ENSEMBLES for Classification

Ensembles

- Methods combining multiple ML models to create low-bias, low-variance, models
- They combine multiple models to create new more accurate models
- Types of ensembles of trees
 - Bagged trees
 - Random Forest
 - Gradient boosting trees

Hyperparameters

Random Forest

- max_features
- n_estimators
- max_depth

Gradient Boosting

- learning_rate
- max_features
- n_estimators
- max_depth

BAGGING

Bootstrap samples (from dataframes)

- A bootstrap sample is a sample with replacement
- May include same row many times
- Bootstrap samples are usually of the same size

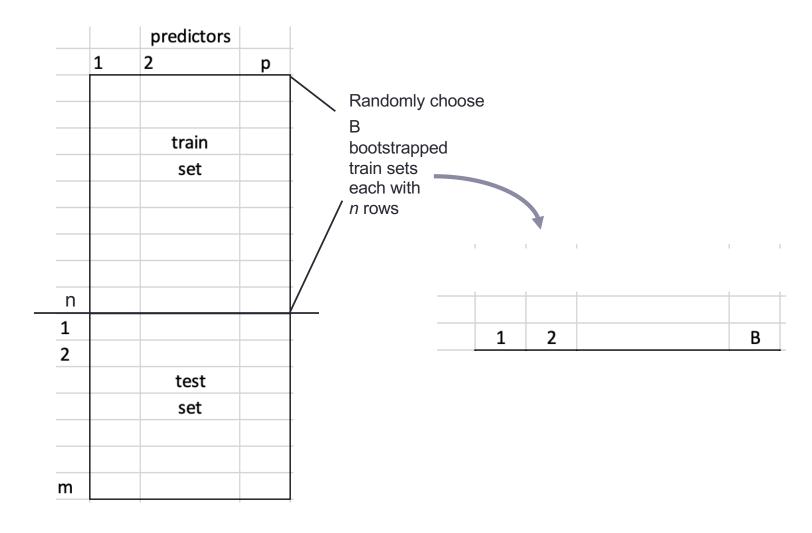
There are two approaches

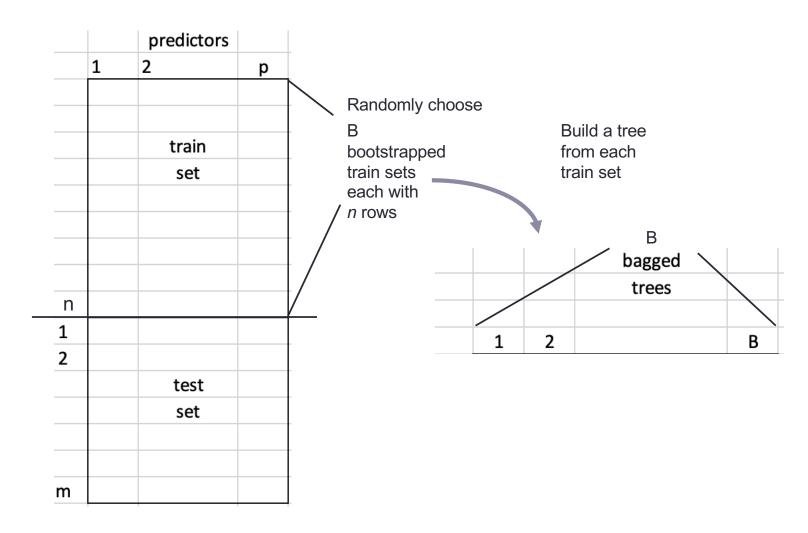
- Predict the most frequent category (majority vote)
- If the model yields probability estimates, average the probabilities for each class, then predict the class with the highest average

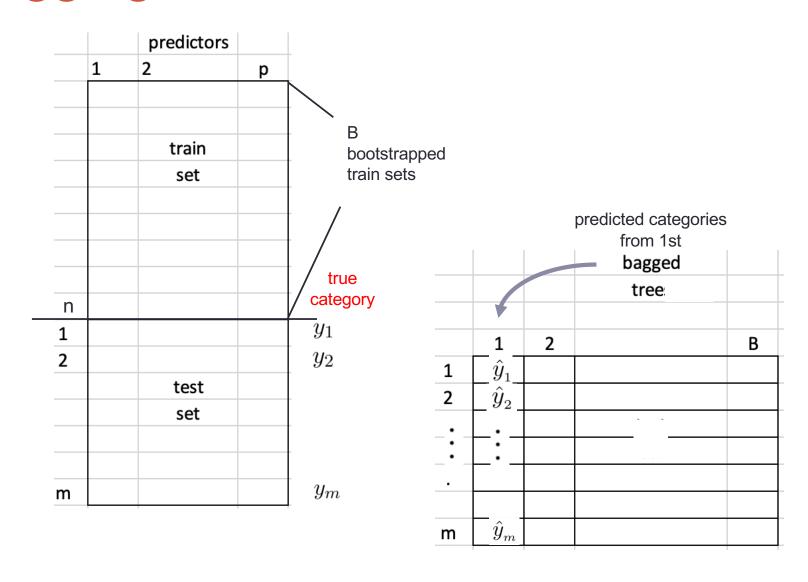
Bagging for Trees

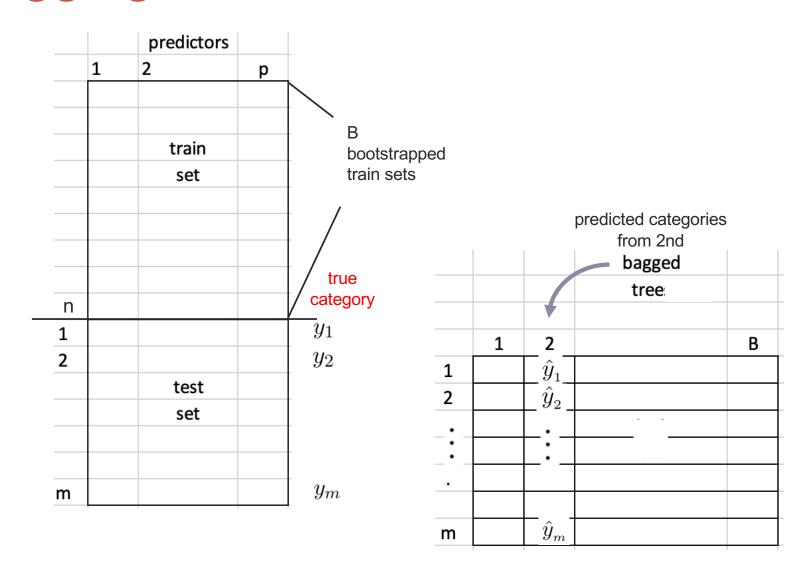
		predictors		
	1	2	р	
		train		
		set		
				-
n				-
1				
2				
		test		
		set		
m				

