Learning Objectives

At the end of the experiment, you will be able to

- understand various boosting methods
- implement AdaBoost, Gradient Boosting and Extreme Gradient Boosting
- implement stacking algorithm

Boosting

Boosting is a general ensemble method that creates a strong model from a number of weak learners.

This is done by building a model from the training data, then creating a second model that attempts to correct the errors from the first model. Models are added until the training set is predicted perfectly or a maximum number of models are added.

There are many boosting methods available, but by far the most popular are AdaBoost (short for Adaptive Boosting) and Gradient Boosting.

AdaBoost

One way for a new predictor to correct its predecessor is to pay a bit more attention to the training instances that the predecessor underfitted. This results in new predictors focusing more and more on the hard cases. This is the technique used by AdaBoost. For example, to build an AdaBoost classifier, a first base classifier (such as a Decision Tree) is trained and used to make predictions on the training set. The relative weight of misclassified training instances is then increased. A second classifier is trained using the updated weights and again it makes predictions on the training set, weights are updated, and so on

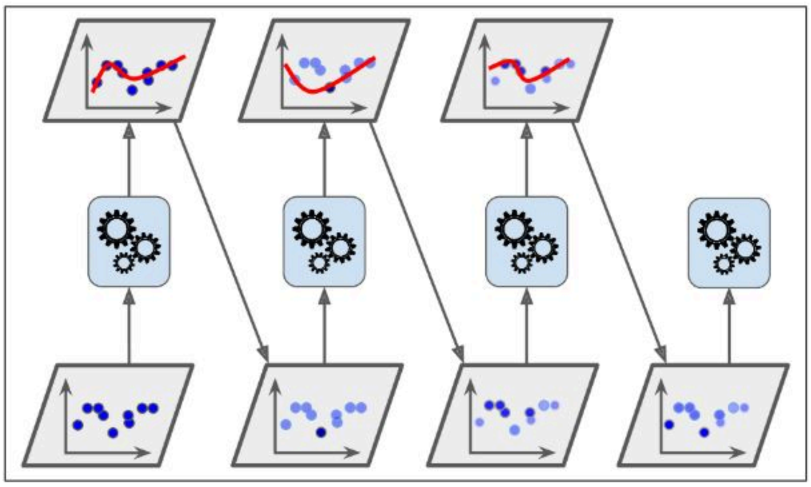

Figure 1: AdaBoost sequential training with instance weight updates

Gradient Boosting

Gradient boosting is known to be one of the leading ensemble algorithms. Gradient boosting algorithm uses gradient descent method to optimize the loss function.

Just like AdaBoost, Gradient Boosting works by sequentially adding predictors to an ensemble, each one correcting its predecessor. However, instead of tweaking the instance weights at every iteration just like AdaBoost does, this method tries to fit the new predictor to the residual errors made by the previous predictor.

A simpler way to train the gradient boosting regression trees ensemble technique is to use Scikit-Learn's Gradient Boosting Regressor class. Much like the Random Forest Regressor class, it has hyperparameters to control the growth of Decision Trees (e.g., max_depth, min_samples_leaf, and so on), as well as hyperparameters to control the ensemble training, such as the number of trees (n_estimators).

How boosting is accomplished?

- Iteratively learning a set of weak models on subsets of the data
- Weighting each weak prediction according to each weak learner's performance
- Combine the weighted predictions to obtain a single weighted prediction

- that is much better than the individual predictions themselves!

Here is a list of essential components required by Gradient Boosting Algorithms:

Additive Model

We try to minimize losses by implementing more decision trees. We can also diminish the error rates by minimizing the parameters. In cases like these, we create the model to ensure there are no changes to the existing tree despite the addition of another one.

Weak Learner

Weak learners are an essential part of gradient boosting for making predictions. We utilize regression trees to extract authentic values. It is essential to develop trees greedily to arrive at the most favorable split point. It is a significant reason why the model mostly overfits the specific dataset.

Loss Function

We must optimize loss functions to reduce prediction-related errors. Contrary to Ada Boost, the wrong result does not receive an increased weight in gradient boosting. Instead, it minimizes the loss function from weak learners by obtaining output averages.

