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Ensemble Learning



Introduction

Ensemble methods combine multiple hypotheses, aiming to form a better one than the best hypothesis alone. Often, ensemble methods use multiple weak learners to build a strong learner.

A weak learner is one that consistently generates better predictions than random.

Ensemble methods use multiple learning algorithms (or instances) to obtain better predictive performance than could be obtained from any of the individual learning algorithms (or instances) alone. A machine learning ensemble can consist of a finite set of alternative models, which are more general classification models discretely.

The common ensemble training scheme employs numerous weaker classifiers that use only subsets of the dataset in terms of rows (data points) or columns (features), and then conducts a majority voting among their resulting predictions to decide on a particular single data point classification.

One important advantage of ensemble methods is the reduction of over-fitting.

Curse of Dimensionality

In machine learning one of the biggest difficulty is dealing with high number of dataset features or lack of enough data points to cover them. As an example, when a naive model requires 5 data points on each feature of a 100 feature dataset, the **joint** density function would ideally necessitate 5^{100} data points, so that the density function could be computed perfectly. This is not only too big of a dataset size, but also it might be impossible to acquire such a dataset. In practice, the curse of dimensionality is avoided by assuming the features are independent, such as the Naive Bayes assumption. The alternative approach is using ensembles of weak classifiers and bagging, so that each classifier would work on a subset of features.

Note that if the features are (asumed to be) independent one would require $5 \cdot 100$ data points to represent the dataset conforming to the same criteria above.

Bagging or Bootstrap Aggregating

Bagging trains each model in the ensemble using a randomly drawn subset of the training set. Then lets each model in the ensemble vote with equal weight. The random forest algorithm combines random decision trees with bagging to achieve high classification

accuracy while preserving model generality, which is one of the reasons why the Random Forest classifier is very popular.

Boosting

Boosting trains several weak learning algorithms and combine (i.e. summation) their weighted results. Boosting builds an ensemble by training each new model instance in such a way to improve upon the previous models mis-classify. The most common implementation of boosting is Adaboost where the classifier is composed of T many classifiers such that $F_T(x) = \sum_{t=1}^T f_t(x)$. The training is done such that the error is minimized at every iteration, $E_T = \sum_i Eig(F_{t-1}(x_i) + lpha_t h(x_i)ig)$

Decision Tree Learning

Introduction

A decision tree is a layout of various outcomes associated with a series of choices related to each other. They can be utilized to weight their actions based on multiple factors such as benefits, probabilities, and costs. In machine learning the outcomes could be class predictions or new nodes that can result in class predictions eventually.

Most decision tree building algorithms split nodes into two via a comparison operator, such as a binary tree. Training a decision tree can be costly ($\mathcal{O}(n^k)$ complexity) since the problem is non-convex and a greedy algorithm has to be employed. However, using a DT model is very fast such as traversing the tree until the final leaf, class prediction is reached ($\mathcal{O}(\log n)$ complexity).

Method

Given: Collection of examples (x, f(x))

Return: a function h (hypothesis) that approximates f, where h is a decision tree

Note that f(x) is not generally known and a dataset (of observations or records) is considered. In our common problems, we have X as the dataset and y as the observations (ground truth labels).

Input: An object or situation described by a set of attributes (or features), i.e. the dataset XOutput: a "decision" \longrightarrow predicts the output value for the input, i.e. y

For a decision tree learner, the input attributes can be nominal (discrete) or numerical (continuous).

A decision tree is a tree with two types of nodes

1. Decision nodes, specifies a test on a feature (attribute) with 2 or more alternatives

- Every decision node is in the path to a leaf node
- 2. Leaf nodes, indicates a classification of a data point (example, test)

Example

Food	Speedy	Price	Will Tip	Decision Tree
good good good ok bad good good ok good	yes no yes no yes yes yes yes yes	ok high ok ok ok ok high ok	yes no yes yes no no yes yes no	Speedy no no no pad pad no no no price ok high yes yes

Given the observations (table) from 10 customers in a restaurant. According to three questions, customers are stating they tipped or not. The problem is to model this behavior in a decision tree. The following decision tree can be fit to the data. Note that this tree is consistent to the input data, i.e. no contradictions, non-overlapping classification, a decision surface divides the classes perfectly.

