```

Output

The below output has images showing clusters centers learned by K-Means Clustering.



Next, the Python script below will match the learned cluster labels (by K-Means) with the true labels found in them:

```
from scipy.stats import mode
labels = np.zeros_like(clusters)
for i in range(10):
    mask = (clusters == i)
    labels[mask] = mode(digits.target[mask])[0]
```

We can also check the accuracy with the help of the below mentioned command.

```
from sklearn.metrics import accuracy_score
accuracy_score(digits.target, labels)
```

Output

```
0.7935447968836951
```

Complete Implementation Example

```
%matplotlib inline
import matplotlib.pyplot as plt
import seaborn as sns; sns.set()
import numpy as np

from sklearn.cluster import KMeans
from sklearn.datasets import load_digits
digits = load_digits()
digits.data.shape
kmeans = KMeans(n_clusters=10, random_state=0)
clusters = kmeans.fit_predict(digits.data)
kmeans.cluster_centers_.shape
fig, ax = plt.subplots(2, 5, figsize=(8, 3))
centers = kmeans.cluster_centers_.reshape(10, 8, 8)
for axi, center in zip(ax.flat, centers):
    axi.set(xticks=[], yticks=[])
    axi.imshow(center, interpolation='nearest', cmap=plt.cm.binary)
from scipy.stats import mode
labels = np.zeros_like(clusters)
for i in range(10):
    mask = (clusters == i)
    labels[mask] = mode(digits.target[mask])[0]
from sklearn.metrics import accuracy_score
```

```
accuracy_score(digits.target, labels)
```

18. Scikit-Learn — Clustering Performance Evaluation

There are various functions with the help of which we can evaluate the performance of clustering algorithms.

Following are some important and mostly used functions given by the Scikit-learn for evaluating clustering performance:

Adjusted Rand Index

Rand Index is a function that computes a similarity measure between two clustering. For this computation rand index considers all pairs of samples and counting pairs that are assigned in the similar or different clusters in the predicted and true clustering. Afterwards, the raw Rand Index score is 'adjusted for chance' into the Adjusted Rand Index score by using the following formula:

$$Adjusted\ RI\ =\ (RI - Expected\_RI)/(max(RI) - Expected\_RI)$$

It has two parameters namely **labels_true**, which is ground truth class labels, and **labels_pred**, which are clusters label to evaluate.

Example

```
from sklearn.metrics.cluster import adjusted_rand_score

 labels_true = [0, 0, 1, 1, 1, 1]
 labels_pred = [0, 0, 2, 2, 3, 3]

adjusted_rand_score(labels_true, labels_pred)
```

Output

```
0.4444444444444445
```

Perfect labeling would be scored 1 and bad labelling or independent labelling is scored 0 or negative.

Mutual Information Based Score

Mutual Information is a function that computes the agreement of the two assignments. It ignores the permutations. There are following versions available:

Normalized Mutual Information (NMI)

Scikit learn have **sklearn.metrics.normalized_mutual_info_score** module.

Example

```
from sklearn.metrics.cluster import normalized_mutual_info_score

 labels_true = [0, 0, 1, 1, 1, 1]
 labels_pred = [0, 0, 2, 2, 3, 3]

normalized_mutual_info_score (labels_true, labels_pred)
```

Output

```
0.7611702597222881
```

Adjusted Mutual Information (AMI)

Scikit learn have **sklearn.metrics.adjusted_mutual_info_score** module.

Example

```
from sklearn.metrics.cluster import adjusted_mutual_info_score

 labels_true = [0, 0, 1, 1, 1, 1]
 labels_pred = [0, 0, 2, 2, 3, 3]

adjusted_mutual_info_score (labels_true, labels_pred)
```

Output

```
0.4444444444444448
```

Fowlkes-Mallows Score

The Fowlkes-Mallows function measures the similarity of two clustering of a set of points. It may be defined as the geometric mean of the pairwise precision and recall.

Mathematically,

$$FMS = \frac{TP}{\sqrt{(TP + FP)(TP + FN)}}$$

Here, ***TP = True Positive;*** number of pair of points belonging to the same clusters in true as well as predicted labels both.

FP = False Positive; number of pair of points belonging to the same clusters in true labels but not in the predicted labels.

FN = False Negative; number of pair of points belonging to the same clusters in the predicted labels but not in the true labels.

The Scikit learn has **sklearn.metrics.fowlkes_mallows_score** module:

Example