Setup Steps:

Import required packages

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
# Import support vector regressor algorithm
from sklearn.svm import SVR
from sklearn.linear_model import Ridge, Lasso
from sklearn.preprocessing import StandardScaler, LabelEncoder
# Import modelling methods
from sklearn.model_selection import train_test_split, RepeatedStratifiedKFold, cross_val_score
# Import the model performance evaluation metrics
from sklearn import metrics
# Import Adaboost, Gradient Boost, Random Forest and Stacking algorithm
from sklearn.ensemble import AdaBoostClassifier, GradientBoostingRegressor, RandomForestRegressor, StackingRegressor
import warnings
warnings.filterwarnings('ignore')
from sklearn.tree import DecisionTreeClassifier, plot_tree
from sklearn.datasets import fetch_california_housing   # to import boston housing dataset
# to visualize decision boundaries
import graphviz
import xgboost as xgb
from xgboost import XGBRegressor
```

Define the AdaBoost classifier

Let’s take a closer look at the AdaBoost algorithm. Each instance weight $w^{(i)}$ is initially set to $\frac{1}{m}$. A first predictor is trained and its weighted error rate r_1 is computed on the training set

Equation 1: Weighted error rate of the j^{th} predictor

$$r_j = \frac{\sum_{\substack{i=1 \\ \hat{y_j^i} \neq y^i}}^{m} w^i}{\sum_{i=1}^{m} w^i}$$

where $\hat{y_j^i}$ is the j^{th} predictor’s prediction for the i^{th} instance.

The predictor’s weight α_j is then computed using Equation 2, where η is the learning rate hyperparameter. The more accurate the predictor is, the higher its weight will be. If it is just guessing randomly, then its weight will be close to zero. However, if it is most often wrong (i.e., less accurate than random guessing), then its weight will be negative.

Equation 2: Predictor weight

$$\alpha_j = \eta \log \frac{1-r_j}{r_J}$$

Next, the instance weights are updated using Equation 3: the misclassified instances are boosted.

Equation 3: Weight update rule

for $i = 1, 2, \cdots, m$

$$w^{(i)} \leftarrow \begin{cases} w^{(i)} & if\ \hat{y}_j^{(i)} = y^{(i)} \\ w^{(i)} \exp(a_j) & if\ \hat{y}_j^{(i)} \neq y^{(i)} \end{cases}$$

Then all the instance weights are normalized (i.e., divided by $\sum_{i=1}^{m} w_i$).

Finally, a new predictor is trained using the updated weights, and the whole process is repeated (the new predictor's weight is computed, the instance weights are updated, then another predictor is trained, and so on). The algorithm stops when the desired number of predictors is reached, or when a perfect predictor is found. To make predictions, AdaBoost simply computes the predictions of all the predictors and weighs them using the predictor weights α_j. The predicted class is the one that receives the majority of weighted votes (see Equation 4).

Equation 4: AdaBoost predictions

$$\hat{y}(X) = \underset{k}{\operatorname{argmax}} \sum_{\substack{j=1 \\ \hat{y}_j(X)=k}}^{N} \alpha_j$$ Where N is the number of predictors.

In the following exercises, we will use the [Indian Liver Patient] dataset. The task is to predict whether a patient suffers from a liver disease using 10 features including Albumin, age, and gender. We will be training an AdaBoost ensemble to perform the classification task. In addition, given that this dataset is imbalanced, we will be using the ROC AUC score as a metric instead of accuracy.

As a first step, we will start by instantiating an AdaBoost classifier.

```
df = pd.read_csv('indian_liver_patient.csv')
df.head()
```

	Age	Gender	Total_Bilirubin	Direct_Bilirubin	Alkaline_Phosphotase	Alamine_Aminotransferase	Aspartate_Aminotransferase	Total
0	65	Female	0.7	0.1	187	16	18	
1	62	Male	10.9	5.5	699	64	100	
2	62	Male	7.3	4.1	490	60	68	
3	58	Male	1.0	0.4	182	14	20	
4	72	Male	3.9	2.0	195	27	59	

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Preprocessing

