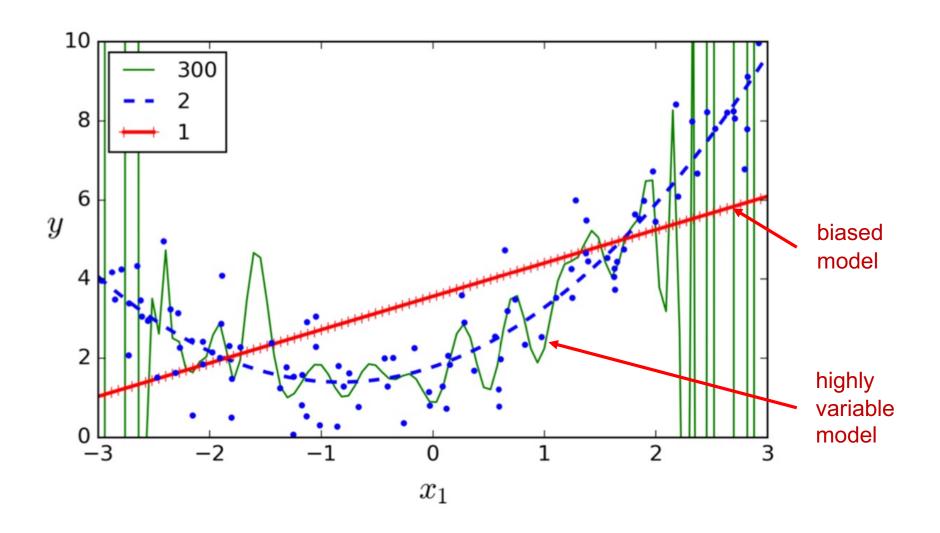
## **ENSEMBLES**

### Outline

- Definition of Ensembles
- Bias-Variance Tradeoff
- Bootstrap samples
- Ensembles
- Bagging
- Random Forest
- Gradient Boosting

### Ensembles

- Methods combining multiple machine learning models to create low-bias, low-variance, prediction models
- What are low-bias and low-variance models?



The model error (MSE, error rate) is the sum of 3 parts

- Bias
- Variance
- Random error

The model error (MSE, error rate) is the sum of 3 parts
• Bias

Model is unable to follow the structural variation underlying the data. (i.e., a linear model used with nonlinear data).

Models with high-bias are likely to underfit the data.

The model error (MSE, error rate) is the sum of 3 parts

• Bias

Model is unable to follow the structural variation underlying the data. (i.e., a linear model used with nonlinear data).

Models with high-bias are likely to underfit the data.

#### Variance

Model is highly sensitive, trying to capture random variations in the data. (i.e., a high-degree polynomial model).

Models with high-variance are likely to overfit the data.

The model error (MSE, error rate) is the sum of 3 parts

Random error

Data portion that cannot be predicted

We look for models that do not underfit or overfit the data

These are low-bias, low-variance models

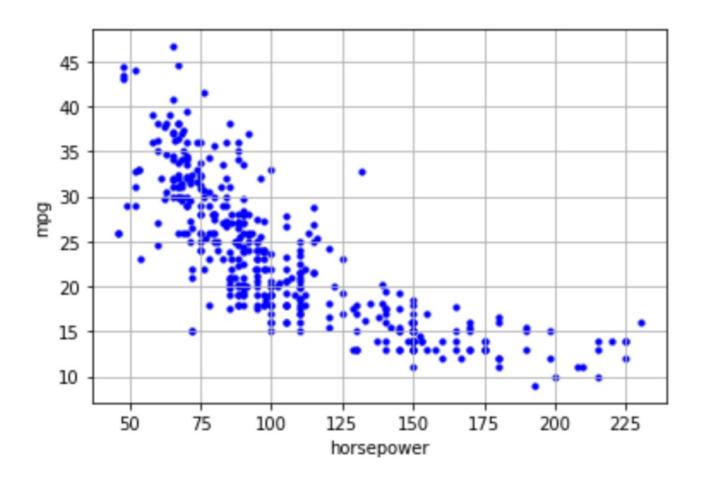
## Model Complexity

- Model Complexity is given by the number of predictor columns in the model.
- Adding new predictors, transformed predictors, interactions, and polynomial terms increases the model complexity

## **Model Complexity**

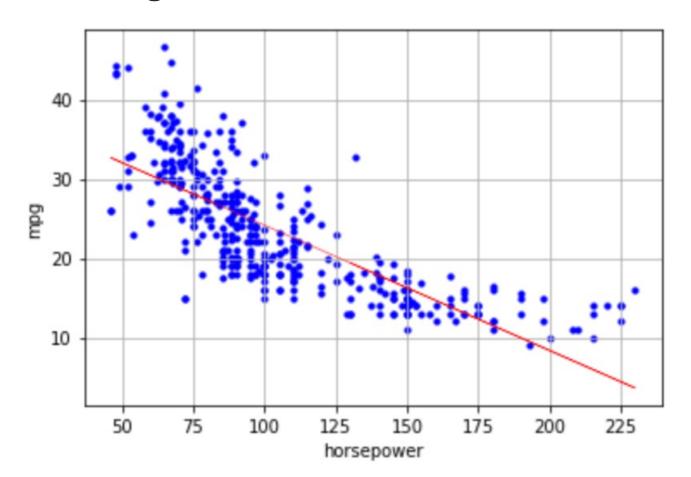
- Increasing model complexity usually increases the model's variance and reduces its bias.
- Decreasing model complexity usually increases the model's bias and reduces its variance.
- This relation between the error portions of a model is called the Bias – Variance Tradeoff

#### Non-linear relation



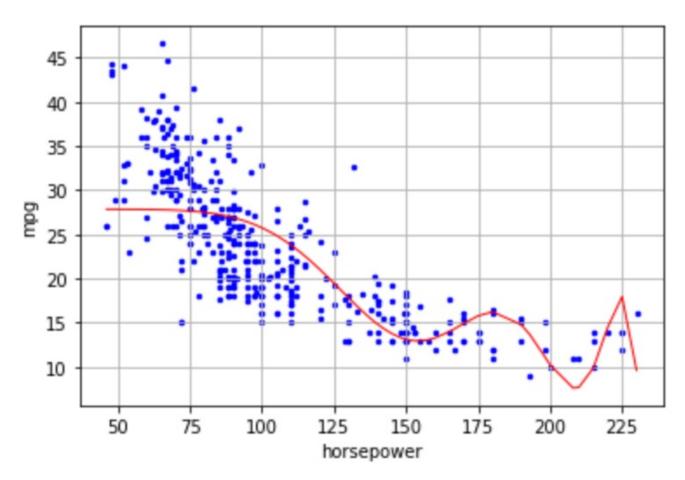
Model with High-Bias

(does not follow underlying pattern)