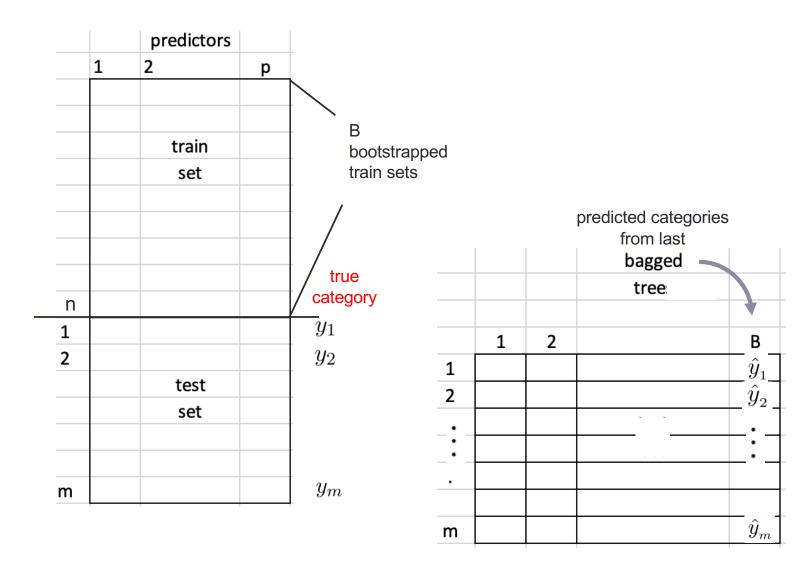
Bagging for Trees

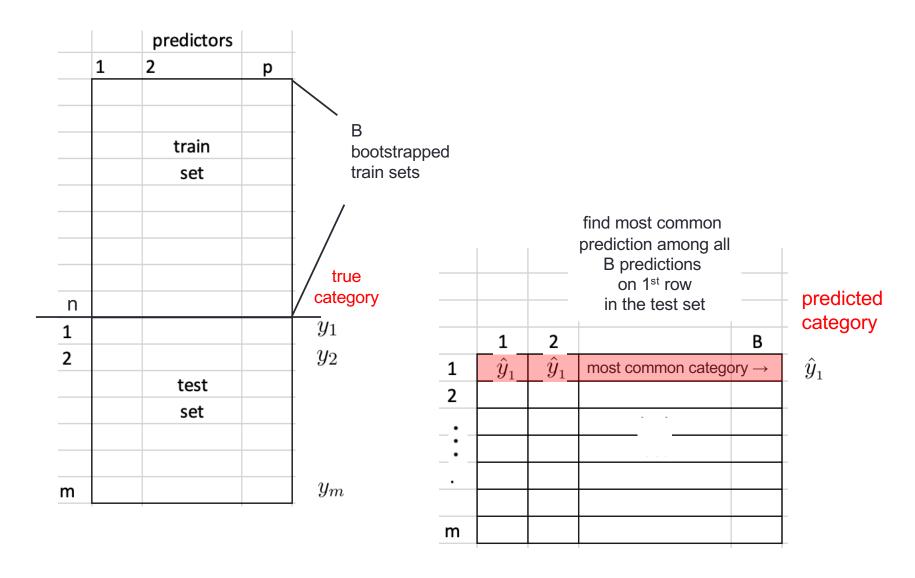


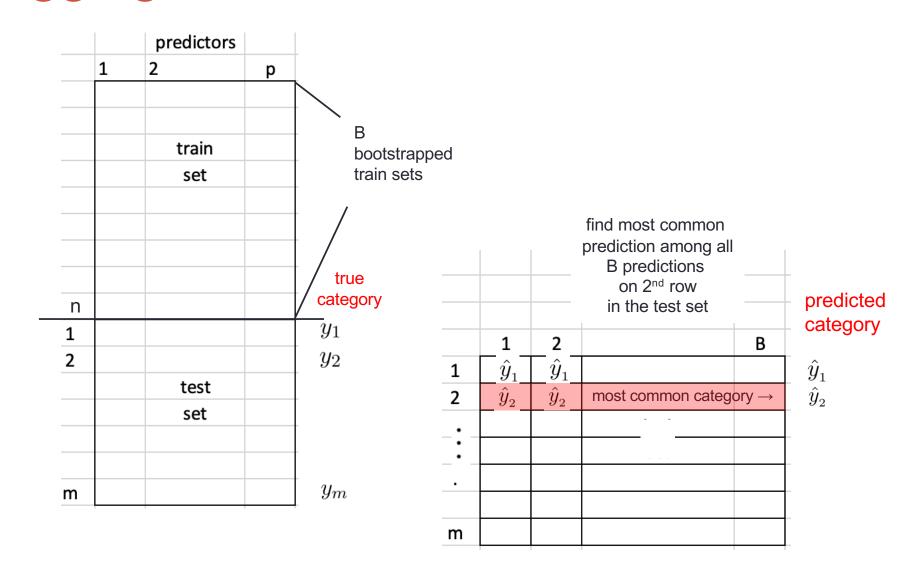


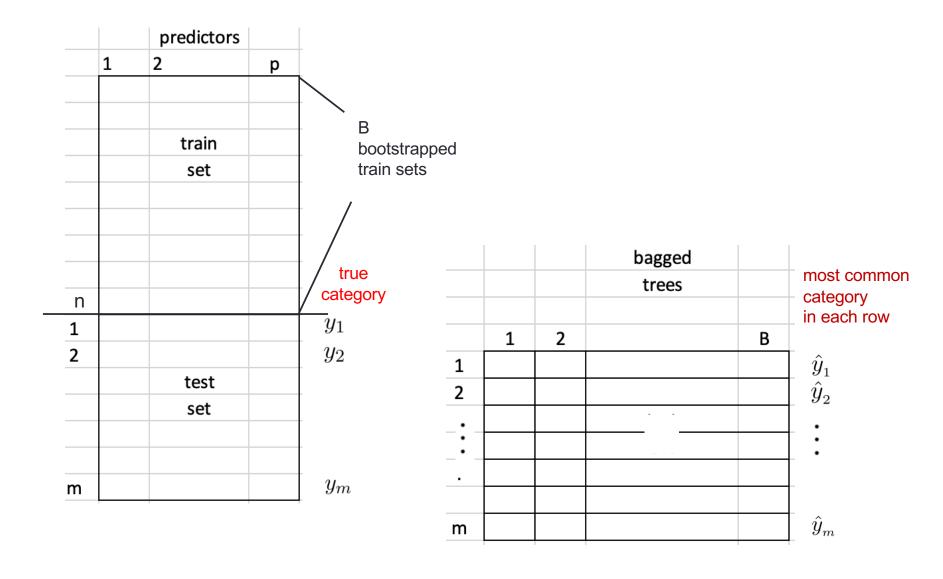


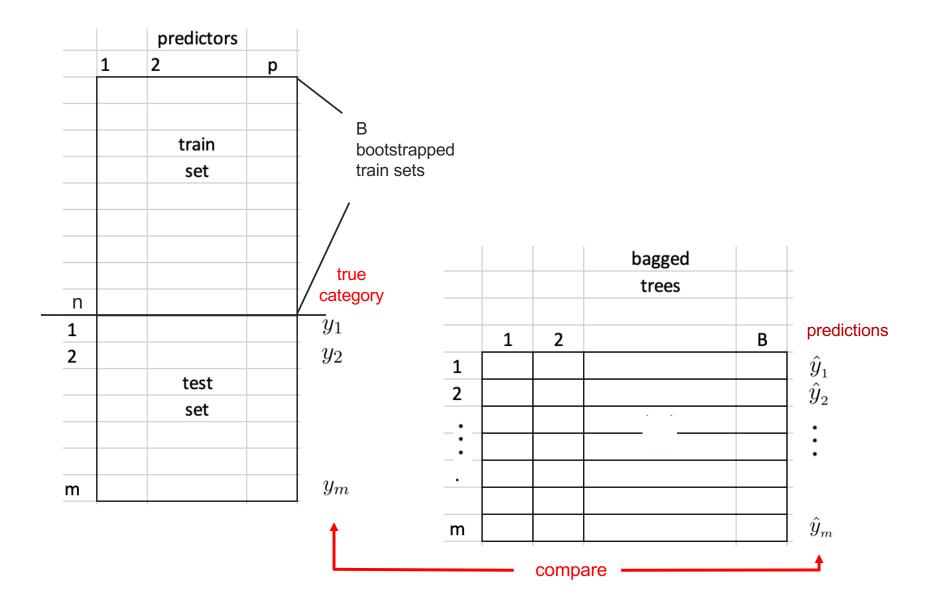


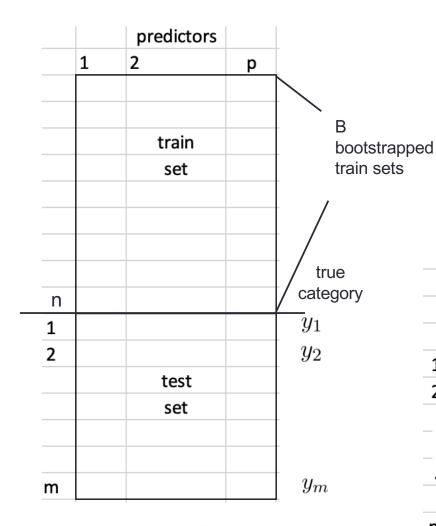












			bagged		
			trees		- predicted
					predictedcategory
	1	2		В	
1					$egin{array}{c} \hat{y}_1 \ \hat{y}_2 \end{array}$
2					\hat{y}_{2}
			test		
:			set		:
m					${\hat y}_m$

