



EXTREME GRADIENT BOOSTING WITH XGBOOST

Regression review

Regression basics

- Outcome is real-valued



Common regression metrics

- Root mean squared error (RMSE)
- Mean absolute error (MAE)

Computing RMSE

Actual	Predicted
10	20
3	8
6	1

Computing RMSE

Actual	Predicted	Error
10	20	-10
3	8	-5
6	1	5

Computing RMSE

Actual	Predicted	Error	Squared Error
10	20	-10	100
3	8	-5	25
6	1	5	25

- Total Squared Error: 150
- Mean Squared Error: 50
- Root Mean Squared Error: 7.07

Computing MAE

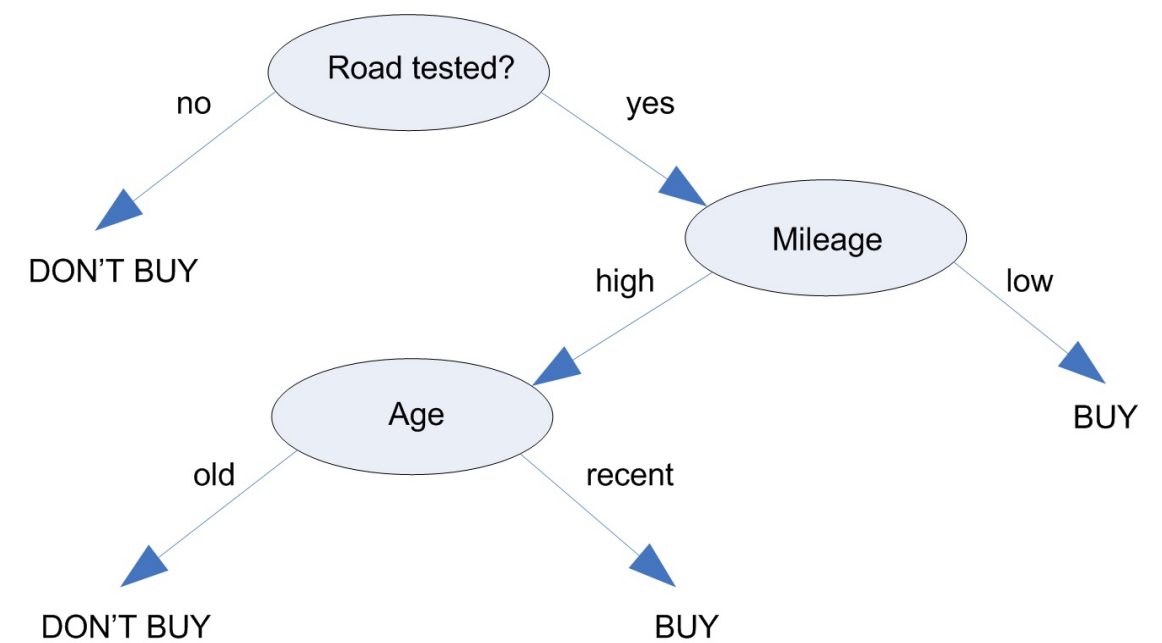
Actual	Predicted	Error
10	20	-10
3	8	-5
6	1	5

- Total Absolute Error: 20
- Mean Absolute Error: 6.67

Common regression algorithms

- Linear regression
- Decision trees

Algorithms for both regression and classification





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Let's practice!



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Objective (loss) functions and base learners

Objective Functions and Why We Use Them

- Quantifies how far off a prediction is from the actual result
- Measures the difference between estimated and true values for some collection of data
- Goal: Find the model that yields the minimum value of the loss function

Common Loss Functions and XGBoost

- Loss function names in xgboost:
 - `reg:linear` - use for regression problems
 - `reg:logistic` - use for classification problems when you want just decision, not probability
 - `binary:logistic` - use when you want probability rather than just decision

Base Learners and Why We Need Them

- XGBoost involves creating a meta-model that is composed of many individual models that combine to give a final prediction
- Individual models = base learners
- Want base learners that when combined create final prediction that is **non-linear**
- Each base learner should be good at distinguishing or predicting different parts of the dataset
- Two kinds of base learners: tree and linear