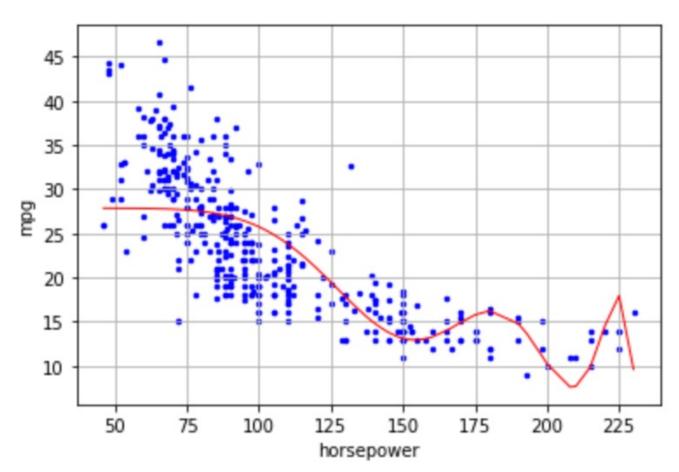
underfits the data

Model with High-Variance (high-degree polynomial)



overfits the data

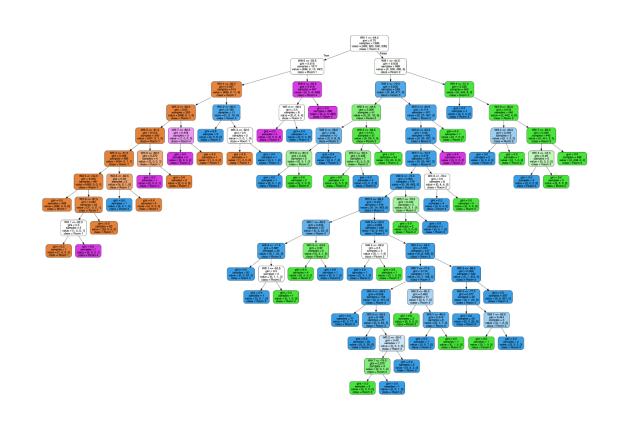
Model with High-Variance (high-degree polynomial)



the model follows both the underlying pattern and the random errors in the data

## Tree complexity

- A decision Tree with a large depth is a high variance model
- To avoid it, we may define a maximum depth
- But then predictions may become less accurate



## **Balancing Tree Complexity**

- Ensembles are combination of models (trees)
- They tend to be low-bias, low-variance models

## ENSEMBLES

### **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**

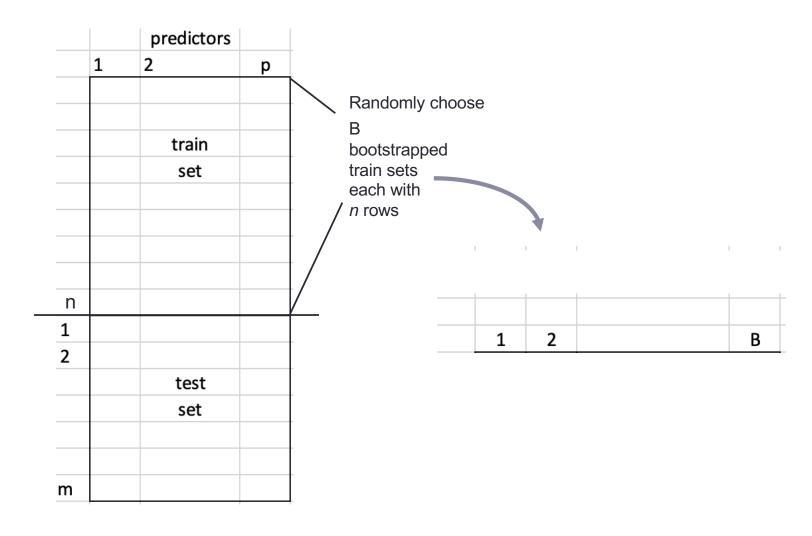
### Bootstrap samples (from dataframes)

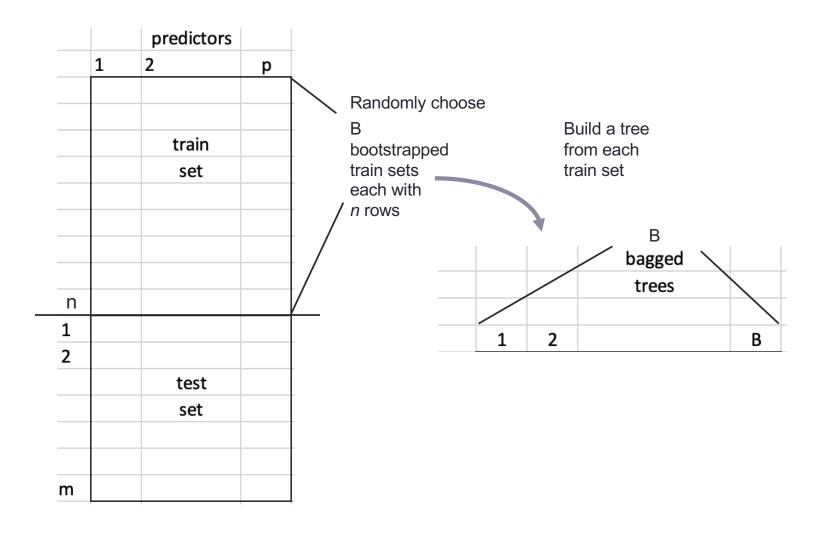
- A bootstrap sample is a sample with replacement
- May include same row many times
- Bootstrap samples are usually of the same size

