

Regression review

EXTREME GRADIENT BOOSTING WITH XGBOOST



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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

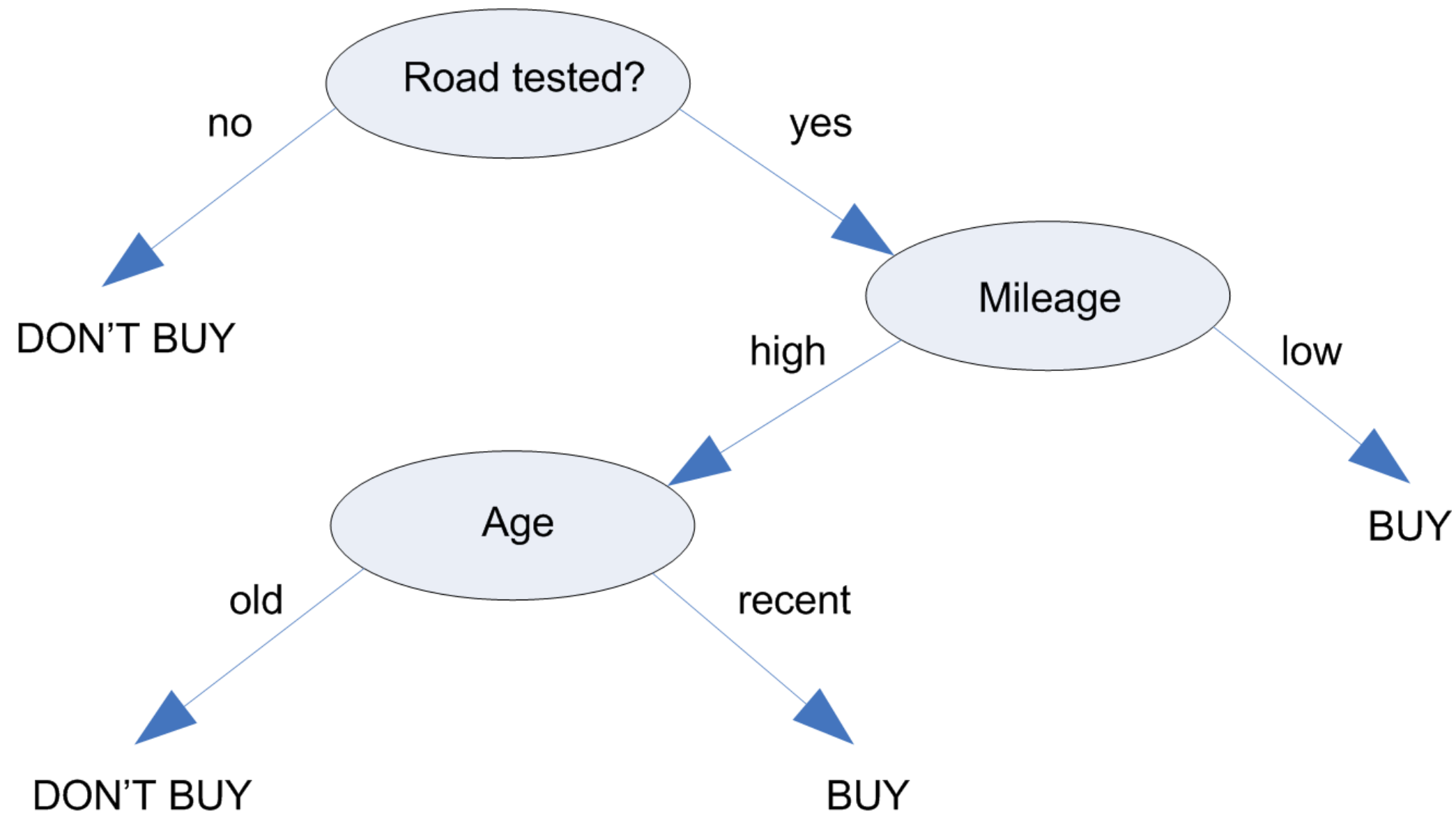
| Actual | Predicted | Error |
|--------|-----------|-------|
| 10 | 20 | -10 |
| 3 | 8 | -5 |
| 6 | 1 | 5 |

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

Common regression algorithms

- Linear regression
- Decision trees

Algorithms for both regression and classification



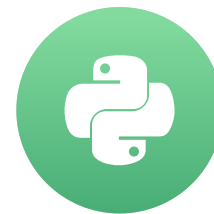
¹ https://www.ibm.com/support/knowledgecenter/en/SS3RA7_15.0.0/com.ibm.spss.modeler.help/nodes_treebuilding.htm

Let's practice!

EXTREME GRADIENT BOOSTING WITH XGBOOST

Objective (loss) functions and base learners

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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

```
import xgboost as xgb
import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split

boston_data = pd.read_csv("boston_housing.csv")
X, y = boston_data.iloc[:, :-1], boston_data.iloc[:, -1]

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

xg_reg = xgb.XGBRegressor(objective='reg:linear', n_estimators=10,
                          seed=123)

xg_reg.fit(X_train, y_train)

preds = xg_reg.predict(X_test)
```

Trees as base learners example: Scikit-learn API

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

```
RMSE: 129043.2314
```


Linear base learners example: learning API only

```
import xgboost as xgb
import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split

boston_data = pd.read_csv("boston_housing.csv")

X, y = boston_data.iloc[:, :-1], boston_data.iloc[:, -1]

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

DM_train = xgb.DMatrix(data=X_train, label=y_train)
DM_test = xgb.DMatrix(data=X_test, label=y_test)

params = {"booster": "gblinear", "objective": "reg:linear"}

xg_reg = xgb.train(params = params, dtrain=DM_train, num_boost_round=10)

preds = xg_reg.predict(DM_test)
```

Linear base learners example: learning API only

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

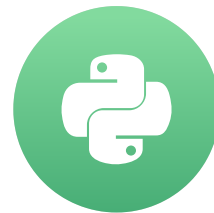
```
RMSE: 124326.24465
```

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

```
import xgboost as xgb
import pandas as pd
boston_data = pd.read_csv("boston_data.csv")
X,y = boston_data.iloc[:, :-1], boston_data.iloc[:, -1]
boston_dmatrix = xgb.DMatrix(data=X, label=y)
params={"objective":"reg:linear", "max_depth":4}
l1_params = [1,10,100]
rmse_l1=[]
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)
    rmse_l1.append(cv_results["test-rmse-mean"].tail(1).values[0])
print("Best rmse as a function of l1:")
print(pd.DataFrame(list(zip(l1_params, rmse_l1)), columns=["l1", "rmse"]))
```

Best rmse as a function of l1:

| | l1 | rmse |
|---|-----|--------------|
| 0 | 1 | 69572.517742 |
| 1 | 10 | 73721.967141 |
| 2 | 100 | 82312.312413 |

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

Let's practice!

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