Lecture 12 k-NN, Decision Tree and Random Forest

In previous lectures, we take linear regression and logistic regression as examples to form a (relatively) rigorous mathematical framework of **supervised learning**:

1. Define the **supervised learning** problem as function fitting problem $y \approx f(x)$:

   Determining the function with **training data** (providing both true x and y), and with this f, making predictions on **test data** (only x is necessary, although sometimes y is also provided to evaluate the performace).
2. Making assumptions about the form of $f(x;\beta)$ by introducting parameters β (or w, W)-- assumptions lead to models;

1. Deriving the concrete form of Loss function $L(\beta)$ -- most common approach is maximum likelihood estimation, which measures "how good" $f(x;\beta)$ fits the actual y given the paramter β;

1. Minimizing (analytically or numerically) the Loss function $L(\beta)$ on **training data**, to find a reasonable parameter $\hat{\beta}$; (this step is called "fit" in sklearn)

1. On the test data, making predictions (called "predict" in sklearn) . If true labels are also known in test dataset, using metrics (R-squared,accuracy) to evaluate the performace (called "score" in sklearn).

Meanwhile, there exists other supervised learning approaches that might not strictly follow this guidline. Sometimes the formula f and loss function L is not explictly used. At first glance, these methods are rather heuristic or even "naive" -- while they can really give surprisingly good results. In this lecture, we are going to introduce some important algorithms of such style.

k-NN (k-nearest neighbor classifier) (https://en.wikipedia.org/wiki/K-nearest_neighbors_algorithm)

Intuitions: To make a prediction of test sample, we don't have to always derive the mapping formula explicitly -- we just look at its "close friends" in training dataset, and follow its friends' label!

Mathematical Description: Given a test sample $\mathbf{x}$ from **test** dataset, the kNN classifier first identifies the neighbors k points in the **training** data that are closest to $\mathbf{x}$, whose indices are represented by $\mathcal{N}_x$. It then estimates the probability that $\mathbf{x}$ belongs to class j by $P\big(y=j|\mathbf{x}\big)$ computing the fraction of points in $\mathcal{N}$ whose label(s) actually equal j:

$$P\big(y=j|\mathbf{x}\big) \approx \frac{1}{k}\sum_{i\in\mathcal{N}_x} 1\{y^{(i)}=j\}.$$

We finally determine its class by picking up the class with largest probability.

Remark: The similar philosophy can also extend to regression problem.

```
In [1]: from sklearn.datasets import load_iris
        X,y = load_iris(return_X_y = True)
```

```
In [2]: 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
        =42)
```

In practice, the challenging question is always choosing the correct k (parameter tuning). Recall that a powerful strategy is to use crosms validation (https://scikit-learn.org/stable/modules/cross_validation.html).

In [3]:
```
from sklearn.neighbors import KNeighborsClassifier
knn_clf = KNeighborsClassifier(n_neighbors = 20)
knn_clf.fit(X_train, y_train)
knn_clf.score(X_test,y_test)
```

Out[3]:
```
1.0
```

In [4]:
```
import pandas as pd
from sklearn.model_selection import cross_val_score

k_list = list(range(1,50,10))
# creating dataframe of cv scores and test scores -- of course you can also use Numpy
array
cv_scores = pd.DataFrame()
test_scores = pd.Series(dtype = 'float64')

# perform 10-fold cross validation
for k in k_list:
    knn_clf.set_params(n_neighbors=k) # update the object
    scores = cross_val_score(knn_clf, X_train, y_train, cv=10, scoring='accuracy')
    cv_scores[str(k)] = scores
    test_scores[str(k)] = knn_clf.score(X_test,y_test)
```

In [5]:
```
cv_scores
```

Out[5]:

	1	11	21	31	41
0	0.888889	0.777778	0.777778	0.777778	0.777778
1	1.000000	1.000000	1.000000	0.888889	0.888889
2	1.000000	0.888889	0.888889	0.888889	0.888889
3	0.666667	0.777778	0.777778	0.777778	0.888889
4	0.888889	1.000000	0.888889	0.888889	0.888889
5	1.000000	1.000000	1.000000	0.888889	0.888889
6	1.000000	1.000000	1.000000	1.000000	1.000000
7	1.000000	1.000000	1.000000	1.000000	1.000000
8	1.000000	1.000000	1.000000	0.777778	0.777778
9	0.888889	0.888889	0.888889	0.888889	0.888889

In [6]:
```
cv_scores.mean()
```

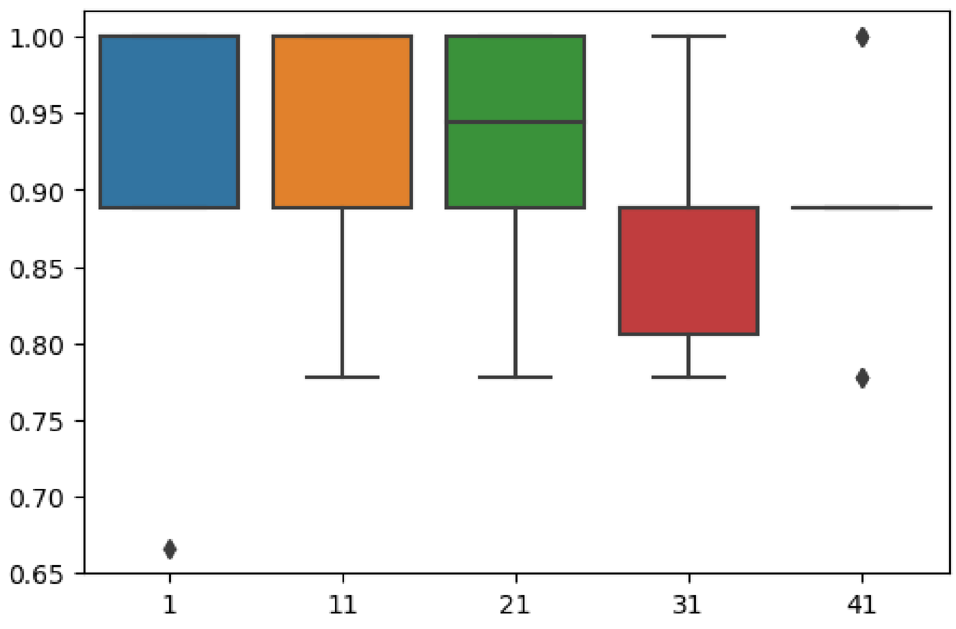
Out[6]:
```
1     0.933333
11    0.933333
21    0.922222
31    0.877778
41    0.888889
dtype: float64
```

In [7]:
```
cv_scores.std()
```

Out[7]:
```
1     0.107344
11    0.093697
21    0.091475
31    0.081985
41    0.074074
dtype: float64
```

In [8]:
```
import seaborn as sns
import matplotlib.pyplot as plt
fig, ax = plt.subplots(dpi=100)
sns.boxplot(data =cv_scores)
```

Out[8]:
```
<AxesSubplot:>
```



In [9]:
```
test_scores
```

Out[9]:
```
1     0.983333
11    1.000000
21    1.000000
31    0.983333
41    0.950000
dtype: float64
```

Decision Tree (https://en.wikipedia.org/wiki/Decision_tree_learning)

How human-being make classifications? Instead of using mathematical equations, we actually make a series of "decisions" based on the important features that are drawn from our past experience.

Intuitions: By repeatedly setting threshold for different features (multiple if-else conditions -- forming a flow-chart or decision tree structure), we can naturally achieve the classification task.