Test Accuracy Rate

$$AR = \frac{1}{m} \sum_{i=1}^{m} I(y_i = \hat{y}_i)$$

Bagging - Notes

- Sometimes a few predictors are very good while many are poor predictors
- If so, many of the trees may contain the same set of powerful predictors
- Then the trees would yield similar predictions
- We say that the predictions are co-rrelated
- We need a way to de-correlate them

RANDOM FORESTS

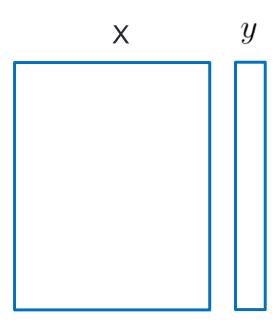
Why are we selecting *m* predictors instead of all *p* predictors for splitting?

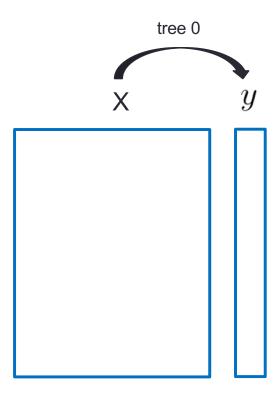
- If there is a single strong predictor, most bagged trees will choose it for the first split (and for the following splits too)
- Most trees will look similar
- As a result their predictions will be highly correlated
- Averaging many highly correlated quantities does not lead to a large variance reduction
- By selecting the predictors for splits, from different subsets of predictors, Random Forest "de-correlates" the bagged trees leading to a reduction in variance

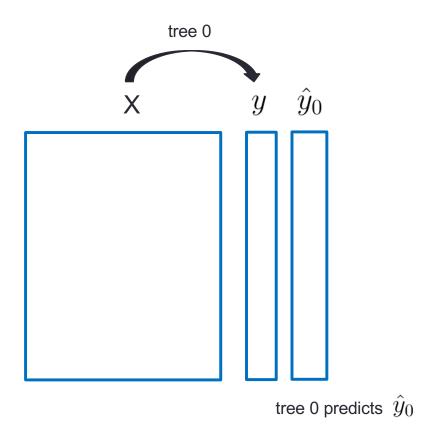
GRADIENT BOOSTING

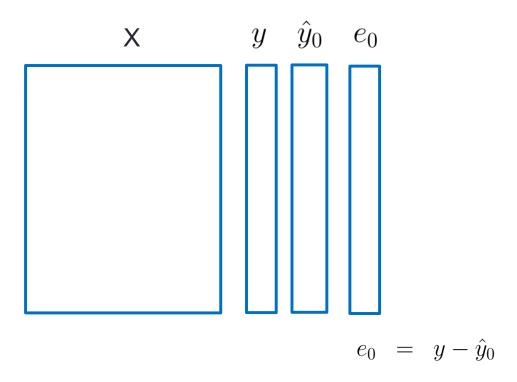
Gradient Boosting

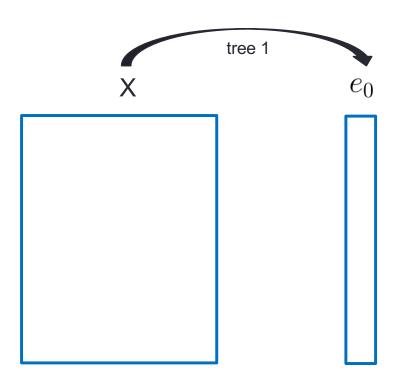
- Trees are built sequentially to improve upon the errors made by their predecessor trees
- Each new tree fits the data to the error made by the previous tree, predicting that error
- The new prediction is equal to the prediction of the previous tree plus α times the predicted error
- Parameter $0 < \alpha < 1$ is called the learning rate

