Statistical Machine Learning with Python Week #3

Ching-Shih Tsou (Ph.D.), Distinguished Prof. at the Department of Mechanical Engineering/Director of the Center for Artifical Intelligence & Data Science, Ming Chi University of Technology

September/2020 at MCUT

Collecting Data

- First of all, just like what you do with any other case, you are going to import the Boston Housing dataset and store it in a variable called boston. To import it from scikit-learn you will need to run this snippet.

```
from sklearn.datasets import load_boston
boston = load_boston()
```

- The boston variable itself is a dictionary, so you can check for its keys using the .keys() method.

```
print(type(boston))
```

```
## <class 'sklearn.utils.Bunch'>
```

```
print(boston.keys())
```

```
## dict_keys(['data', 'target', 'feature_names', 'DESCR', 'filename'])
```

- You can easily check for its shape by using the boston.data.shape attribute, which will return the size of the dataset.

```
print(boston.data.shape)
```

```
## (506, 13)
```

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

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

```
## ['CRIM' 'ZN' 'INDUS' 'CHAS' 'NOX' 'RM' 'AGE' 'DIS' 'RAD' 'TAX' 'PTRATIO'
##  'B' 'LSTAT']
```

- The description of the dataset is available in the dataset itself. You can take a look at it using .DESCR.

```
print(boston.DESCR)
```

```
## .. _boston_dataset:
##
## Boston house prices dataset
## ---------------------------
##
## **Data Set Characteristics:**
##
##     :Number of Instances: 506
##
##     :Number of Attributes: 13 numeric/categorical predictive. Median Value
(attribute 14) is usually the target.
##
##     :Attribute Information (in order):
##         - CRIM     per capita crime rate by town
##         - ZN       proportion of residential land zoned for lots over 25,00
0 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
##         - B        1000(Bk - 0.63)^2 where Bk is the proportion of blacks b
y town
##         - LSTAT    % lower status of the population
##         - MEDV     Median value of owner-occupied homes in $1000's
##
##     :Missing Attribute Values: None
##
##     :Creator: Harrison, D. and Rubinfeld, D.L.
##
## This is a copy of UCI ML housing dataset.
## https://archive.ics.uci.edu/ml/machine-learning-databases/housing/
##
##
## This dataset was taken from the StatLib library which is maintained at Carn
egie Mellon University.
##
## The Boston house-price data of Harrison, D. and Rubinfeld, D.L. 'Hedonic
## prices and the demand for clean air', J. Environ. Economics & Management,
## vol.5, 81-102, 1978.   Used in Belsley, Kuh & Welsch, 'Regression diagnosti
cs
## ...', Wiley, 1980.   N.B. Various transformations are used in the table on
## pages 244-261 of the latter.
##
## The Boston house-price data has been used in many machine learning papers t
hat address regression
## problems.
```

```
##
## .. topic:: References
##
##    - Belsley, Kuh & Welsch, 'Regression diagnostics: Identifying Influentia
l Data and Sources of Collinearity', Wiley, 1980. 244-261.
##    - Quinlan,R. (1993). Combining Instance-Based and Model-Based Learning.
In Proceedings on the Tenth International Conference of Machine Learning, 236-
243, University of Massachusetts, Amherst. Morgan Kaufmann.
```

- Now let's convert it into a pandas DataFrame! For that you need to import the pandas library and call the DataFrame() function passing the argument boston.data. To label the names of the columns, please use the .columnns attribute of the pandas DataFrame and assign it to boston.feature_names.

```
import pandas as pd
pd.set_option('display.max_columns', 500)
pd.set_option('display.max_rows', 500)

type(boston.data)
```

```
## <class 'numpy.ndarray'>
```

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

- Explore the top 5 rows of the dataset by using head() method on your pandas DataFrame.

```
data.head()
```

```
##       CRIM    ZN  INDUS  CHAS    NOX     RM   AGE     DIS  RAD    TAX  \
## 0  0.00632  18.0   2.31   0.0  0.538  6.575  65.2  4.0900  1.0  296.0
## 1  0.02731   0.0   7.07   0.0  0.469  6.421  78.9  4.9671  2.0  242.0
## 2  0.02729   0.0   7.07   0.0  0.469  7.185  61.1  4.9671  2.0  242.0
## 3  0.03237   0.0   2.18   0.0  0.458  6.998  45.8  6.0622  3.0  222.0
## 4  0.06905   0.0   2.18   0.0  0.458  7.147  54.2  6.0622  3.0  222.0
##
##    PTRATIO       B  LSTAT
## 0     15.3  396.90   4.98
## 1     17.8  396.90   9.14
## 2     17.8  392.83   4.03
## 3     18.7  394.63   2.94
## 4     18.7  396.90   5.33
```

- You'll 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 your pandas DataFrame.

