# Welcome to the course!

EXTREME GRADIENT BOOSTING WITH XGBOOST

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# Before we get to XGBoost...

- Need to understand the basics of
    - Supervised classification
    - Decision trees
    - Boosting

# Supervised learning

- Relies on labeled data
- Have some understanding of past behavior

# Supervised learning example

- Does a specific image contain a person's face?


- Training data: vectors of pixel values
- Labels: 1 or 0

# Supervised learning: Classification

- Outcome can be binary or multi-class

# Binary classification example

- Will a person purchase the insurance package given some quote?

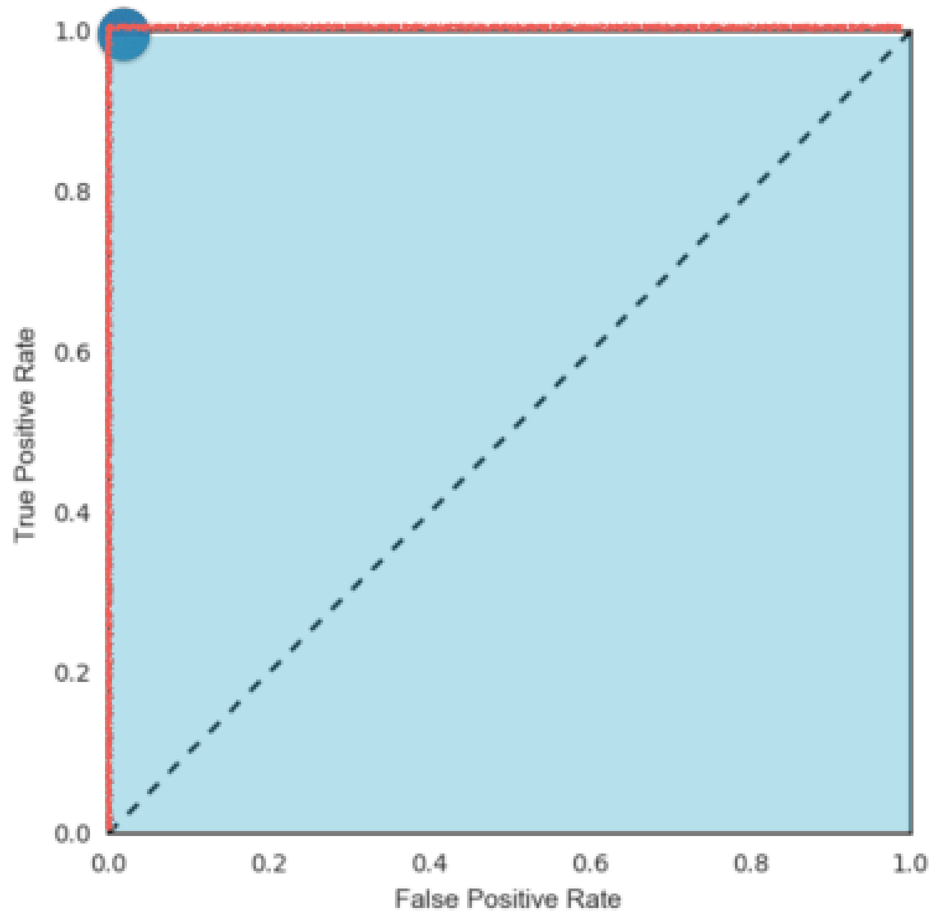
# Multi-class classification example

- Classifying the species of a given bird

# AUC: Metric for binary classification models

## Area under the ROC curve (AUC)

- Larger area under the ROC curve = better model



# Accuracy score and confusion matrix

- Confusion matrix

| | Predicted: Spam Email | Predicted: Real Email |
|---|---|---|
| Actual: Spam Email | True Positive | False Negative |
| Actual: Real Email | False Positive | True Negative |