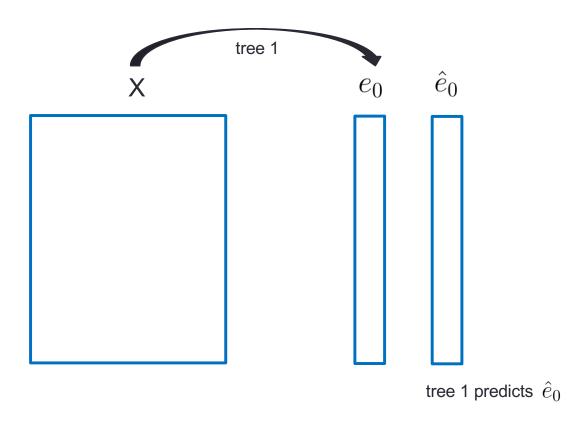


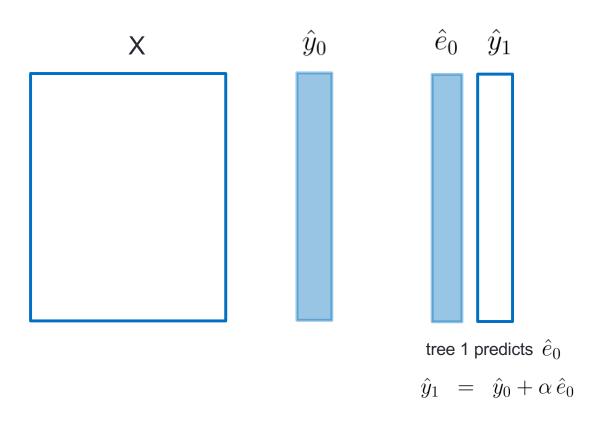


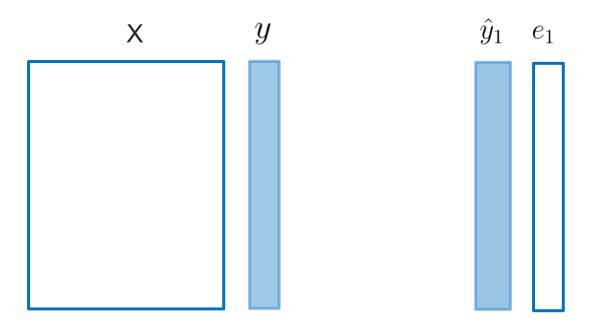




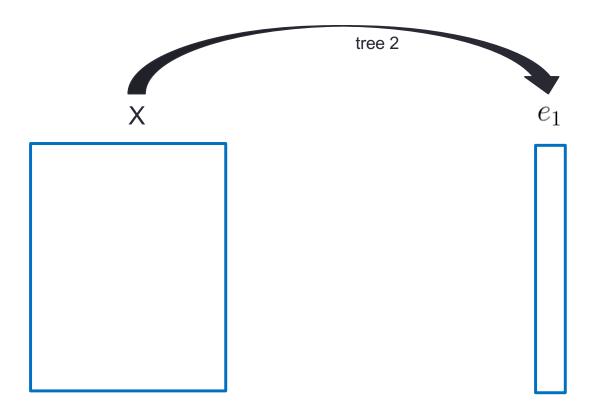


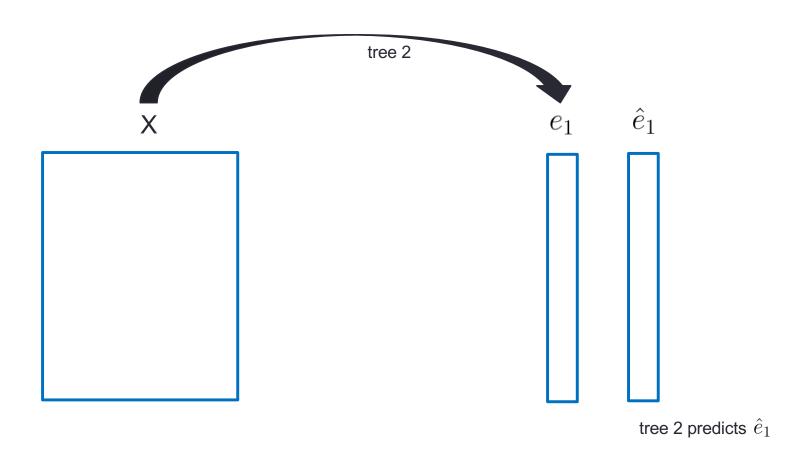


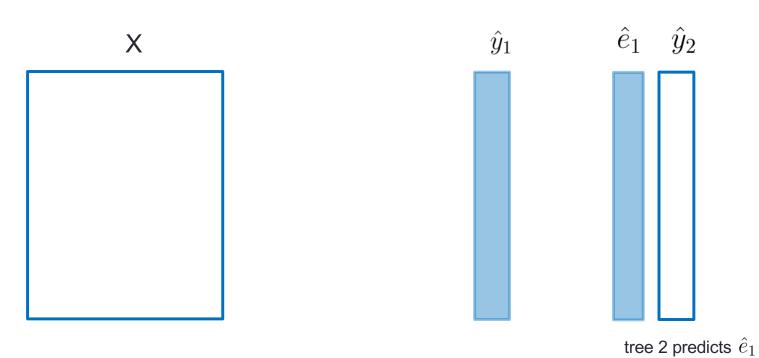




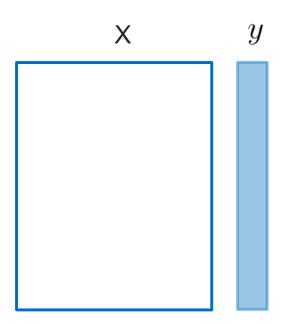
$$e_1 = y - \hat{y}_1$$

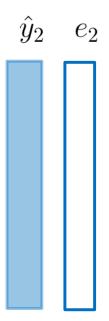




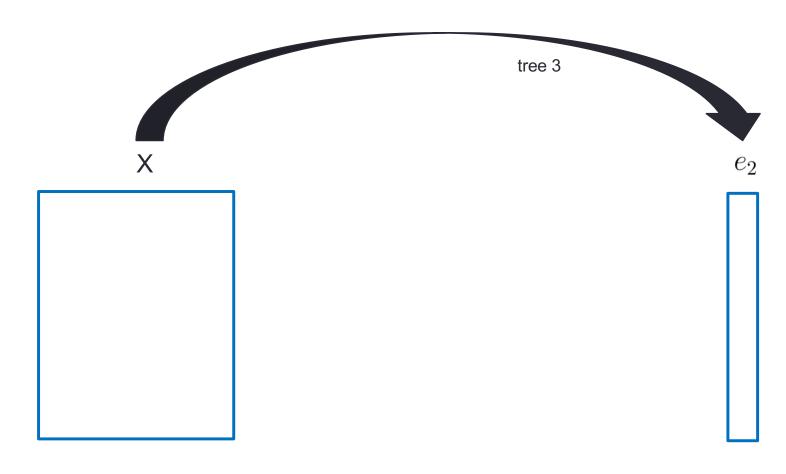


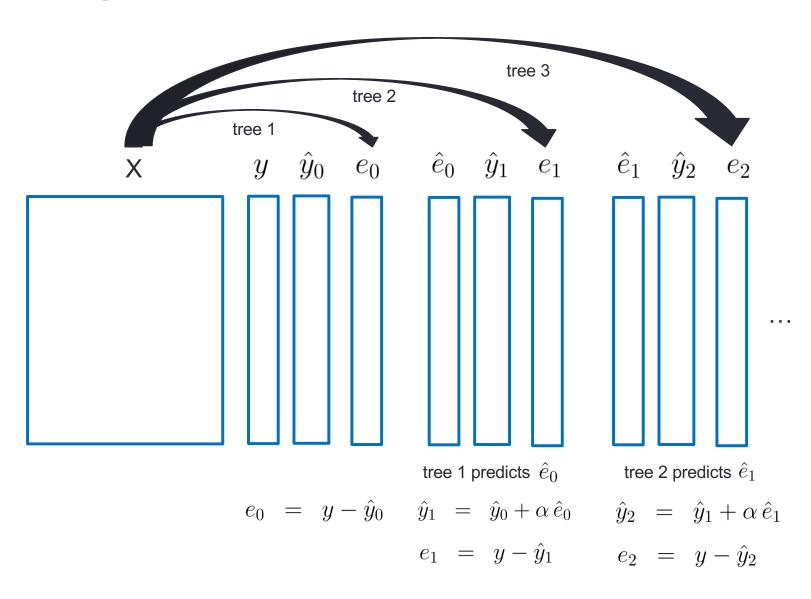
 $\hat{y}_2 = \hat{y}_1 + \alpha \, \hat{e}_1$





$$e_2 = y - \hat{y}_2$$





Example 1

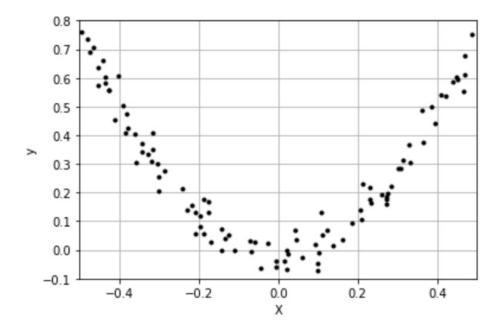
Example – Polynomial data

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import GradientBoostingRegressor
df = pd.read csv('dataset.csv')
df[:5]
        X
0 -0.125460 0.051573
   0.450714 0.594480
2 0.231994 0.166052
                                                df.shape
3 0.098658 -0.070178
4 -0.343981 0.343986
                                                (100, 2)
y = df.y
X = df.drop(['y'],axis =1)
```

Example – Polynomial data

```
plt.plot(X, y, 'k.')

