Lec.2. XGBoost

Machine Learning II

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XGBoost

Before to get started w/ XGB you have to know:

1. What supervised learning is
2. Decision trees
3. Boosting

Supervised learning

- Relies on the labeled data
- Have some understanding of past behaviour

Supervised learning example

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

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

Supervised learning

In majority of the cases you have either a classification or a regression problem

- Classification does a binary or multiclass classification
- Regression predicts a real value

Supervised learning. Binary classification

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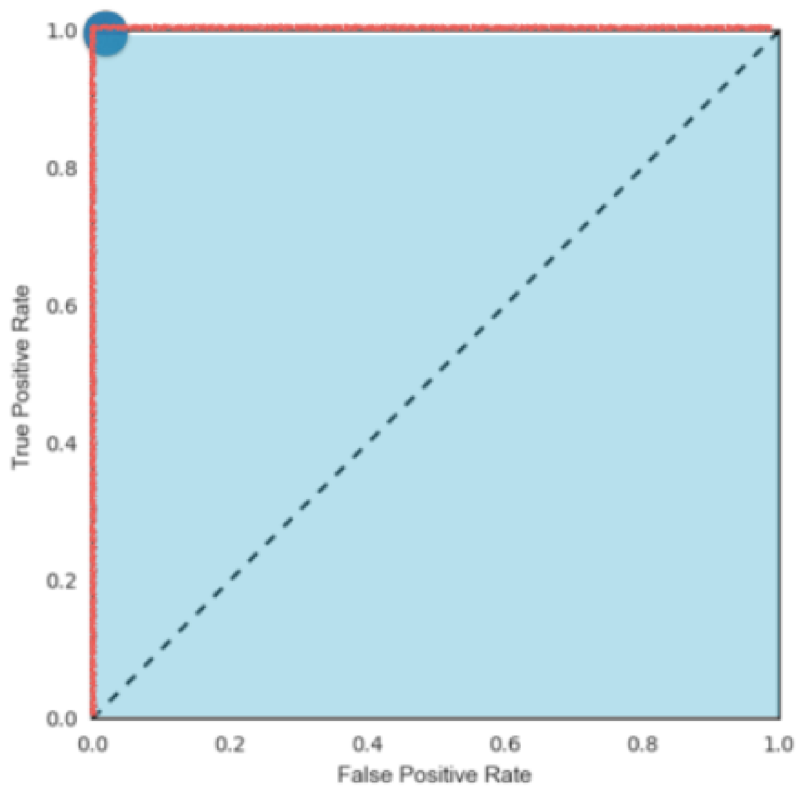
AUC is simply the probability that a randomly chosen positive data point will have a higher rank than a randomly chosen negative data point for your learning problem

Supervised learning. AUC.

Larger area under the ROC curve = better model



Supervised learning. AUC.

Some useful readings:

- https://towardsdatascience.com/understanding-auc-roc-curve-68b2303cc9c5
- https://towardsdatascience.com/data-science-performance-metrics-for-everyone-4d68f4859eef