Trees as Base Learners example: Scikit-learn API

```
In [1]: import xgboost as xgb
In [2]: import pandas as pd
In [3]: import numpy as np
In [4]: from sklearn.model_selection import train_test_split
In [5]: boston_data = pd.read_csv("boston_housing.csv")
In [6]: X, y = boston_data.iloc[:, :-1], boston_data.iloc[:, -1]
In [7]: X_train, X_test, y_train, y_test = train_test_split(X, y,
    test_size=0.2, random_state=123)
In [8]: xg_reg = xgb.XGBRegressor(objective='reg:linear',
    n_estimators=10, seed=123)
In [9]: xg_reg.fit(X_train, y_train)
```

Trees as base learners example: Scikit-learn API

```
In [11]: rmse = np.sqrt(mean_squared_error(y_test, preds))
```

```
In [12]: print("RMSE: %f" % (rmse))  
RMSE: 129043.2314
```


Linear Base Learners Example: Learning API Only

```
In [1]: import xgboost as xgb
In [2]: import pandas as pd
In [3]: import numpy as np
In [4]: from sklearn.model_selection import train_test_split
In [5]: boston_data = pd.read_csv("boston_housing.csv")
In [6]: X, y = boston_data.iloc[:, :-1], boston_data.iloc[:, -1]
In [7]: X_train, X_test, y_train, y_test = train_test_split(X, y,
    test_size=0.2, random_state=123)
In [8]: DM_train = xgb.DMatrix(data=X_train, label=y_train)
In [9]: DM_test = xgb.DMatrix(data=X_test, label=y_test)
In [10]: params = {"booster": "gblinear", "objective": "reg:linear"}
```

Linear base learners example: Learning API only

```
In [13]: rmse = np.sqrt(mean_squared_error(y_test,preds))
```

```
In [14]: print("RMSE: %f" % (rmse))  
RMSE: 124326.24465
```



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Let's get to work!



EXTREME GRADIENT BOOSTING WITH XGBOOST

Regularization and base learners in XGBoost

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Regularization in XGBoost

- Regularization is a control on model complexity
- Want models that are both accurate and as simple as possible
- Regularization parameters in XGBoost:
 - gamma - minimum loss reduction allowed for a split to occur
 - alpha - l1 regularization on leaf weights, larger values mean more regularization
 - lambda - l2 regularization on leaf weights

L1 Regularization in XGBoost example

```
In [1]: import xgboost as xgb
In [2]: import pandas as pd
In [3]: boston_data = pd.read_csv("boston_data.csv")
In [4]: X,y = boston_data.iloc[:, :-1], boston_data.iloc[:, -1]

In [5]: boston_dmatrix = xgb.DMatrix(data=X, label=y)
In [6]: params={"objective": "reg:linear", "max_depth": 4}

In [7]: l1_params = [1, 10, 100]
In [8]: rmses_l1=[]

In [9]: for reg in l1_params:
...:     params["alpha"] = reg
...:     cv_results = xgb.cv(dtrain=boston_dmatrix,
...:         params=params, nfold=4,
...:         num_boost_round=10, metrics="rmse", as_pandas=True, seed=123)
...:     rmses_l1.append(cv_results["test-rmse-mean"] \
...:         .tail(1).values[0])

In [10]: print("Best rmse as a function of l1:")
In [11]: print(pd.DataFrame(list(zip(l1_params, rmses_l1))
```

Base Learners in XGBoost

- Linear Base Learner:
 - Sum of linear terms
 - Boosted model is weighted sum of linear models (thus is itself linear)
 - Rarely used
- Tree Base Learner:
 - Decision tree
 - Boosted model is weighted sum of decision trees (nonlinear)
 - Almost exclusively used in XGBoost

Creating DataFrames from multiple equal-length lists

- `pd.DataFrame(list(zip(list1,list2)),columns=["list1","list2"]))`
- `zip` creates a generator of parallel values:
 - `zip([1,2,3],["a","b","c"]) = [1,"a"],[2,"b"],[3,"c"]`
 - generators need to be completely instantiated before they can be used in DataFrame objects
- `list()` instantiates the full generator and passing that into the DataFrame converts the whole expression



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Let's practice!