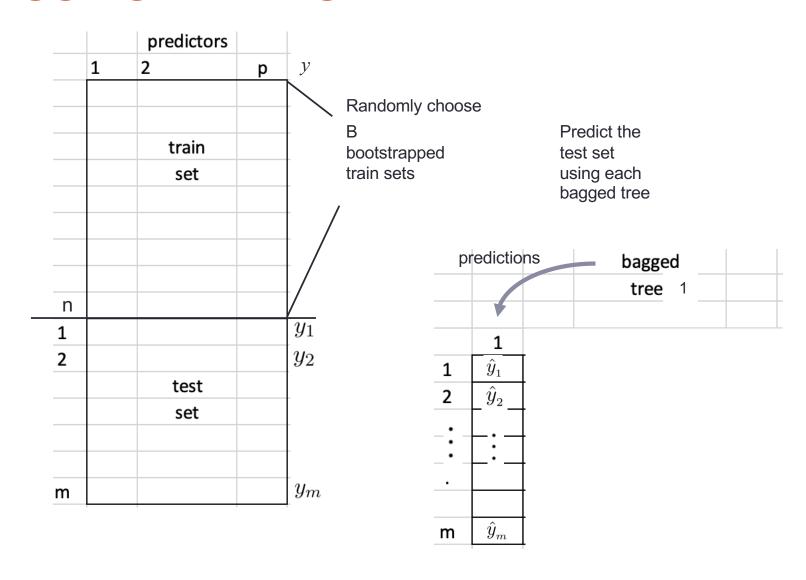
## Bagging

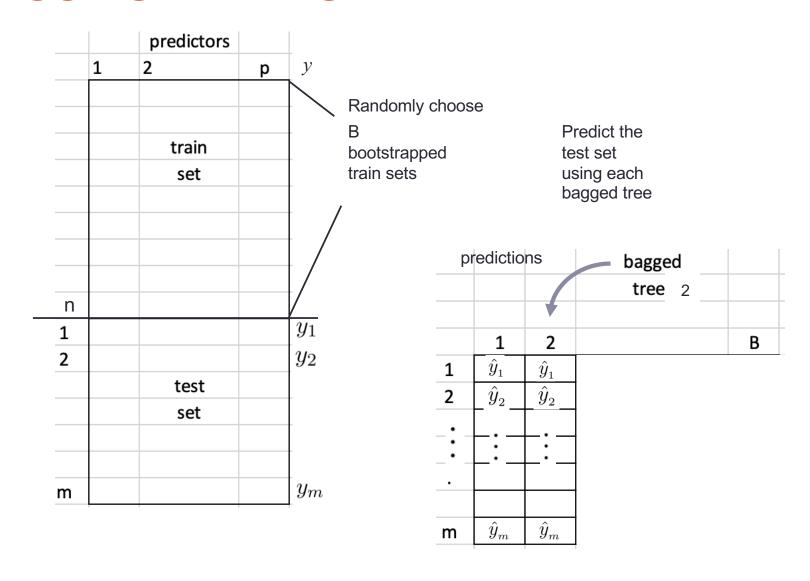
- Individual trees suffer from high variance
- That is, if a dataset is randomly split into 2 sets and a tree is fit to each half, the predictions may be *very* different
- On the other hand, a low-variance model would yield predictions that are not much different
- Averaging trees predictions help avoid high-variance models

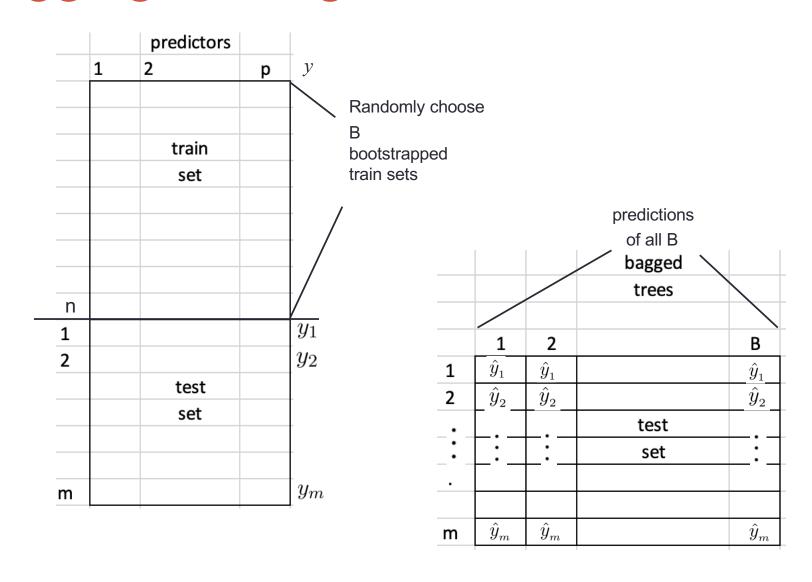
		predictors	
	1	2	р
		train	
		set	
n			
2			
2			
		test	
		set	
m			