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

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

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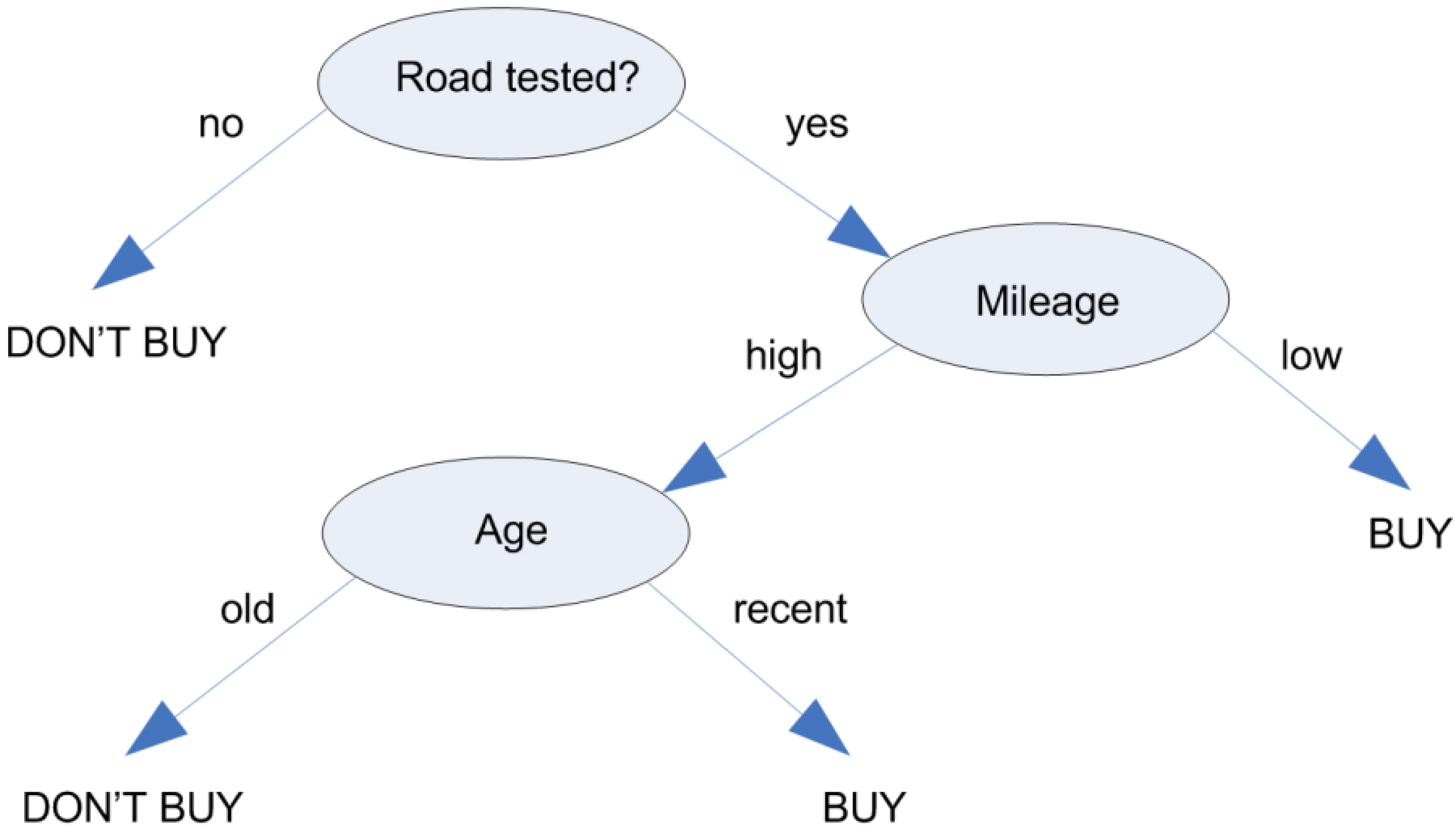
- Numeric features should be scaled (Z-scored, standardized)
- Categorical features should be encoded ((label) one-hot)