- Accuracy: $\frac{tp + tn}{tp + tn + fp + fn}$

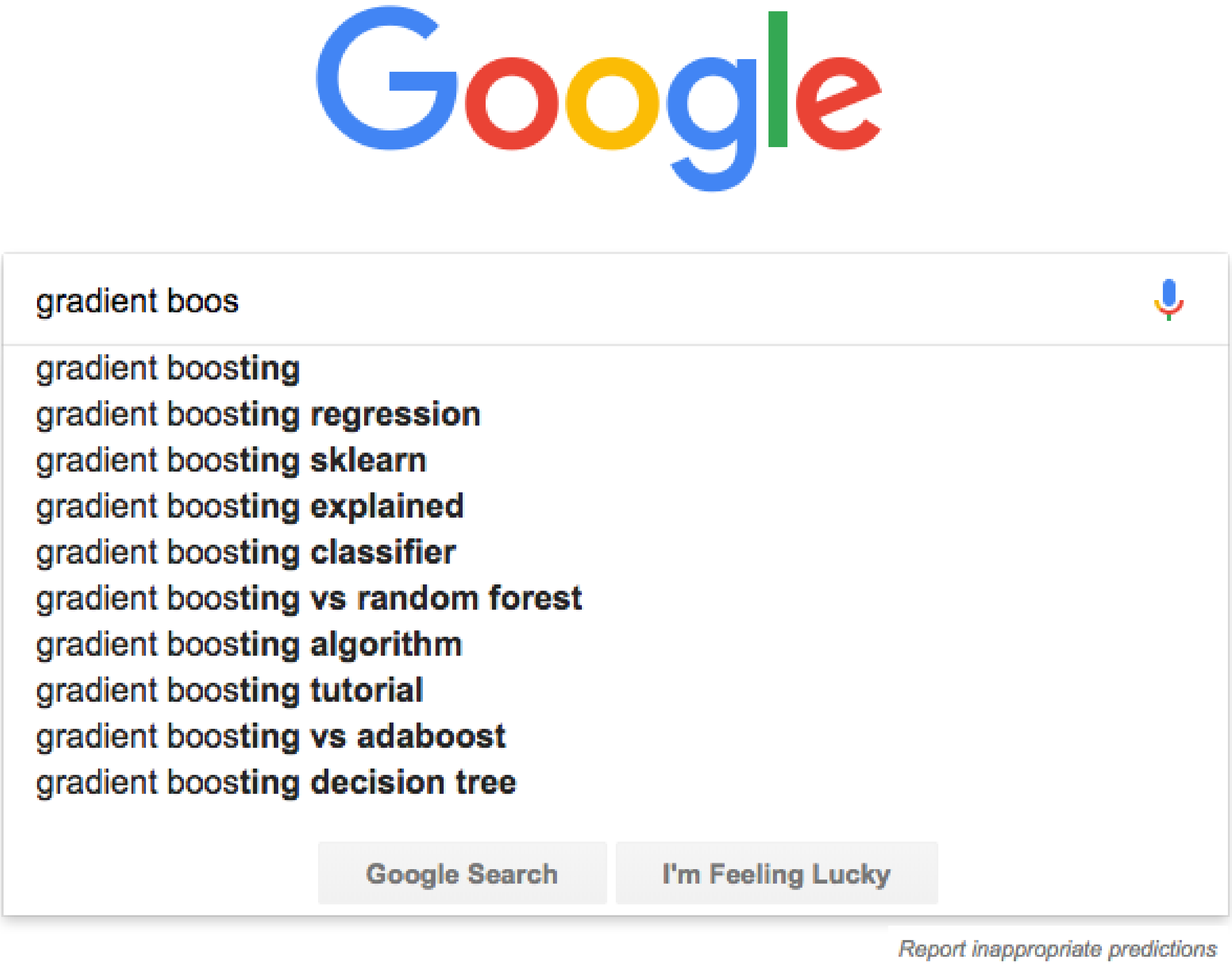
# Supervised learning with scikit-learn

# Other supervised learning considerations

- Features can be either numeric or categorical
- Numeric features should be scaled (Z-scored)
- Categorical features should be encoded (one-hot)

# Ranking

- Predicting an ordering on a set of choices



# Recommendation

- Recommending an item to a user
- Based on consumption history and profile
- Example: Netflix

# Let's practice!

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# Introducing XGBoost

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# What is XGBoost?

- Optimized gradient-boosting machine learning library
- Originally written in C++
- Has APIs in several languages:
  - **Python**
  - R
  - Scala
  - Julia
  - Java

# What makes XGBoost so popular?

- Speed and performance
- Core algorithm is parallelizable
- Consistently outperforms single-algorithm methods
- State-of-the-art performance in many ML tasks

# Using XGBoost: a quick example

```python
import xgboost as xgb
import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split
class_data = pd.read_csv("classification_data.csv")

X, y = class_data.iloc[:,:-1], class_data.iloc[:,-1]
X_train, X_test, y_train, y_test= train_test_split(X, y,
        test_size=0.2, random_state=123)
xg_cl = xgb.XGBClassifier(objective='binary:logistic',
        n_estimators=10, seed=123)
xg_cl.fit(X_train, y_train)

preds = xg_cl.predict(X_test)
accuracy = float(np.sum(preds==y_test))/y_test.shape[0]

print("accuracy: %f" % (accuracy))
```

```
accuracy: 0.78333
```

# Let's begin using XGBoost!

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# What is a decision tree?

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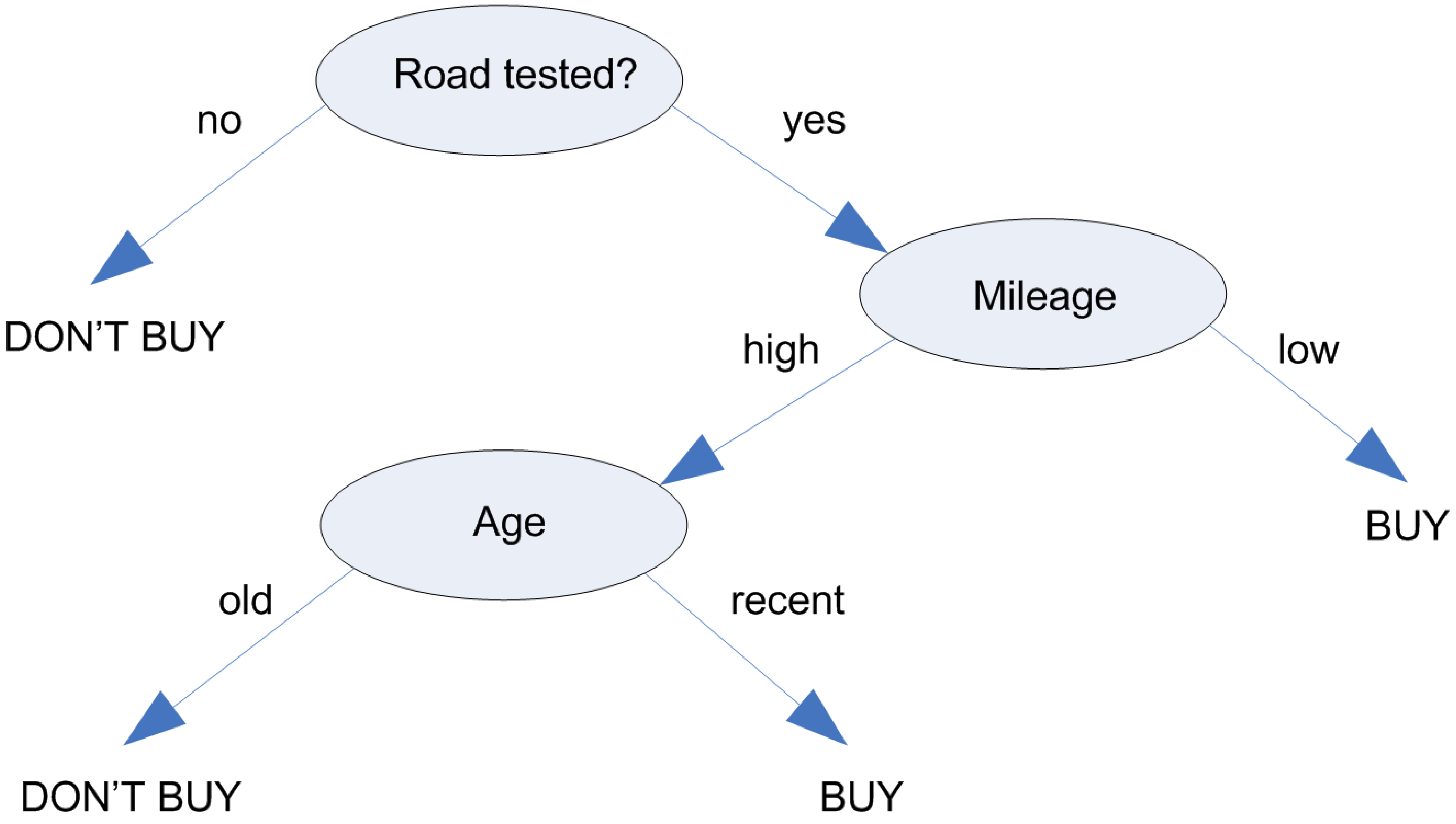
# Visualizing a decision tree