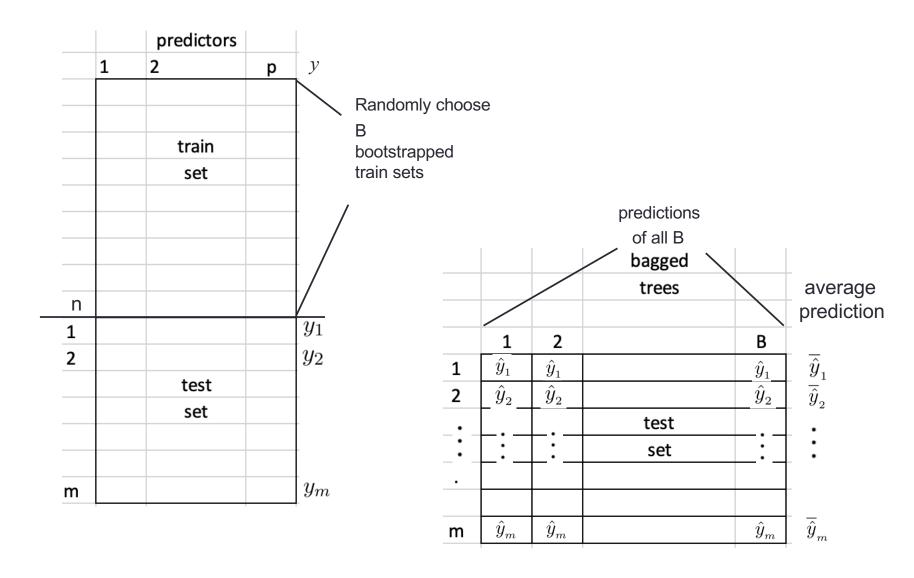


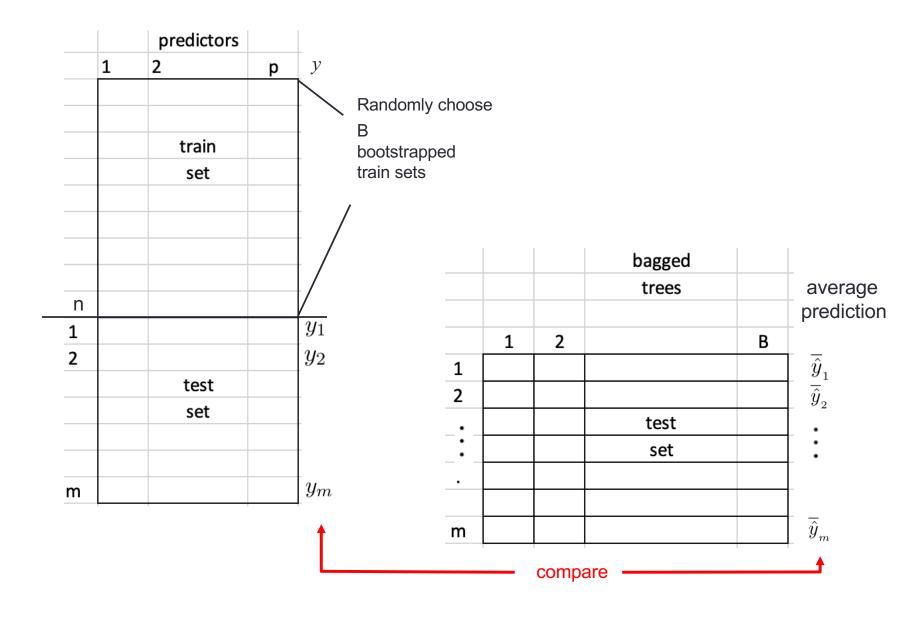


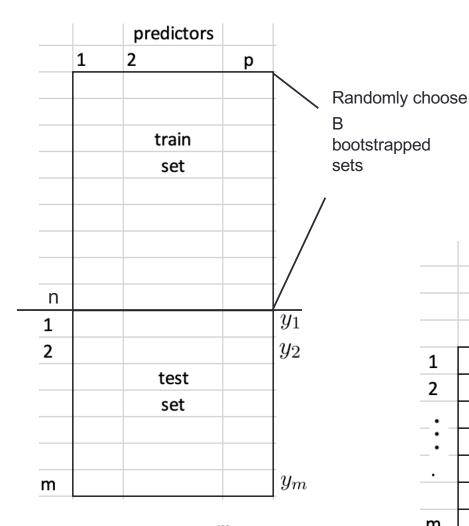












MSPE =	$\frac{1}{m}$	$\sum_{i=1}^{m} (y_i -$	$\overline{\hat{y}}_i)^2$
--------	---------------	-------------------------	---------------------------

			bagged		
			trees		average
					prediction
	1	2		В	
1					$\left[ egin{array}{c} rac{\widehat{\hat{y}}}{\widehat{\hat{y}}_2} \end{array}  ight]$
2					$\overline{\hat{y}}_2$
			test		•
:			set		:
m					$\overline{\hat{y}}_m$

### 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

### Random Forests

It is a simple modification on bagging How does it work?

- Before each split, randomly select a subset with m of the p predictors as candidates to make the split
- then choose the predictor giving the largest MSE reduction

### Random Forests

It is a simple modification on bagging How does it work?

- Before each split, randomly select a subset with m of the p predictors as candidates to make the split
- then choose the predictor giving the largest MSE reduction
- Bagging uses m = p (all the predictors)
- Random Forest m < p predictors

# 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  $\alpha$  times the predicted error
- Parameter  $0 < \alpha < 1$  is called the learning rate

## Example 1 – Ensembles on Regression

## Example – Boston dataset

Data of 506 houses in the area of Boston

- Want to predict the price of houses and to identify which variables are most important for prediction
- Split the dataset into a training (50%) and a test set
- Fit and compare bagged trees with 25 and 500 trees. Find the test MSPE.
- Fit a Random Forest with 500 trees and max\_features = 6.
   Which predictors are most important?
- Fit 500 Gradient boosted trees with  $max_{depth} = 4$ , and  $\alpha = 0.01$ , 0.20. Which predictors are most important?

# Boston dataset -13 features, 1 target

- CRIM per capita crime rate by town
- ZN proportion of residential land zoned for lots over 25,000 sq.ft.
- INDUS proportion of non-retail business acres per town.
- CHAS Charles River dummy variable (1 if tract bounds river; 0 otherwise)
- NOX nitric oxides concentration (parts per 10 million)
- RM average number of rooms per dwelling
- AGE proportion of owner-occupied units built prior to 1940
- DIS weighted distances to five Boston employment centres
- RAD index of accessibility to radial highways
- TAX full-value property-tax rate per \$10,000
- PTRATIO pupil-teacher ratio by town
- BLACK proportion of blacks by town
- LSTAT % lower status of the population
- MEDV Median price of owner-occupied homes in \$1000's

# Example – libraries

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

```
from sklearn.model_selection import train_test_split
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import mean_squared_error
```

```
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.ensemble import RandomForestRegressor
```

Use RandomForestRegressor for both Bagging and Random Forest

## Example – Boston dataset variables

```
boston_df = pd.read_csv('Boston.csv')
boston_df[:5]
```

	crim	zn	indus	chas	nox	rm	age	dis	rad	tax	ptratio	black	Istat	medv
0	0.00632	18.0	2.31	0	0.538	6.575	65.2	4.0900	1	296	15.3	396.90	4.98	24.0
1	0.02731	0.0	7.07	0	0.469	6.421	78.9	4.9671	2	242	17.8	396.90	9.14	21.6
2	0.02729	0.0	7.07	0	0.469	7.185	61.1	4.9671	2	242	17.8	392.83	4.03	34.7
3	0.03237	0.0	2.18	0	0.458	6.998	45.8	6.0622	3	222	18.7	394.63	2.94	33.4
4	0.06905	0.0	2.18	0	0.458	7.147	54.2	6.0622	3	222	18.7	396.90	5.33	36.2

```
X = boston_df.drop('medv',axis =1)
y = boston_df.medv
```

# Ensembles on Regression – Bagging

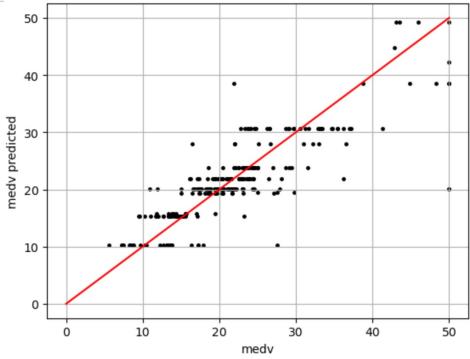
# Boston dataset – Single tree

```
X_train,X_test,y_train,y_test =\
train_test_split(X,y,train_size=0.5,random_state=0)

tree1 = DecisionTreeRegressor(max_depth=4)
tree1.fit(X_train,y_train)
pred1 = tree1.predict(X_test)
mspe = mean_squared_error(y_test,pred1)
mspe
```