```
# Check for missing values
df.isnull().sum()
```

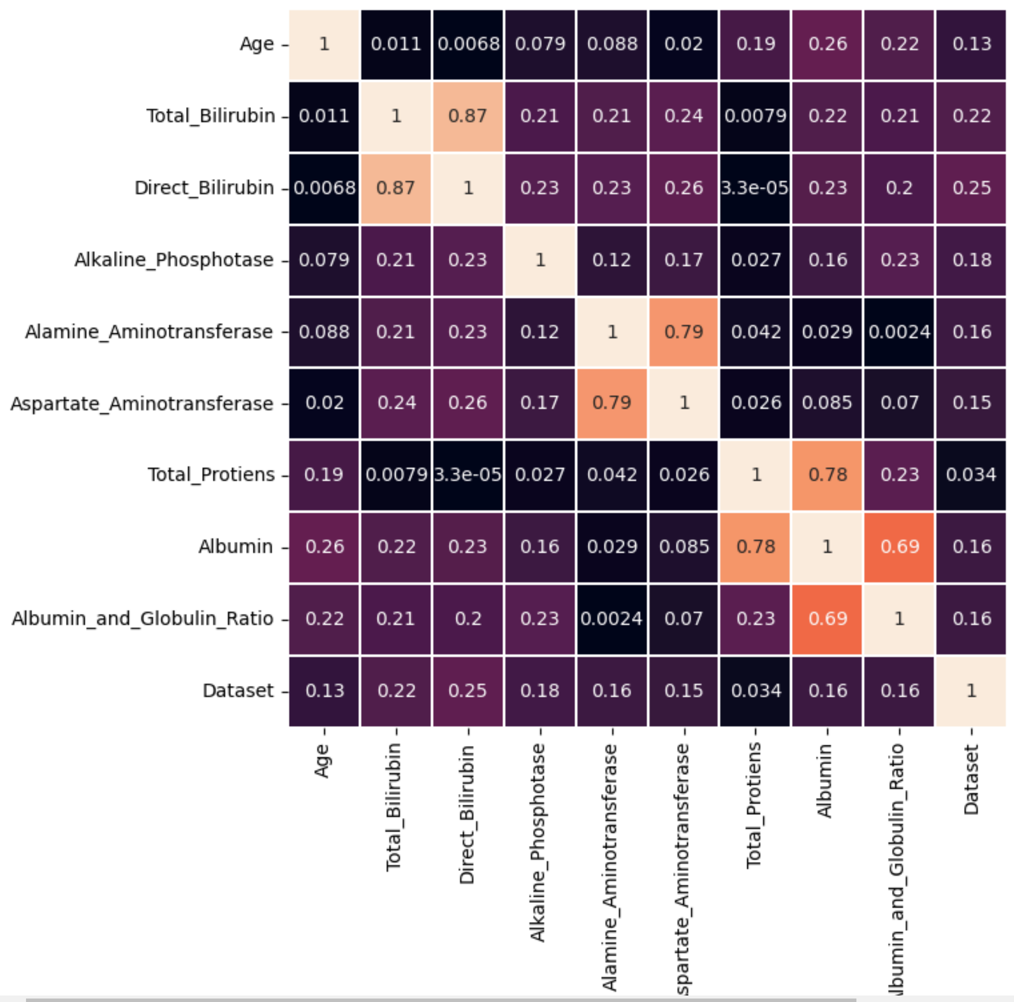
	0
Age	0
Gender	0
Total_Bilirubin	0
Direct_Bilirubin	0
Alkaline_Phosphotase	0
Alamine_Aminotransferase	0
Aspartate_Aminotransferase	0
Total_Protiens	0
Albumin	0
Albumin_and_Globulin_Ratio	4
Dataset	0

```
# Drop missing values
df1 = df.dropna()
df1.isnull().any()
```

	0
Age	False
Gender	False
Total_Bilirubin	False
Direct_Bilirubin	False
Alkaline_Phosphotase	False
Alamine_Aminotransferase	False
Aspartate_Aminotransferase	False
Total_Protiens	False
Albumin	False
Albumin_and_Globulin_Ratio	False
Dataset	False

Now, we plot a correlation matrix and see how the attributes are correlated to each other.

```
# Visualize correlation matrix
numeric_df = df1.select_dtypes(include=['number'])
fig, ax = plt.subplots(figsize=(7,7))
sns.heatmap(abs(numeric_df.corr()), annot=True, square=True, cbar=False, ax=ax, linewidths=0.25);
```



```
# Drop correlated features
df2 = df1.drop(columns= ['Direct_Bilirubin', 'Alamine_Aminotransferase', 'Total_Protiens'])
```

As we can see there is a correlation between

- *Total_Bilirubin* and *Direct_Bilirubin*
- *Alamine_Aminotransferase* and ^Aspartate_Aminotransferase*

- *Total_Protiens* and *Albumin*

The features we drop from data are: *Direct_Bilirubin*, *Alamine_Aminotransferase* and *Total_Protiens*.

There is only one column *Gender* of categorical type and remaining below are continuous data.

- Age
- Total_Bilirubin
- Alkaline_Phosphotase
- Aspartate_Aminotransferase
- Albumin
- Albumin_and_Globulin_Ratio

```
df2['Dataset'] = df2['Dataset'].replace(1,0)
df2['Dataset'] = df2['Dataset'].replace(2,1)
print(df2.columns)
```

```
Index(['Age', 'Gender', 'Total_Bilirubin', 'Alkaline_Phosphotase',
       'Aspartate_Aminotransferase', 'Albumin', 'Albumin_and_Globulin_Ratio',
       'Dataset'],
      dtype='object')
```

Now, we will segregate the disease according to gender and total people who participated in this study.