# boundary for x and y axes
axes=[-0.5, 0.5, -0.1, 0.8]
plt.axis(axes)
plt.xlabel('X')
plt.ylabel('y')
plt.grid();
```



```
# make sequence of x-coordinate values
seq = np.linspace(-0.5,0.5, 500)
```

```
# transform seq to a dataframe
x1 = pd.DataFrame()
x1['X'] = seq
x1[:5]
```

0 -0.500000

1 -0.497996

2 -0.495992

3 -0.493988

4 -0.491984

```
x1.shape
(500, 1)
```

0.4

0.3

0.2

0.1

0.0

-0.1

-0.4

-0.2

```
# build the regression tree
tree = DecisionTreeRegressor(max_depth=2, random_state=42)

tree.fit(X,y)
red_linel = tree.predict(x1)

plt.plot(X,y,"k.",markersize=4)
plt.plot(x1,red_line1,"r-", linewidth=2)
plt.axis(axes)
plt.grid();

0.8

0.7

0.8

0.7

0.6

0.5
```

0.2

0.0

0.4

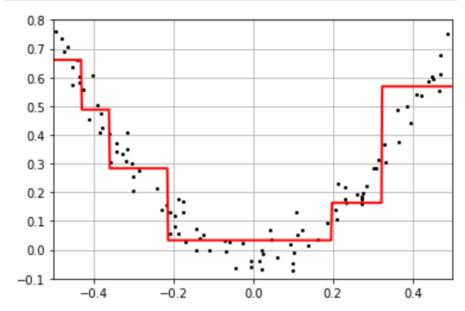
```
yhat1 = tree.predict(X)
e1 = y - yhat1
```

```
e_hat1

tree.fit(X, e1)

red_line2 = red_line1 + tree.predict(x1)
```

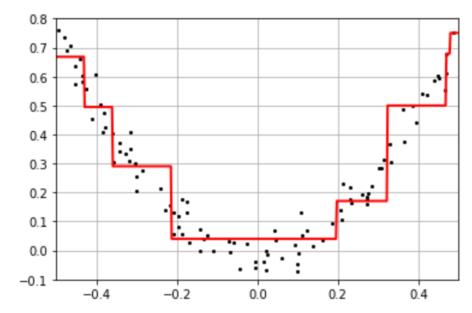
```
plt.plot(X, y, "k.", markersize=4)
plt.plot(x1, red_line2, "r-", linewidth=2)
plt.axis(axes)
plt.grid();
```



```
yhat2 = tree.predict(X)
e2 = e1 - yhat2
```

```
tree.fit(X, e2);
red_line3 = red_line2 + tree.predict(x1)
```

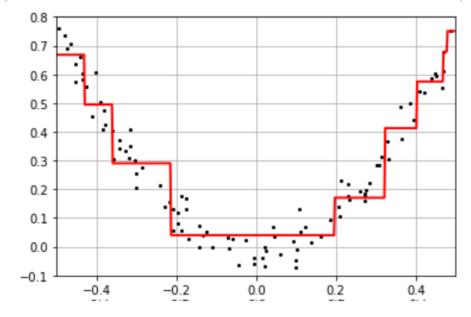
```
plt.plot(X, y, "k.", markersize=4)
plt.plot(x1,red_line3, "r-", linewidth=2)
plt.axis(axes)
plt.grid();
```



```
yhat3 = tree.predict(X)
e3 = e2 - yhat3
```

```
tree.fit(X,e3)
red_line4 = red_line3 + tree.predict(x1)
```

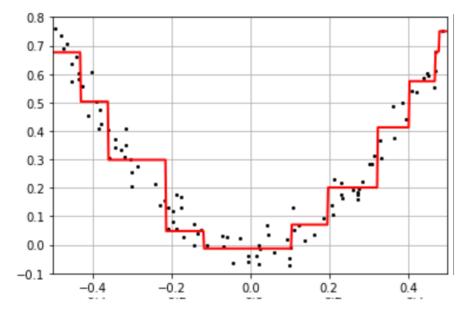
```
plt.plot(X, y, "k.", markersize=4)
plt.plot(x1,red_line4,"r-", linewidth=2)
plt.axis(axes)
plt.grid();
```



```
yhat4 = tree.predict(X)
e4 = e3 - yhat4
```

```
tree.fit(X,e4)
red_line5 = red_line4 + tree.predict(x1)
```

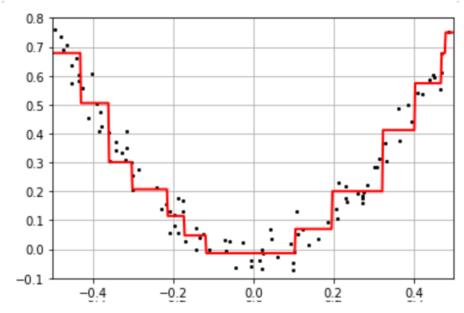
```
plt.plot(X, y, "k.", markersize=4)
plt.plot(x1, red_line5, "r-", linewidth=2)
plt.axis(axes)
plt.grid();
```



```
yhat5 = tree.predict(X)
e5 = e4 - yhat5
```

```
tree.fit(X,e5)
red_line6 = red_line5 + tree.predict(x1)
```

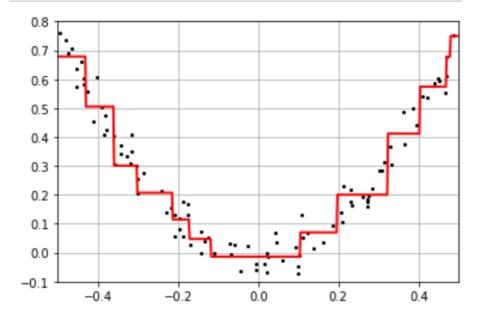
```
plt.plot(X, y, "k.", markersize=4)
plt.plot(x1,red_line6, "r-", linewidth=2)
plt.axis(axes)
plt.grid();
```



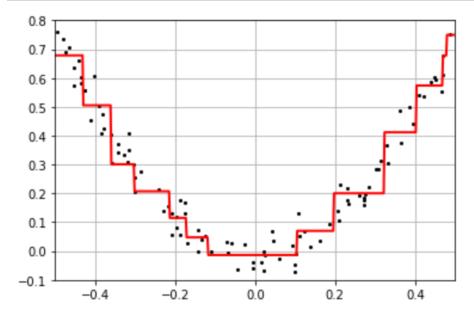
Example

```
tree.fit(X,e5)
red_line6 = red_line5 + tree.predict(x1)
```

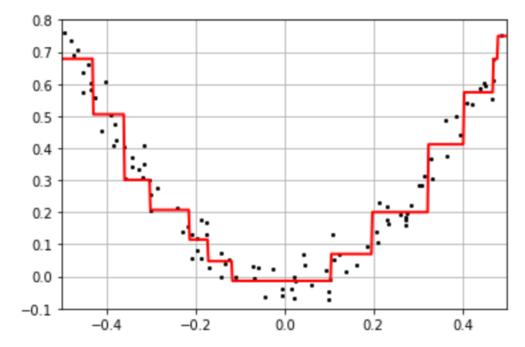
```
plt.plot(X, y, "k.",markersize=4)
plt.plot(x1,red_line6,"r-", linewidth=2)
plt.axis(axes)
plt.grid();
```



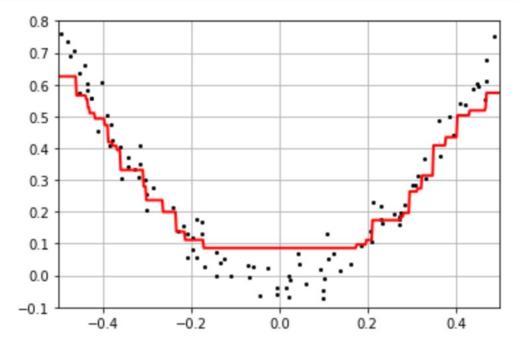
Gradient Boosting with 6 steps



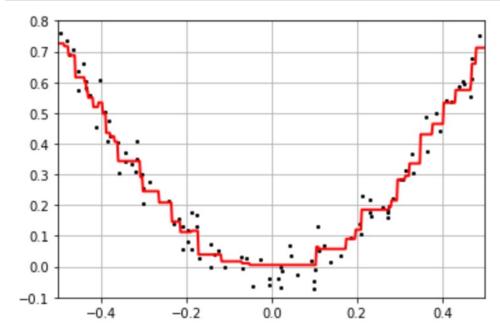
Example – Gradient Boosting with 6 steps



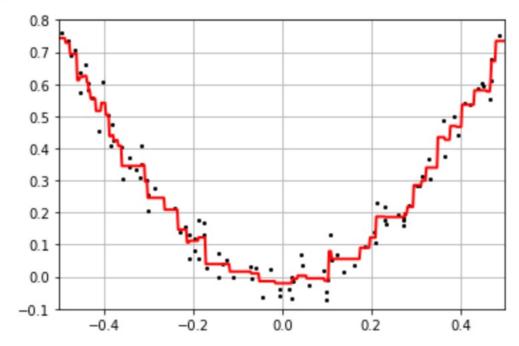
Example – Gradient Boosting with 20 steps



Example – Gradient Boosting with 50 steps



Example – Gradient Boosting with 80 steps



Example 2 – Ensembles on Classification

Example – Cancer dataset

The Cancer data from *sklearn* contains data from 569 patients with breast tumors. It is of interest to predict whether the tumor of a patient is malignant.

- Compare test AR of bagged trees with 25 and 500 trees.
 Find the test accuracy rate.
- Fit Random Forest models with 25 and 500 trees (and max_features = 4). Which predictors are most important?
- Fit 500 Gradient boosted trees with max_depth = 4, and α = 0.01, 0.20. Which predictors are found most important?

Example – libraries

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt

from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
from sklearn.model_selection import StratifiedKFold
from sklearn.model_selection import GridSearchCV

from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier
from sklearn.ensemble import GradientBoostingClassifier
```