23.817371513828622

```
xaxis = np.linspace(0,50,100)
plt.scatter(y_test,pred1,s = 6,color='k')
plt.plot(xaxis,xaxis,color='r')
plt.xlabel('medv')
plt.ylabel('medv predicted')
```

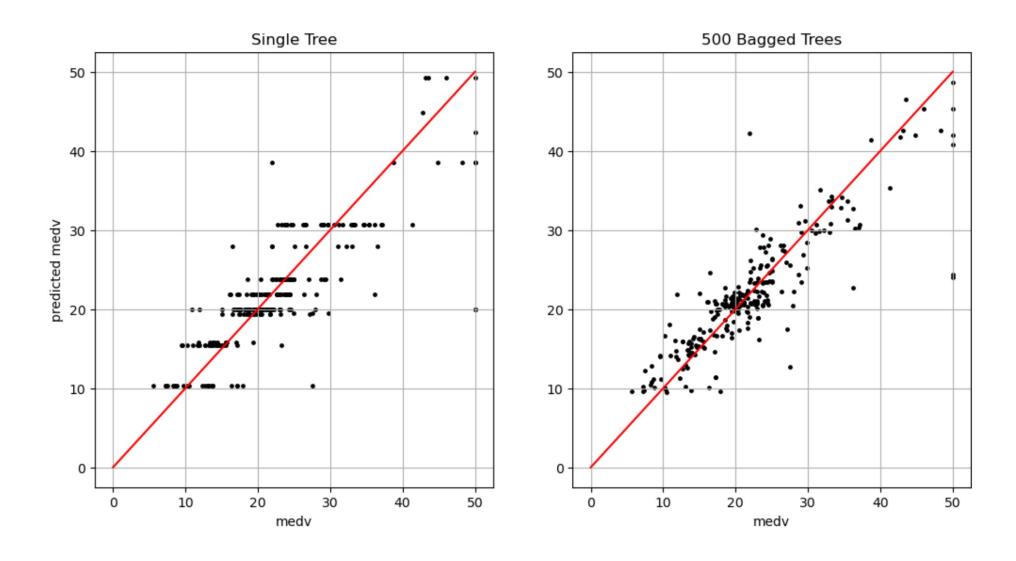


# Boston dataset – Bagging 500 trees

17.511475948091437

```
50
                                                    40
                                                 nedv predicted
                                                   30
plt.scatter(y_test,pred2,s = 6,color='k')
                                                   20
plt.plot(xaxis,xaxis,color='r')
plt.xlabel('medv')
plt.ylabel('medv predicted')
                                                    10
                                                     0
                                                                  10
                                                                            20
                                                                                      30
                                                                                                          50
                                                                                medv
```

# Single tree vs. Bagging 500 trees



### Holdout CV – Finding best n\_estimators

```
X_nontest, X_test, y_nontest, y_test = train_test_split(X, y, test_size=0.5,
                                                    random state=0)
X train, X validation, y train, y validation = train_test_split(X nontest, y nontest,
                                                    train size=0.5,
                                                    random_state=0)
                                                          try 25 <= n estimators <= 1100
nn = range(25, 1100, 50)
mses = []
for k in nn:
    model = RandomForestRegressor(max_features=13, max_depth=4,
                                        n_{estimators} = k
                                        random state=1)
    model.fit(X_train,y_train);
    yhat = model.predict(X validation)
    mse = mean_squared_error(y_validation,yhat)
    mses.append(mse)
```

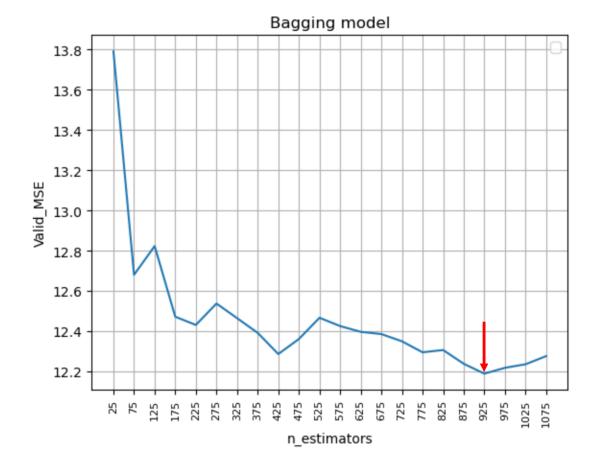
## Holdout CV – Finding best n\_estimators

```
df = pd.DataFrame(mses,columns = ['Valid_MSE'])
df.index = nn
df.index.name = 'n_estimators'
```

#### Valid MSE

n	es	tir	na	to	rs
••-	~~	•		•••	

n_estimators			
25	13.790862	575	12.425720
75	12.680501	625	12.397227
125	12.823402	675	12.385996
175	12.472117	725	12.350061
225	12.431220	775	12.295512
275	12.537799	825	12.306713
325	12.465000	875	12.238240
375	12.392024	925	12.189376
425	12.286661	975	12.218270
475	12.361468	1025	12.235890
525	12.466939	1075	12.276540



### Holdout CV – Finding best n\_estimators

```
df = pd.DataFrame(mses,columns = ['Valid_MSE'])
df.index = nn
df.index.name = 'n_estimators'
```

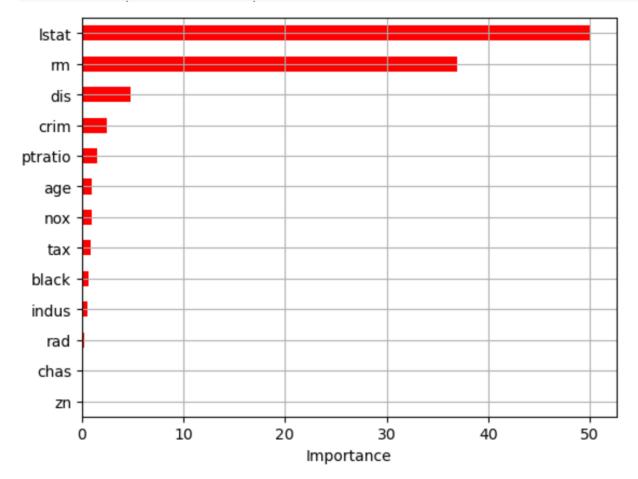
#### Valid\_MSE

#### n\_estimators

25	13.790862	575	12.425720
75	12.680501	625	12.397227
125	12.823402	675	12.385996
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275	12.537799	825	12.306713
325	12.465000	875	12.238240
375	12.392024	925	12.189376
425	12.286661	975	12.218270
475	12.361468	1025	12.235890
525	12.466939	1075	12.276540

