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?



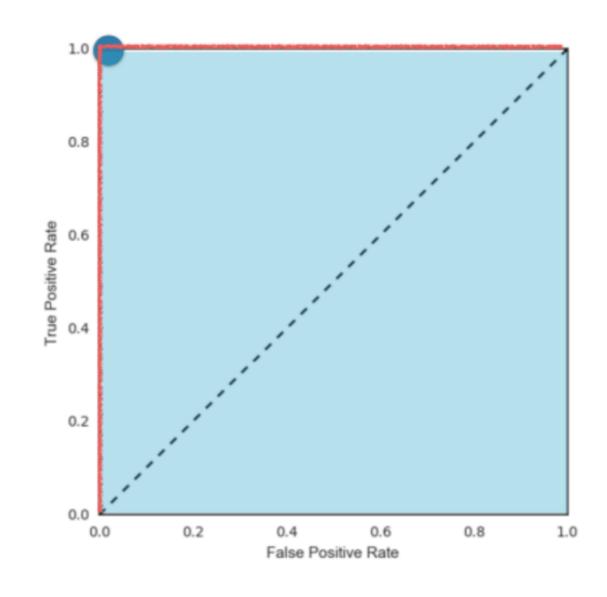
Multi-class classification example

• 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

Actual: Spam Email

Actual: Real Email

Predicted: Spam Email	Predicted: Real Email
True Positive	False Negative
False Positive	True Negative

Accuracy

$$\frac{tp+tn}{tp+tn+fp+fn}$$

Review

• Supervised Learning with scikit-learn



Other supervised learning considerations

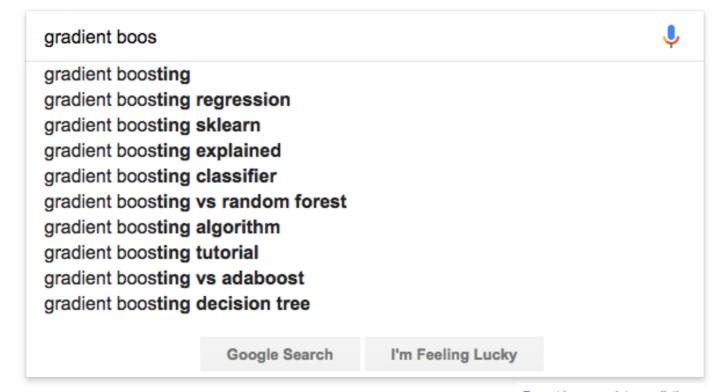
- Features can be either numeric or categorical
- Numeric features should be scaled (Z-scored)
- Categorical features should be encoded (one-hot)