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

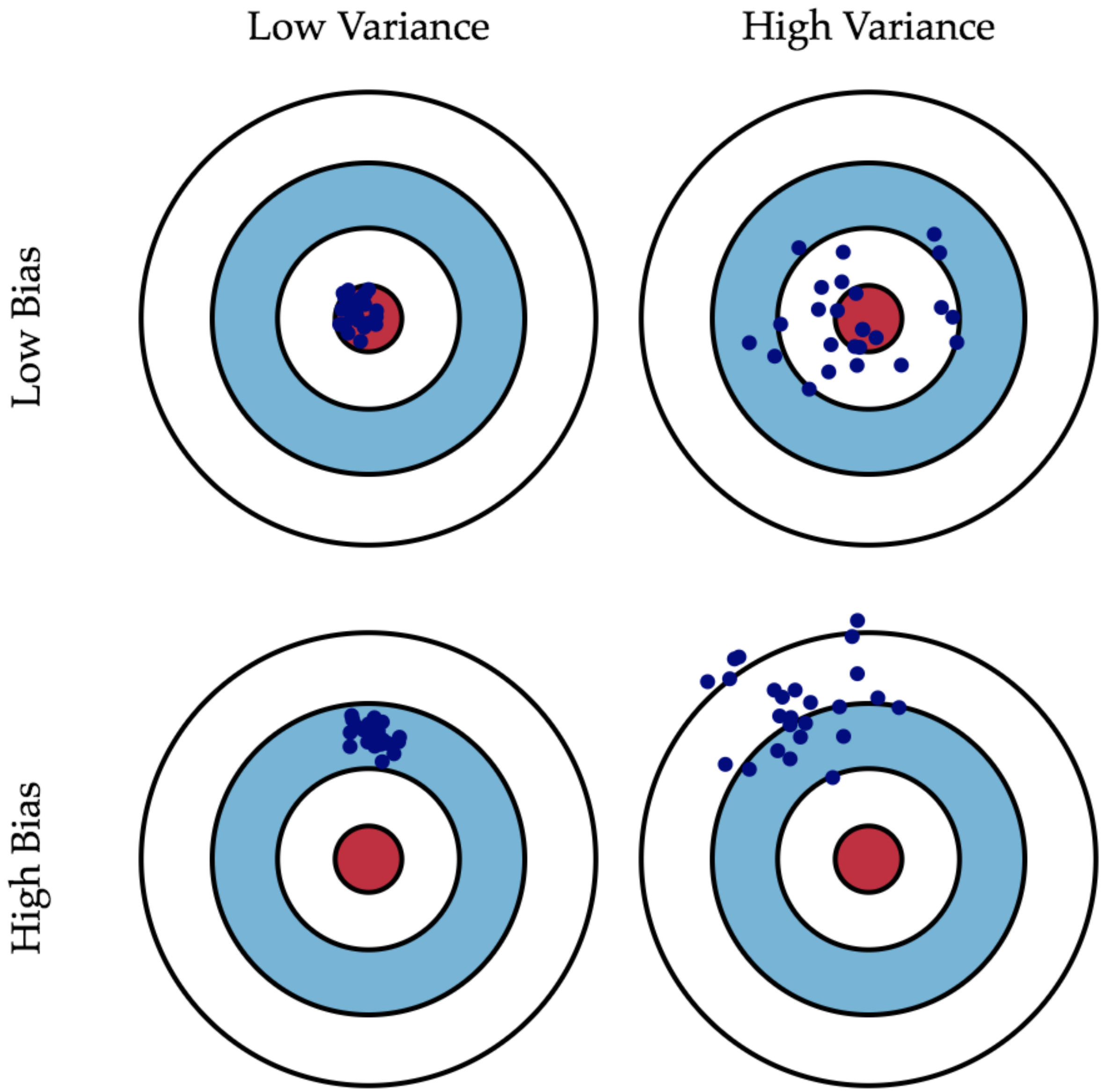
# Decision trees as base learners

- Base learner - Individual learning algorithm in an ensemble algorithm
- Composed of a series of binary questions
- Predictions happen at the "leaves" of the tree