### **Test MSE**

## Feature Importance – Bagging 500 trees

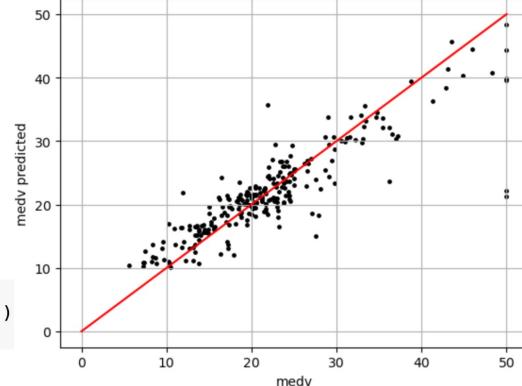


The wealth level of the community ('Istat') and the house size ('rm') are the 2 most important predictors

### Ensembles on Regression – Random Forest

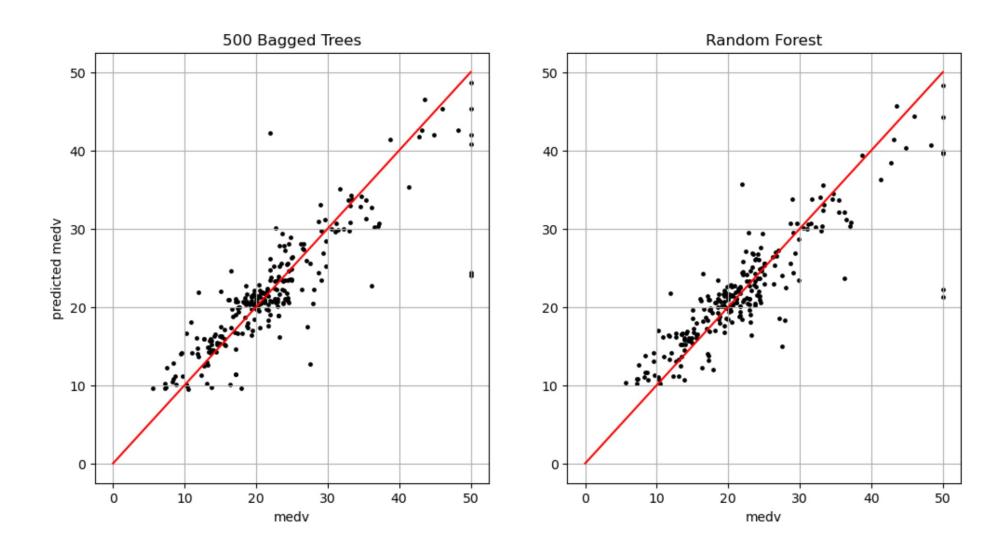
### Random Forest with 500 trees

17.434233348241854



xaxis = np.linspace(0,50,100)
plt.scatter(y\_test,pred,s = 6,color='k')
plt.plot(xaxis,xaxis,color='r')

# Bagging vs. Random Forest



### Holdout CV – Finding best max\_features

```
X_nontest, X_test, y_nontest, y_test = train_test_split(X, y, test_size=0.5,
                                                    random_state=0)
X_train, X_validation, y_train, y_validation = train_test_split(X_nontest, y_nontest,
                                                   train_size=0.5,
                                                    random state=0)
                                                          trv 1 <= m <= 13
nn = range(1,14)
mses = []
for k in nn:
    model = RandomForestRegressor(max_features=k, max_depth=4,
                                        n_{estimators} = 500,
                                        random state=1)
    model.fit(X_train,y_train)
    yhat = model.predict(X validation)
    mse = mean_squared_error(y_validation,yhat)
    mses.append(mse)
```

## Holdout CV – Finding best max\_features

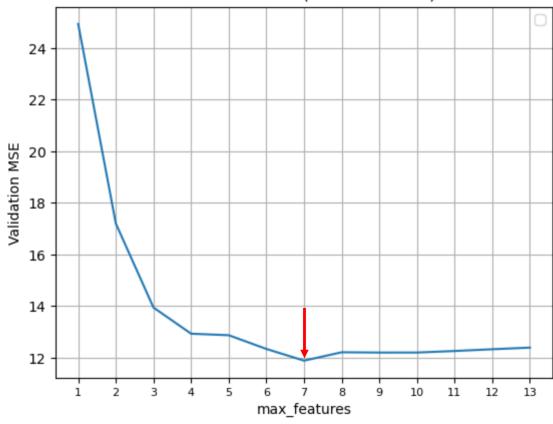
```
df = pd.DataFrame(mses,columns = ['Valid_MSE'])
df.index = nn
df.index.name = 'max_features'
```

#### Valid MSE

#### max\_features

1	24.939713	7	11.886289
2	17.200655	8	12.210822
3	13.943997	9	12.199773
4	12.930648	10	12.200606
5	12.871667	11	12.260297
6	12.339600	12	12.328083
		13	12.391338

### Random Forest (with 500 trees)



### Holdout CV – Finding best max\_features

```
df = pd.DataFrame(mses,columns = ['Valid_MSE'])
df.index = nn
df.index.name = 'max_features'
```

#### Valid MSE

#### max\_features

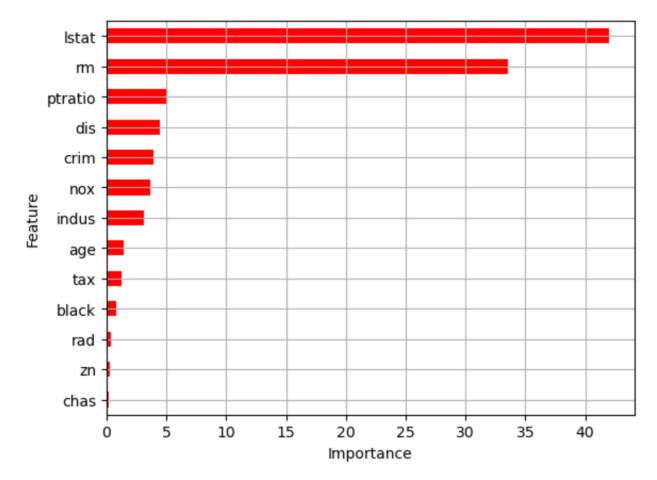
1	24.939713	7	11.886289
2	17.200655	8	12.210822
3	13.943997	9	12.199773
4	12.930648	10	12.200606
5	12.871667	11	12.260297
6	12.339600	12	12.328083
		13	12.391338