The following cells demonstrate how to use this data in a regular classifier.

```
In [1]: import numpy as np
         import pandas as pd
         from sklearn.preprocessing import LabelEncoder # Generally used for supervised
        df = pd.DataFrame(
             np.array([['good', 'yes', 'ok'],
                        ['good', 'no', 'high'],
                        ['good', 'yes', 'high'],
['good', 'no', 'ok'],
                        ['ok', 'yes', 'ok'],
['bad', 'yes', 'ok'],
                        ['good', 'yes', 'ok'],
                        ['good', 'yes', 'high'],
                        ['ok', 'yes', 'ok'],
                        ['good', 'yes', 'ok']
                       ]),
             columns=['Food', 'Speedy', 'Price'])
        df['Will Tip'] = pd.Series(np.array(['yes', 'no', 'yes', 'yes', 'no', 'no', 'ye
         # Convert nominals to numerical keeping the order - sklearn requirement for Dec
        df['Food'] = df['Food'].replace({'bad':0, 'ok':1, 'good':2})
        df['Speedy'] = df['Speedy'].replace({'no':0, 'yes':1})
        df['Price'] = df['Price'].replace({'high':0, 'ok':1})
         # Prepare X and y
        X = df.loc[:, df.columns != 'Will Tip'].values
        y = df.loc[:, df.columns == 'Will Tip'].values.ravel()
```

```
# Convert y values to 0, 1 for sklearn
y_le = LabelEncoder()
y = y_le.fit_transform(y)
# Sanity
df.head()
```

```
Food Speedy Price Will_Tip
Out[1]:
          0
                 2
                          1
                                 1
                                         yes
          1
                 2
                          0
                                 0
                                         no
          2
                 2
                          1
                                 0
                                        yes
          3
                 2
                          0
                                 1
                                         yes
          4
                          1
                                 1
                 1
                                         no
```

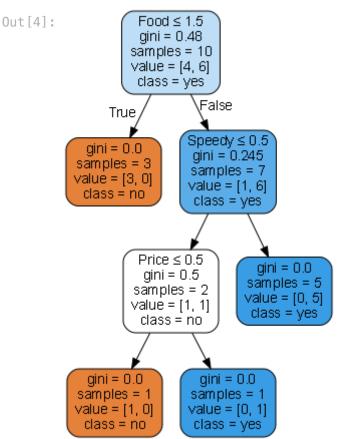
```
In [2]: from sklearn.tree import DecisionTreeClassifier
        willtip_clf = DecisionTreeClassifier(random_state=0)
        model = willtip_clf.fit(X, y)
```

The following visualization requires graphviz which can be installed by, conda install python-graphviz

```
In [3]: %matplotlib inline
        import matplotlib.pyplot as plt
        plt.rcParams["figure.dpi"] = 72
        from IPython.display import display
        from sklearn.tree import export graphviz
        from IPython.display import Image
        from subprocess import run, PIPE
        import graphviz
        print(f'graphviz version= {graphviz.__version__})')
```

graphviz version= 0.20.1

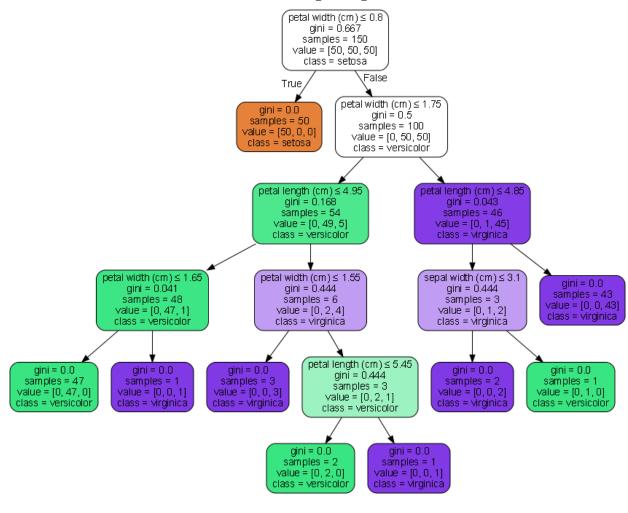
```
In [4]: # export graphviz will generate a DOT image file in the folder with this notebo
        dot data = export graphviz(willtip clf,
                                    out file='wt tree.dot',
                                    feature names=df.columns[:-1],
                                    class names=y le.classes ,
                                    filled=True,
                                    rounded=True,
                                    special characters=True)
        # Convert the DOT file to PNG
        run(['dot', '-Tpng', 'wt_tree.dot', '-o', 'wt_tree.png', '-Gdpi=72'], shell=Tru
        # Display the decision tree
        Image(filename = 'wt_tree.png')
```



Example

Following is another decision tree example using the Iris dataset.

```
In [5]: from sklearn import datasets
        # Load the data
        iris = datasets.load iris()
        iris clf = DecisionTreeClassifier(random state=0)
        model = iris clf.fit(iris.data, iris.target)
        # Generate the learned tree using DOT language and graphviz
        dot data = export graphviz(iris clf,
                                    out file='iris tree.dot',
                                    feature names=iris.feature names,
                                    class names=iris.target names,
                                    filled=True,
                                    rounded=True,
                                    special characters=True)
        # Convert the DOT file to PNG
        run(['dot', '-Tpng', 'iris tree.dot', '-o', 'iris tree.png', '-Gdpi=72'], shell
        # Display the decision tree
        Image(filename = 'iris tree.png')
```



ID3 Algorithm: Building a Decision Tree

Following algorithms can build decision trees.

