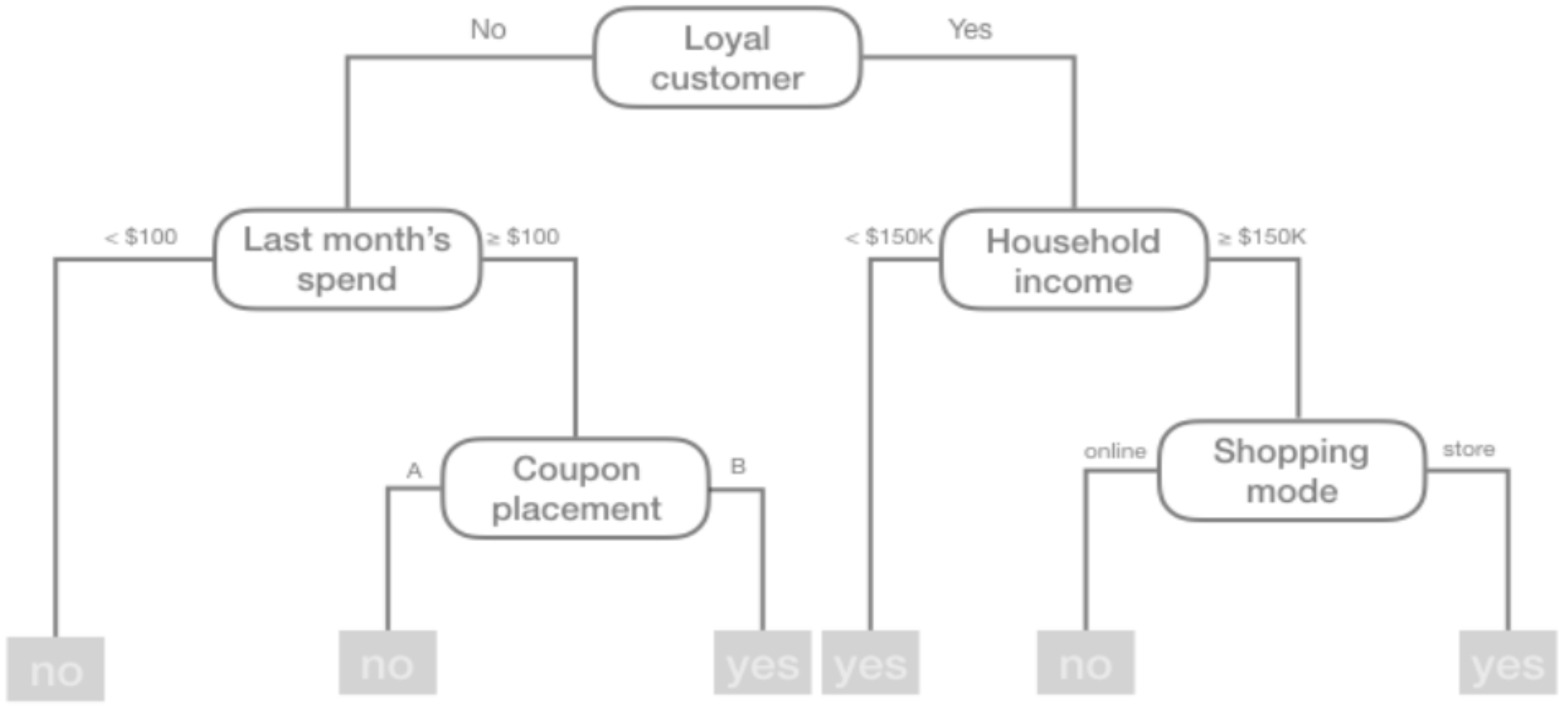
CS135
Introduction to Machine Learning

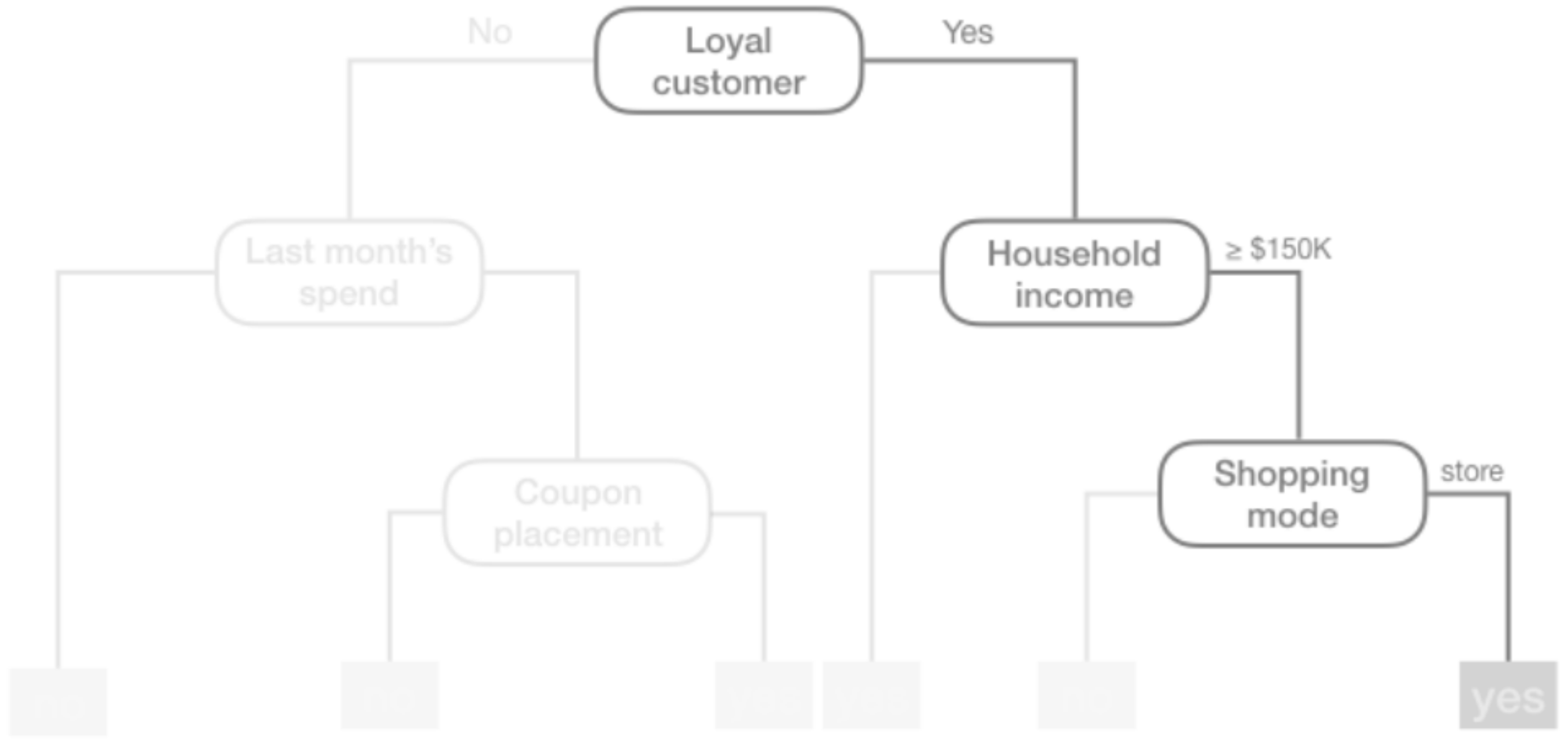
Lecture 10: Classifiers (Decision Tree, Random Forest)