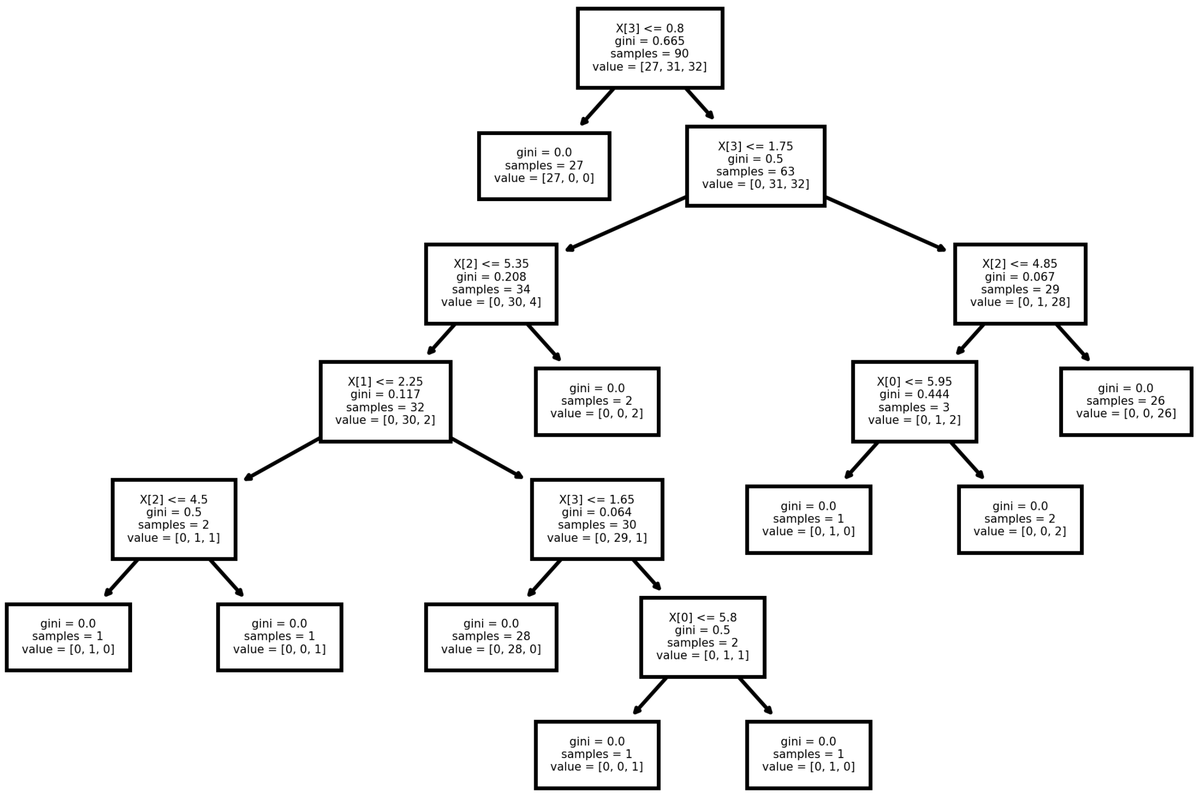
Mathematical Considerations: How to decide the appropriate thresholds and the order of if-else conditions? **Gini impurity** or **Entropy** (not required in this class). You only need to know that these tresholds/order of conditions are determined by the training dataset, using certain metrics to select. Different concerete strategies lead to various algorithms, known as ID3, CART, C4.5...

For the basic requirements, in this course we only ask you to call the package and understand how to interpret the results.

In [10]:
```
from sklearn import tree
dt_clf = tree.DecisionTreeClassifier()
dt_clf.fit(X_train,y_train)
dt_clf.score(X_test,y_test)
```