- 1. Iterative Dichotomiser 3 (ID3) algorithm is used for selecting the splitting value by information gain, recursively for each level of the tree.
- 2. C4.5 algorithm is a modified version of the ID3 algorithm. Utilizes information gain and gain ratio for selecting the feature. It can handle numerical features and missing values.
- 3. CART (Classification and Regression Tree) algorithm can produce classification as well as a regression tree.

Hard Problem

If the dataset has M binary features then there are 2^M rows in the complete truth table. In addition, if the outcome, i.e. target variable, is binary then each row can have a {0, 1} output. The number of possible ways to build this truth table is 2^{2^M} . Thus, the solution space is exponential, and the decision tree algorithms are always have to be greedy as there is no known method to solve them in polynomial time.

All greedy algorithms have a **strategy**.

Occam's Razor

The principle of parsimony, is the principle that one should not make more assumptions than the minimum needed.

All scientific modeling and theory building is based on this principle.

Another interpretationis that all other things being equal, pick the smallest explanation.

Building a decision tree using Occam's Razor principle results in the smallest tree possible. The approach also minimizes overfitting.

Algorithm idea: Recursively pick the most significant attribute as root of the (sub)tree

- Use a top-down greedy search through the space of possible decision trees
- Greedy strategy pick the highest/best values first

Measure of the worthiness of an attribute: Information Gain

$$\mathtt{I} = -\sum\limits_{i=1}^K P(y_i) \log_2ig(P(y_i)ig)$$

$$\mathtt{I}\left(\frac{p}{p+n},\frac{n}{p+n}\right) = -\frac{p}{p+n} \log_2\left(\frac{p}{p+n}\right) - \frac{n}{p+n} \log_2\left(\frac{n}{p+n}\right)$$

I is also called **entropy** of the prior, p and n are positive and negative class labels.

A good strategy is starting with the feature that has the highest entropy of the dependent variable.

 Information answers questions. The more clueless I am about a question, the more information the answer contains.

Gini Index, also known as Gini impurity, corresponds to the probability of a specific feature that is classified incorrectly when selected randomly. As an example, if all data points could be classified into one particular class then it would be called pure.

The features with the lowest Gini Index would be preferred during the tree building.

Gini Index =
$$1 - \sum_{i=1}^{C} P(i)^2$$

Intuition

Pick the attribute that reduces the entropy (uncertainity) the most.

$$\mathtt{IG}(\mathrm{A}) = \mathtt{I} - \mathrm{remainder}(\mathrm{A})$$

remainder(A) is the remaining uncertainity after getting info (i.e. using on a decision tree to decide, split)

$$\operatorname{remainder}(\mathrm{A}) = \sum\limits_{i=1}^{K} rac{p_i + n_i}{p+n} \mathtt{I}\Big(rac{p_i}{p+n}, rac{n_i}{p+n}\Big)$$

Gini Index vs Information Gain

- Gini Index favors bigger partitions
- Information Gain favors smaller partitions having smaller counts with multiple specific values
- · CART uses Gini
- ID3 and C4.5 uses IG
- Gini is computed by correct/incorrect target values
- IG computes the difference between entropy before and after the split and indicates the impurity in classes of elements
- Pick the lowest Gini
- Pick the highest IG

Random Forest

The Random Forest classifier is a method that combines the decision trees and ensemble learning. The forest is composed of many trees that use randomly picked data features (attributes) as their input. The forest generation process constructs a collection of trees with controlled variance. The resulting prediction can be decided by majority voting or weighted voting. Random Forests have several advantages, such as a low number of control and model parameters, resistance to overfitting, no requirement for feature selection or feature reduction because they can use a large number of potential attributes. If some features are not useful for prediction, the algorithm will simply ignore them. One important advantage of Random Forest is that the variance of the model decreases as the number of trees in the forest increase, whereas the bias remains the same.

Random Forests have some disadvantages such as low model interpretability, performance loss due to correlated (dependent) variables, and dependence on the random number generator of the implementation. Note that all these disadvantages (except for the third one which is relatively easy to fix) are inherent to several other popular classifiers.