Example – Cancer dataset

```
cancer = load_breast_cancer()

list1 = list(cancer.feature_names)

df0 = pd.DataFrame(cancer.data,columns = list1)
df0[:5]
```

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry	mean fractal dimension	
0	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	0.2419	0.07871	
1	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	0.1812	0.05667	
2	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	0.2069	0.05999	
3	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	0.2597	0.09744	
4	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	0.1809	0.05883	

5 rows × 30 columns

```
y = cancer.target
X = cancer.data
```

X.shape

(569, 30)

Example 2 – Bagging Model

Decision Tree vs. Bagging

Single Tree

```
X_train,X_test,y_train,y_test = train_test_split(X,y,stratify = y,
                                                  random_state = 0)
tree1 = DecisionTreeClassifier(max_depth = 4)
tree1.fit(X_train,y_train)
tree1.score(X_test,y_test)
0.9230769230769231
```

Bagging model (500 Trees)

```
X_train,X_test,y_train,y_test = train_test_split(X,y,stratify = y,
                                                  random_state = 0)
bag_model = RandomForestClassifier(max_features = 30,
                                    max_depth = 4,
                                    n_{estimators} = 500,
                                    random_state=0)
bag model.fit(X train,y train)
bag_model.score(X_test,y_test)
```

0.9300699300699301

Decision Tree vs. Bagging

Single Tree

```
X_train,X_test,y_train,y_test = train_test_split(X,y,stratify = y, random_state = 0)

tree1 = DecisionTreeClassifier(max_depth = 4)
tree1.fit(X_train,y_train)
tree1.score(X_test,y_test)

0.9230769230769231
```

Bagging model (25 Trees)

0.9230769230769231

Bagging – Find best n_estimators

GridSearchCV on n_estimators

Bagging – Find best n_estimators

GridSearchCV on n_estimators

```
X train, X test, y train, y test = train test split(X, y, stratify = y,
                                                  random state = 0)
model1 = RandomForestClassifier(max depth=4, random state=1)
kfold = StratifiedKFold(n_splits=5,shuffle = True,
                                     random_state = 1)
estimators = range(100,1000,100)
params = dict(n estimators = estimators)
grid1 = GridSearchCV(model1,param grid = params,cv = kfold)
grid1.fit(X train, y train);
# Best Validation Accuracy rate
grid1.best_score_
                                                                   Test Accuracy rate
0.9647058823529413
                                                                   grid1.score(X test, y test)
grid1.best params
{'n_estimators': 500}
                                                                   0.9440559440559441
```

Bagging – Feature Importance

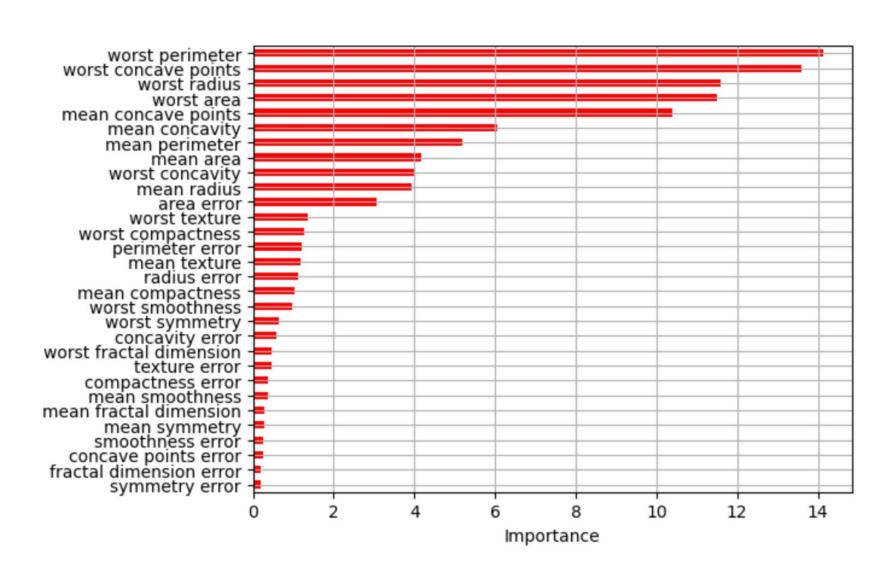
Feature Importance

worst perimeter	14.129173
worst concave points	13.576649
worst radius	11.579474
worst area	11.495622
mean concave points	10.388860
mean concavity	6.064789
mean perimeter	5.184134
mean area	4.173711
worst concavity	4.033597
mean radius	3.920080

area error	3.068875
worst texture	1.350636
worst compactness	1.269216
perimeter error	1.208892
mean texture	1.166103
radius error	1.117846
mean compactness	1.016690
worst smoothness	0.969281
worst symmetry	0.626952
concavity error	0.567973

worst fractal dimension	0.473491
texture error	0.446715
compactness error	0.383106
mean smoothness	0.359460
mean fractal dimension	0.280126
mean symmetry	0.269401
smoothness error	0.265304
concave points error	0.259535
fractal dimension error	0.177464
symmetry error	0.176844

Bagging – Feature Importance



Example 2 – Random Forest

Random Forest 500 vs 25 trees

RandomForest on 500 Trees (max_features = 5)

RandomForest on 25 Trees

0.9370629370629371

Random Forest vs Bagging (25 trees)

Bagging model (25 Trees)

RandomForest on 25 Trees

0.9370629370629371

Random Forest – Find best max_features

GridSearchCV on max_features

```
X_train,X_test,y_train,y_test = train_test_split(X,y,stratify = y, random_state = 0)

model3 = RandomForestClassifier(max_depth=4,n_estimators = 500, random_state=1)

kfold = StratifiedKFold(n_splits=5,shuffle = True, random_state = 1)

features = range(1,31)
    params = dict(max_features = features)

grid1 = GridSearchCV(model3,param_grid = params,cv = kfold)
    grid1.fit(X_train,y_train);
```