```
from sklearn.metrics.cluster import fowlkes_mallows_score


 labels_true = [0, 0, 1, 1, 1, 1]
 labels_pred = [0, 0, 2, 2, 3, 3]


fowlkes_mallows__score (labels_true, labels_pred)
```

Output

```
0.6546536707079771
```

Silhouette Coefficient

The Silhouette function will compute the mean Silhouette Coefficient of all samples using the mean intra-cluster distance and the mean nearest-cluster distance for each sample.

Mathematically,

$$S = (b - a)/max(a, b)$$

Here, a is intra-cluster distance.

and, b is mean nearest-cluster distance.

The Scikit learn have **sklearn.metrics.silhouette_score** module:

Example

```
from sklearn import metrics.silhouette_score
from sklearn.metrics import pairwise_distances
from sklearn import datasets
import numpy as np
from sklearn.cluster import KMeans
dataset = datasets.load_iris()
X = dataset.data
y = dataset.target


kmeans_model = KMeans(n_clusters=3, random_state=1).fit(X)
labels = kmeans_model.labels_
silhouette_score(X, labels, metric='euclidean')
```

Output

```
0.5528190123564091
```

Contingency Matrix

This matrix will report the intersection cardinality for every trusted pair of (true, predicted). Confusion matrix for classification problems is a square contingency matrix.

The Scikit learn have **sklearn.metrics.contingency_matrix** module.

Example

```
from sklearn.metrics.cluster import contingency_matrix
x = ["a", "a", "a", "b", "b", "b"]
y = [1, 1, 2, 0, 1, 2]
contingency_matrix(x, y)
```

Output

```
array([[0, 2, 1],
       [1, 1, 1]])
```

The first row of above output shows that among three samples whose true cluster is “a”, none of them is in 0, two of the are in 1 and 1 is in 2. On the other hand, second row shows that among three samples whose true cluster is “b”, 1 is in 0, 1 is in 1 and 1 is in 2.

19. Scikit-Learn — Dimensionality Reduction using PCA

Dimensionality reduction, an unsupervised machine learning method is used to reduce the number of feature variables for each data sample selecting set of principal features. Principal Component Analysis (PCA) is one of the popular algorithms for dimensionality reduction.

Exact PCA

Principal Component Analysis (PCA) is used for linear dimensionality reduction using **Singular Value Decomposition** (SVD) of the data to project it to a lower dimensional space. While decomposition using PCA, input data is centered but not scaled for each feature before applying the SVD.

The Scikit-learn ML library provides **sklearn.decomposition.PCA** module that is implemented as a transformer object which learns n components in its **fit()** method. It can also be used on new data to project it on these components.

Example

The below example will use sklearn.decomposition.PCA module to find best 5 Principal components from Pima Indians Diabetes dataset.

```
 from pandas import read_csv
from sklearn.decomposition import PCA
path = r'C:\Users\Leekha\Desktop\pima-indians-diabetes.csv'
names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age',
‘class']
dataframe = read_csv(path, names=names)
array = dataframe.values
X = array[:,0:8]
Y = array[:,8]
pca = PCA(n_components=5)
fit = pca.fit(X)
print(("Explained Variance: %s") % (fit.explained_variance_ratio_))
print(fit.components_)
```

Output

```
Explained Variance: [0.88854663 0.06159078 0.02579012 0.01308614 0.00744094]


[[-2.02176587e-03  9.78115765e-02  1.60930503e-02  6.07566861e-02
```

```
  9.93110844e-01  1.40108085e-02  5.37167919e-04 -3.56474430e-03]
[-2.26488861e-02 -9.72210040e-01 -1.41909330e-01  5.78614699e-02
  9.46266913e-02 -4.69729766e-02 -8.16804621e-04 -1.40168181e-01]
[-2.24649003e-02  1.43428710e-01 -9.22467192e-01 -3.07013055e-01
  2.09773019e-02 -1.32444542e-01 -6.39983017e-04 -1.25454310e-01]
[-4.90459604e-02  1.19830016e-01 -2.62742788e-01  8.84369380e-01
 -6.55503615e-02  1.92801728e-01  2.69908637e-03 -3.01024330e-01]
[ 1.51612874e-01 -8.79407680e-02 -2.32165009e-01  2.59973487e-01
 -1.72312241e-04  2.14744823e-02  1.64080684e-03  9.20504903e-01]]
```

Incremental PCA

Incremental Principal Component Analysis (IPCA) is used to address the biggest limitation of Principal Component Analysis (PCA) and that is PCA only supports batch processing, means all the input data to be processed should fit in the memory.

The Scikit-learn ML library provides **sklearn.decomposition.IPCA** module that makes it possible to implement Out-of-Core PCA either by using its **partial_fit** method on sequentially fetched chunks of data or by enabling use of **np.memmap**, a memory mapped file, without loading the entire file into memory.

Same as PCA, while decomposition using IPCA, input data is centered but not scaled for each feature before applying the SVD.

Example

The below example will use **sklearn.decomposition.IPCA** module on Sklearn digit dataset.

