EXTREME GRADIENT BOOSTING WITH XGBOOST

Regression review

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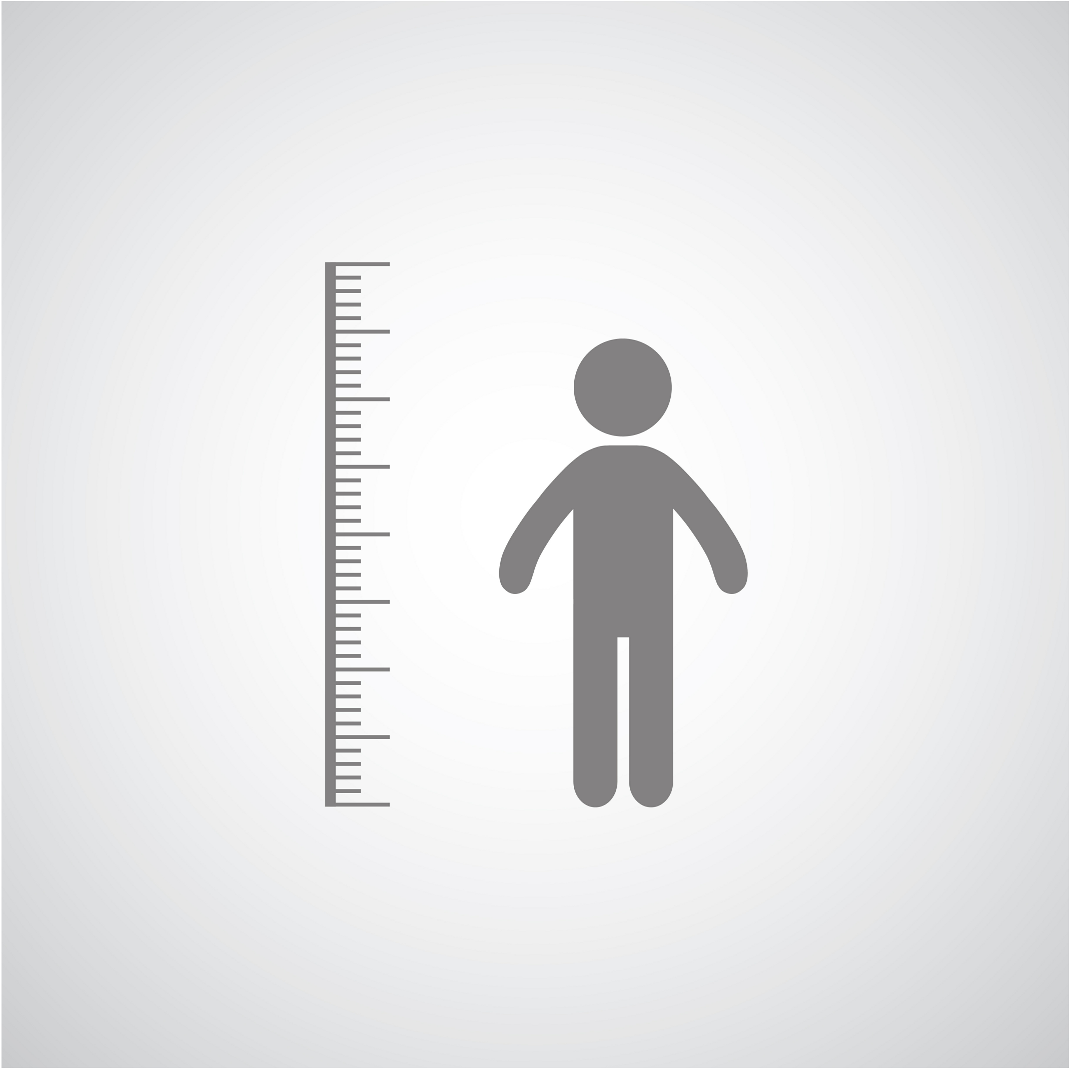
Regression basics