# Decision trees and CART

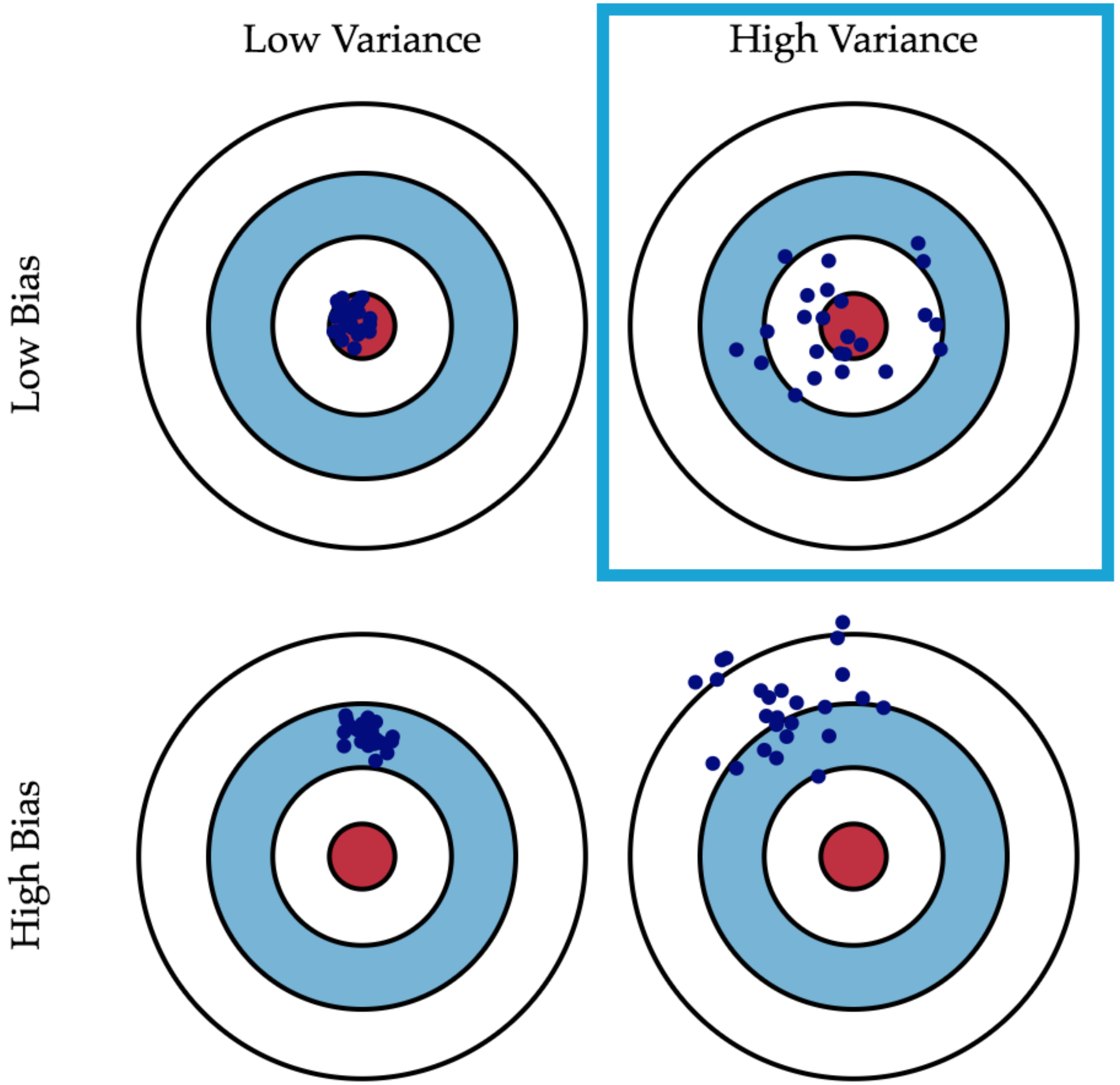
- Constructed iteratively (one decision at a time)
  - Until a stopping criterion is met

# Individual decision trees tend to overfit




[1] http://scott.fortmann [2] roe.com/docs/BiasVariance.html

# Individual decision trees tend to overfit




[1] http://scott.fortmann [2] roe.com/docs/BiasVariance.html

# CART: Classification and Regression Trees

- Each leaf **always** contains a real-valued score
- Can later be converted into categories

# Let's work with some decision trees!

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# What is Boosting?

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# Boosting overview

- Not a specific machine learning algorithm
- 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