Random Forest Implementation Details

Number of features in each tree can be set to either \sqrt{M} , or $\log_2{(M+1)}$ for a dataset $X \in \mathbb{R}^{N imes M}$

Ensemble size determination remains to be a challenge. In practice a size is picked subjectively according to the number of features and data points.

Demonstrating the Power of Numerous Weak Classifiers as a Team

Note that not all datasets would benefit an ensemble classifier. The following cells demonstrate the power of the ensemble classifier with the following steps.

- Data exploration
- · Evaluating regular classifiers on the dataset
- · Building an ensemble

Recall that a few strategies to build a weak learner:

- Use a subset of dataset in training
- Use a subset of features in training
- Use a weak learner (generally more primitive and have higher generalization, or abstraction)

Note that the test on the weak learner has to match the subset features that the learning model uses.

```
In [6]: # Locate and load the data file
        df = pd.read csv('../../EP datasets/titanic preprocessed.csv')
        # Sanity check
        print(f'#rows={len(df)}, #columns={len(df.columns)}')
        df.head()
```

#rows=891, #columns=69

Out[6]:		Sex	Age	SibSp	Parch	Fare	Title_Master	Title_Miss	Title_Mr	Title_Mrs	Title_Officer
	0	1	22.0	1	0	7.2500	0	0	1	0	0
	1	0	38.0	1	0	71.2833	0	0	0	1	0
	2	0	26.0	0	0	7.9250	0	1	0	0	0
	3	0	35.0	1	0	53.1000	0	0	0	1	0
	4	1	35.0	0	0	8.0500	0	0	1	0	0

5 rows × 69 columns

```
In [7]: # Data exploration, a few plots
        def plt var( col):
            plt.hist([df[df['Survived']==1][ col],df[df['Survived']==0][ col]], label=[
            plt.xlabel( col)
            plt.legend()
        plt.figure(figsize=(18, 3), dpi=72)
        plt.subplot(1, 5, 1)
        plt var('Age')
        plt.subplot(1, 5, 2)
```

```
plt_var('Sex')
plt.subplot(1, 5, 3)
plt_var('Fare')
plt.subplot(1, 5, 4)
plt_var('Pclass_1')
plt.subplot(1, 5, 5)
plt_var('Pclass_3')
plt.show()
                             Suvd
                                                             Suvd
                                                                                     Suvd
                                                                                            350
               Not Suvd
                                                              Not Suvd
                                                                                     Not Suvd
                       400
                                                                     400
                                                                                            300
                                              400
                                                                                            250
                       300
                                                                     300
                                              300
                                                                                            200
                                              200
                                                                                            150
                                                                                            100
                       100
                                                                     100
                                                                                             50
                             0.25
                                  0.50
                                      0.75
                                                        200
                                                                       0.00
                                                                            0.25
                                                                                0.50
                                                                                     0.75
                                                                                                   0.25
                                                                                                        0.50
                                                                                         1.00
```