Example Decision Tree – Retail Data



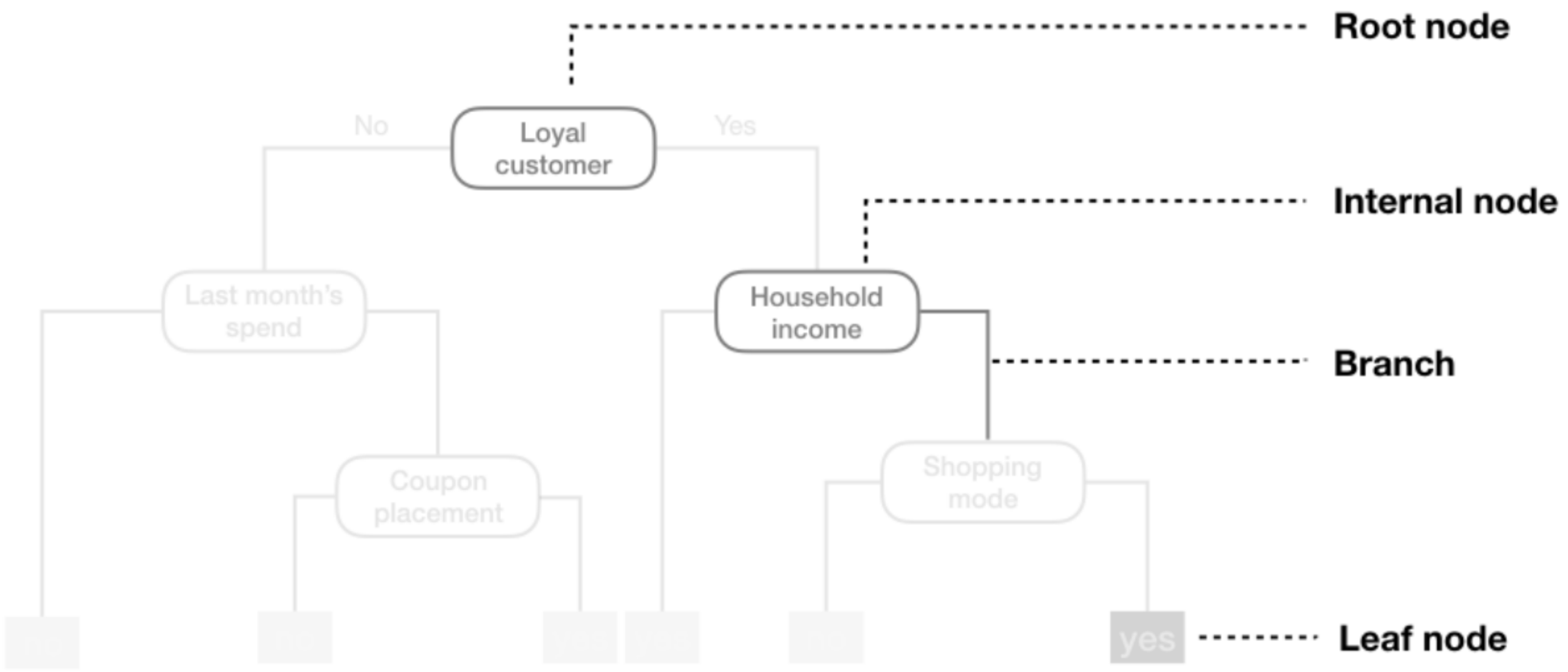
Will a customer redeem a coupon

Decision Tree - Ruleset Model



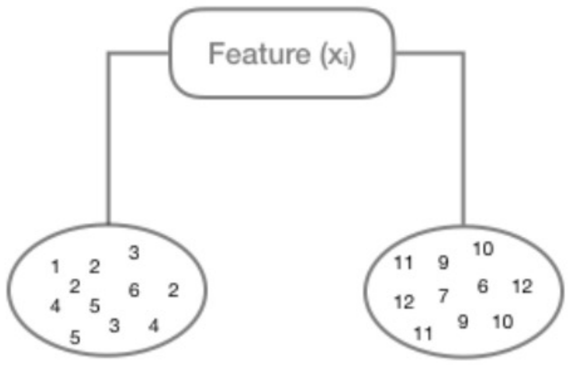
```
if Loyal Customer = Yes and Household income >= $150K and Shopping mode = store then coupon redemption = Yes
```

Terminology



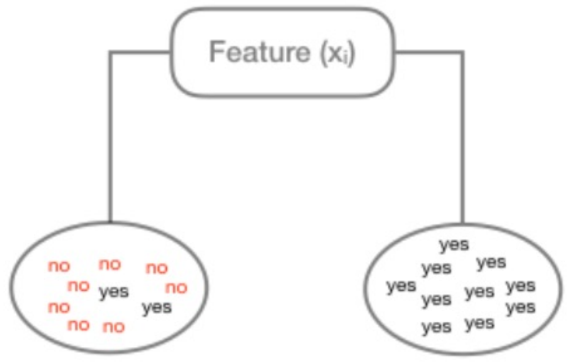
Best Binary Partitioning

Regression tree



Prediction:	3.36	9.7
SSE:	24.55	36.1

Classification tree



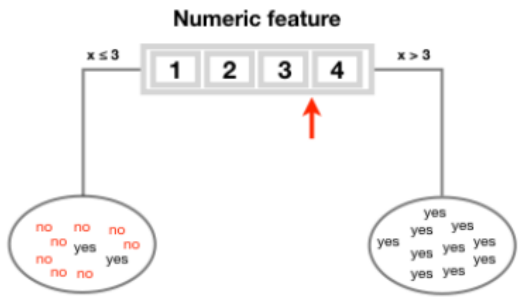
Feature (x_i)
no no no no yes no no yes no no
yes yes yes yes yes yes yes yes yes yes

Prediction:	no	yes
Gini:	.16	0

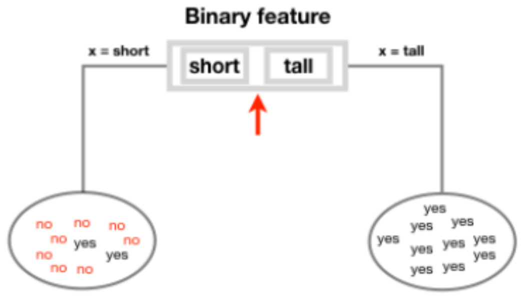
Objective: Minimize disimilarity in terminal nodes

Best Binary Partitioning

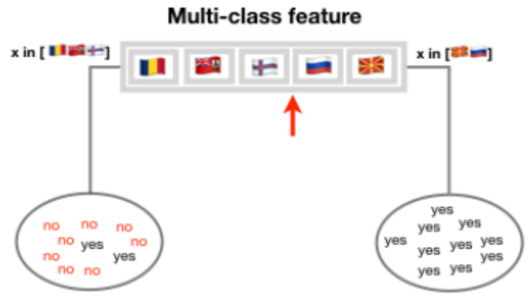
- **Numeric feature**: Numeric split to minimize loss function


Numeric feature
x ≤ 3
x > 3
1
2
3
4
no no no no yes no no yes no no
yes yes yes yes yes yes yes yes yes yes

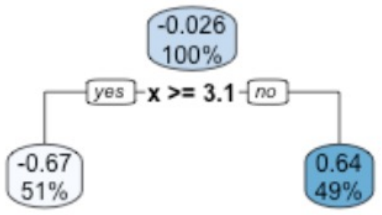
- **Binary feature**: Category split to minimize loss function


Binary feature
x = short
x = tall
short
tall
no no no no yes no no yes no no
yes yes yes yes yes yes yes yes yes yes