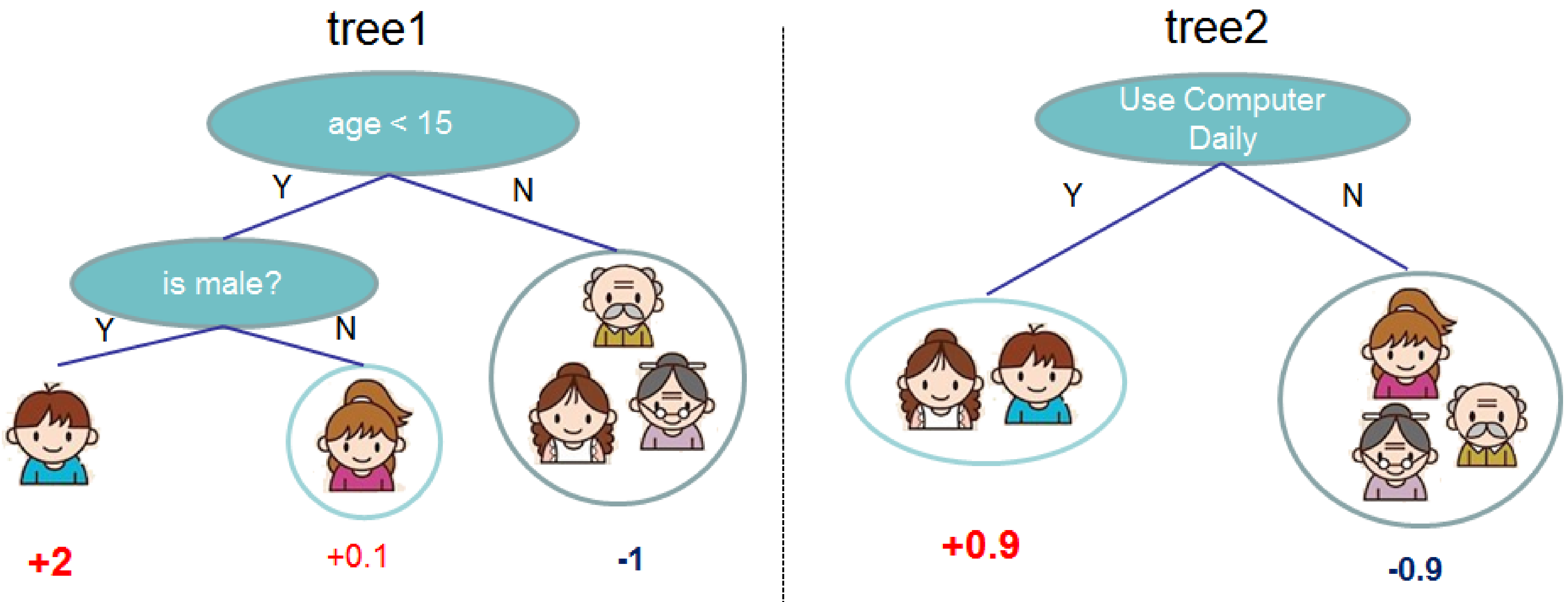
# Weak learners and strong learners

- Weak learner: ML algorithm that is slightly better than chance
  - Example: Decision tree 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 the data
- Weighing each weak prediction according to each weak learner's performance
- Combine the weighted predictions to obtain a single weighted prediction
- ... that is much better than the individual predictions themselves!

# Boosting example




f(  ) = 2 + 0.9= 2.9     f(  )= -1 - 0.9 = -1.9

[1] https://xgboost.readthedocs.io/en/latest/model.html

# Model evaluation through cross-validation

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

# Cross-validation in XGBoost example

```python
import xgboost as xgb
import pandas as pd
churn_data = pd.read_csv("classification_data.csv")
churn_dmatrix = xgb.DMatrix(data=churn_data.iloc[:,:-1],
        label=churn_data.month_5_still_here)
params={"objective":"binary:logistic","max_depth":4}
cv_results = xgb.cv(dtrain=churn_dmatrix, params=params, nfold=4,
        num_boost_round=10, metrics="error", as_pandas=True)
print("Accuracy: %f" %((1-cv_results["test-error-mean"]).iloc[-1]))
```

```
Accuracy: 0.88315
```

# Let's practice!

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# When should I use XGBoost?

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# When to use XGBoost

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

# When to NOT use XGBoost

- Image recognition
- Computer vision
- Natural language processing and understanding problems
- When the number of training samples is significantly smaller than the number of features

# Let's practice!

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# Regression review

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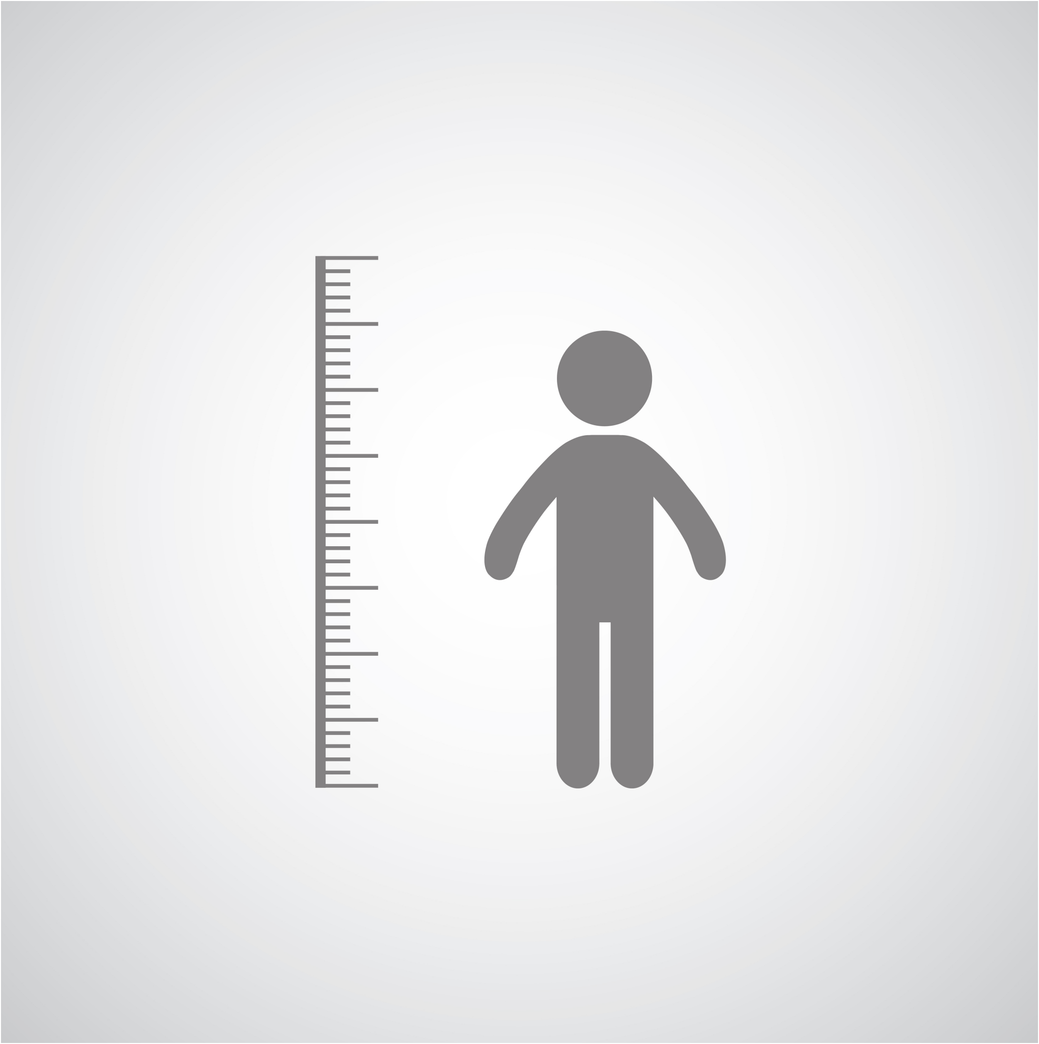
# Regression basics