Decision Trees



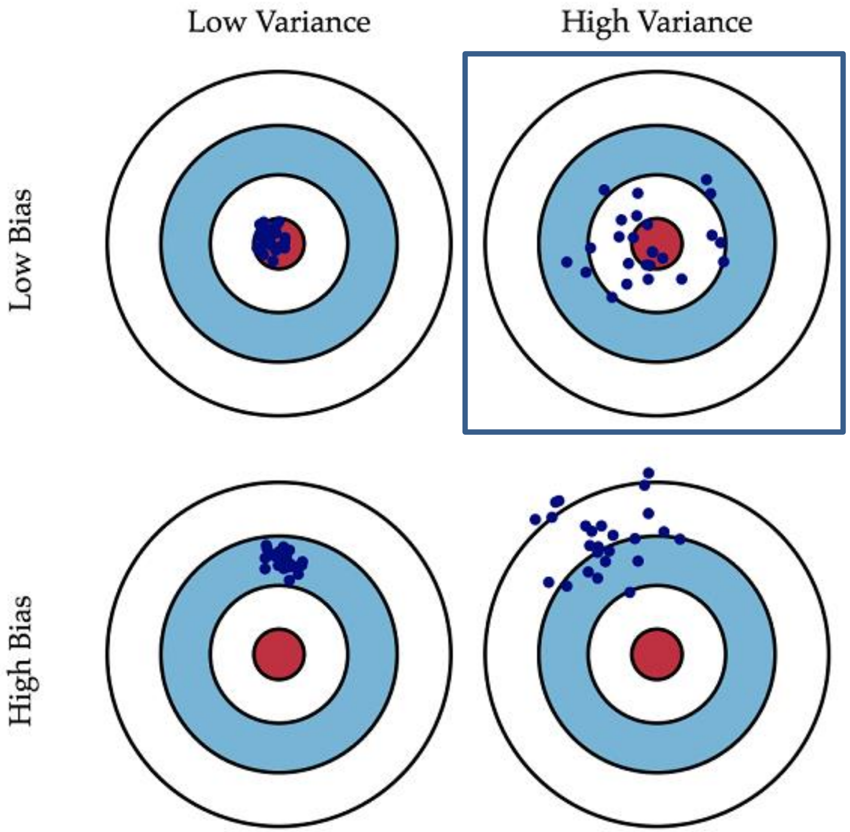
Decision trees as base learners

- 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



This means that they train good at some data you provide it with, but **<u>generalize very poorly</u>** on it. Therefore, it predicts not very well on new data.

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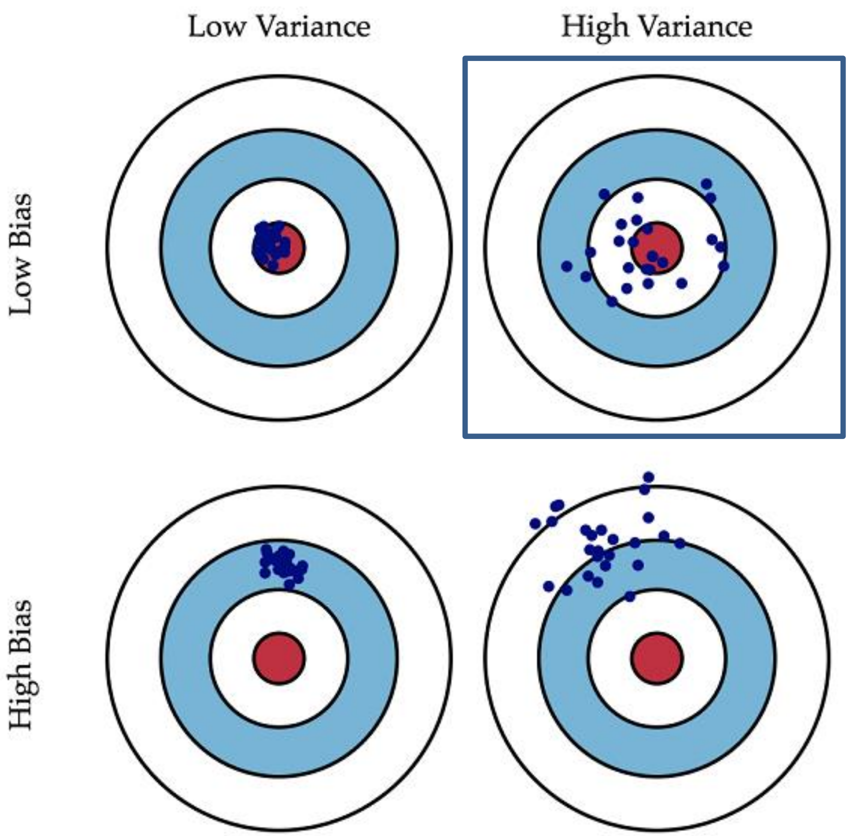