```
print('How many people have disease:', '\n', df2.groupby('Gender')[['Dataset']].sum(), '\n')
print('How many people participated in the study:', '\n', df2.groupby('Gender')[['Dataset']].count())
```

```
How many people have disease:
          Dataset
Gender
Female        49
Male         116

How many people participated in the study:
          Dataset
Gender
Female       140
Male         439
```

Now, we will see the percentage of male and female having disease.

```
print('Percentage of people with the disease depending on gender:')
df2.groupby('Gender')[['Dataset']].sum()/ df2.groupby('Gender')[['Dataset']].count()
```

```
Percentage of people with the disease depending on gender:
          Dataset
Gender
Female   0.350000
```

Women have a higher percentage of the disease, so we will conduct a separate study, depending on the gender of the person.

```
# defining the X and y variables
X = df2[['Gender', 'Total_Bilirubin','Alkaline_Phosphotase','Aspartate_Aminotransferase','Albumin','Albumin_and_Globulin_Ratio']]
y = pd.Series(df2['Dataset'])
```

We will apply label encoding for categorical data (Gender).

```
labelencoder = LabelEncoder()
X['Gender'] = labelencoder.fit_transform(X['Gender'])
```

Now, we will split the data into training and testing datasets. After, that we scale the data.

```
x_train, x_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
scaler = StandardScaler()
X_train = scaler.fit_transform(x_train)
X_test = scaler.transform(x_test)
```

Train the model Using AdaBoost Classifier

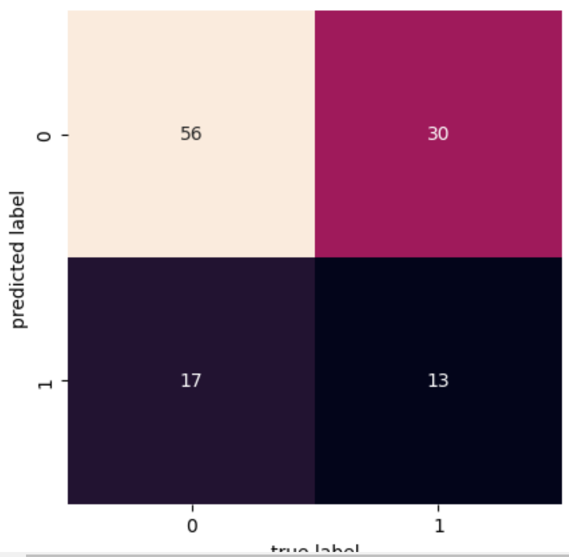
```
ADB = AdaBoostClassifier(DecisionTreeClassifier(max_depth=2),
                         n_estimators=125,
                         learning_rate = 0.6,
                         random_state=42)

ADB.fit(X_train, y_train)
cv = RepeatedStratifiedKFold(n_splits=10, n_repeats=3, random_state=1)
```

Repeated k-fold cross-validation provides a way to improve the estimated performance of a machine learning model. This involves simply repeating the cross-validation procedure multiple times and reporting the mean result across all folds from all runs. This mean result is expected to be a more accurate estimate of the true unknown underlying mean performance of the model on the dataset, as calculated using the standard error.