- 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

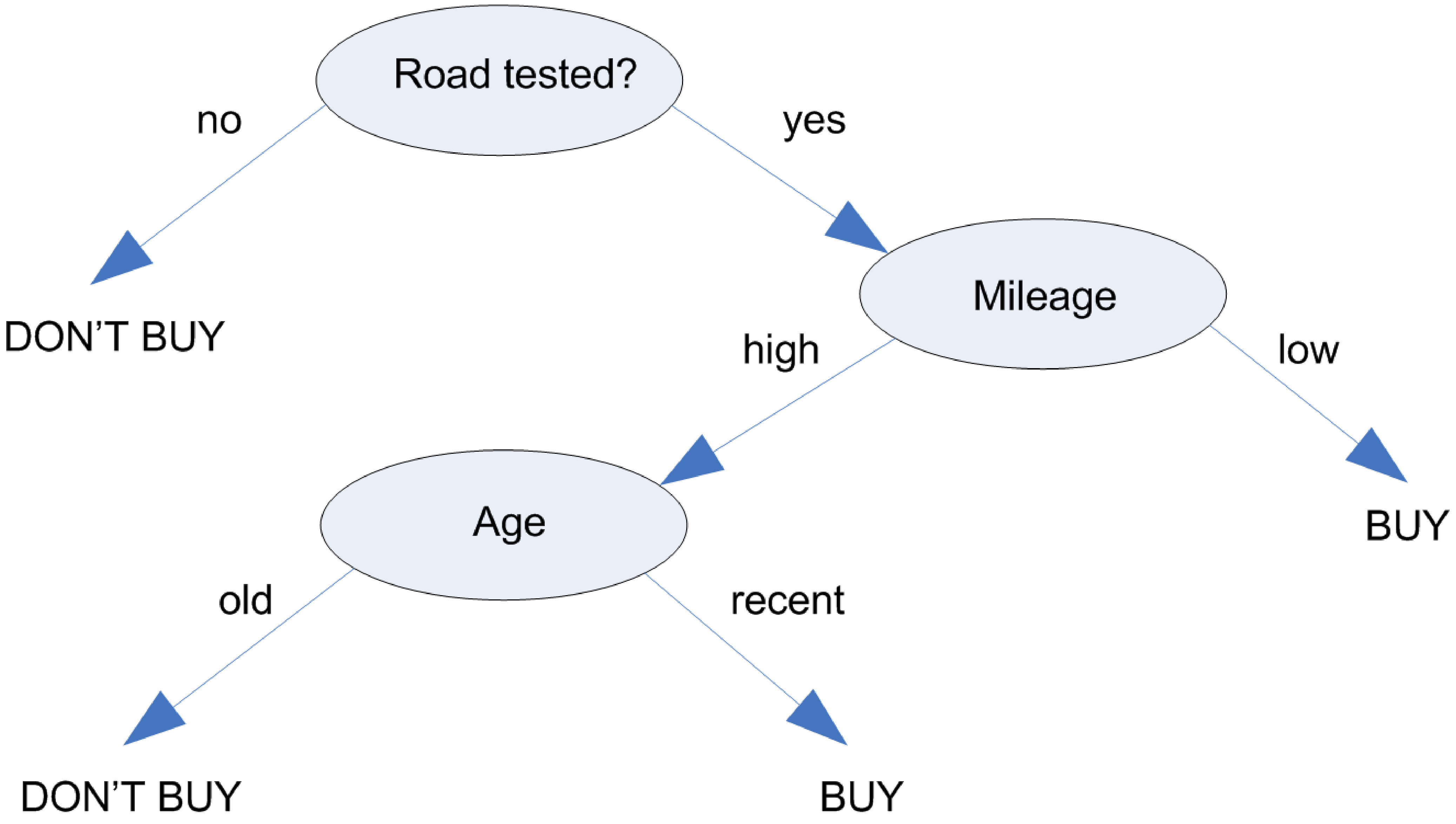
| Actual | Predicted | Error |
|---|---|---|
| 10 | 20 | -10 |
| 3 | 8 | -5 |
| 6 | 1 | 5 |

- 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

# 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

```
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
                                                       random_state
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!

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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

```
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]
rmses_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)
    rmses_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,rmses_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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# Why tune your model?