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

- Run the .info() method on your DataFrame to get useful information about the data.

```
data.info()
```

```
## <class 'pandas.core.frame.DataFrame'>
## RangeIndex: 506 entries, 0 to 505
## Data columns (total 14 columns):
## CRIM       506 non-null float64
## ZN         506 non-null float64
## INDUS      506 non-null float64
## CHAS       506 non-null float64
## NOX        506 non-null float64
## RM         506 non-null float64
## AGE        506 non-null float64
## DIS        506 non-null float64
## RAD        506 non-null float64
## TAX        506 non-null float64
## PTRATIO    506 non-null float64
## B          506 non-null float64
## LSTAT      506 non-null float64
## PRICE      506 non-null float64
## dtypes: float64(14)
## memory usage: 55.4 KB
```

Exploring and Preparing the Data

- Turns out that this dataset has 14 columns (including the target variable PRICE) and 506 rows. Notice that the columns are of float data-type indicating the presence of only continuous features with no missing values in any of the columns. To get more summary statistics of the different features in the dataset you will use the describe() method on your DataFrame.
- Note that describe() only gives summary statistics of columns which are continuous in nature and not categorical.

```
data.describe()
```

```
##              CRIM          ZN       INDUS        CHAS         NOX
RM  \
## count  506.000000  506.000000  506.000000  506.000000  506.000000  506.0000
00
## mean     3.613524   11.363636   11.136779    0.069170    0.554695    6.2846
34
## std      8.601545   23.322453    6.860353    0.253994    0.115878    0.7026
17
## min      0.006320    0.000000    0.460000    0.000000    0.385000    3.5610
00
## 25%      0.082045    0.000000    5.190000    0.000000    0.449000    5.8855
00
## 50%      0.256510    0.000000    9.690000    0.000000    0.538000    6.2085
00
## 75%      3.677083   12.500000   18.100000    0.000000    0.624000    6.6235
00
## max     88.976200  100.000000   27.740000    1.000000    0.871000    8.7800
00
##
##               AGE         DIS         RAD         TAX     PTRATIO
B  \
## count  506.000000  506.000000  506.000000  506.000000  506.000000  506.0000
00
## mean    68.574901    3.795043    9.549407  408.237154   18.455534  356.6740
32
## std     28.148861    2.105710    8.707259  168.537116    2.164946   91.2948
64
## min      2.900000    1.129600    1.000000  187.000000   12.600000    0.3200
00
## 25%     45.025000    2.100175    4.000000  279.000000   17.400000  375.3775
00
## 50%     77.500000    3.207450    5.000000  330.000000   19.050000  391.4400
00
## 75%     94.075000    5.188425   24.000000  666.000000   20.200000  396.2250
00
## max    100.000000   12.126500   24.000000  711.000000   22.000000  396.9000
00
##
##             LSTAT       PRICE
## count  506.000000  506.000000
## mean    12.653063   22.532806
## std      7.141062    9.197104
## min      1.730000    5.000000
## 25%      6.950000   17.025000
## 50%     11.360000   21.200000
## 75%     16.955000   25.000000
## max     37.970000   50.000000
```

- If you plan to use XGBoost on a dataset which has categorical features you may want to consider applying some encoding (like one-hot encoding) to such features before training the model. Also, if you have some missing values such as NA in the dataset you may or may not do a separate treatment for them, because XGBoost is capable of handling missing values internally. You can check out this link if you wish to know more on this.