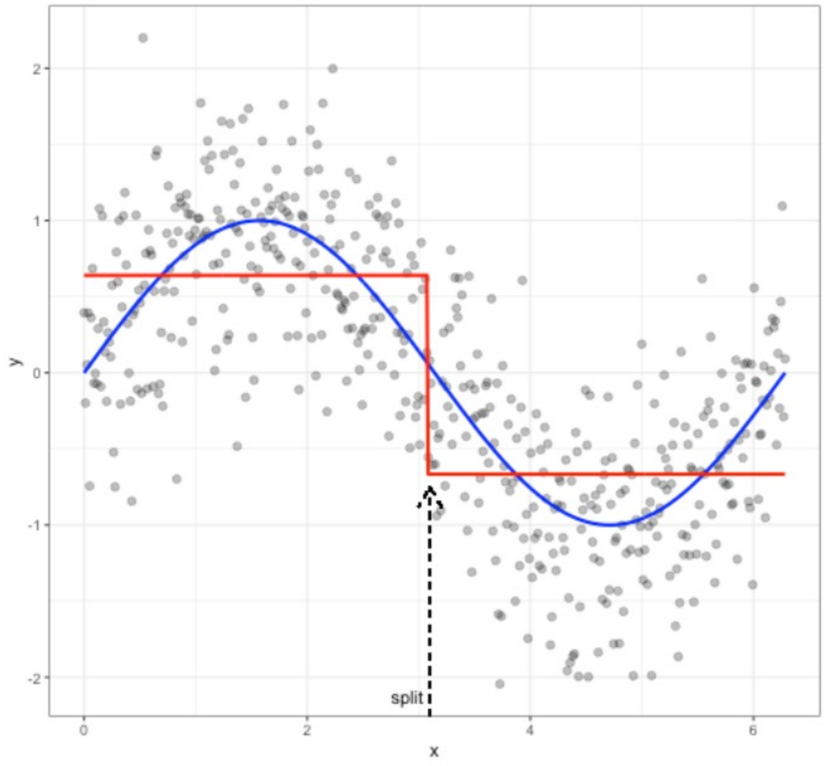
- **Multiclass feature**: Order feature classes based on mean target variable (regression) or class proportion (classification) and choose split to minimize loss function


Multi-class feature
x in [ ]
x in [ ]
no no no no yes no no yes no no
yes yes yes yes yes yes yes yes yes yes

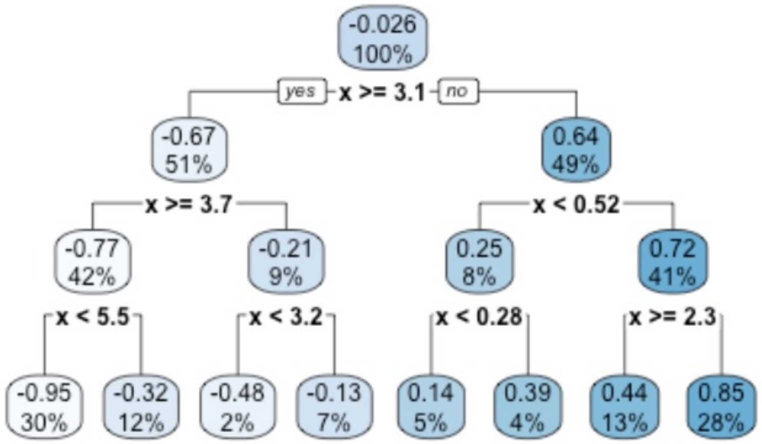
Tree Depth = 1 (Decision Stump)

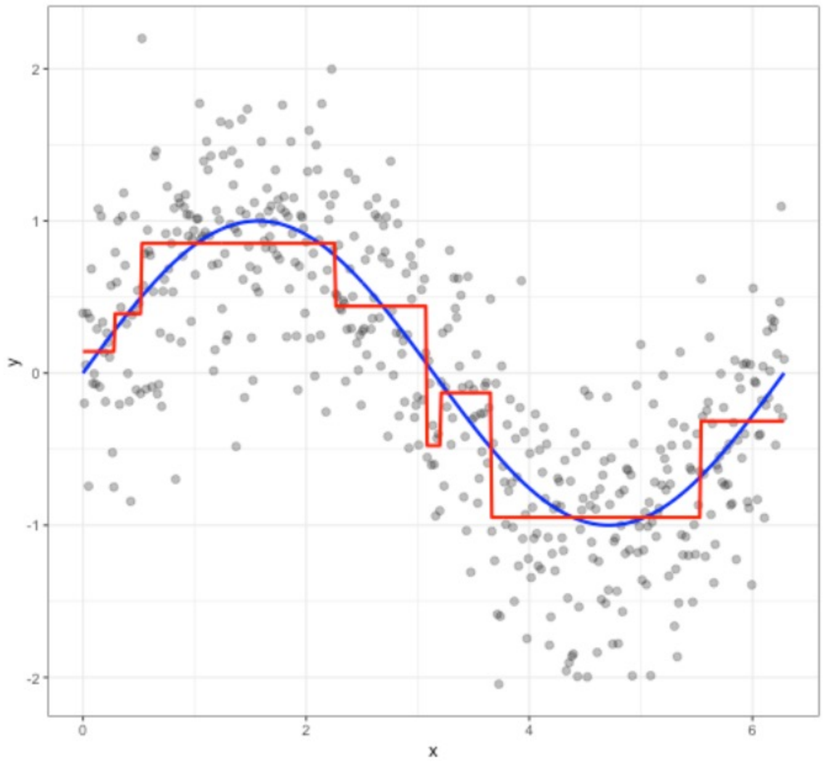


```
##
## Model formula:
## y ~ x
##
## Fitted party:
## [1] root
## |   [2] x >= 3.07863: -0.665 (n = 255, err = 95.5)
## |   [3] x < 3.07863: 0.640 (n = 245, err = 75.9)
##
## Number of inner nodes:    1
## Number of terminal nodes: 2
```