Ranking

Predicting an ordering on a set of choices





Report inappropriate predictions



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

```
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?

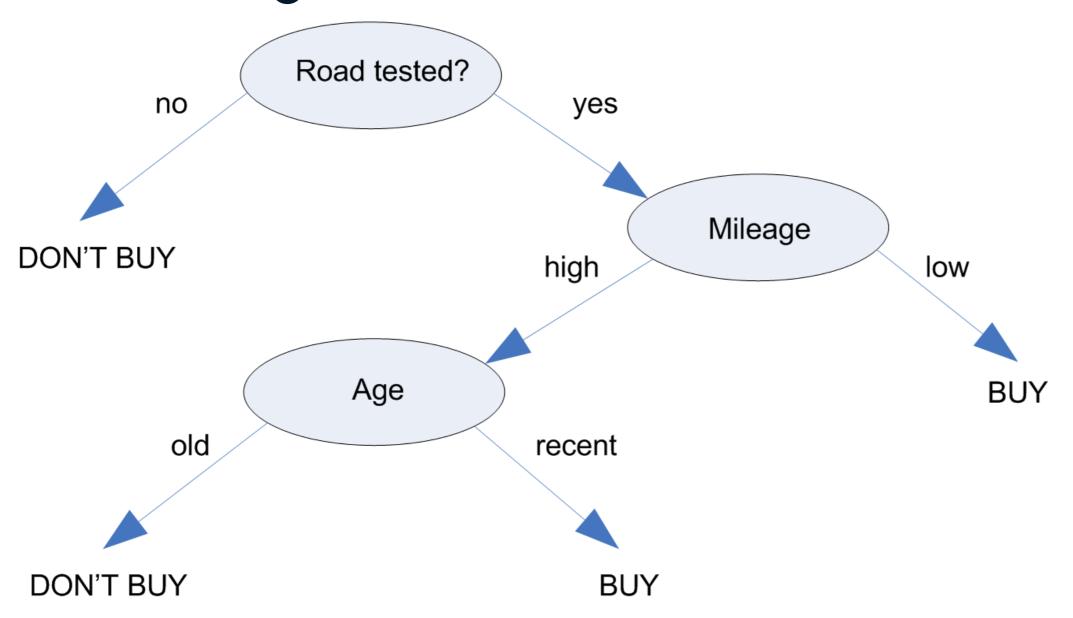
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Visualizing a decision tree



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

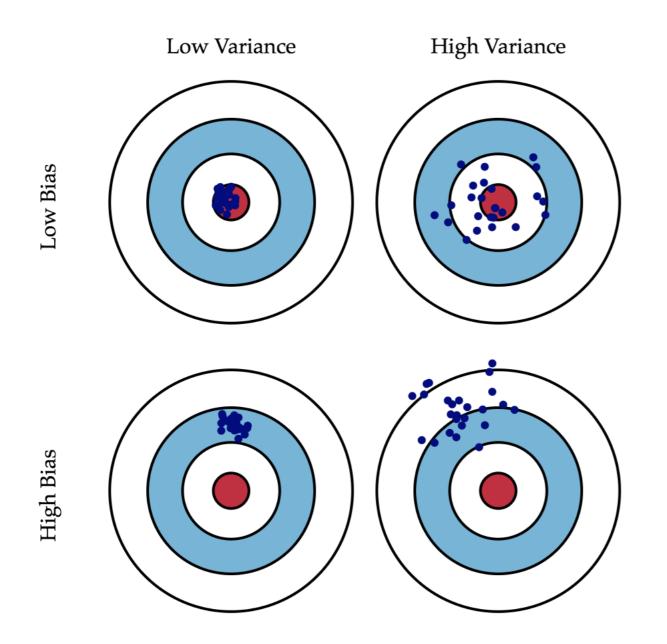


Decision trees and CART

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



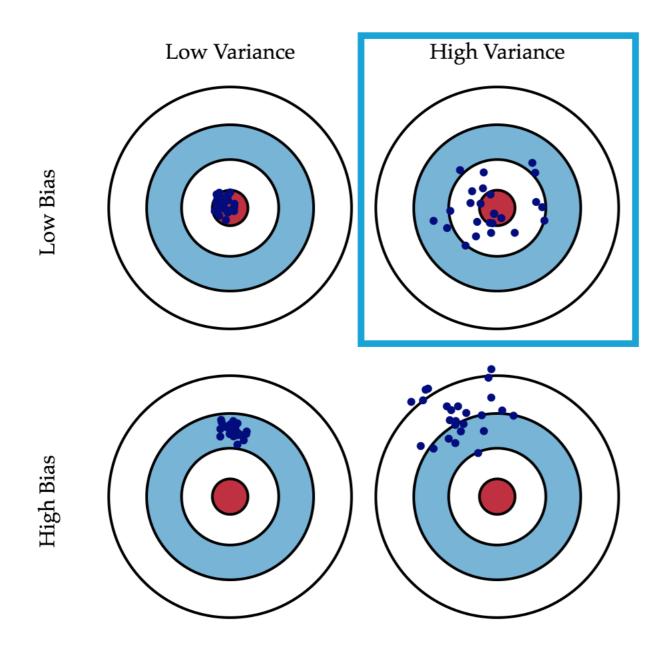
Individual decision trees tend to overfit



¹ http://scott.fortmann-roe.com/docs/BiasVariance.html



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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

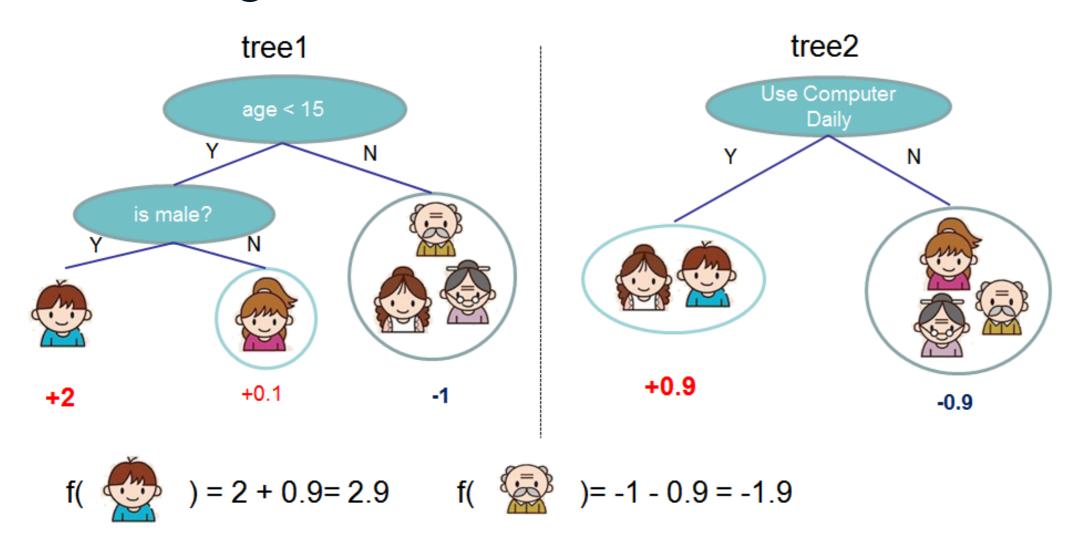
- Weak learner: ML algorithm that is slightly better than chance
 - Example: Decision tree whose predictions are slightly better than 50%
- Boosting converts a collection of weak learners into a strong learner
- Strong learner: Any algorithm that can be tuned to achieve good performance

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



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

Accuracy: 0.88315



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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

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