- Without delving into more exploratory analysis and feature engineering, you will now focus on applying the algorithm to train the model on this data.
- You will build the model using Trees as base learners (which are the default base learners) using XGBoost's scikit-learn compatible API. Along the way, you will also learn some of the common tuning parameters which XGBoost provides in order to improve the model's performance, and using the root mean squared error (RMSE) performance metric to check the performance of the trained model on the test set. Root mean Squared error is the square root of the mean of the squared differences between the actual and the predicted values. As usual, you start by importing the library xgboost and other important libraries that you will be using for building the model.
- Note you can install python libraries like xgboost on your system using pip install xgboost on cmd.

```
import xgboost as xgb
from sklearn.metrics import mean_squared_error
import pandas as pd
import numpy as np
```

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

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

- Now you will convert the dataset into an optimized data structure called Dmatrix that XGBoost supports and gives it acclaimed performance and efficiency gains. You will use this later in the tutorial.

```
data_dmatrix = xgb.DMatrix(data=X,label=y)
```

XGBoost's hyperparameters

- At this point, before building the model, you should be aware of the tuning parameters that XGBoost provides. Well, there are a plethora of tuning parameters for tree-based learners in XGBoost and you can read all about them here. But the most common ones that you should know are:
- learning_rate: step size shrinkage used to prevent overfitting. Range is [0,1]
- max_depth: determines how deeply each tree is allowed to grow during any boosting round.
- subsample: percentage of samples used per tree. Low value can lead to underfitting.
- colsample_bytree: percentage of features used per tree. High value can lead to overfitting.
- n_estimators: number of trees you want to build.
- objective: determines the loss function to be used like reg:linear for regression problems, reg:logistic for classification problems with only decision, binary:logistic for classification problems with probability.

- XGBoost also supports regularization parameters to penalize models as they become more complex and reduce them to simple (parsimonious) models.
- gamma: controls whether a given node will split based on the expected reduction in loss after the split. A higher value leads to fewer splits. Supported only for tree-based learners.
- alpha: L1 regularization on leaf weights. A large value leads to more regularization.
- lambda: L2 regularization on leaf weights and is smoother than L1 regularization.
- It's also worth mentioning that though you are using trees as your base learners, you can also use XGBoost's relatively less popular linear base learners and one other tree learner known as dart. All you have to do is set the booster parameter to either gbtree (default),gblinear or dart.

Training a Model on the Data

- Now, you 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 reproducibility of the results, a random_state is also assigned.

```
from sklearn.model_selection import train_test_split

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

- 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, you would have used the XGBClassifier() class.

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

- Fit the regressor to the training set and make predictions on the test set using the familiar .fit() and .predict() methods.

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

```
## [18:18:14] WARNING: /Users/travis/build/dmlc/xgboost/src/objective/regressi
on_obj.cu:174: reg:linear is now deprecated in favor of reg:squarederror.
## [18:18:14] WARNING: /Users/travis/build/dmlc/xgboost/src/objective/regressi
on_obj.cu:174: reg:linear is now deprecated in favor of reg:squarederror.
## XGBRegressor(alpha=10, base_score=0.5, booster='gbtree', colsample_bylevel=
1,
##              colsample_bynode=1, colsample_bytree=0.3, gamma=0, gpu_id=-1,
##              importance_type='gain', interaction_constraints='',
##              learning_rate=0.1, max_delta_step=0, max_depth=5,
##              min_child_weight=1, missing=nan, monotone_constraints='()',
##              n_estimators=10, n_jobs=0, num_parallel_tree=1,
##              objective='reg:linear', random_state=0, reg_alpha=10, reg_lamb
da=1,
##              scale_pos_weight=1, subsample=1, tree_method='exact',
##              validate_parameters=1, verbosity=None)
```

```
preds = xg_reg.predict(X_test)
```

- Compute the rmse by invoking the mean_sqaured_error function from sklearn's metrics module.