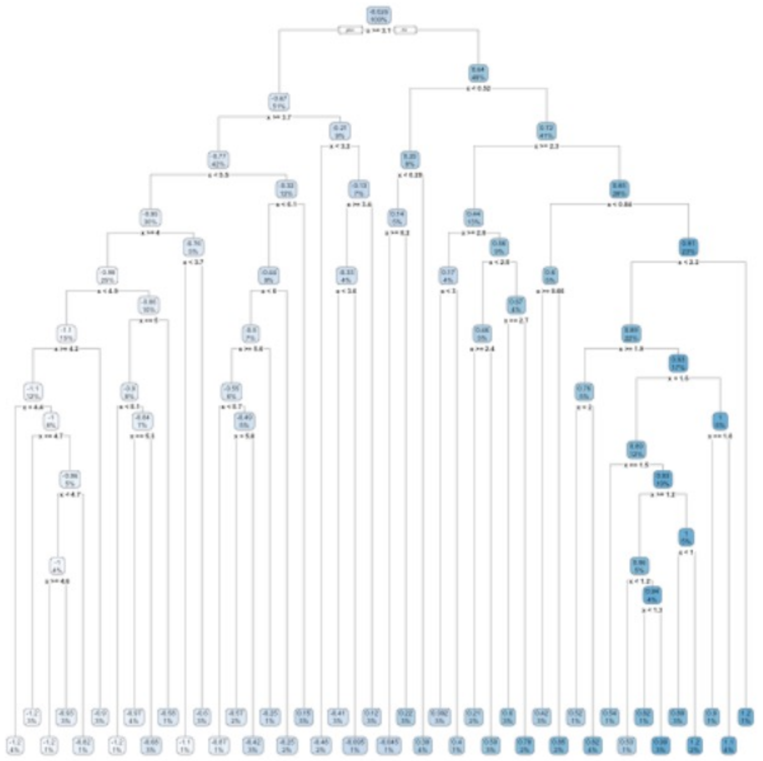
Tree Depth = 3

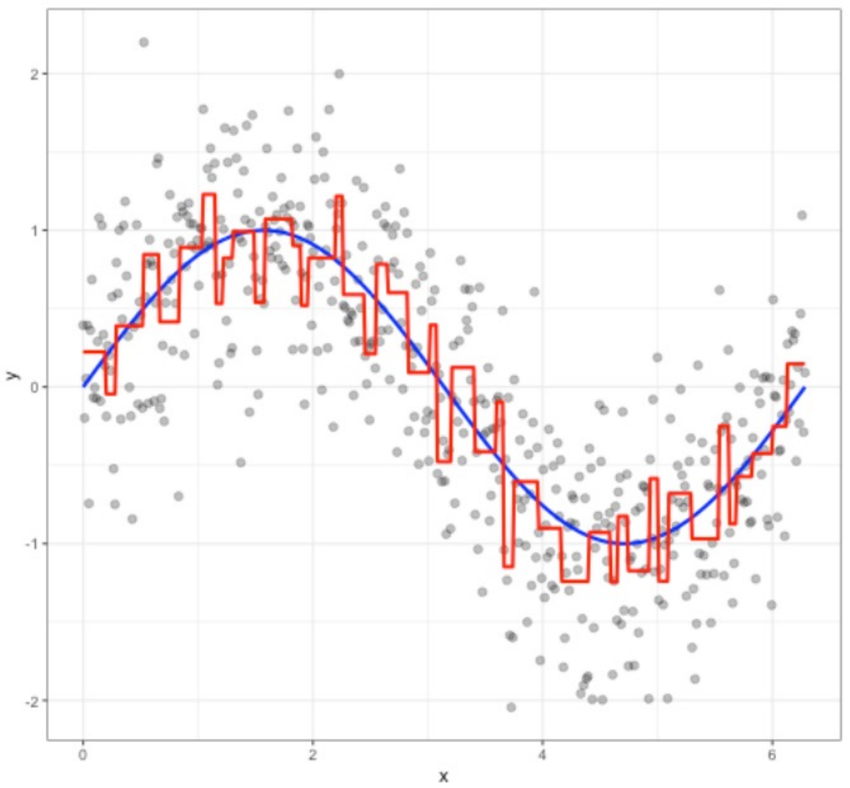




```
##
## Model formula:
## y ~ x
##
## Fitted party:
## [1] root
```

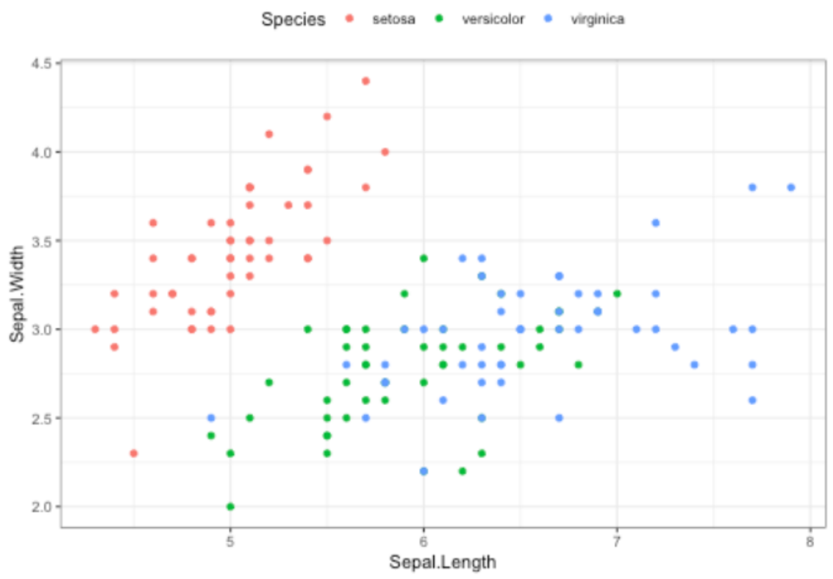
Tree Depth = 20 (Complex Tree)





Two Predictor Decision Boundaries

Classification problem: Iris data



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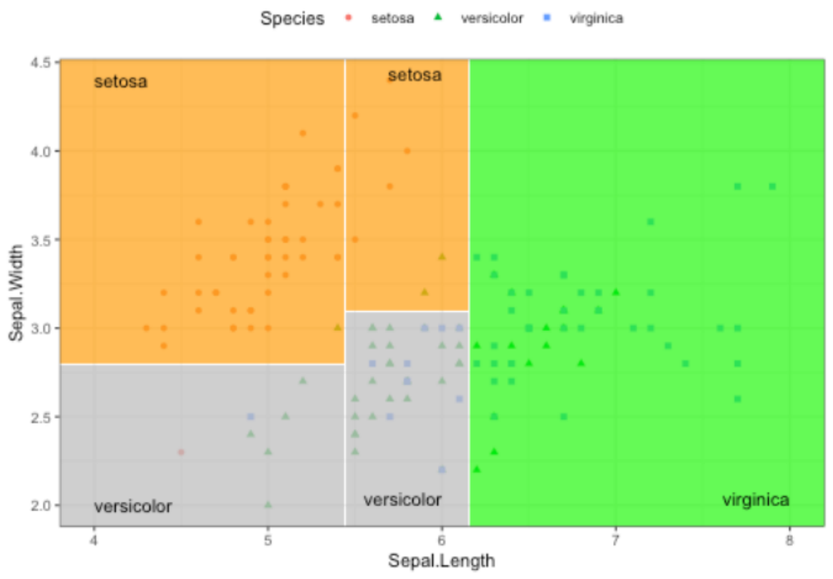
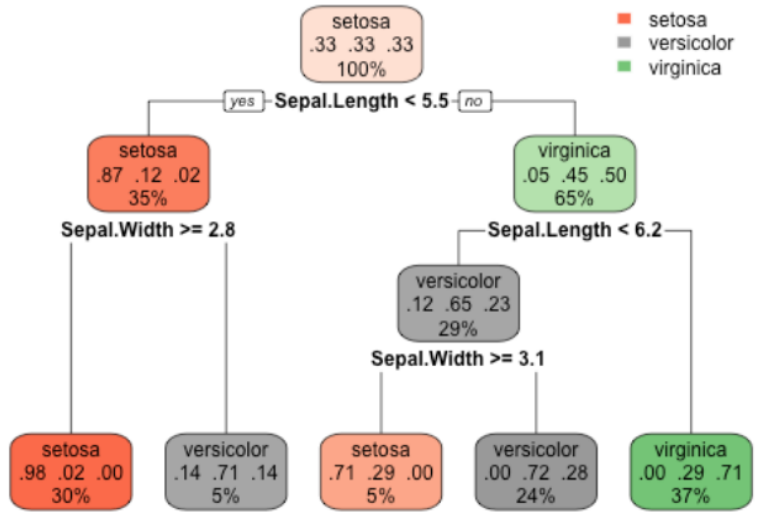
Two Predictor Decision Boundaries

