## xgboost-1-Introduction

May 8, 2019

## 1 Extreme gradient boosting with xgboost

#### This is an online course provided by datacamp

XGBoost (Extreme Gradient Boosting) belongs to a family of boosting algorithms and uses the gradient boosting framework at its core.

- optimized gradient-boosting machine learning library
- Originally written in C++

Why xgboost?

- speed and performance
- core algorithm is parallelizable
- consistently outperforms single-algorithm methods
- state-of-the-art performance in many ML task

you can use the scikit-learn .fit() / .predict() paradigm that you are already familiar to build your XGBoost models, as the xgboost library has a scikit-learn compatible API!

**Boosting** is a sequential technique which works on the principle of an ensemble. It combines a set of weak learners and delivers improved prediction accuracy. At any instant t, the model outcomes are weighted based on the outcomes of previous instant t-1. The outcomes predicted correctly are given a lower weight and the ones miss-classified are weighted higher. Note that a **weak learner** is one which is slightly better than random guessing.

```
In [1]: import textwrap
    import os
    import sys
    import pandas as pd
    import numpy as np
    import xgboost as xgb
    import sklearn as sk
    from sklearn.model_selection import train_test_split

    print("Python version: {0}".format(sys.version))
    print("pandas version: {0}".format(pd.__version__))
    print("numpy version:{0}".format(np.__version__))
    print("sklearn version:{0}".format(sk.__version__))
    print("xgboost version: {0}".format(xgb.__version__))
    print("Working directory: \n" + os.getcwd())
```

```
[Clang 4.0.1 (tags/RELEASE_401/final)]
pandas version: 0.23.4
numpy version:1.15.4
sklearn version:0.20.1
xgboost version: 0.82
Working directory:
/Users/miaocai/Dropbox/RprojectMiao/xgboost
In [2]: # from sk.model_selection import train_test_split
        train_url = "http://s3.amazonaws.com/assets.datacamp.com/course/Kaggle/train.csv"
        train = pd.read_csv(train_url)
        train.head()
        # y: survived
Out[2]:
           PassengerId Survived Pclass
        0
                     1
                               0
        1
                     2
                               1
                                        1
        2
                     3
                                        3
        3
                     4
                               1
                                        1
        4
                     5
                               0
                                        3
                                                         Name
                                                                  Sex
                                                                             SibSp \
                                                                         Age
        0
                                      Braund, Mr. Owen Harris
                                                                 male
                                                                       22.0
                                                                                  1
        1
           Cumings, Mrs. John Bradley (Florence Briggs Th...
                                                               female
                                                                       38.0
                                                                                  1
                                       Heikkinen, Miss. Laina
                                                               female
                                                                       26.0
                                                                                  0
        3
                Futrelle, Mrs. Jacques Heath (Lily May Peel)
                                                               female
                                                                       35.0
                                                                                  1
        4
                                     Allen, Mr. William Henry
                                                                 male
                                                                       35.0
           Parch
                            Ticket
                                        Fare Cabin Embarked
        0
               0
                         A/5 21171
                                      7.2500
                                               NaN
                                                          S
        1
                                               C85
                                                          С
               0
                          PC 17599
                                    71.2833
        2
                  STON/02. 3101282
                                     7.9250
                                                          S
               0
                                               NaN
        3
               0
                            113803
                                    53.1000 C123
                                                          S
        4
                            373450
                                      8.0500
                                               NaN
In [3]: train.columns
Out[3]: Index(['PassengerId', 'Survived', 'Pclass', 'Name', 'Sex', 'Age', 'SibSp',
               'Parch', 'Ticket', 'Fare', 'Cabin', 'Embarked'],
              dtype='object')
In [4]: test_url = "http://s3.amazonaws.com/assets.datacamp.com/course/Kaggle/test.csv"
        test = pd.read_csv(test_url)
        test.head()
Out[4]:
           PassengerId Pclass
                                                                         Name
                                                                                   Sex \
        0
                   892
                                                             Kelly, Mr. James
                             3
                                                                                  male
```