Evaluate numerous classifiers by a stratified 10-fold CV as in the following cells.

```
In [8]: # Prepare the input X and y
         dfX = df.loc[:, df.columns != 'Survived']
         dfy = df.loc[:, df.columns == 'Survived'].values.ravel()
         # Sanity check
         print(f'N={len(dfX)}, M={len(dfX.columns)}')
         N=891, M=68
 In [9]: # Set our main data structures X and y
         X = dfX.values
         y = dfy
In [10]; from sklearn.model selection import StratifiedKFold
         from sklearn.metrics import accuracy score
         # 10-fold CV evaluation of a classifier
         def eval classifier( clf, X, y):
             accuracies = []
             kf = StratifiedKFold(n splits=10, shuffle=True, random state=0)
             for train index, test index in kf.split( X, y):
                 _clf.fit(_X[train_index], _y[train_index])
                 y pred = clf.predict( X[test index])
                 accuracies += [accuracy_score(_y[test_index], y_pred)]
             return np.array(accuracies)
In [11]: from sklearn.naive bayes import GaussianNB
         acc = eval classifier(GaussianNB(),
         print(f'Naive Bayes CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3f}
         Naive Bayes CV accuracy=0.45 ±0.016
```

```
In [12]: from sklearn.svm import LinearSVC
                   # Problem is difficult and LinearSVC does not converge
                   # Increase the convergence tolerance to a very high number
                   acc = eval_classifier(LinearSVC(tol=10),
                                                                 X, y)
                   print(f'Linear SVC CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3f}'
                   Linear SVC CV accuracy=0.72 ±0.137
In [13]: from sklearn.svm import LinearSVC
                   # See balancing the classes with penalties help or not
                   acc = eval_classifier(LinearSVC(class_weight='balanced', tol=10),
                   print(f'Linear SVC CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3f}'
                   Linear SVC CV accuracy=0.75 ±0.092
In [14]: from sklearn.svm import SVC
                   acc = eval_classifier(SVC(kernel='rbf', gamma=.5, C=2),
                   print(f'SVM RBF CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3f}')
                   SVM RBF CV accuracy=0.68 ±0.039
In [15]: from sklearn.svm import SVC
                   acc = eval classifier(SVC(kernel='rbf', gamma=.05, C=2),
                                                                 X, y)
                   print(f'SVM RBF CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3f}')
                   SVM RBF CV accuracy=0.73 ±0.045
In [16]: from sklearn.linear model import LogisticRegression
                   acc = eval classifier(LogisticRegression(solver='lbfgs', multi class='auto', ma
                   print(f'Logistic Regression CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(accuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.deccuracy=fine.
                   Logistic Regression CV accuracy=0.81 ±0.040
In [17]: from sklearn.neural network import MLPClassifier
                   acc = eval classifier(MLPClassifier(hidden layer sizes=(50,100), max iter=500),
                   print(f'Neural Network CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3
                   Neural Network CV accuracy=0.77 ±0.059
In [18]; acc = eval classifier(MLPClassifier(hidden layer sizes=(20,50,50,20), max iter=2
                   print(f'Neural Network CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3
                   Neural Network CV accuracy=0.78 ±0.078
In [19]: from sklearn.neighbors import KNeighborsClassifier
                   acc = eval classifier(KNeighborsClassifier(n neighbors=1),
```

```
print(f'K Nearest Neighbor CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc
         K Nearest Neighbor CV accuracy=0.71 ±0.038
In [20]: | acc = eval_classifier(DecisionTreeClassifier(),
         print(f'Decision Tree CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3f
         Decision Tree CV accuracy=0.81 ±0.037
In [21]: from sklearn.ensemble import RandomForestClassifier
         acc = eval_classifier(RandomForestClassifier(n_estimators=200, max_depth=5, rar
         print(f'Random Forest CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3f
         Random Forest CV accuracy=0.83 ±0.041
         Best result so far.
```

Ensemble

Build an ensemble using regular Naive Bayes (NB) classifier as the weak learner. As can be seen above, its performance is almost half of the Random Forest ensemble classifier.

The following approach uses a subset of features to generate a Naive Bayes classifier. Note that clf is the weak classifier model and its predict function will be used. It is only called a weak model because a subset of the features is passed for learning.

Note that the first step below, has a single NB estimator and uses its single prediction value. On the contrary, a RandomForestClassifier would have n estimators many decision tree classifiers, and it would use majority-vote their predictions as its prediction.

We also compute the original class Priors from the full dataset to be fair to the NB learner.

Note on Prediction using predict_proba

The ensemble scores/probabilities generated fby every model might have a large variation, therefore it is better to sum up the scores and apply np.argmax. For example consider the situation of an ensemble of 100 models where sixty predictions had class₀ with a P of 0.55 and forty predictions with $class_1$ with a P of 0.95.

```
In [22]: # Main Priors
         counts = np.unique(y, return_counts=True)
         NBpriors = [counts[1][0]/len(y), counts[1][1]/len(y)]
         print(NBpriors)
         [0.6161616161616161, 0.3838383838383838]
```

```
In [23]: acc = eval_classifier(GaussianNB(priors=NBpriors), X, y)
         print(f'Naive Bayes CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3f}
         # For reference
         acc = eval classifier(RandomForestClassifier(n estimators=200, max depth=5, ran
         print(f'Random Forest CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3f
         Naive Bayes CV accuracy=0.45 ±0.016
         Random Forest CV accuracy=0.83 ±0.041
In [24]: # Let's build a single weak learner using GaussianNB by subset of features
         def weakNB_fit(_list_cols, _X, y):
             Xs = _X[:,_list_cols]
             return GaussianNB(priors=NBpriors).fit(Xs, _y) # return a single NaiveBaye
         def weakNB_predict(_clf, _list_cols, _X):
             Xs = X[:, list cols]
             return _clf.predict(Xs), _clf.predict_proba(Xs)
         # Use m features randomly selected from M features
         # a total of n estimators many weak learners
         def features_randomsubset(_M, _m, n_estimators=1):
             from numpy.random import choice
             # returns a list of list of column choices - subset features
             return [choice(_M, _m, replace=False) for _ in range(n_estimators)]
In [25]: | %%time
         def eval_singleweak(_X, _y, _niters, _nfeatures):
             accuracies = []
             for in range( niters):
                 # Keep the subset features (i.e. columns) the same for a 10-fold
                 cols = features_randomsubset(_X.shape[1], _nfeatures, n_estimators=1)
                 # 10-fold CV
                 kf = StratifiedKFold(n splits=10, shuffle=True, random state=0)
                 for train index, test index in kf.split( X, y):
                     clf = weakNB fit(cols[0], X[train index], y[train index])
                     y_pred, y_prob = weakNB_predict(clf, cols[0], _X[test_index])
                     accuracies += [accuracy score( y[test index], y pred)]
             return np.array(accuracies)
         # Measure individual weak learner performance
         acc = eval singleweak(X, y, 100, 5)
         # Sanity
         print(f'total #results= {len(acc)}')
         print(f'Weak learners average Acc= {np.mean(acc):.2f} {chr(177)}{np.std(acc):.3
         total #results= 1000
         Weak learners average Acc= 0.50 ±0.135
         CPU times: total: 1.03 s
         Wall time: 1.03 s
```