```
from sklearn.datasets import load_digits
from sklearn.decomposition import IncrementalPCA
X, _ = load_digits(return_X_y=True)
transformer = IncrementalPCA(n_components=10, batch_size=100)
transformer.partial_fit(X[:100, :])
X_transformed = transformer.fit_transform(X)
X_transformed.shape
```

Output

```
(1797, 10)
```

Here, we can partially fit on smaller batches of data (as we did on 100 per batch) or you can let the **fit()** function to divide the data into batches.

Kernel PCA

Kernel Principal Component Analysis, an extension of PCA, achieves non-linear dimensionality reduction using kernels. It supports both **transform and inverse_transform.**

The Scikit-learn ML library provides **sklearn.decomposition.KernelPCA** module.

Example

The below example will use **sklearn.decomposition.KernelPCA** module on Sklearn digit dataset. We are using sigmoid kernel.

```
from sklearn.datasets import load_digits
from sklearn.decomposition import KernelPCA
X, _ = load_digits(return_X_y=True)
transformer = KernelPCA(n_components=10, kernel='sigmoid')
X_transformed = transformer.fit_transform(X)
X_transformed.shape
```

Output

```
(1797, 10)
```

PCA using randomized SVD

Principal Component Analysis (PCA) using randomized SVD is used to project data to a lower-dimensional space preserving most of the variance by dropping the singular vector of components associated with lower singular values. Here, the **sklearn.decomposition.PCA** module with the optional parameter **svd_solver='randomized'** is going to be very useful.

Example

The below example will use **sklearn.decomposition.PCA** module with the optional parameter svd_solver='randomized' to find best 7 Principal components from Pima Indians Diabetes dataset.

```
from pandas import read_csv
from sklearn.decomposition import PCA
path = r'C:\Users\Leekha\Desktop\pima-indians-diabetes.csv'
names = ['preg', 'plas', 'pres', 'skin', 'test', 'mass', 'pedi', 'age',
'class']
 dataframe = read_csv(path, names=names)
 array = dataframe.values

 X = array[:,0:8]
```

```
Y = array[:,8]
pca = PCA(n_components=7,svd_solver= 'randomized')
fit = pca.fit(X)
print(("Explained Variance: %s") % (fit.explained_variance_ratio_))
print(fit.components_)
```

Output

```
Explained Variance: [8.88546635e-01 6.15907837e-02 2.57901189e-02 1.30861374e-
02
 7.44093864e-03 3.02614919e-03 5.12444875e-04]
[[-2.02176587e-03  9.78115765e-02  1.60930503e-02  6.07566861e-02
   9.93110844e-01  1.40108085e-02  5.37167919e-04 -3.56474430e-03]
 [-2.26488861e-02 -9.72210040e-01 -1.41909330e-01  5.78614699e-02
   9.46266913e-02 -4.69729766e-02 -8.16804621e-04 -1.40168181e-01]
 [-2.24649003e-02  1.43428710e-01 -9.22467192e-01 -3.07013055e-01
   2.09773019e-02 -1.32444542e-01 -6.39983017e-04 -1.25454310e-01]
 [-4.90459604e-02  1.19830016e-01 -2.62742788e-01  8.84369380e-01
  -6.55503615e-02  1.92801728e-01  2.69908637e-03 -3.01024330e-01]
 [ 1.51612874e-01 -8.79407680e-02 -2.32165009e-01  2.59973487e-01
  -1.72312241e-04  2.14744823e-02  1.64080684e-03  9.20504903e-01]
 [-5.04730888e-03  5.07391813e-02  7.56365525e-02  2.21363068e-01
  -6.13326472e-03 -9.70776708e-01 -2.02903702e-03 -1.51133239e-02]
 [ 9.86672995e-01  8.83426114e-04 -1.22975947e-03 -3.76444746e-04
   1.42307394e-03 -2.73046214e-03 -6.34402965e-03 -1.62555343e-01]]
```