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# Untuned model example

```
import pandas as pd
import xgboost as xgb
import numpy as np
housing_data = pd.read_csv("ames_housing_trimmed_processed.csv")
X,y = housing_data[housing_data.columns.tolist()[:-1]],
        housing_data[housing_data.columns.tolist()[-1]]
housing_dmatrix = xgb.DMatrix(data=X,label=y)
untuned_params={"objective":"reg:linear"}
untuned_cv_results_rmse = xgb.cv(dtrain=housing_dmatrix,
        params=untuned_params,nfold=4,
        metrics="rmse",as_pandas=True,seed=123)
print("Untuned rmse: %f" %((untuned_cv_results_rmse["test-rmse-mean"]).tail(1)))
```

```
Untuned rmse: 34624.229980
```

# Tuned model example

```python
import pandas as pd
import xgboost as xgb
import numpy as np
housing_data = pd.read_csv("ames_housing_trimmed_processed.csv")
X,y = housing_data[housing_data.columns.tolist()[:-1]],
     housing_data[housing_data.columns.tolist()[-1]]
housing_dmatrix = xgb.DMatrix(data=X,label=y)
tuned_params = {"objective":"reg:linear",'colsample_bytree': 0.3,
    'learning_rate': 0.1, 'max_depth': 5}
tuned_cv_results_rmse = xgb.cv(dtrain=housing_dmatrix,
     params=tuned_params, nfold=4, num_boost_round=200, metrics="rmse",
     as_pandas=True, seed=123)
print("Tuned rmse: %f" %((tuned_cv_results_rmse["test-rmse-mean"]).tail(1)))
```

```
Tuned rmse: 29812.683594
```

# Let's tune some models!

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# Tunable parameters in XGBoost

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# Common tree tunable parameters

- **learning rate:** learning rate/eta
- **gamma:** min loss reduction to create new tree split
- **lambda:** L2 reg on leaf weights
- **alpha:** L1 reg on leaf weights
- **max_depth:** max depth per tree
- **subsample:** % samples used per tree
- **colsample_bytree:** % features used per tree

# Linear tunable parameters

- **lambda:** L2 reg on weights
- **alpha:** L1 reg on weights
- **lambda_bias:** L2 reg term on bias
- You can also tune the number of estimators used for both base model types!

# Let's get to some tuning!

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# Review of grid search and random search

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# Grid search: review

- Search exhaustively over a given set of hyperparameters, once per set of hyperparameters
- Number of models = number of distinct values per hyperparameter multiplied across each hyperparameter
- Pick final model hyperparameter values that give best cross-validated evaluation metric value

# Grid search: example

```
import pandas as pd
import xgboost as xgb
import numpy as np
from sklearn.model_selection import GridSearchCV
housing_data = pd.read_csv("ames_housing_trimmed_processed.csv")
X, y = housing_data[housing_data.columns.tolist()[:-1]],
       housing_data[housing_data.columns.tolist()[-1]
housing_dmatrix = xgb.DMatrix(data=X,label=y)
gbm_param_grid = {'learning_rate': [0.01,0.1,0.5,0.9],
                  'n_estimators': [200],
                  'subsample': [0.3, 0.5, 0.9]}
gbm = xgb.XGBRegressor()
grid_mse = GridSearchCV(estimator=gbm,param_grid=gbm_param_grid,
            scoring='neg_mean_squared_error', cv=4, verbose=1)
grid_mse.fit(X, y)
print("Best parameters found: ",grid_mse.best_params_)
print("Lowest RMSE found: ", np.sqrt(np.abs(grid_mse.best_score_)))
```

```
Best parameters found: {'learning_rate': 0.1,
'n_estimators': 200, 'subsample': 0.5}
Lowest RMSE found:  28530.1829341
```

# Random search: review

- Create a (possibly infinite) range of hyperparameter values per hyperparameter that you would like to search over
- Set the number of iterations you would like for the random search to continue
- During each iteration, randomly draw a value in the range of specified values for each hyperparameter searched over and train/evaluate a model with those hyperparameters
- After you've reached the maximum number of iterations, select the hyperparameter configuration with the best evaluated score

# Random search: example

```
import pandas as pd
import xgboost as xgb
import numpy as np
from sklearn.model_selection import RandomizedSearchCV
housing_data = pd.read_csv("ames_housing_trimmed_processed.csv")
X,y = housing_data[housing_data.columns.tolist()[:-1]],
      housing_data[housing_data.columns.tolist()[-1]]
housing_dmatrix = xgb.DMatrix(data=X,label=y)
gbm_param_grid = {'learning_rate': np.arange(0.05,1.05,.05),
                  'n_estimators': [200],
                  'subsample': np.arange(0.05,1.05,.05)}
gbm = xgb.XGBRegressor()
randomized_mse = RandomizedSearchCV(estimator=gbm, param_distributions=gbm_param_grid,
                        n_iter=25, scoring='neg_mean_squared_error', cv=4, verbose=1)
randomized_mse.fit(X, y)
print("Best parameters found: ",randomized_mse.best_params_)
print("Lowest RMSE found: ", np.sqrt(np.abs(randomized_mse.best_score_)))
```

```
Best parameters found: {'subsample': 0.6000000000000009,
'n_estimators': 200, 'learning_rate': 0.20000000000000001}
Lowest RMSE found: 28300.2374291
```

# Let's practice!

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# Limits of grid search and random search

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# Grid search and random search limitations

- Grid Search
  - Number of models you must build with every additional new parameter grows very quickly
- Random Search
  - Parameter space to explore can be massive
  - Randomly jumping throughout the space looking for a "best" result becomes a waiting game

# Let's practice!

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# Review of pipelines using sklearn

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# Pipeline review

- Takes a list of named 2-tuples (name, pipeline_step) as input
- Tuples can contain any arbitrary scikit-learn compatible estimator or transformer object
- Pipeline implements fit/predict methods
- Can be used as input estimator into grid/randomized search and cross_val_score methods