Classification problem: Iris data

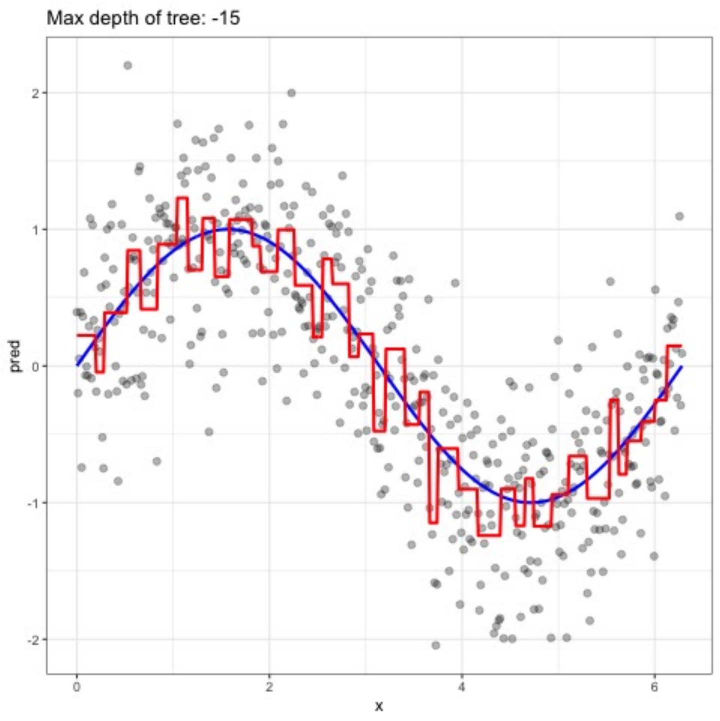


Classification tree

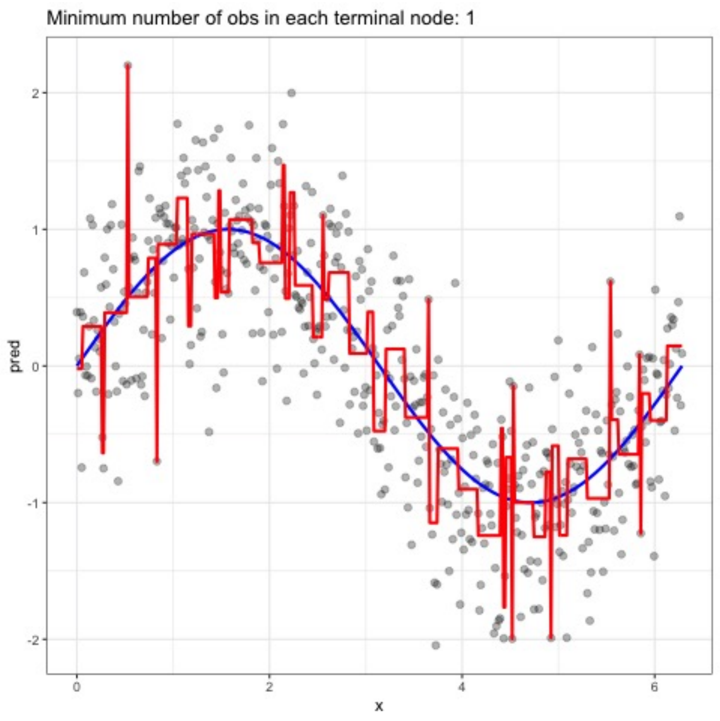


Minimize overfitting: Early stopping

Limit tree depth: Stop splitting after a certain depth



Minimum node "size": Do not split intermediate node which contains too few data points

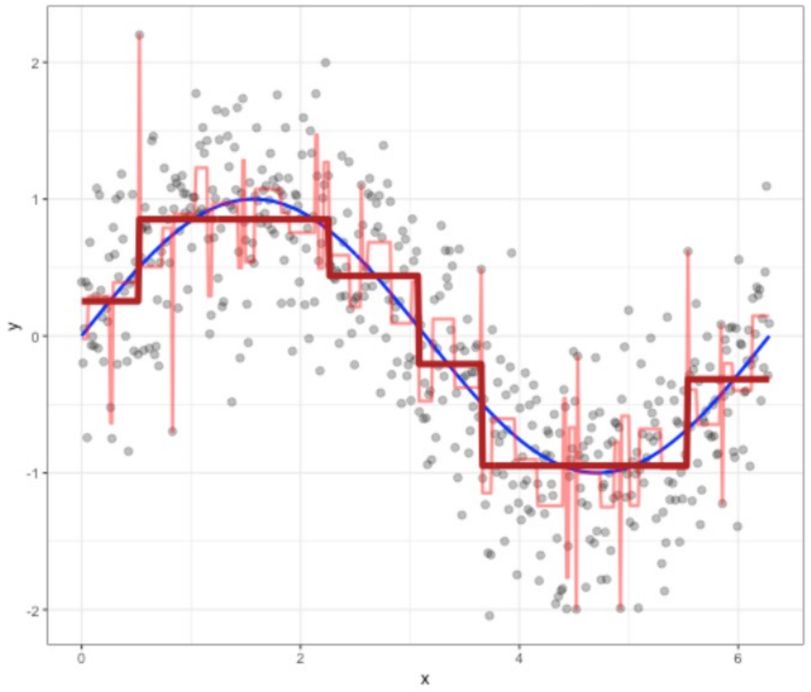


Minimize overfitting: Pruning

1. Grow a very large tree
2. Prune it back with a *cost complexity parameter* (α) × number of terminal nodes (T) to find an optimal subtree:
   - Very similar to lasso penalty in regularized regression
   - Large α = small tree
   - Small α = large tree
   - Find optimal α with cross validation

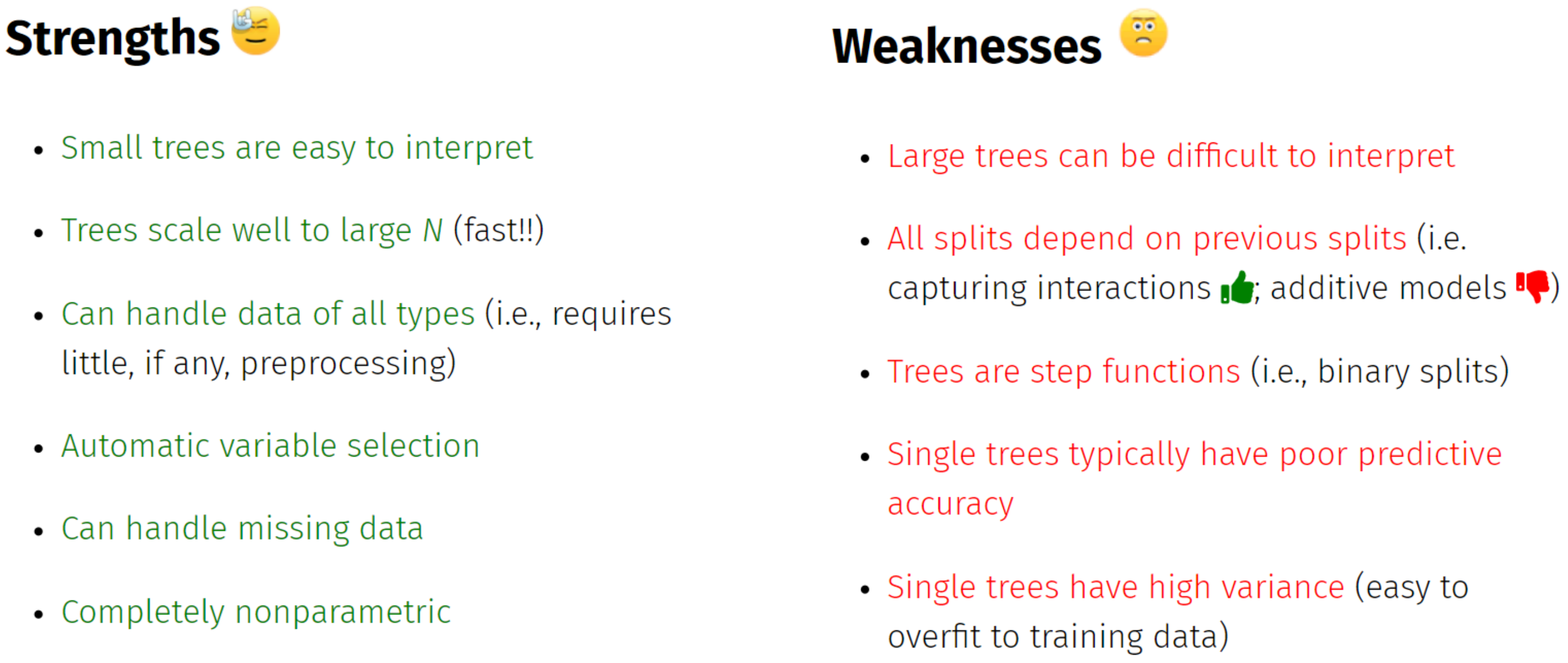
$$\text{minimize: loss function} + \alpha|T|$$