Interestingly, by using the good old GaussianNB with a small dataset and accumulating its accuracy shows a jump in performance compared to the plain NB using all features at the same time.

Question 1: Why does the performance increase?

Question 2: Why there is an increase in the standard deviation?

Note: Attempting number of features nfeatures =3 or so might cause individual GaussianNB classifier to fail due to data problems with that particular subset of features (such as no data point for the target, or all same values for a column).

```
In [26]: # Generate numerous trained NB classifiers as weak learners
         def ensembleNB_fit(_ensemble_cols, _X, _y):
             # the list of ensemble columns have a column list for every member of the
             n estimators = len( ensemble cols)
             # list of weak learners
             ensemble_clf = []
             for j in range(n_estimators):
                 ensemble_clf += [weakNB_fit(_ensemble_cols[j], _X, _y)]
             return ensemble clf
         # Using trained ensemble, predict the outcome by majority voting
         def ensembleNB_predict(_ensemble_clf, _ensemble_cols, _Xtest):
             from collections import defaultdict
             n_estimators = len(_ensemble_clf)
             assert n_estimators==len(_ensemble_cols) # Error check
             # weak learner predictions
             ypred_e, yprob_e = [], []
             for j in range(n estimators):
                 res = weakNB_predict(_ensemble_clf[j], _ensemble_cols[j], _Xtest)
                 ypred e += [res[0]]
                 yprob_e += [res[1]] # score/probability of the prediction
             # majority voting for each data point in Xtest
             ypred = []
             for i in range(_Xtest.shape[0]):
                 ypred scores = defaultdict(float)
                 for j in range(n estimators):
                     for c, p in enumerate(yprob e[j][i]):
                         # a proper score is necessary
                         ypred_scores[c] += p
                 ix = max(ypred scores.items(), key=lambda a: a[1])
                 ypred += [ix[0]]
             return np.array(ypred)
```

```
In [27]: | %%time
         # Attemp 10-fold CV using ensemble fit, ensemble predict
         # _nfeatures: feature subset size
         def eval_ensemble(_X, _y, _niter, _n_estimators, _nfeatures):
             accuracies = []
             for i in range( niter):
                 # Keep subset features, columns same for a 10-fold
                 cols = features randomsubset( X.shape[1], nfeatures, n estimators= n e
                 # 10-fold CV
                 kf = StratifiedKFold(n splits=10, shuffle=True, random state=i)
                 for train index, test index in kf.split( X, y):
                     e_clf = ensembleNB_fit(cols, _X[train_index], _y[train_index])
                     y pred = ensembleNB predict(e clf, cols, X[test index])
                     accuracies += [accuracy score( y[test index], y pred)]
```

```
return np.array(accuracies)
# Measure ensemble weak learners performance
acc = eval\_ensemble(X, y, 10, 200, 7)
print(f'Ensemble learners average Acc= {np.mean(acc):.2f} {chr(177)}{np.std(acc
Ensemble learners average Acc= 0.39 ±0.012
CPU times: total: 13.9 s
Wall time: 13.9 s
```

Question: Above performance results are not very promising, so do you think we have a bug in the scripts?

Improvements

More or less half of the features are not useful in this dataset. So, subsets of them are not useful either. Random Forest classifier ignores many of these by employing entropy or information gain strategy. However, such capability does not exist for a plain NB classifier. NB classifier has to use all features that it was provided. Thus, we need to do some kind of feature ranking.

Use a simple approach and check the **correlation** between X columns and the target variable y. Drop the bottom performers.