Random Forest – Find best max_features

GridSearchCV on max_features

```
X_train, X_test, y_train, y_test = train_test_split(X, y, stratify = y,
                                                  random state = 0)
model3 = RandomForestClassifier(max_depth=4,n_estimators = 500,
                                 random state=1)
kfold = StratifiedKFold(n_splits=5,shuffle = True, random_state = 1)
features = range(1,31)
params = dict(max_features = features)
grid1 = GridSearchCV(model3,param_grid = params,cv = kfold)
grid1.fit(X train, y train);
# Best Validation Accuracy rate
grid1.best_score_
0.9670861833105336
                                                                      Test Accuracy rate
                                                                      grid1.score(X_test,y_test)
grid1.best params
                                                                      0.9440559440559441
{'max features': 14}
```

Random Forest – Feature Importance

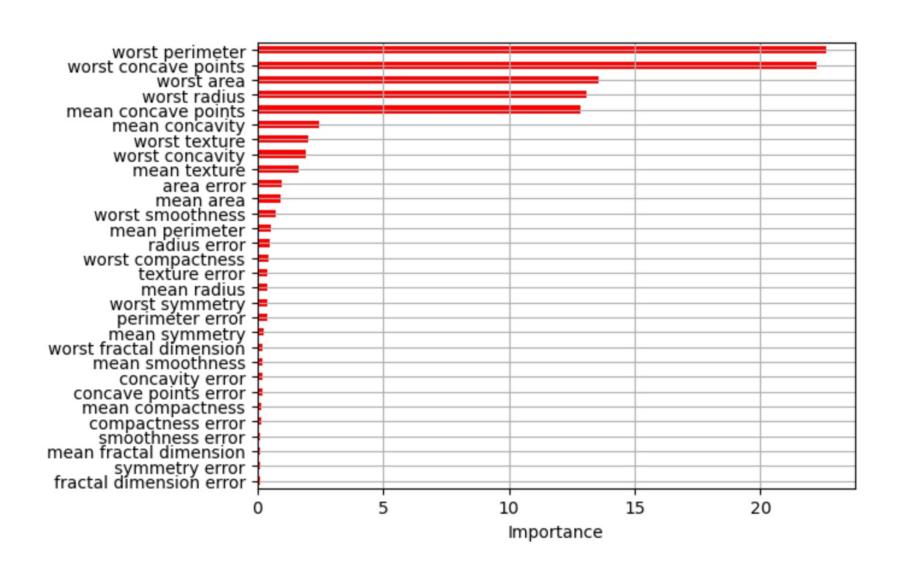
Feature Importance

worst perimeter	22.611353
worst concave points	22.232967
worst area	13.548250
worst radius	13.065276
mean concave points	12.862108
mean concavity	2.457333
worst texture	2.010432
worst concavity	1.912220
mean texture	1.644063
area error	0.999653

mean area	0.937828
worst smoothness	0.758059
mean perimeter	0.569221
radius error	0.511625
worst compactness	0.450272
texture error	0.397110
mean radius	0.392667
worst symmetry	0.387934
perimeter error	0.382765
mean symmetry	0.263526

worst fractal dimension	0.225117
mean smoothness	0.202968
concavity error	0.197187
concave points error	0.193128
mean compactness	0.149347
compactness error	0.144200
smoothness error	0.133866
mean fractal dimension	0.131247
symmetry error	0.125688
fractal dimension error	0.102590

Random Forest – Feature Importance



Example 2 – Gradient Boosting

Gradient Boosting Classification Trees

learning rate to 0.60

0.9370629370629371

learning rate to 0.10

0.951048951048951

Gradient Boosting – Find best learning_rate

GridSearchCV on learning_rate

```
X train, X test, y train, y test = train test split(X, y, stratify = y,
                                                  random state = 0)
model3 = GradientBoostingClassifier(n_estimators = 25,
                                      \max depth = 4, random state =1)
lrates = np.linspace(0.0,1.0,20)
lrates
array([0.
                 , 0.05263158, 0.10526316, 0.15789474, 0.21052632,
       0.26315789, 0.31578947, 0.36842105, 0.42105263, 0.47368421,
       0.52631579, 0.57894737, 0.63157895, 0.68421053, 0.73684211,
       0.78947368, 0.84210526, 0.89473684, 0.94736842, 1.
                                                                  ])
kfold = StratifiedKFold(n splits=5,shuffle = True, random state = 1)
params = dict(learning rate = lrates)
grid1 = GridSearchCV(model3,param grid = params,cv = kfold)
grid1.fit(X_train,y_train);
```

Gradient Boosting – Find best learning_rate

GridSearchCV on learning_rate

```
X train, X test, y train, y test = train test split(X, y, stratify = y,
                                                  random state = 0)
model3 = GradientBoostingClassifier(n estimators = 25,
                                      max_depth = 4, random_state =1)
lrates = np.linspace(0.0,1.0,20)
lrates
array([0.
                 , 0.05263158, 0.10526316, 0.15789474, 0.21052632,
       0.26315789, 0.31578947, 0.36842105, 0.42105263, 0.47368421,
       0.52631579, 0.57894737, 0.63157895, 0.68421053, 0.73684211,
       0.78947368, 0.84210526, 0.89473684, 0.94736842, 1.
kfold = StratifiedKFold(n splits=5,shuffle = True, random state = 1)
params = dict(learning rate = lrates)
grid1 = GridSearchCV(model3,param grid = params,cv = kfold)
grid1.fit(X_train,y_train);
```

```
# Best Validation Accuracy rate
grid1.best_score_
0.9671135430916553
grid1.best_params_
{'learning_rate': 0.63157894736
```

Test Accuracy rate

```
grid1.score(X_test,y_test)
```

0.9300699300699301

Gradient Boosting-Feature Importance

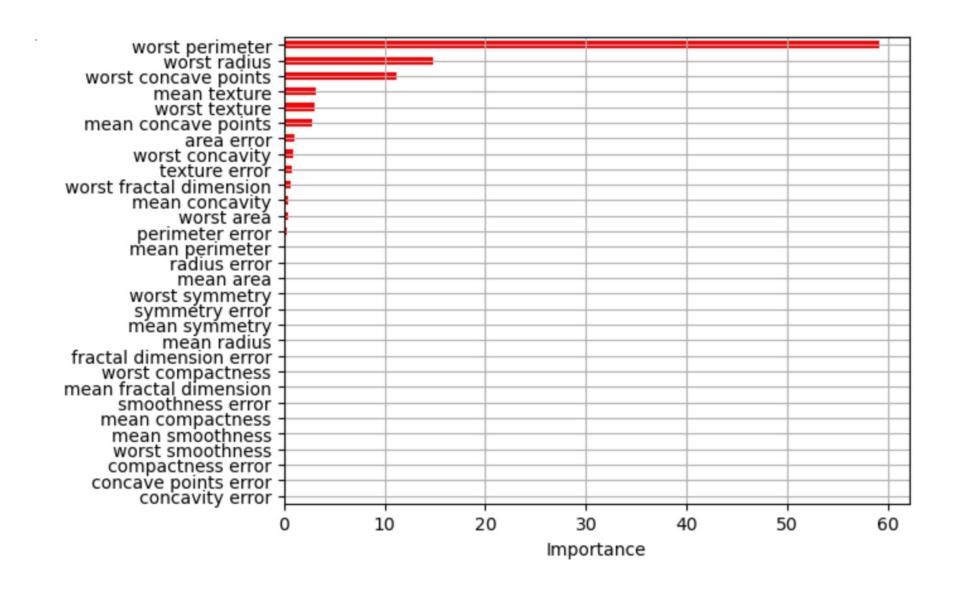
Importance

worst perimeter	59.099340
worst radius	14.847550
worst concave points	11.161615
mean texture	3.231188
worst texture	3.098257
mean concave points	2.843215
area error	1.067154
worst concavity	0.949111
texture error	0.799159
worst fractal dimension	0.725911

mean concavity	0.453931
worst area	0.452600
perimeter error	0.332176
mean perimeter	0.217580
radius error	0.204401
mean area	0.165851
worst symmetry	0.148986
symmetry error	0.089275
mean symmetry	0.062010
mean radius	0.020612

fractal dimension error	0.013000
worst compactness	0.008984
mean fractal dimension	0.003803
smoothness error	0.002376
mean compactness	0.000650
mean smoothness	0.000562
worst smoothness	0.000505
compactness error	0.000130
concave points error	0.000067
concavity error	0.000003