```
# calculating model evaluation metrics using cross_val_score like accuracy, R2 score, etc.
n_scores = cross_val_score(ADB, X, y, scoring='accuracy', cv=cv, n_jobs=-1, error_score='raise')
('Accuracy: %.3f' % (np.mean(n_scores)*100))
```

Create a Confusion Matrix

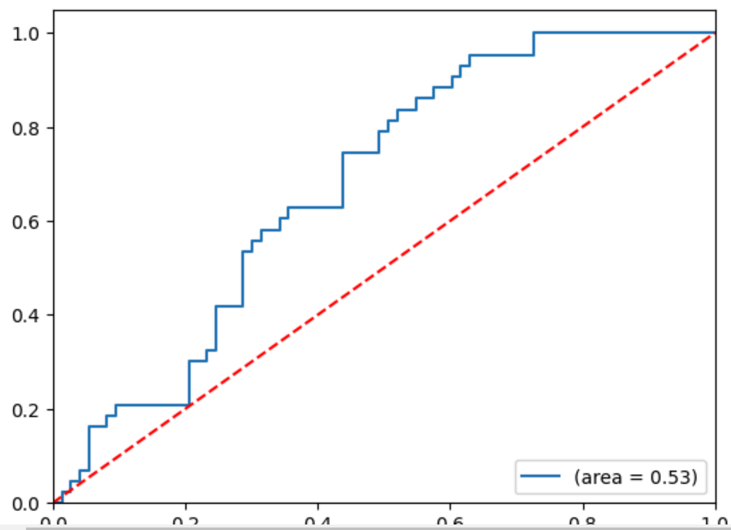
```
labels = ADB.predict(X_test)
matrix = metrics.confusion_matrix(y_test, labels)
# creating a heat map to visualize confusion matrix
sns.heatmap(matrix.T, square=True, annot=True, fmt='d', cbar=False)
plt.xlabel('true label')
plt.ylabel('predicted label');
```



From the above plot of the confusion matrix, we can say that the AdaBoost classifier model predicts 56 'no disease' and 13 'with disease' values correctly.

Now, we plot ROC and AUC curve for the predictions.

```
logit_roc_auc = metrics.roc_auc_score(y_test, labels)
fpr, tpr, thresholds = metrics.roc_curve(y_test, ADB.predict_proba(X_test)[:,1])
plt.figure()
plt.plot(fpr, tpr, label='(area = %0.2f)' % logit_roc_auc)
plt.plot([0, 1], [0, 1],'r--')
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.legend(loc="lower right")
plt.savefig('Log_ROC')
plt.show()
```



So, we get an Area under the curve value (AUC) of 0.53.

When we need to check or visualize the performance of the multi-class classification problem, we use the AUC (Area Under The Curve) ROC (Receiver Operating Characteristics) curve. It is one of the most important evaluation metrics for checking any classification model's performance.

To know more about AUC-ROC, click here.

Gradient Boosting Implementation

We use Boston house-price dataset as a regression dataset in this example. After loading the dataset, first, we will separate data into x and y parts.

```
boston = fetch_california_housing()
print(boston.keys())
print("shape of dataset",boston.data.shape)
```

```
dict_keys(['data', 'target', 'frame', 'target_names', 'feature_names', 'DESCR'])
shape of dataset (20640, 8)
```

As we can see it returned (506, 13), that means there are 506 rows of data with 13 columns. Now, if we want to know what the 13 columns are, we can simply use the `.feature_names` attribute and it will return the feature names.

```
print(boston.feature_names)
```

```
['MedInc', 'HouseAge', 'AveRooms', 'AveBedrms', 'Population', 'AveOccup', 'Latitude', 'Longitude']
```

Now let's convert it into a pandas DataFrame.

```
df = pd.DataFrame(boston.data)
df.columns = boston.feature_names
```

Explore the top 5 rows of the dataset by using head() method.

```
df.head()
```

	MedInc	HouseAge	AveRooms	AveBedrms	Population	AveOccup	Latitude	Longitude
0	8.3252	41.0	6.984127	1.023810	322.0	2.555556	37.88	-122.23
1	8.3014	21.0	6.238137	0.971880	2401.0	2.109842	37.86	-122.22
2	7.2574	52.0	8.288136	1.073446	496.0	2.802260	37.85	-122.24
3	5.6431	52.0	5.817352	1.073059	558.0	2.547945	37.85	-122.25
4	3.8462	52.0	6.281853	1.081081	565.0	2.181467	37.85	-122.25

Next steps: Generate code with df View recommended plots New interactive sheet

Here, we will notice that there is no column called `PRICE` in the DataFrame. This is because the target column is available in another attribute called `boston.target`. Append `boston.target` to the pandas DataFrame.

```
df['PRICE'] = boston.target
```

Now, we will run the `.info()` method on our DataFrame to get useful information about the data.

```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 20640 entries, 0 to 20639
Data columns (total 9 columns):
 #   Column      Non-Null Count  Dtype  
---  ------      --------------  -----  
 0   MedInc      20640 non-null  float64
 1   HouseAge    20640 non-null  float64
 2   AveRooms    20640 non-null  float64
 3   AveBedrms   20640 non-null  float64
 4   Population  20640 non-null  float64
 5   AveOccup    20640 non-null  float64
 6   Latitude    20640 non-null  float64
 7   Longitude   20640 non-null  float64
 8   PRICE       20640 non-null  float64
dtypes: float64(9)
memory usage: 1.4 MB
```

Separate the target variable and rest of the variables using .iloc to subset the data.