Out[10]:
```
0.9833333333333333
```

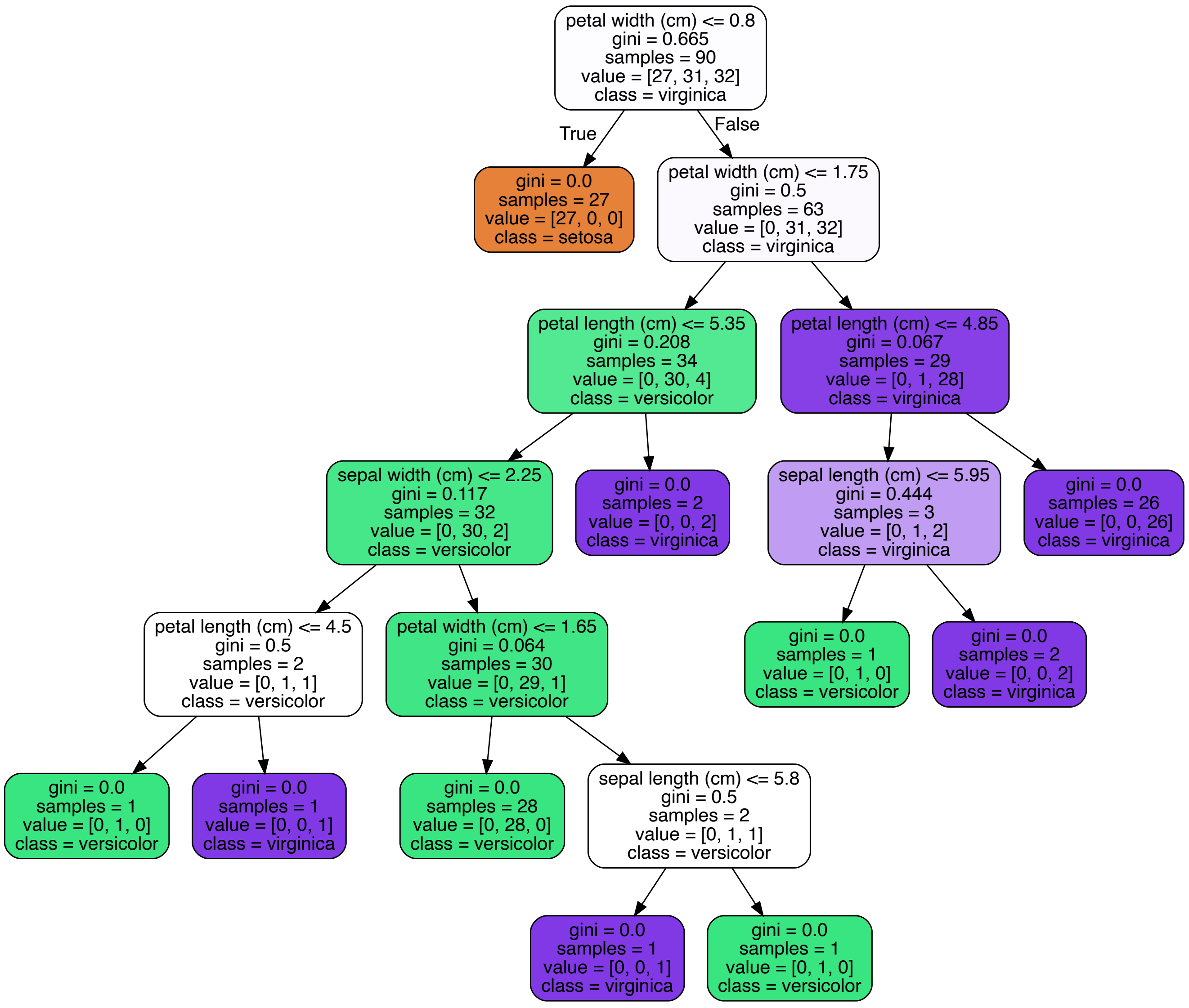
```
In [11]: fig, ax = plt.subplots(dpi=500)
         tree.plot_tree(dt_clf,fontsize=3)
         plt.show()
```



To visualize the trees more elegantly, we can use the graphviz package (installment (https://scikit-learn.org/stable/modules/tree.html) is not basic requirement of our course, and the easiest way is through conda command line (https://tljh.jupyter.org/en/latest/howto/env/user-environment.html)).