Gradient Boosting – Feature Importance



GridSearchCV - Tuning 2 hyperparameters

```
# Consider 6 values for each parameter
params = {'learning_rate': np.linspace(0.2,0.7,6),
              'max features': list(range(3,9))}
params
{'learning_rate': array([0.2, 0.3, 0.4, 0.5, 0.6, 0.7]),
 'max_features': [3, 4, 5, 6, 7, 8]}
grid2 = GridSearchCV(model3, param_grid = params,cv = kfold)
grid2.fit(X train,y train);
# Best Validation Accuracy rate
grid2.best_score_
0.9741723666210671
grid2.best_params_
{'learning rate': 0.6, 'max features': 6}
```

cv_results_ has the accuracy rates of each fold and their average in column mean_test_score

```
# store the results into dataframe
results = pd.DataFrame(grid2.cv results)
results.dtypes
                       float64
mean fit time
std fit time
                       float64
mean score time
                       float64
std score time
                       float64
param learning rate
                        object
                        object
param max features
                        object
params
                       float64
split0 test score
                       float64
split1 test score
split2 test score
                       float64
split3 test score
                       float64
split4 test score
                       float64
mean test score
                       float64
std_test_score
                       float64
rank test score
                          int32
```

cv_results_ has the accuracy rates of each fold and their average in column mean_test_score

```
# store the results into dataframe
results = pd.DataFrame(grid2.cv results)
results.dtypes
                       float64
mean fit time
std fit time
                       float64
mean score time
                       float64
std score time
                       float64
param learning rate
                        object
                        object
param max features
                        object
params
split0 test score
                       float64
                       float64
split1 test score
split2 test score
                       float64
split3 test score
                       float64
split4_test_score
                       float64
mean test score
                       float64
                       float64
std test score
rank test score
                          int32
```

0.955458

0.946101

8

3

```
list1 = list([4,5,12])
df9 = results.iloc[:,list1].copy()
df9[:13]
                                                 Validation
                                               Accuracy rate
    param_learning_rate param_max_features mean_test_score
                   0.02
 0
                                          3
                                                    0.941423
  1
                   0.02
                                                    0.953160
 2
                   0.02
                                          5
                                                    0.950807
  3
                   0.02
                                          6
                                                    0.950752
  4
                   0.02
                                          7
                                                    0.941341
                   0.02
                                          8
                                                    0.948372
  5
                  0.025
                                                    0.943776
 6
                                          3
                  0.025
                                                    0.953160
 7
                                          4
                                                    0.953133
 8
                  0.025
                                          5
                  0.025
                                                    0.953105
 9
                                          6
10
                  0.025
                                                    0.948372
                                          7
```

0.025

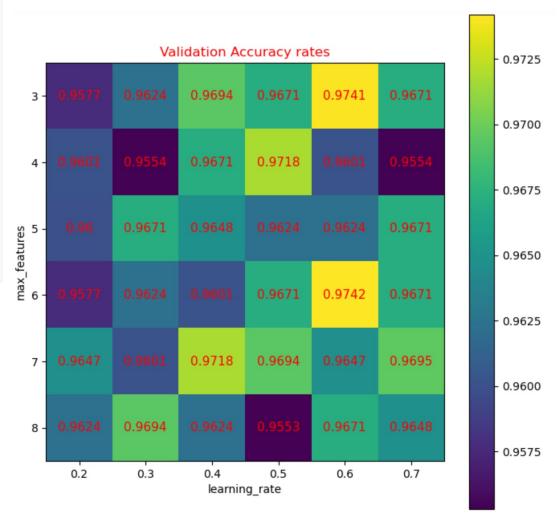
0.03

11

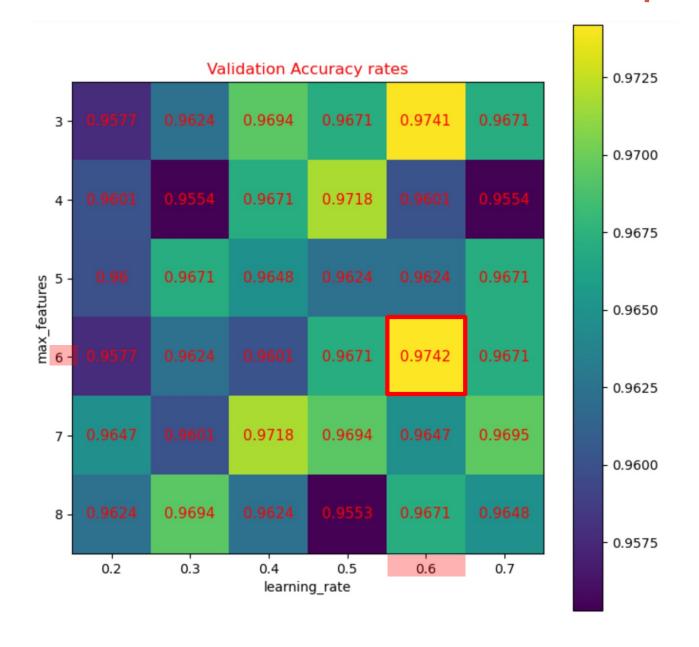
12

```
df1 = df9.pivot_table('mean_test_score',
                          columns = 'param_learning_rate',
                           index = 'param max features')
df1
                        0.2
                                 0.3
                                                   0.5
                                                            0.6
                                                                     0.7
 param_learning_rate
                                          0.4
param_max_features
                 3 0.957674 0.962408 0.969412 0.967059 0.974118 0.967086
                   0.960055 0.955376 0.967086 0.971792 0.960055
                                                                0.955376
                   0.960027 0.967086 0.964761 0.962408 0.962435 0.967059
                   0.957729  0.962435  0.960055  0.967114  0.974172
                                                                0.967086
                 7 0.964733 0.960109 0.971765 0.969439 0.964733 0.969466
                 8 0.962380 0.969412 0.962408 0.955349 0.967114 0.964761
```

GridSearchCV results on a Heatmap



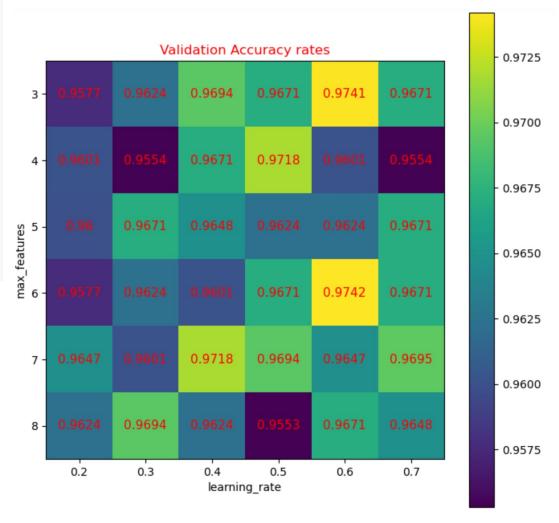
GridSearchCV results on a Heatmap



GridSearchCV results on a Heatmap

Test Accuracy rate

```
grid2.score(X_test,y_test)
0.9440559440559441
```



Gradient Boosting – Feature Importance