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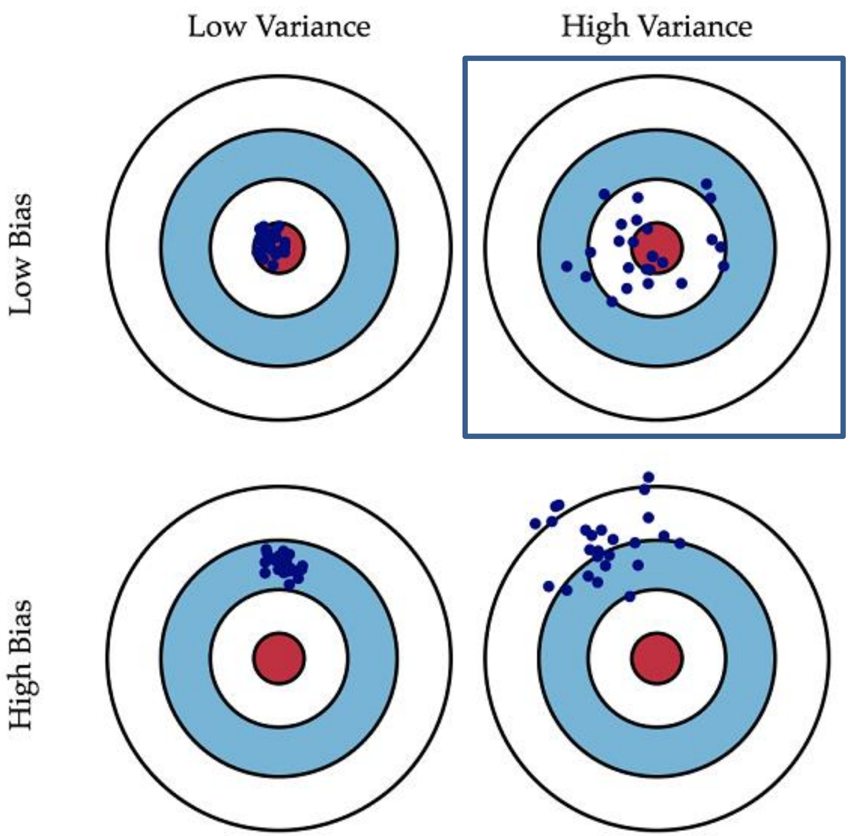

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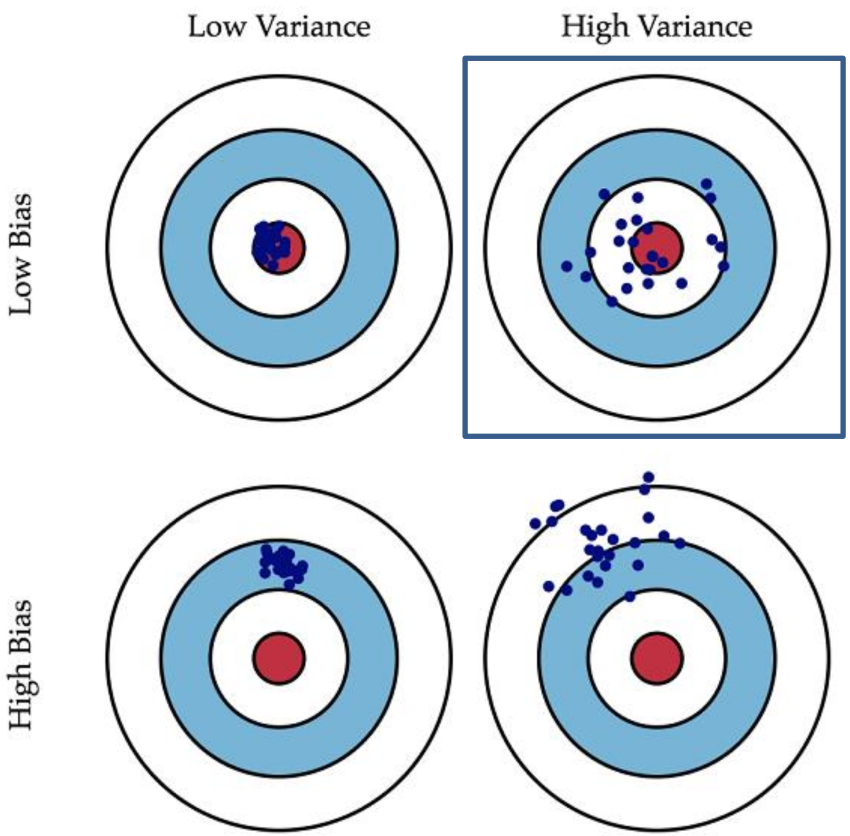