Note: Normalization of features would help the correlation analytic

```
In [28]: # Direct correlation between each column of X and the target y
         corrs = np.array([np.correlate(X[:,j], y)[0] for j in range(X.shape[1])])
          # Reverse sort, numpy array negation reverses the order
         ranks = np.argsort((-corrs))
          # Display top-9 and bot-5
         rankings = [(f'{corrs[j]:.1f}', df.columns[j]) for j in ranks]
         display(rankings[:9])
         display(rankings[-5:])
         [('16551.2', 'Fare'),
           ('9639.2', 'Age'),
           ('663.0', 'FamilySize'),
           ('254.0', 'Ticket_XXX'),
('219.0', 'Embarked_S'),
           ('206.0', 'Cabin U'),
           ('169.0', 'SmallFamily'),
           ('162.0', 'SibSp'),
           ('159.0', 'Parch')]
         [('0.0', 'Ticket_SCA4'),
           ('0.0', 'Ticket_SCA3'),
           ('0.0', 'Ticket_Fa'),
           ('0.0', 'Ticket LP'),
           ('0.0', 'Ticket A')]
```

```
In [29]: # Find columns with correlation=2.0 or less and then delete them from X
          delcols = [(j, f'{corrs[j]:.1f}', df.columns[j]) for j in ranks if corrs[j]<=2]</pre>
          print(delcols)
          [(47, '2.0', 'Ticket_SCAH'), (60, '2.0', 'Ticket_SWPP'), (55, '2.0', 'Ticket_S
          OTONOQ'), (50, '2.0', 'Ticket_SCParis'), (42, '2.0', 'Ticket_PP'), (33, '2.0',
          'Ticket_C'), (29, '2.0', 'Ticket_A5'), (20, '2.0', 'Cabin_G'), (39, '1.0', 'Ti
          cket_LINE'), (43, '1.0', 'Ticket_PPP'), (44, '1.0', 'Ticket_SC'), (62, '1.0', 'Ticket_WEP'), (61, '1.0', 'Ticket_WC'), (51, '1.0', 'Ticket_SOC'), (65, '0.
          0', 'Singleton'), (28, '0.0', 'Ticket A4'), (30, '0.0', 'Ticket AQ3'), (59,
          '0.0', 'Ticket_STONOQ'), (31, '0.0', 'Ticket_AQ4'), (32, '0.0', 'Ticket_AS'), (56, '0.0', 'Ticket_SP'), (54, '0.0', 'Ticket_SOTONO2'), (53, '0.0', 'Ticket_S
          OPP'), (52, '0.0', 'Ticket_SOP'), (35, '0.0', 'Ticket_CASOTON'), (36, '0.0',
          'Ticket_FC'), (48, '0.0', 'Ticket_SCOW'), (21, '0.0', 'Cabin_T'), (46, '0.0',
          'Ticket_SCA4'), (45, '0.0', 'Ticket_SCA3'), (38, '0.0', 'Ticket_Fa'), (40, '0.
          0', 'Ticket_LP'), (27, '0.0', 'Ticket_A')]
In [30]: # Column numbers to delete
          dd = [d[0]  for d  in delcols]
          # Drop those columns, axis=1
          Xpp = np.delete(np.array(X, copy=True), dd, axis=1)
          # Xpp is new pre-processed X
          # Sanity check
          print(f'{X.shape}, {Xpp.shape}')
          (891, 68), (891, 35)
In [31]: # Base classifier
          acc = eval classifier(GaussianNB(priors=NBpriors), Xpp, y)
          accNB, stdevNB = np.mean(acc), np.std(acc)
          print(f'Naive Bayes CV accuracy={accNB:.2f} {chr(177)}{stdevNB:.3f}')
          # Reference
          acc = eval classifier(RandomForestClassifier(n estimators=200, max depth=5, rar
          print(f'Random Forest CV accuracy={np.mean(acc):.2f} {chr(177)}{np.std(acc):.3f
          Naive Bayes CV accuracy=0.75 ±0.065
          Random Forest CV accuracy=0.83 ±0.042
          Notice: The plain Naive Bayes has an improved performance now, since we are helping NB
          with the removal of uncorrelated features. Random Forest uses the information gain metric
          to do this by itself.
```

```
In [32]: %%time
         # Measure weak learners performance on updated X
         acc = eval_singleweak(Xpp, y, 100, 5)
         print(f'Weak learners average Acc= {np.mean(acc):.2f} {chr(177)}{np.std(acc):.3
         Weak learners average Acc= 0.70 ±0.072
         CPU times: total: 953 ms
         Wall time: 949 ms
In [33]: acc = eval_ensemble(Xpp, y, 10, 200, 11)
         print(f'Ensemble learners average Acc= {np.mean(acc):.2f} {chr(177)}{np.std(acc
```