- 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

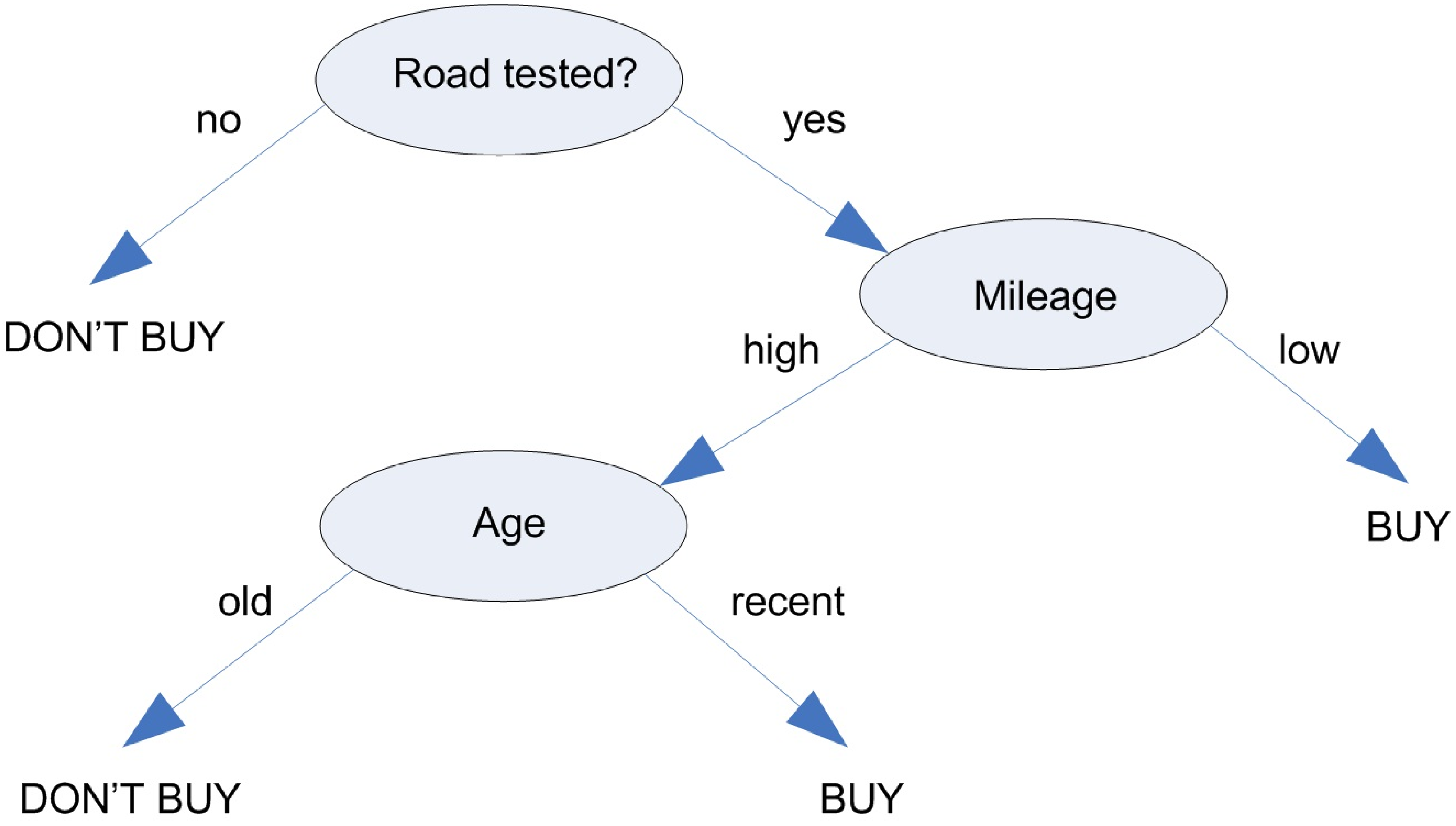
Actual	Predicted	Error
10	20	-10
3	8	-5
6	1	5

- 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

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Let's practice!

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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

```
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)

In [10]: preds = xg_reg.predict(X_test)
```

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"}

In [11]: xg_reg = xgb.train(params = params, dtrain=DM_train,
         num_boost_round=10)

In [12]: preds = xg_reg.predict(DM_test)
```

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!

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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)),
         columns=["l1","rmse"]))
Best rmse as a function of l1:
        l1          rmse
    0    1  69572.517742
    1   10  73721.967141
```

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!