In [12]:
```
from sklearn.datasets import load_iris
iris = load_iris()
import graphviz
dot_data = tree.export_graphviz(dt_clf, out_file=None,class_names = iris.target_names
,feature_names=iris.feature_names,filled=True, rounded=True)
graph = graphviz.Source(dot_data)
graph
```

Out[12]:



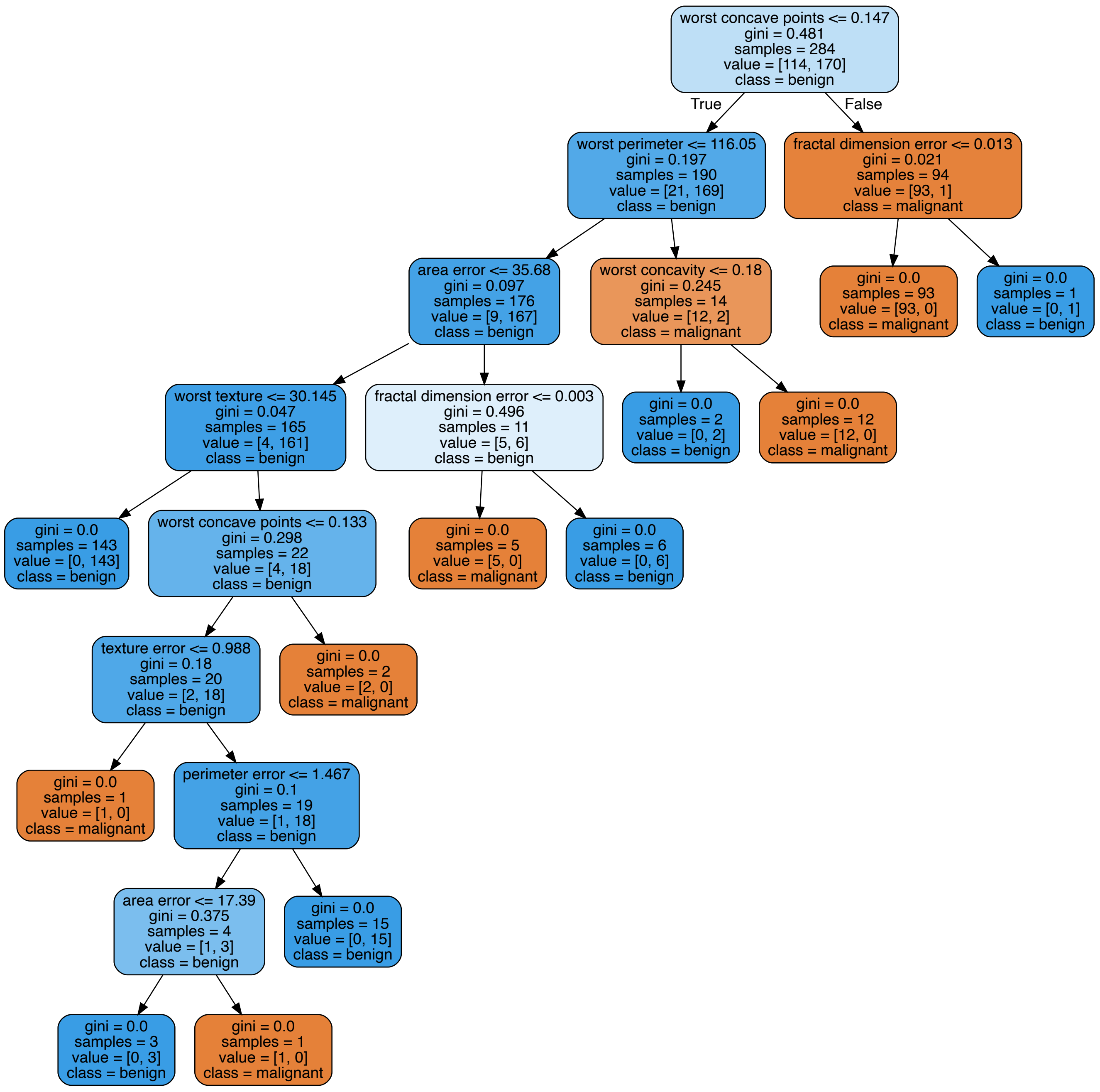
To get you more familiar with the concept of decision tree, let's try another dataset of breast cancer.