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XGBoost uses slightly different kind of a decision tree, called as CART. The individual decision trees leafs always contain decision values. Whereas CART contain only real-valued score in each leaf, regardless of whether they are used of regression or classification. The real-valued scores can then be thresholded to convert into categories for classification, if necessary

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- 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%

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- 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

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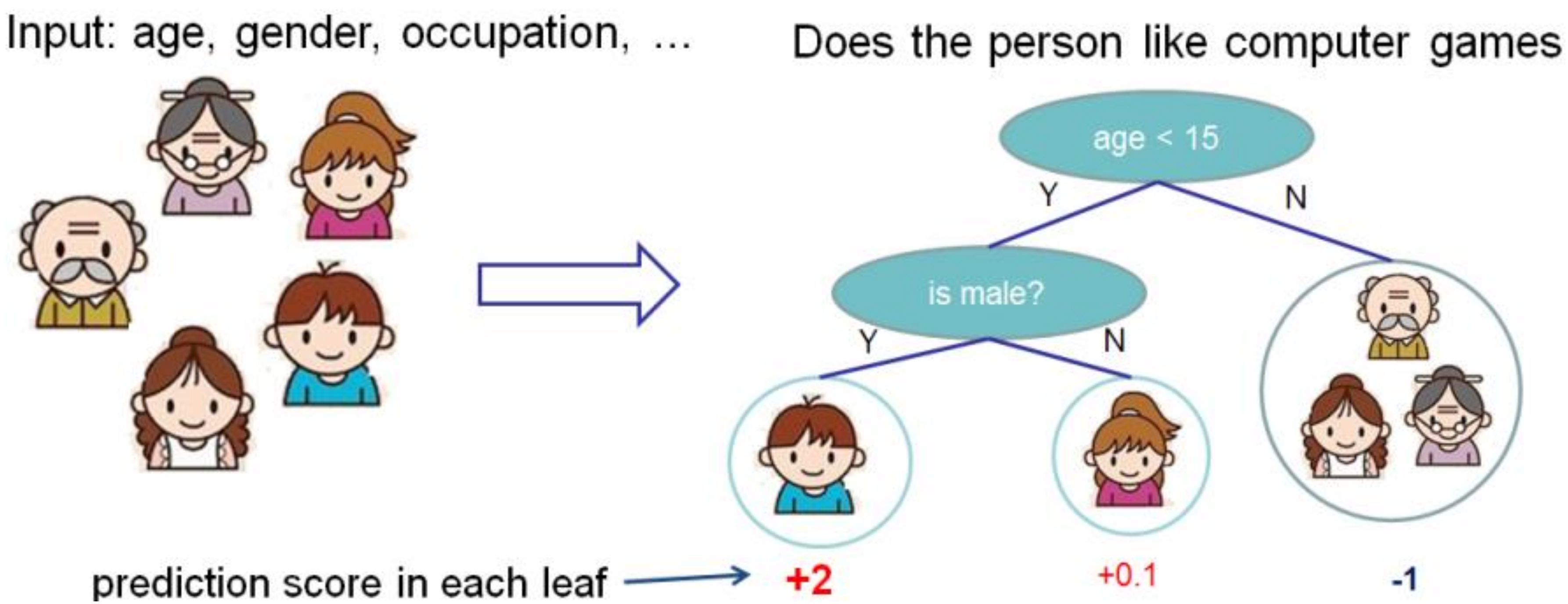
- Iteratively learning a set of weak models on subsets of the data
- Weighing each weak prediction according to each weak learner's performance
- Combine the weighted predictions to obtain a single weighted prediction
- ... that is much better than the individual predictions themselves!