```
X, y = df.iloc[:,:-1],df.iloc[:,-1]
```

```
xtrain, xtest, ytrain, ytest=train_test_split(X, y, random_state=12, test_size=0.15)
```

Defining the model

We can define the model with its default parameters or set the new parameter values.

```
# with new parameters
gbr1 = GradientBoostingRegressor(alpha=0.9, criterion='friedman_mse', n_estimators=600,
    max_depth=5,
    learning_rate=0.01,
    min_samples_split=4)
# with default parameters
gbr = GradientBoostingRegressor()
```

Fit the model with default parameters and predict the data

```
# fit with default parameters
gbr.fit(xtrain, ytrain)

ypred = gbr.predict(xtest)

# calculating Mean Squared Error
mse = metrics.mean_squared_error(ytest,ypred)
# mse for default model
print("MSE: %.2f" % mse)
```

```
MSE: 0.27
```

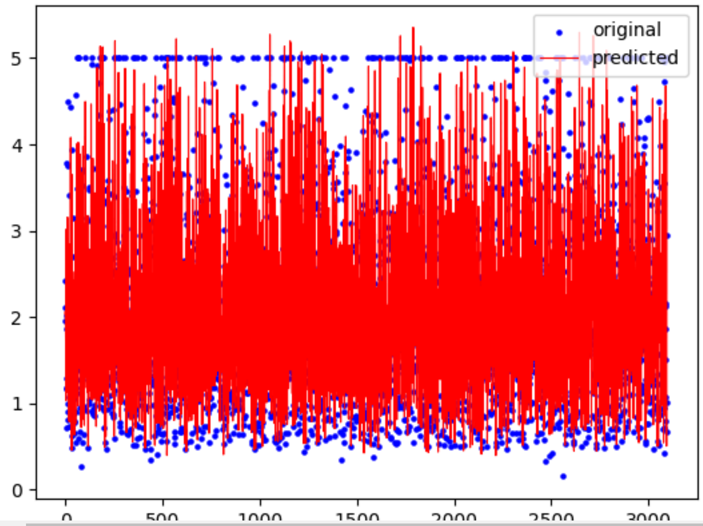
Fit the model by passing parameters and predict the data

```
# fit by passing hyperparameters
gbr1.fit(xtrain, ytrain)

ypred1 = gbr1.predict(xtest)
# calculating Mean Squared Error
mse1 = metrics.mean_squared_error(ytest, ypred1)

# mse for regularized model
print("MSE: %.2f" % mse1)
```

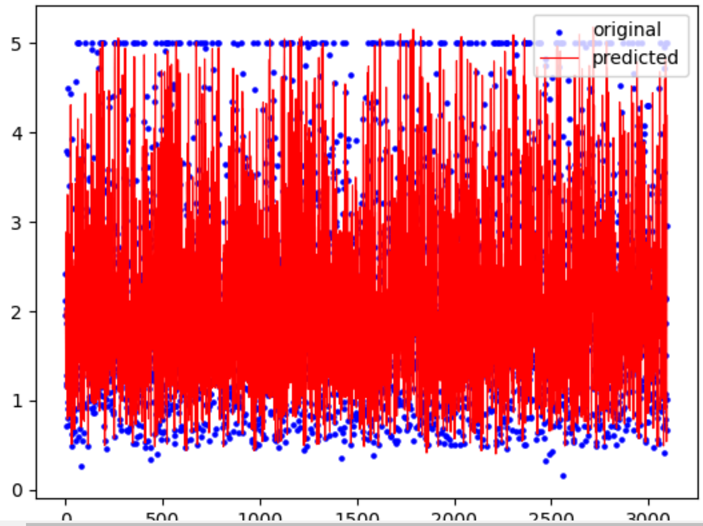
```
MSE: 0.24
```

Finally, we will visualize the actual and predicted values in a plot for both models.