Python version: 3.7.1 (default, Dec 14 2018, 13:28:58)

```
2
                    894
                               2
                                                       Myles, Mr. Thomas Francis
                                                                                      male
        3
                    895
                               3
                                                                Wirz, Mr. Albert
                                                                                      male
        4
                    896
                                  Hirvonen, Mrs. Alexander (Helga E Lindqvist)
                                                                                    female
                                  Ticket
                                              Fare Cabin Embarked
             Age
                 SibSp
                         Parch
        0
           34.5
                      0
                                  330911
                                            7.8292
                                                      NaN
           47.0
        1
                      1
                              0
                                  363272
                                            7.0000
                                                      NaN
                                                                 S
        2
          62.0
                      0
                                  240276
                                            9.6875
                                                      NaN
                                                                 Q
                              0
                                                                 S
        3
           27.0
                      0
                              0
                                  315154
                                            8.6625
                                                      NaN
           22.0
                      1
                                                                 S
                              1
                                 3101298
                                           12.2875
                                                      {\tt NaN}
   split into train and test using scikit learn
   from sklearn.model_selection import train_test_split xTrain, xTest, yTrain,
ySplit = train_test_split(x, y, test_size = 0.2, radom_state = 0)
In [5]: X_columns = ['Pclass', 'Sex', 'Age', 'SibSp', 'Parch',
                     'Fare', 'Cabin', 'Embarked']
        X_train = train[X_columns].fillna(0)
        X_train = pd.get_dummies(X_train, columns =
                                   ['Pclass', 'Sex', 'Cabin', 'Embarked'])
        y_train = train['Survived']
        X test = test[X columns].fillna(0)
        X_train.head()
Out [5]:
             Age
                 SibSp
                         Parch
                                    Fare
                                           Pclass_1 Pclass_2 Pclass_3
                                                                           Sex female
           22.0
        0
                              0
                                  7.2500
                                                  0
                                                             0
                                                                        1
                                                                                     0
        1
           38.0
                                71.2833
                      1
                              0
                                                  1
                                                             0
                                                                        0
                                                                                     1
        2 26.0
                      0
                              0
                                  7.9250
                                                  0
                                                             0
                                                                        1
                                                                                     1
           35.0
                                 53.1000
        3
                      1
                              0
                                                  1
                                                             0
                                                                        0
                                                                                     1
           35.0
                      0
                                  8.0500
                                                  0
                                                             0
                                                                        1
                                                                                     0
           Sex_male
                      Cabin_0
                                             Cabin_F2 Cabin_F33
                                                                   Cabin_F38
                                                                               Cabin_F4
        0
                   1
                                                     0
                                                                0
                                                                            0
                                                                                       0
        1
                   0
                             0
                                                     0
                                                                0
                                                                            0
                                                                                       0
                                    . . .
        2
                   0
                                                     0
                                                                0
                                                                            0
                                                                                       0
                             1
        3
                   0
                             0
                                                     0
                                                                0
                                                                            0
                                                                                       0
        4
                                                     0
                                                                0
                   1
                             1
                                                                                       0
                      Cabin_T Embarked_O Embarked_C Embarked_Q Embarked_S
           Cabin G6
        0
                   0
                             0
                                          0
                                                       0
                                                                    0
                                                                                 1
        1
                   0
                             0
                                                       1
                                                                    0
                                                                                 0
                                          0
        2
                   0
                             0
                                          0
                                                       0
                                                                    0
                                                                                 1
        3
                   0
                             0
                                          0
                                                       0
                                                                    0
                                                                                 1
                   0
                             0
                                          0
                                                                    0
        4
                                                                                 1
```

Wilkes, Mrs. James (Ellen Needs)

female

[5 rows x 161 columns]

# 1.1 Decision tree

Decision trees as base learners:

- Base learner individual learning algorithm in an ensemble algorithm
- Composed of a series of binary questions
- Predictions happen at the "leaves" of the tree
- Constructed iteratively (one decision at a time)
  - Until a stopping criterion is met (such as predefined tree depth)
  - Individual tree: tend to be low bias but high variance
  - Also, low training error but high test error (overfit)

#### **CART: Classification and Regression Trees**

- Decision trees: the leaf nodes always contain decision values,
- CART: contain a **real-valued score** in each leaf, regardless of whether they are used for classification or regression.
  - The real-valued scores can be thresholded to convert into categories for classifiction problems if necessary.

```
In [7]: from sklearn.tree import DecisionTreeClassifier
    dt_clf_4 = DecisionTreeClassifier(max_depth = 4)
    dt_clf_4.fit(X_train, y_train)
    y_pred_4 = dt_clf_4.predict(X_train)
    accuracy= float(np.sum(y_pred_4 == y_train)/y_train.shape[0])
    print("Prediction accuracy on train set:", np.round(accuracy*100, 2), "%")
```

Prediction accuracy on train set: 83.05 %

#### 1.2 Boosting

- Not a specific machine learning algorithm
- It is actually a concept that can be applied to a set of machine learning models
  - "Meta-algorithm"
- Ensemble meta-algorithm used to convert many weak learners into a strong learner
- Used to reduce any given single learner's variance and to convert any weak learner into an arbitrarily strong learner.

#### Weak learner and strong learners

- Weak leaner: ML algorithm that is slightly better than chance
  - Example: Decision trees whose predictions are slightly better than 50%
- Boosting converts a collection of weak learners into a strong learner
- Strong learner: any algorithm that can be tuned to achieve good performance.

#### How boosting is accomplished

- Iteratively learning a set of weak models on subsets of data
- Weighing each weak prediction according to each weak learner's performance
- Combined the weighted predictions to obtain a single weighted prediction
- The prediction is much better than the individual predictions themselves!

The prediction scores for each possibility are summed across trees, and the prediction is simply the sum of the scores across both trees.

#### Model evaluation through cross-validation

- Cross-validation: a robust method for estimating the performance of a model on unseen data
- Generating many non-overlapping train/test splits on training data
- Report the average test set performance across all data splits

We can convert the dataset into an optimized data structure that the creators of XGBoost made that gives the package its lauded performance and efficiency gains called a DMatrix.

If we use the XGBoost cv object, which is a part of XGBoost's learning api, we have to first explicitly convert our data into a DMatrix.

#### 1.3 When should I use XGBoost

#### Occasions when you should use XGBoost

- A large number of training examples
  - Greater than 1000 training samples and less than 100 features
  - The number of features < number of training samples
- A mixture of categorical and numeric features
  - Or just numeric features

### Occassions when you should NOT use XGBoost

- If you can success using other state-of-the-art algorithms or those that suffer from data size issues.
  - Image recognition
  - Computer vision
  - Natural language processing and understanding problems
  - These problems can be much better tackled using deep learning approaches
- When you have very small data sets (<100 observations, or the number of training samples is significantly smaller than the number of features)