Boosting example



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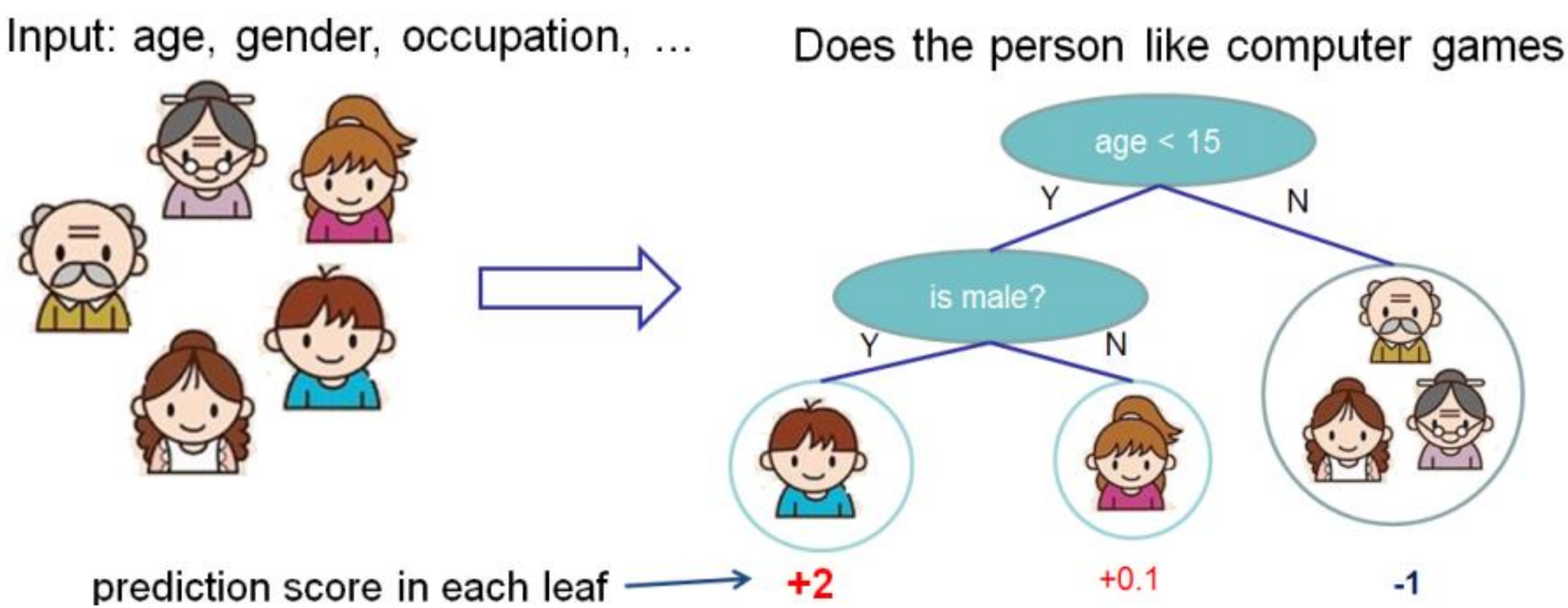