```
x_ax = range(len(ytest))
plt.scatter(x_ax, ytest, s=5, color="blue", label="original")
plt.plot(x_ax, ypred, lw=0.8, color="red", label="predicted")
plt.legend()
plt.show()
```



```
x_ax = range(len(ytest))
plt.scatter(x_ax, ytest, s=5, color="blue", label="original")
plt.plot(x_ax, ypred1, lw=0.8, color="red", label="predicted")
plt.legend()
plt.show()
```



From the above plots, we can see that the mean square error is less for the regularized model than the default model.

Implementation of XGBoost

An optimized implementation of Gradient Boosting is available in the popular python library `XGBoost`, which stands for Extreme Gradient Boosting. This package aims at being extremely fast, scalable, and portable. In fact, XGBoost is often an important component of winning entries in ML competitions. XGBoost's API is quite similar to Scikit-Learn's:

Here, we also going to import the Boston Housing dataset and store it in a variable called boston.

The next step is to instantiate an `XGBoost regressor` object by calling the `XGBRegressor()` class from the `XGBoost` library with the hyper-parameters passed as arguments. For classification problems, we would have used the `XGBClassifier()` class.

```
xgb_reg = xgb.XGBRegressor(objective ='reg:linear', colsample_bytree = 0.3, learning_rate = 0.1,
                           max_depth = 5, alpha = 10, n_estimators = 10)
```

Now, we will create the train and test set for cross-validation of the results using the `train_test_split` function from sklearn's `model_selection` module with `test_size` size equal to 20% of the data. Also, to maintain the reproducibility of the results, a random_state is also assigned.

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=123)
```

```
xgb_reg.fit(X_train,y_train)
```

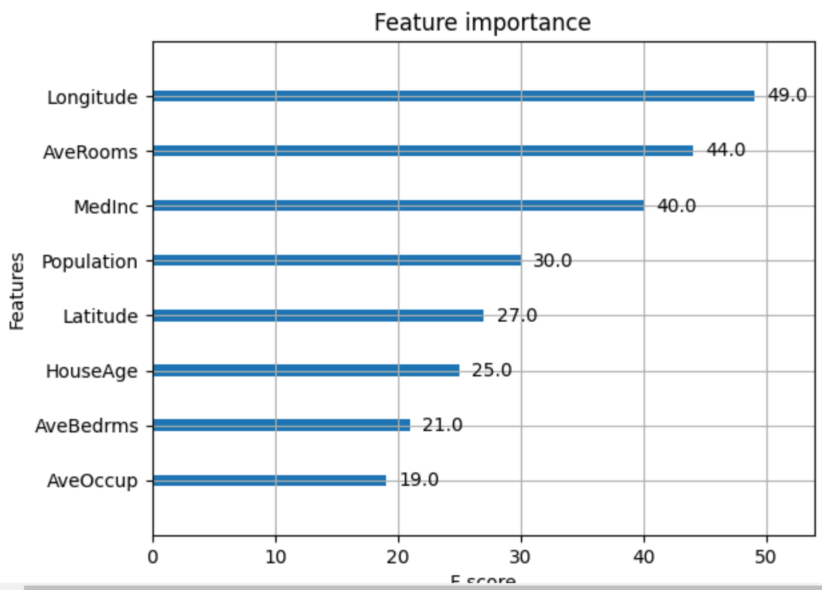
```
y_pred = xgb_reg.predict(X_test)
```

```
mse2 = metrics.mean_squared_error(y_test, y_pred)
print("MSE: %f" % (mse))
```

```
MSE: 0.270435
```

Plotting the `feature importance` graph with the matplotlib library:

```
xgb.plot_importance(xgb_reg)
plt.rcParams['figure.figsize'] = [5, 5]
plt.show()
```



As we can see the feature `LSTAT` and `RM` have been given the highest importance score among all the features. Thus XGBoost also gives us a way to do Feature Selection.

To know more about XGboost, click here.

Stacking (Optional)

The overall idea of the stacking ensemble method is to train several models with different algorithm types (i.e. base-learners), on the train data, and then aggregate all the models using another model (meta learner), to make the final prediction. The inputs for the meta-learner are the prediction outputs of the base-learners.