Deep trees overfit



Penalize depth to generalize

Decision Tree - Strengths & Weaknesses



Strengths

- Small trees are easy to interpret
- Trees scale well to large *N* (fast!!)
- Can handle data of all types (i.e., requires little, if any, preprocessing)
- Automatic variable selection
- Can handle missing data
- Completely nonparametric

Weaknesses

- Large trees can be difficult to interpret
- All splits depend on previous splits (i.e. capturing interactions 👍; additive models 👎)
- Trees are step functions (i.e., binary splits)
- Single trees typically have poor predictive accuracy
- Single trees have high variance (easy to overfit to training data)

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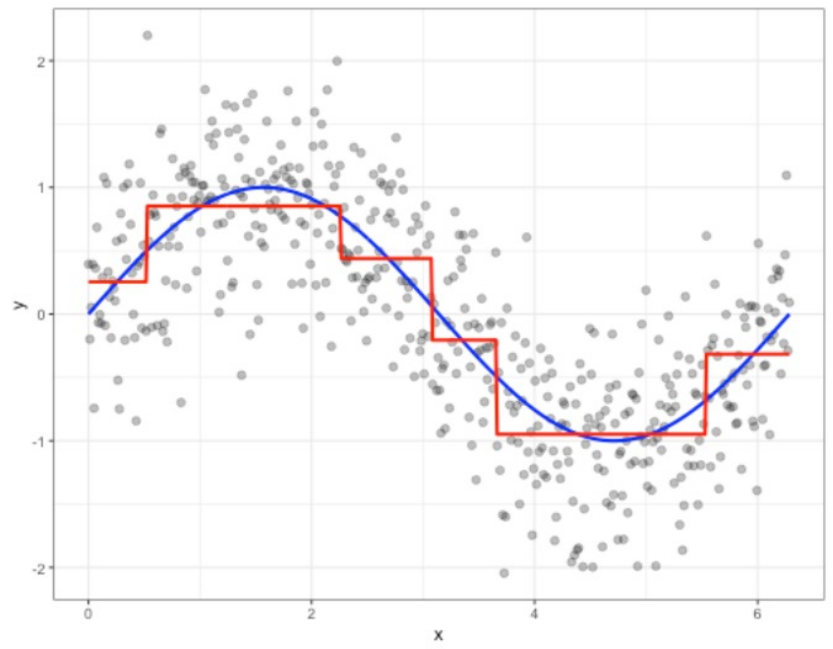
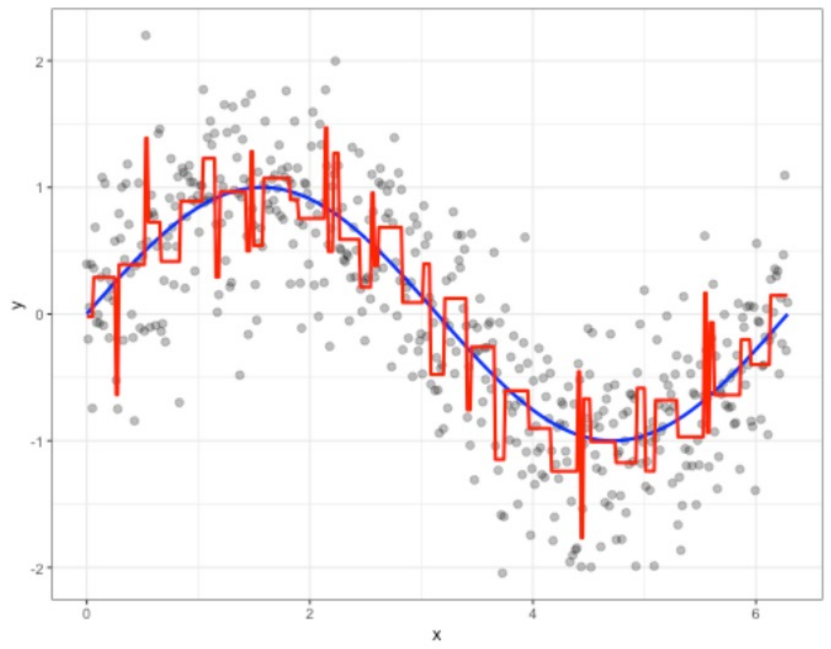
The Problem with Single Decision Trees

Single pruned trees are poor predictors



Single deep trees are noisy



Bagging uses this high variance to our advantage ↑

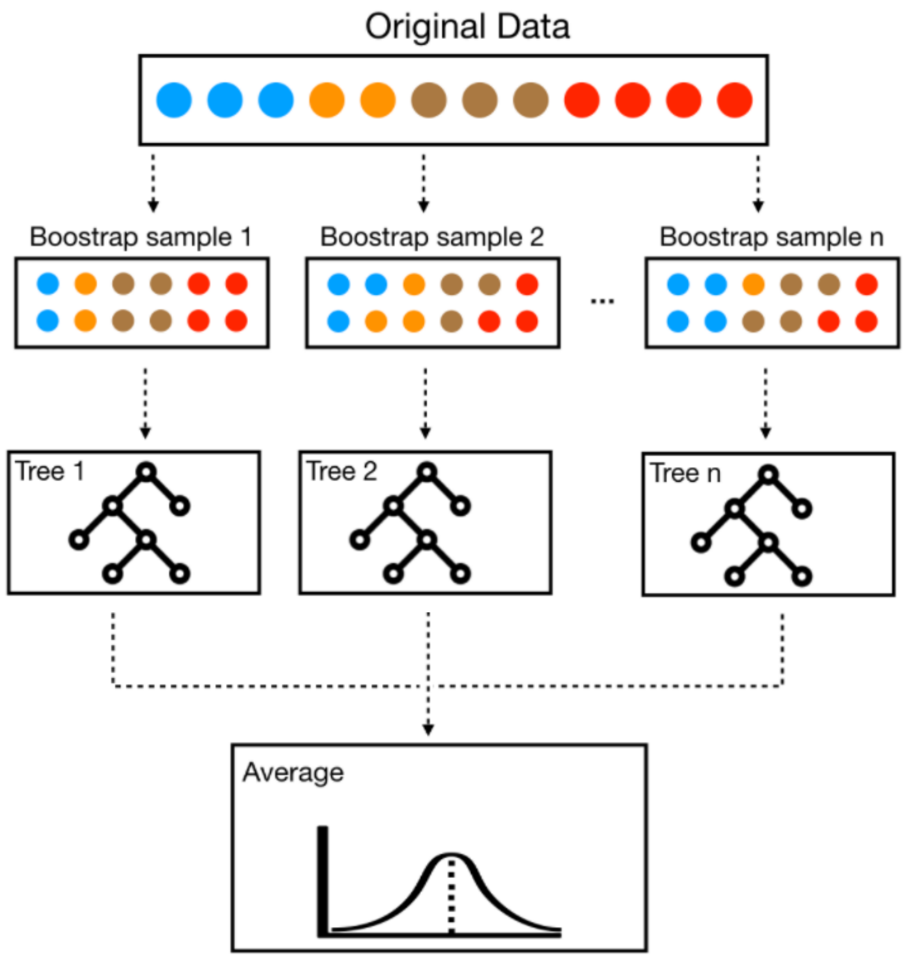
Bagging : Bootstrap Aggregating : wisdom of the crowd

1. Sample records w replacement (aka "bootstrap" the training data)

Sampling is selecting a subset of items from a vast collection of items.
Bootstrap = Sampling with replacement. It means a data point in a drawn sample can reappear in future drawn samples as well.