```
rmse = np.sqrt(mean_squared_error(y_test, preds))
print("RMSE: %f" % (rmse))
```

```
## RMSE: 10.517005
```

- Well, you can see that your RMSE for the price prediction came out to be around 10.8 per 1000$.

Improving Model Performance

k-fold Cross Validation using XGBoost

- In order to build more robust models, it is common to do a k-fold cross validation where all the entries in the original training dataset are used for both training as well as validation. Also, each entry is used for validation just once. XGBoost supports k-fold cross validation via the cv() method. All you have to do is specify the nfolds parameter, which is the number of cross validation sets you want to build. Also, it supports many other parameters (check out this link) like:

- num_boost_round: denotes the number of trees you build (analogous to n_estimators)

- metrics: tells the evaluation metrics to be watched during CV

- as_pandas: to return the results in a pandas DataFrame.

- early_stopping_rounds: finishes training of the model early if the hold-out metric ("rmse" in our case) does not improve for a given number of rounds.

- seed: for reproducibility of results.

- This time you will create a hyper-parameter dictionary params which holds all the hyper-parameters and their values as key-value pairs but will exclude the n_estimators from the hyper-parameter dictionary because you will use num_boost_rounds instead.
- You will use these parameters to build a 3-fold cross validation model by invoking XGBoost's cv() method and store the results in a cv_results DataFrame. Note that here you are using the Dmatrix object you created before.

```
params = {"objective":"reg:linear",'colsample_bytree': 0.3,'learning_rate': 0.
1,
                'max_depth': 5, 'alpha': 10}

cv_results = xgb.cv(dtrain=data_dmatrix, params=params, nfold=3,
                    num_boost_round=50,early_stopping_rounds=10,metrics="rms
e", as_pandas=True, seed=123)
```

```
## [18:18:14] WARNING: /Users/travis/build/dmlc/xgboost/src/objective/regressi
on_obj.cu:174: reg:linear is now deprecated in favor of reg:squarederror.
## [18:18:14] WARNING: /Users/travis/build/dmlc/xgboost/src/objective/regressi
on_obj.cu:174: reg:linear is now deprecated in favor of reg:squarederror.
## [18:18:14] WARNING: /Users/travis/build/dmlc/xgboost/src/objective/regressi
on_obj.cu:174: reg:linear is now deprecated in favor of reg:squarederror.
```

- cv_results contains train and test RMSE metrics for each boosting round.

```
cv_results.head()
```

```
##    train-rmse-mean  train-rmse-std  test-rmse-mean  test-rmse-std
## 0        21.680257        0.025607       21.719121       0.019025
## 1        19.740500        0.072068       19.818879       0.061769
## 2        18.007202        0.119744       18.109862       0.129375
## 3        16.463924        0.115086       16.587236       0.182339
## 4        14.990313        0.112001       15.132976       0.166282
```

```
cv_results.tail()
```

```
##     train-rmse-mean  train-rmse-std  test-rmse-mean  test-rmse-std
## 45         2.303110        0.095324        3.929727       0.418970
## 46         2.284013        0.099422        3.921385       0.420554
## 47         2.262122        0.099400        3.914916       0.421881
## 48         2.233371        0.089460        3.884679       0.438200
## 49         2.202443        0.085125        3.862102       0.439726
```

- Extract and print the final boosting round metric.