Ensemble learners average Acc= 0.77 ±0.043

```
In [34]: # The final number of features
         M = Xpp.shape[1]
```

Notice: The following experiment takes around 12 minutes on my machine to run.

```
In [35]: %%time
         # Run an experiment for a full scale of number of features
         valsF, accF, stdevF = np.arange(1,M+1), [], []
         for nf in valsF:
             acc = eval_ensemble(Xpp, y, 10, 200, nf)
             accF += [np.mean(acc)]
             stdevF += [np.std(acc)]
         CPU times: total: 8min 54s
         Wall time: 8min 54s
```

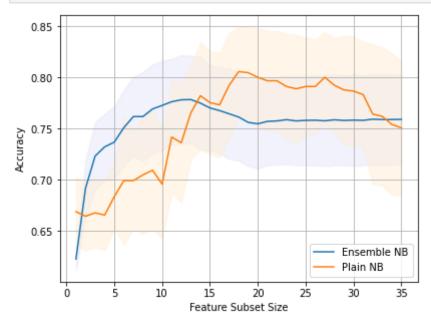
Performance Comparison

Since we are varying the feature subset size for the ensemble NB, we can do something similar for the plain NB. Let's vary the features added for classification using the ranked features and plot the 10-fold CV performance. By ranking the features we are helping the plain Naive Bayes immensely.

Note that both the ensemble test and plain NB test have 10 iterations to collect sufficient statistics.

```
In [36]: %%time
          # Add number of iterations - better statistics
         def eval classifier_niter(_clf, _X, _y, _niter):
              return np.array([eval_classifier(_clf, _X, _y) for _ in range(_niter)])
          # Get the X matrix starting from the high-ranked variables
         def getX( X, ncols, ranks):
              cols = [j for n, j in enumerate( ranks) if n < ncols]</pre>
              return np.array( X[:,cols])
          # Iterate over the features, adding 1 by 1 by starting from the first (the best
         valsNB, accNB, stdevNB = np.arange(1,M+1), [], []
          for nc in valsNB:
              # feature order is coming from ranks
              X \text{ nb} = \text{get}X(X, \text{nc}, \text{ranks})
              acc = eval classifier niter(GaussianNB(priors=NBpriors), X nb, y, 10)
              accNB += [np.mean(acc)]
              stdevNB += [np.std(acc)]
         CPU times: total: 3.02 s
         Wall time: 3.01 s
In [37]: # Ease of computation for the plotting of the error band
         accF, stdevF = np.array(accF), np.array(stdevF)
         accNB, stdevNB = np.array(accNB), np.array(stdevNB)
          # Plot
```

```
plt.plot(valsF, accF, label='Ensemble NB')
plt.plot(valsNB, accNB, label='Plain NB')
plt.fill_between(valsF, accF-stdevF, accF+stdevF, color='lavender', alpha=0.5)
plt.fill_between(valsNB, accNB-stdevNB, accNB+stdevNB, color='papayawhip', alph
plt.xlabel('Feature Subset Size')
plt.ylabel('Accuracy')
plt.legend(loc='lower right')
plt.grid()
plt.show()
```



Conclusions

- 1. Ensemble performance is better than the plain NB when all features are added
- 2. Ensemble has better generalization performance (why?)
- 3. Ensemble performance has smaller error variance
- 4. Ensemble uses all features randomly picked
- 5. Since we ranked the features, plain NB starts adding the best features first, thus even with 1 feature its performance is 67%
- 6. There is an optimum number of features for the NB for this dataset
- 7. The plain NB performance sensitivity to the features included is high (why?)
- 8. The ensemble performance sensitivity to the features included is lower (why?)

Question: From the above plot, the performance of the ensemble looks a bit less than the plain NB, do you agree with this statement? Why?

References

1. Breiman, Leo. "Random forests." Machine learning 45.1 (2001): 5-32.

Exercises

Exercise 1. Add the data points ['good', 'yes', 'ok', 'no'] to the data and rebuild the Will_Tip tree. Observe the difference between the previous and the current.

Exercise 2. Using above dataset compare the AdaBoostClassifier performance to the RandomForestClassifier performance.

Exercise 3. Normalize features so the ranking would be more proper for the ensemble. Report improvements.

```
In [38]: %%html
         <style>
             table {margin-left: 0 !important;}
         <!-- Display markdown tables left oriented in this notebook. -->
```