### **Test MSE**

17.31901376537634

```
# similar to Bagging Test MSE
```

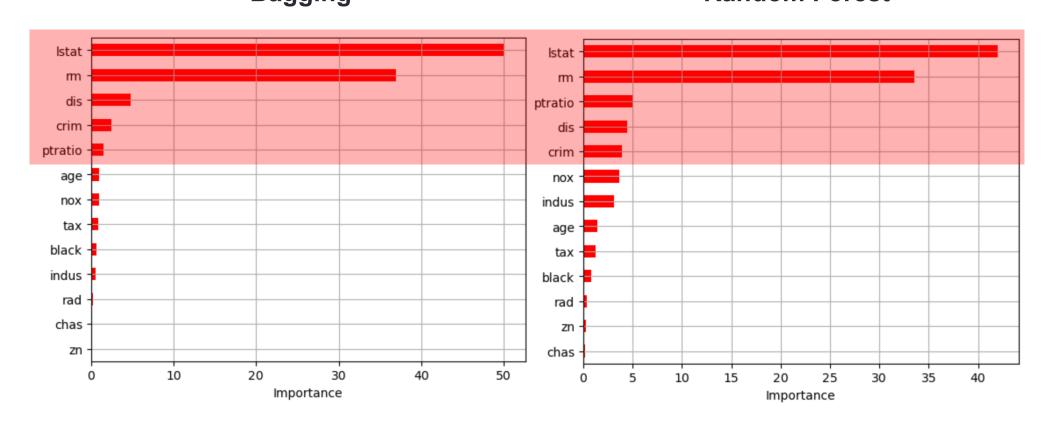
## Feature Importance – Random Forest



The wealth level of the community ('Istat') and the house size ('rm') are the 2 most important predictors

# Feature Importance





Both models agree on the best 5 predictors



## Gradient Boosting Trees - learning\_rate

### learning\_rate to 0.10

### learning\_rate to 0.40

16.580039404288993

### GridSearchCV on the learning\_rate

```
X train, X test, y train, y test = train test split(X, y, train size=0.5,
                                                  random_state=0)
                                                              ← try these learning rates
lrates = np.linspace(0.01,1,20)
lrates
array([0.01
                 , 0.06210526, 0.11421053, 0.16631579, 0.21842105,
       0.27052632, 0.32263158, 0.37473684, 0.42684211, 0.47894737,
       0.53105263, 0.58315789, 0.63526316, 0.68736842, 0.73947368,
       0.79157895, 0.84368421, 0.89578947, 0.94789474, 1.
                                                           use the sklearn parameter name
params = dict(learning_rate = lrates)
params
{'learning_rate': array([0.01 , 0.06210526, 0.11421053, 0.16631579, 0.21842105,
        0.27052632, 0.32263158, 0.37473684, 0.42684211, 0.47894737,
        0.53105263, 0.58315789, 0.63526316, 0.68736842, 0.73947368,
        0.79157895, 0.84368421, 0.89578947, 0.94789474, 1.
                                                                   1)}
```

## GridSearchCV on the learning rate

```
model = GradientBoostingRegressor(n_estimators = 500,
                                   max_depth = 4,
                                   random state=1)
grid1 = GridSearchCV(model,param_grid = params,
                    scoring = 'neg mean squared error', cv = 5)
grid1.fit(X train,y train);
grid1.best_params_
{'learning_rate': 0.11421052631578947}
-grid1.score(X_test,y_test)
                                                    ← Test MSE
```

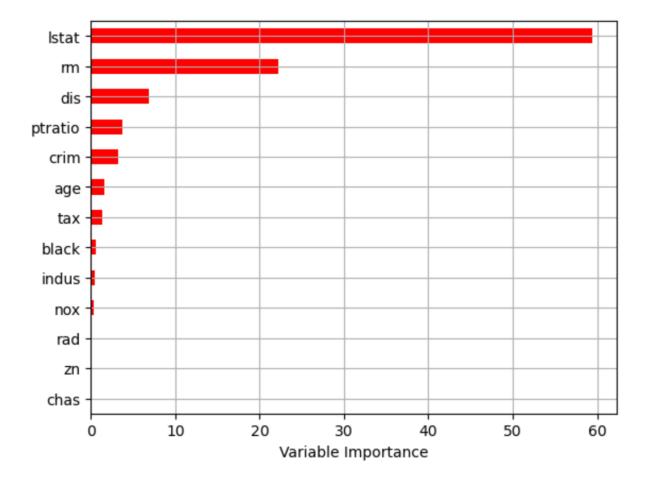
17.525614916769054

## GridSearchCV on the learning\_rate

```
# Refine params values
                                                    ← now try these learning rates
lrates = np.linspace(0.05, 0.15, 20)
params = dict(learning_rate = lrates)
lrates
array([0.05 , 0.05526316, 0.06052632, 0.06578947, 0.07105263,
       0.07631579, 0.08157895, 0.08684211, 0.09210526, 0.09736842,
       0.10263158, 0.10789474, 0.11315789, 0.11842105, 0.12368421,
       0.12894737, 0.13421053, 0.13947368, 0.14473684, 0.15
grid2 = GridSearchCV(model,param_grid = params,
                    scoring = 'neg mean squared error', cv = 5)
grid2.fit(X train,y train);
grid2.best_params_
{'learning rate': 0.10263157894736842}
-grid2.score(X_test,y_test)
                                                        ← Test MSE
16.879372503369037
```

### Feature Importance – Gradient Boosting

```
Importance2 = grid2.best_estimator_.feature_importances_*100
Importance2 = pd.DataFrame({'Importance':Importance2},index = X.columns)
df9 = Importance2.sort_values(by = 'Importance',axis = 0,ascending = True)
df9.plot(kind = 'barh',color = 'r',legend = False)
```



The wealth level of the community ('Istat') and the house size ('rm') are the 2 most important predictors