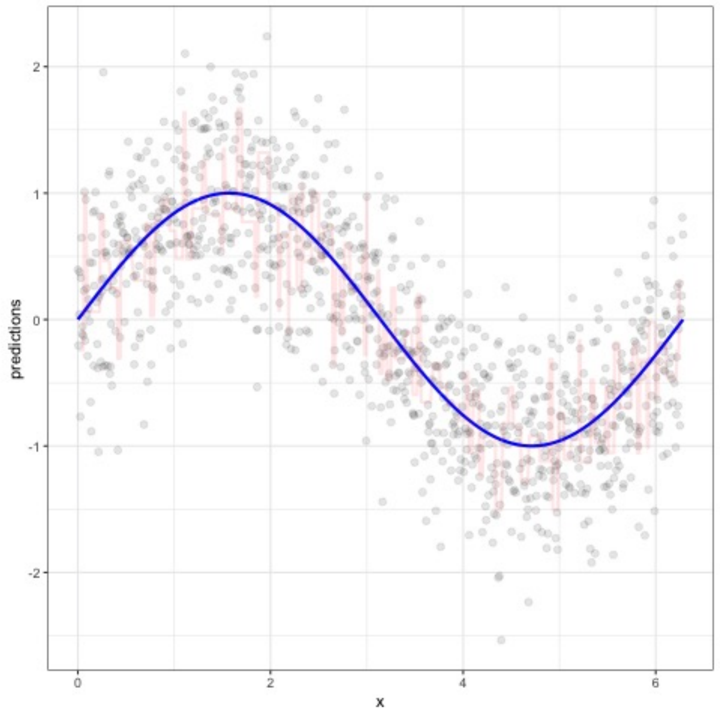
2. Fit an overgrown tree to each resampled data set

3. Average predictions

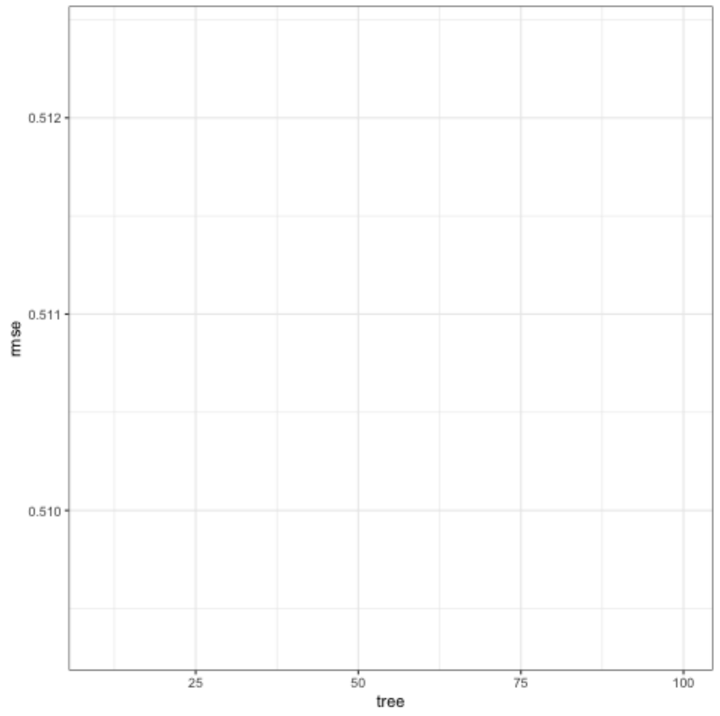


Bagging : Bootstrap Aggregating : wisdom of the crowd

As we add more trees…

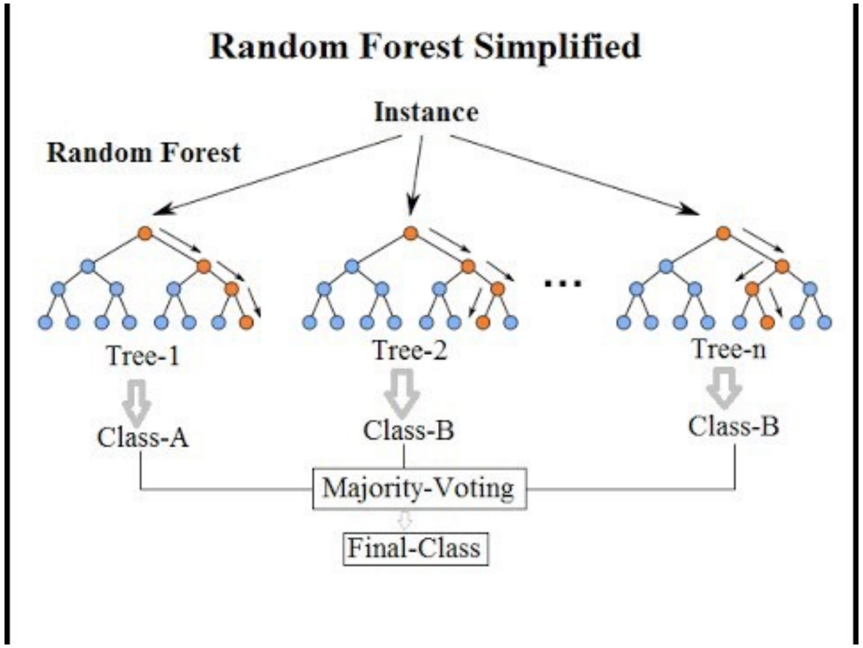


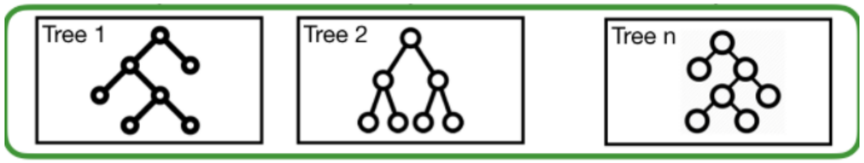
our average prediction error reduces



Random Forest

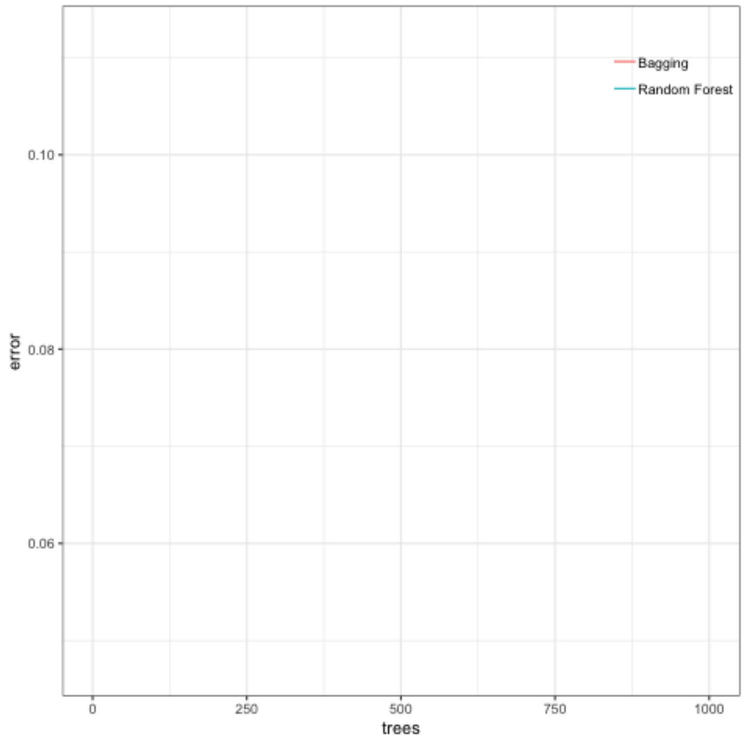
- Random forest is identified as a collection of decision trees. Each tree estimates a classification, and this is called a "vote". Ideally, we consider each vote from every tree and chose the most voted classification (Majority-Voting).
- Random Forest follow the same bagging process as the decision trees but each time a split is to be performed, the search for the split variable is limited to a random subset of m of the p attributes (variables or features) aka Split-Attribute Randomization :
  - classification trees: $m = \sqrt{p}$
  - regression trees: $m = p/3$
  - m is commonly referred to as mtry
- Random Forests produce many unique trees.