# Scikit-learn pipeline example

```
import pandas as pd
from sklearn.ensemble import RandomForestRegressor
import numpy as np
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import Pipeline
from sklearn.model_selection import cross_val_score
names = ["crime","zone","industry","charles","no","rooms",
        "age", "distance","radial","tax","pupil","aam","lower","med_price"]

data = pd.read_csv("boston_housing.csv",names=names)

X, y = data.iloc[:,:-1], data.iloc[:,-1]
rf_pipeline = Pipeline[("st_scaler",
                StandardScaler()),
                ("rf_model",RandomForestRegressor())]

scores = cross_val_score(rf_pipeline,X,y,
scoring="neg_mean_squared_error",cv=10)
```

# Scikit-learn pipeline example

```
final_avg_rmse = np.mean(np.sqrt(np.abs(scores)))

print("Final RMSE:", final_avg_rmse)
```

```
Final RMSE: 4.54530686529
```

# Preprocessing I: LabelEncoder and OneHotEncoder

- `LabelEncoder` : Converts a categorical column of strings into integers
- `OneHotEncoder` : Takes the column of integers and encodes them as dummy variables
- Cannot be done within a pipeline

# Preprocessing II: DictVectorizer

- Traditionally used in text processing
- Converts lists of feature mappings into vectors
- Need to convert DataFrame into a list of dictionary entries
- Explore the **scikit-learn documentation**

# Let's build pipelines!

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# Incorporating xgboost into pipelines

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# Scikit-learn pipeline example with XGBoost

```
import pandas as pd
import xgboost as xgb
import numpy as np
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import Pipeline
from sklearn.model_selection import cross_val_score
names = ["crime","zone","industry","charles","no","rooms","age",
        "distance","radial","tax","pupil","aam","lower","med_price"]
data = pd.read_csv("boston_housing.csv",names=names)
X, y = data.iloc[:,:-1], data.iloc[:,-1]
xgb_pipeline = Pipeline[("st_scaler", StandardScaler()),
                        ("xgb_model",xgb.XGBRegressor())]
scores = cross_val_score(xgb_pipeline, X, y,
                         scoring="neg_mean_squared_error",cv=10)
final_avg_rmse = np.mean(np.sqrt(np.abs(scores)))
print("Final XGB RMSE:", final_avg_rmse)
```

```
Final RMSE: 4.02719593323
```

# Additional components introduced for pipelines

- `sklearn_pandas` :
  - `DataFrameMapper` - Interoperability between `pandas` and `scikit-learn`
  - `CategoricalImputer` - Allow for imputation of categorical variables before conversion to integers
- `sklearn.preprocessing` :
  - `Imputer` - Native imputation of numerical columns in scikit-learn
- `sklearn.pipeline` :
  - `FeatureUnion` - combine multiple pipelines of features into a single pipeline of features

# Let's practice!

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# Tuning xgboost hyperparameters in a pipeline

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# Tuning XGBoost hyperparameters in a pipeline

```
import pandas as pd
   ...: import xgboost as xgb
   ...: import numpy as np
   ...: from sklearn.preprocessing import StandardScaler
   ...: from sklearn.pipeline import Pipeline
   ...: from sklearn.model_selection import RandomizedSearchCV
names = ["crime","zone","industry","charles","no",
   ...: "rooms","age", "distance","radial","tax",
   ...: "pupil","aam","lower","med_price"]
data = pd.read_csv("boston_housing.csv",names=names)
X, y = data.iloc[:,:-1],data.iloc[:,-1]
xgb_pipeline = Pipeline[("st_scaler",
   ...: StandardScaler()), ("xgb_model",xgb.XGBRegressor())]
gbm_param_grid = {
   ...:     'xgb_model__subsample': np.arange(.05, 1, .05),
   ...:     'xgb_model__max_depth': np.arange(3,20,1),
   ...:     'xgb_model__colsample_bytree': np.arange(.1,1.05,.05) }
randomized_neg_mse = RandomizedSearchCV(estimator=xgb_pipeline,
   ...: param_distributions=gbm_param_grid, n_iter=10,
   ...: scoring='neg_mean_squared_error', cv=4)
randomized_neg_mse.fit(X, y)
```

# Tuning XGBoost hyperparameters in a pipeline II

```
print("Best rmse: ", np.sqrt(np.abs(randomized_neg_mse.best_score_)))
```

```
Best rmse: 3.9966784203040677
```

```
print("Best model: ", randomized_neg_mse.best_estimator_)
```

```
Best model:  Pipeline(steps=[('st_scaler', StandardScaler(copy=True,
with_mean=True, with_std=True)),
('xgb_model', XGBRegressor(base_score=0.5, colsample_bylevel=1,
       colsample_bytree=0.95000000000000029, gamma=0, learning_rate=
       max_delta_step=0, max_depth=8, min_child_weight=1, missing=No
       n_estimators=100, nthread=-1, objective='reg:linear', reg_alp
       reg_lambda=1, scale_pos_weight=1, seed=0, silent=True,
       subsample=0.90000000000000013))])
```

# Let's finish this up!

EXTREME GRADIENT BOOSTING WITH XGBOOST

# Final Thoughts

EXTREME GRADIENT BOOSTING WITH XGBOOST

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# What We Have Covered And You Have Learned

- Using XGBoost for classification tasks
- Using XGBoost for regression tasks
- Tuning XGBoost's most important hyperparameters
- Incorporating XGBoost into sklearn pipelines

# What We Have Not Covered (And How You Can Proceed)

- Using XGBoost for ranking/recommendation problems (Netflix/Amazon problem)
- Using more sophisticated hyperparameter tuning strategies for tuning XGBoost models (Bayesian Optimization)
- Using XGBoost as part of an ensemble of other models for regression/classification

# Congratulations!

EXTREME GRADIENT BOOSTING WITH XGBOOST