### GridSearchCV on learning\_rate and max\_features

```
# Consider 6 values for each parameter
params = {'learning_rate': np.linspace(0.01,1,6),
              'max features': list(range(3,9))}
params
{'learning_rate': array([0.01 , 0.208, 0.406, 0.604, 0.802, 1.
                                                                  1).
 'max_features': [3, 4, 5, 6, 7, 8]}
model = GradientBoostingRegressor(n estimators = 500,
                                  max_depth = 4,
                                  random state=1)
grid1 = GridSearchCV(model,param_grid = params,
                    scoring = 'neg mean squared error',cv = 5)
grid1.fit(X train,y train);
grid1.best_params_
{'learning rate': 0.2080000000000002, 'max features': 6}
```

df1 = pd.DataFrame(grid1.cv\_results\_)

0.000010

0.000904

mean_score_time	std_score_time	param_learning_rate	param_max_features
0.001017	0.000075	0.01	3
0.001019	0.000030	0.01	4
0.001120	0.000120	0.01	5
0.001040	0.000090	0.01	6
0.000947	0.000008	0.01	7
0.001069	0.000097	0.01	8

0.208

mean_test_score	sta_test_score	rank_test_score
-11.615787	4.872017	6
-11.435279	5.473211	3
-11.159788	4.803937	2
-11.556346	5.215419	4
-11.891890	5.843181	7
-12.263327	6.333880	9

7.018744

12

-12.377763

Validation MSE

```
params
{'learning_rate': array([0.01 , 0.208, 0.406, 0.604, 0.802, 1. ]),
   'max_features': [3, 4, 5, 6, 7, 8]}
```

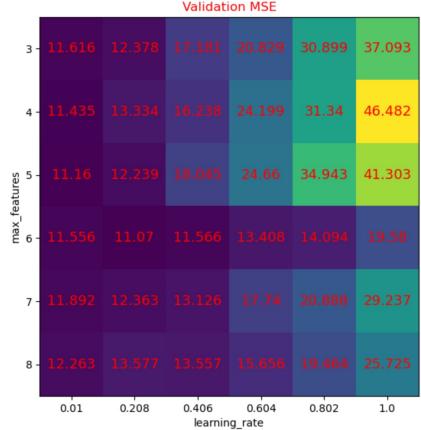
```
df2 = df1.iloc[:,[4,5,12]].copy()
df2.mean_test_score = -df2.mean_test_score
df2[:9]
```

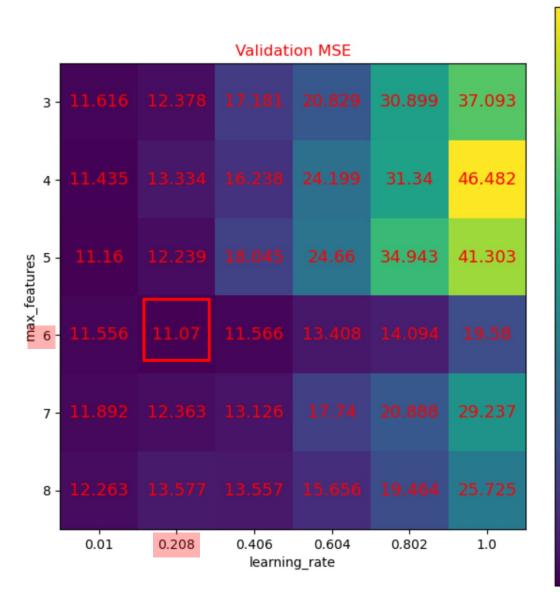
df2[-9:]

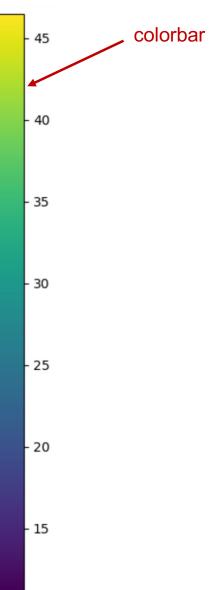
	param_learning_rate	param_max_features	mean_test_score		param_learning_rate	param_max_features	mean_test_score
0	0.01	3	11.615787	27	0.802	6	14.094091
1	0.01	4	11.435279	28	0.802	7	20.887565
2	0.01	5	11.159788	29	0.802	8	19.463552
3	0.01	6	11.556346	30	1.000	3	37.093306
4	0.01	7	11.891890	31	1.000	4	46.481536
5	0.01	8	12.263327	32	1.000	5	41.303353
6	0.208	3	12.377763	33	1.000	6	19.580221
7	0.208	4	13.334128	34	1.000	7	29.236760
8	0.208	5	12.239297	35	1.000	8	25.724720

param_learning_rate	0.010	0.208	0.406	0.604	0.802	1.000
param_max_features						
3	11.615787	12.377763	17.180822	20.829473	30.899405	37.093306
4	11.435279	13.334128	16.238018	24.198933	31.339964	46.481536
5	11.159788	12.239297	18.045442	24.659544	34.942586	41.303353
6	11.556346	11.070416	11.565877	13.408052	14.094091	19.580221
7	11.891890	12.363371	13.125690	17.740055	20.887565	29.236760
8	12.263327	13.577059	13.556925	15.655501	19.463552	25.724720

param_learning_rate	0.010	0.208	0.406	0.604	0.802	1.000
param_max_features						
3	11.615787	12.377763	17.180822	20.829473	30.899405	37.093306
4	11.435279	13.334128	16.238018	24.198933	31.339964	46.481536
5	11.159788	12.239297	18.045442	24.659544	34.942586	41.303353
6	11.556346	11.070416	11.565877	13.408052	14.094091	19.580221
7	11.891890	12.363371	13.125690	17.740055	20.887565	29.236760
8	12.263327	13.577059	13.556925	15.655501	19.463552	25.724720







### **Test MSE**

15.688938784290462

### **Test MSE**

```
model = GradientBoostingRegressor(n_estimators = 500,
                                   \max features = 6,
                                   max depth = 4,
                learning_rate = 0.208000000000000002,
                                   random_state=1)
model.fit(X_train,y_train)
pred2 = model.predict(X test)
mean squared error(y test,pred2)
15.688938784290462
-grid1.score(X test, y test)
15.688938784290462
model = GradientBoostingRegressor(n estimators = 500,
                                   max features = 6,
                                   max_depth = 4,
                                   learning_rate = 0.208,
                                   random_state=1)
model.fit(X train,y train)
pred2 = model.predict(X test)
mean squared error(y test,pred2)
                                            ← Best Test MSF
15.127755055051313
```