Bagging vs Random Forest

- Bagging introduces randomness into the rows of the data.
- Random forest introduces randomness into the rows and columns of the data
- Combined, this provides a more diverse set of trees that almost always lowers our prediction error.



Split-Attribute Randomization : Prediction Erro

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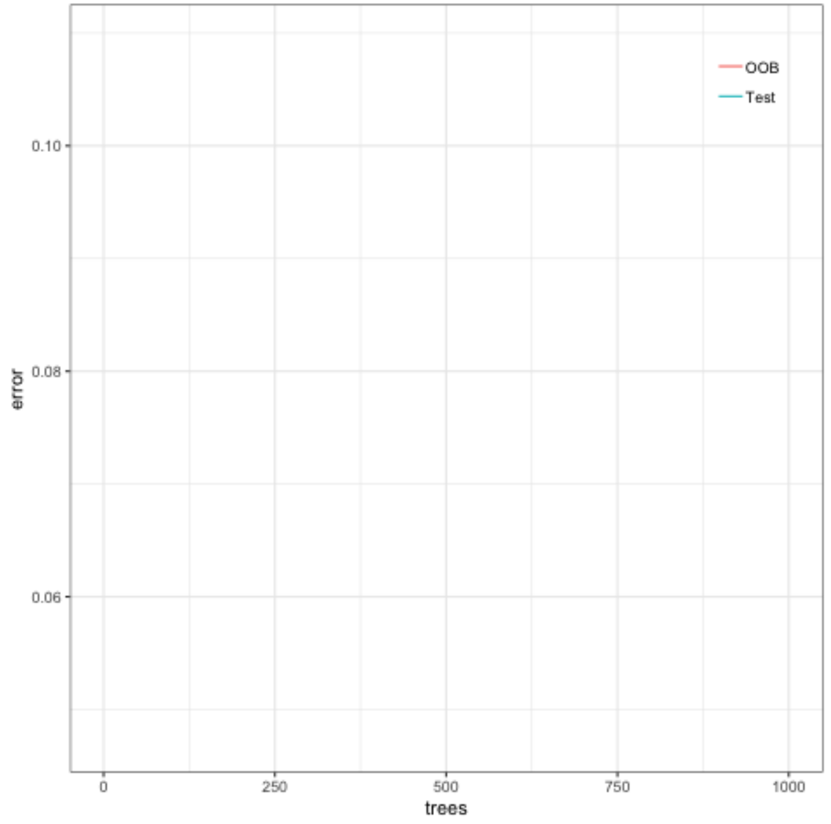
Random Forest: Out-of-Bag (OOB) Observations

- For large enough N, on average, 63.21% or the original records end up in any bootstrap sample
- Roughly 36.79% of the observations are not used in the construction of a particular tree
- These observations are considered out-of-bag (OOB) and can be used for efficient assessment of model performance (**unstructured, but free, cross-validation**)

Pro tip:

- When N is small, OOB is less reliable than validation
- As N increases, OOB is far more efficient than *k*-fold CV
- When the number of trees are about 3x the number needed for the random forest to stabilize, the OOB error estimate is equivalent to leave-one-out cross-validation error.



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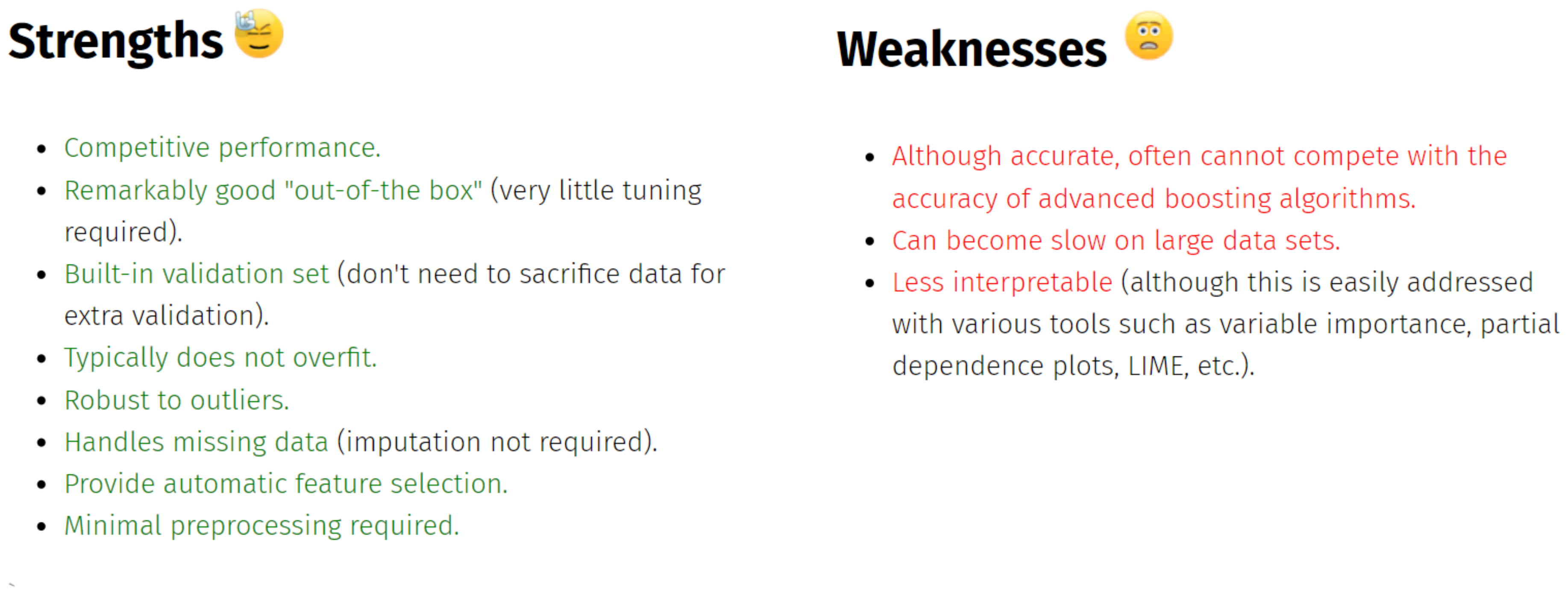
Random Forest : Tuning

Random forests provide good "out-of-the-📦" performance but there are a few parameters we can tune to increase performance.

- Number of trees
- mtry
- Node size
- Sampling scheme
- Split rule

- Typically have the largest impact on predictive accuracy.
- Tend to have marginal impact on predictive accuracy but still worth exploring. Can also increase computational efficiency.
- Generally used to increase computational efficiency

Random Forest - Strengths & Weaknesses



Strengths

- Competitive performance.
- Remarkably good "out-of-the box" (very little tuning required).
- Built-in validation set (don't need to sacrifice data for extra validation).
- Typically does not overfit.
- Robust to outliers.
- Handles missing data (imputation not required).
- Provide automatic feature selection.
- Minimal preprocessing required.

Weaknesses

- Although accurate, often cannot compete with the accuracy of advanced boosting algorithms.
- Can become slow on large data sets.
- Less interpretable (although this is easily addressed with various tools such as variable importance, partial dependence plots, LIME, etc.).