https://xgboost.readthedocs.io/en/latest/tutorials/model.html

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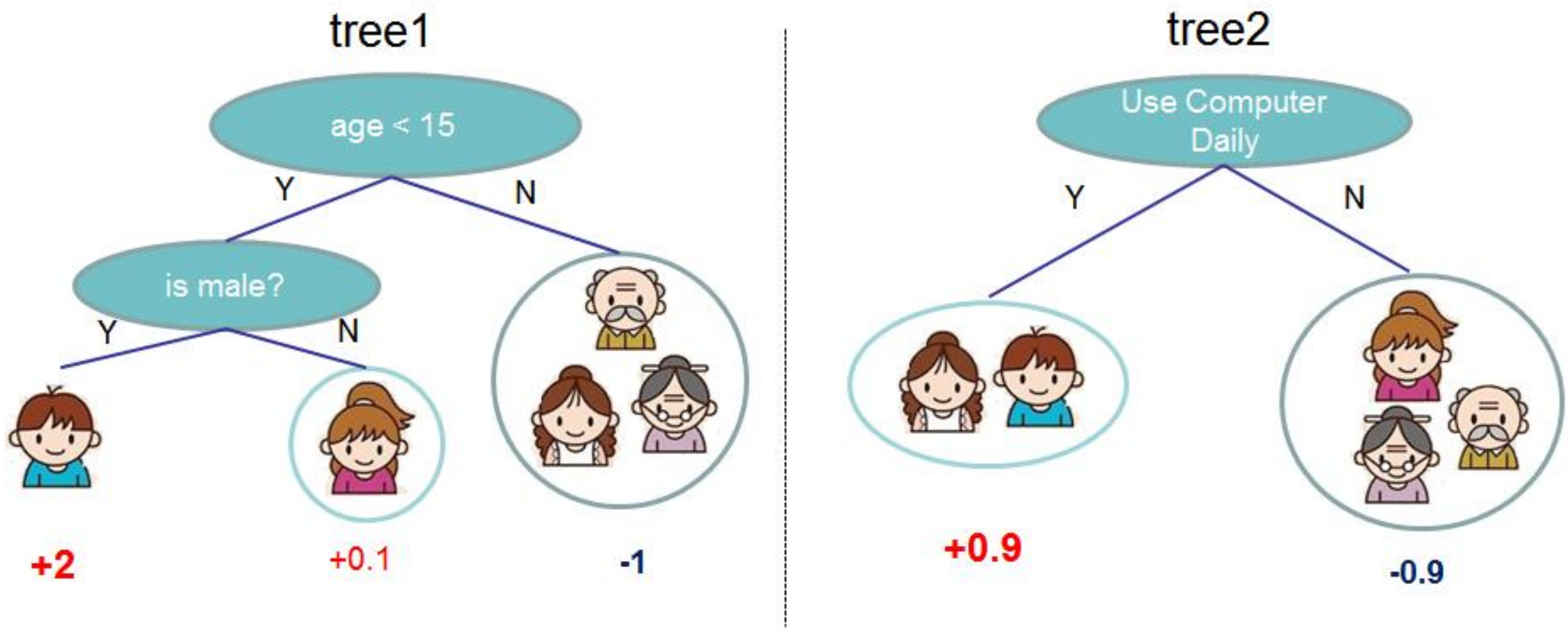

f() = 2 + 0.9= 2.9 f()= -1 - 0.9 = -1.9

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Boosting example

$$\hat{y}_i = \sum_{k=1}^{K} f_k(x_i), f_k \in \mathcal{F}$$

where K is the number of trees, f is a function in the functional space F, and F is the set of all possible CARTs. The objective function to be optimized is given by

$$\text{obj}(\theta) = \sum_{i}^{n} l(y_i, \hat{y}_i) + \sum_{k=1}^{K} \Omega(f_k)$$

where l is a loss and Ω is a complexity regularization

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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

```
In [1]: import xgboost as xgb

In [2]: import pandas as pd

In [3]: class_data = pd.read_csv("classification_data.csv")

In [4]: churn_dmatrix = xgb.DMatrix(data=churn_data.iloc[:,:-1],
        label=churn_data.month_5_still_here)

In [5]: params={"objective":"binary:logistic","max_depth":4}

In [6]: cv_results = xgb.cv(dtrain=churn_dmatrix, params=params, nfold=4,
        num_boost_round=10, metrics="error", as_pandas=True)

In [7]: print("Accuracy: %f" %((1-cv_results["test-error-mean"]).iloc[-1]))
Accuracy: 0.88315
```

XGBoost

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

XGBoost is popular for

- Speed and performance
- Core algorithm is parallelizable
- State-of-the-art performance in many ML task comparing to many other single-algorithm models

XGBoost. Simple example

```
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]: class_data = pd.read_csv("classification_data.csv")

In [6]: X, y = class_data.iloc[:,:-1], class_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_cl = xgb.XGBClassifier(objective='binary:logistic',
        n_estimators=10, seed=123)

In [9]: xg_cl.fit(X_train, y_train)

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

In [11]: accuracy = float(np.sum(preds==y_test))/y_test.shape[0]

In [12]: print("accuracy: %f" % (accuracy))
accuracy: 0.78333
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It uses the fit/predict pattern

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To achieve better results you have to tune the parameters

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

To be continued.

Thanks!