```
print((cv_results["test-rmse-mean"]).tail(1))
```

```
## 49    3.862102
## Name: test-rmse-mean, dtype: float64
```

- You can see that your RMSE for the price prediction has reduced as compared to last time and came out to be around 4.03 per 1000$. You can reach an even lower RMSE for a different set of hyper-parameters. You may consider applying techniques like Grid Search, Random Search and Bayesian Optimization to reach the optimal set of hyper-parameters.

Visualize Boosting Trees and Feature Importance

- You can also visualize individual trees from the fully boosted model that XGBoost creates using the entire housing dataset. XGBoost has a plot_tree() function that makes this type of visualization easy. Once you train a model using the XGBoost learning API, you can pass it to the plot_tree() function along with the number of trees you want to plot using the num_trees argument.

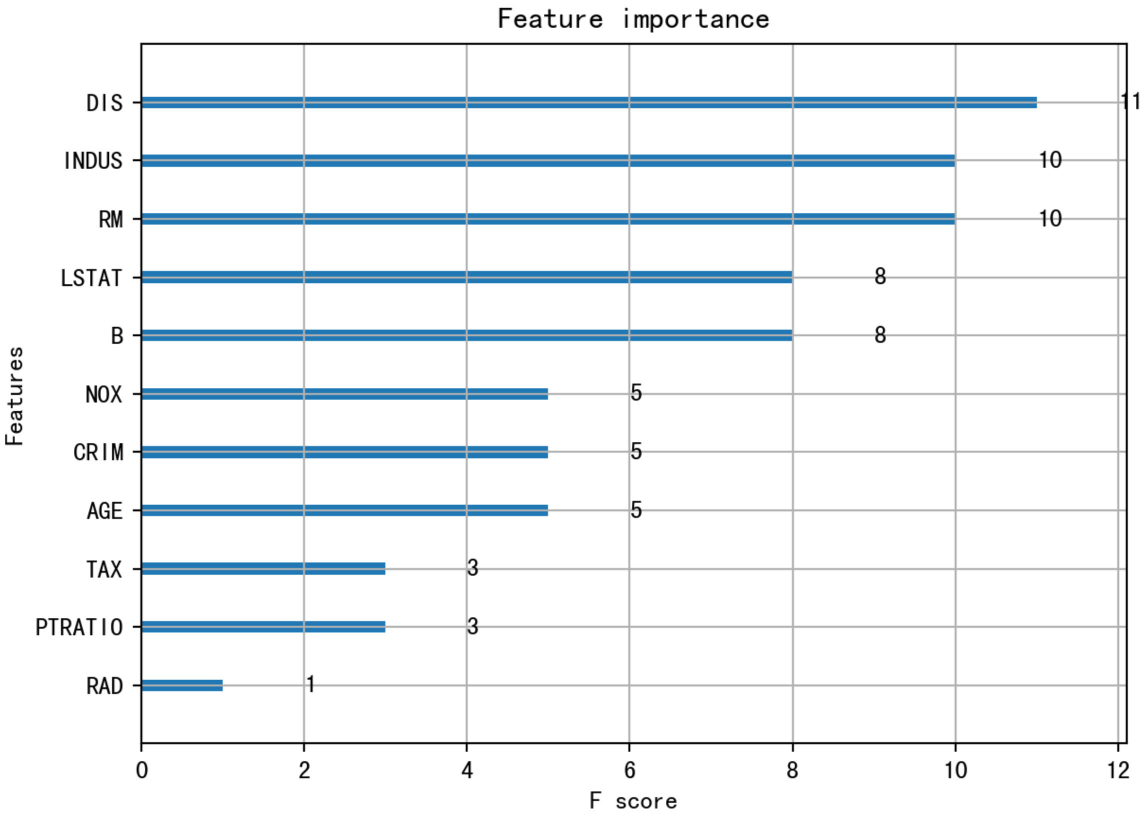
```
# Set the number of boosting round to 10
xg_reg = xgb.train(params=params, dtrain=data_dmatrix, num_boost_round=10)
```

```
## [18:18:14] WARNING: /Users/travis/build/dmlc/xgboost/src/objective/regressi
on_obj.cu:174: reg:linear is now deprecated in favor of reg:squarederror.
## [18:18:14] WARNING: /Users/travis/build/dmlc/xgboost/src/objective/regressi
on_obj.cu:174: reg:linear is now deprecated in favor of reg:squarederror.
```

- Another way to visualize your XGBoost models is to examine the importance of each feature column in the original dataset within the model.
- One simple way of doing this involves counting the number of times each feature is split on across all boosting rounds (trees) in the model, and then visualizing the result as a bar graph, with the features ordered according to how many times they appear. XGBoost has a plot_importance() function that allows you to do exactly this.

```
import matplotlib.pyplot as plt

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



- As you can see the feature RM has been given the highest importance score among all the features. Thus XGBoost also gives you a way to do Feature Selection. Isn't this brilliant?

Conclusion

- You have reached the end of this tutorial. I hope this might have or will help you in some way or the other. You started off with understanding how Boosting works in general and then narrowed down to XGBoost specifically. You also practiced applying XGBoost on an open source dataset and along the way you learned about its hyper-parameters, doing cross-validation, visualizing the trees and in the end how it can also be used as a Feature Selection technique. Whoa!! that's something for starters, but there is so much to explore in XGBoost that it can't be covered in a single tutorial. If you would like to learn more, be sure to take a look at our Extreme Gradient Boosting with XGBoost course on DataCamp.