In [13]:
```
from sklearn.datasets import load_breast_cancer
bc = load_breast_cancer()
X = bc.data
y = bc.target
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.5, random_state
=42)
dt_clf = tree.DecisionTreeClassifier()
dt_clf.fit(X_train,y_train)
dt_clf.score(X_test,y_test)
```

Out[13]:
```
0.9157894736842105
```

In [14]:
```python
import graphviz
dot_data = tree.export_graphviz(dt_clf, out_file=None,class_names = bc.target_names,f
eature_names=bc.feature_names,filled=True, rounded=True)
graph = graphviz.Source(dot_data)
graph
```

Out[14]:



Random Forest (https://en.wikipedia.org/wiki/Random_forest#:~:text=Random%20forests%20 and Ensemble Methods (https://scikit-learn.org/stable/modules/ensemble.html)

Despite that the idea of decision tree is very straightward, the method is notorious for its over-fitting and high variance.

To make the decision tree more robust, we can construct the "forest" of multiple trees, and let the forest of trees to "vote".

The each decision tree can be "random" (therefore different with each other) in two ways:

```
- In each run, we only pick up a random subset of features as training dataset
- In each run, we only pick up a random subset of samples as training dataset
```

```
In [15]: from sklearn.ensemble import RandomForestClassifier
         rf_clf = RandomForestClassifier(n_estimators=1000, max_samples = 0.5, max_depth=5, ra
         ndom_state=0, n_jobs = -1) # make 1000 decision trees by random picking up 90% of the
         dataset, and each tree has the maximum depth of 5. njobs = -1 means you ask to use al
         l the processors of your computer
         rf_clf.fit(X_train, y_train) # note that we still work on the breast cancer dataset
         rf_clf.score(X_test, y_test)

Out[15]: 0.9614035087719298
```

The same idea can be applied to other supervised methods -- and the strategy is called **"bagging"** in machine learning.

```
In [16]: from sklearn.ensemble import BaggingClassifier
         bagging_knn_clf = BaggingClassifier(KNeighborsClassifier(), n_estimators=100,max_samp
         les=0.8, max_features=0.5, n_jobs = -1)
         bagging_knn_clf.fit(X_train,y_train)
         bagging_knn_clf.score(X_test,y_test)

Out[16]: 0.9543859649122807
```

Besides create random classifiers by subsetting the dataset, another clever strategy is to let different classifiers "vote" -- this relates to the wisdom of crowds (https://www.geeksforgeeks.org/ensemble-methods-and-wisdom-of-the-crowd/).

```
In [ ]: from sklearn.ensemble import VotingClassifier

        from sklearn.linear_model import LogisticRegression
        from sklearn.neighbors import KNeighborsClassifier
        from sklearn.svm import SVC

        clf1 = LogisticRegression(max_iter=5000)
        clf2 = RandomForestClassifier(n_estimators=50, random_state=1)
        clf3 = SVC(kernel='rbf', probability=True)

        eclf = VotingClassifier(estimators=[('lr', clf1), ('rf', clf2), ('svm', clf3)],voting
        ='hard')

        for clf, label in zip([clf1, clf2, clf3, eclf], ['Logistic Regression', 'Random Fores
        t', 'Support Vector Machine', 'Ensemble']):
                scores_cv = cross_val_score(clf, X_train, y_train, scoring='accuracy', cv=5)
                clf.fit(X_train,y_train)
                score_test = clf.score(X_test,y_test)
                print("Accuracy of CV: %0.2f (+/- %0.2f) [%s]" % (scores_cv.mean(), scores_cv
        .std(), label))
                print("Accuracy on Test: %0.2f [%s]" % (score_test, label))
```