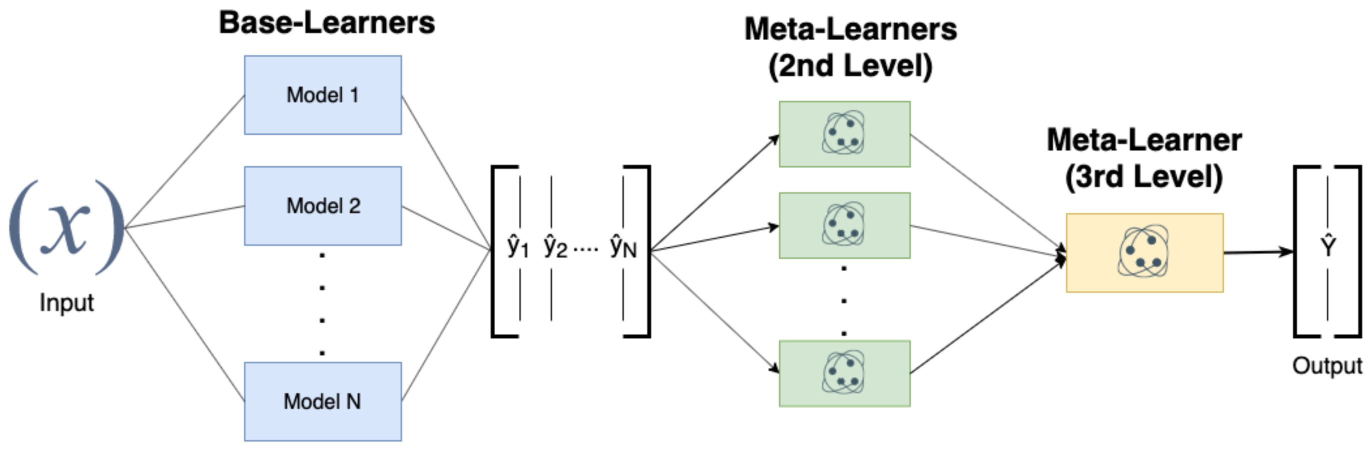


Figure 2: Predictions in a multilayer stacking ensemble

For a given input data point, we pass it through the M base-learners and get M number of predictions, and send those M predictions through the meta-learner as inputs and obtain the final prediction.

Here, we again look at the Boston housing dataset and try to build a regressor model using the stacking method.

Stacking Models

We assume no hyperparameters for the stacking – this means that we use the predefined hyperparameters for each model.

```
xgb = XGBRegressor()
rf = RandomForestRegressor(n_estimators=400, max_depth=5, max_features=6)
ridge = Ridge()
lasso = Lasso()
svr = SVR(kernel='rbf')
```

```
print("X_train columns:", X_train.columns)
print("X_test columns:", X_test.columns)
X_train.columns = X_test.columns
print("X_train columns:", X_train.columns)
print("X_test columns:", X_test.columns)
```

```
X_train columns: Index(['MedInc', 'HouseAge', 'AveRooms', 'AveBedrms', 'Population', 'AveOccup',
       'Latitude', 'Longitude'],
      dtype='object')
X_test columns: Index(['MedInc', 'HouseAge', 'AveRooms', 'AveBedrms', 'Population', 'AveOccup',
       'Latitude', 'Longitude'],
      dtype='object')
X_train columns: Index(['MedInc', 'HouseAge', 'AveRooms', 'AveBedrms', 'Population', 'AveOccup',
       'Latitude', 'Longitude'],
      dtype='object')
X_test columns: Index(['MedInc', 'HouseAge', 'AveRooms', 'AveBedrms', 'Population', 'AveOccup',
       'Latitude', 'Longitude'],
      dtype='object')
```

Now that we have defined all our models, we can begin improving our results by stacking some models. As we can see here, we defined two levels, where the first level has 5 models, and the second level has the meta-learner.

```
estimators = [('ridge', ridge), ('svr', svr), ('rf', rf), ('lasso', lasso)]
reg = StackingRegressor(estimators=estimators,final_estimator=xgb)
# fit the model
reg.fit(X_train, y_train)
#X_test.columns = ['f0', 'f1', 'f2', 'f3', 'f4', 'f5', 'f6', 'f7']
pred = reg.predict(X_test)
```

```
score = metrics.r2_score(y_test, pred)
print(score)
```

```
0.723691663391
```

Theory Questions

1. If your AdaBoost ensemble underfits the training data, what hyperparameters should you tweak and how?

If your AdaBoost ensemble underfits the training data, you can try increasing the number of estimators or reducing the regularization hyperparameters of the base estimator. You may also try slightly increasing the learning rate.

2. If your Gradient Boosting ensemble overfits the training set, should you increase or decrease the learning rate?

   If your Gradient Boosting ensemble overfits the training set, you should try decreasing the learning rate. You could also use early stopping to find the right number of predictors (you probably have too many).

Please answer the questions below to complete the experiment:

Select the False Statement:

`Answer:`

Show code

How was the experiment?

`Complexity:`

Show code

If it was too easy, what more would you have liked to be added? If it was very difficult, what would you have liked to have been removed?

`Additional:` " Insert text here "

Show code

Can you identify the concepts from the lecture which this experiment covered?

`Concepts:`

Show code

Text and image description/explanation and code comments within the experiment:

`Comments:`

Show code