STAT5003

Week 9 : Tree and Ensemble methods

Dr. Qiuzhuang Sun

THE UNIVERSITY OF SYDNEY

Readings 🏛 and Ⓡ functions covered

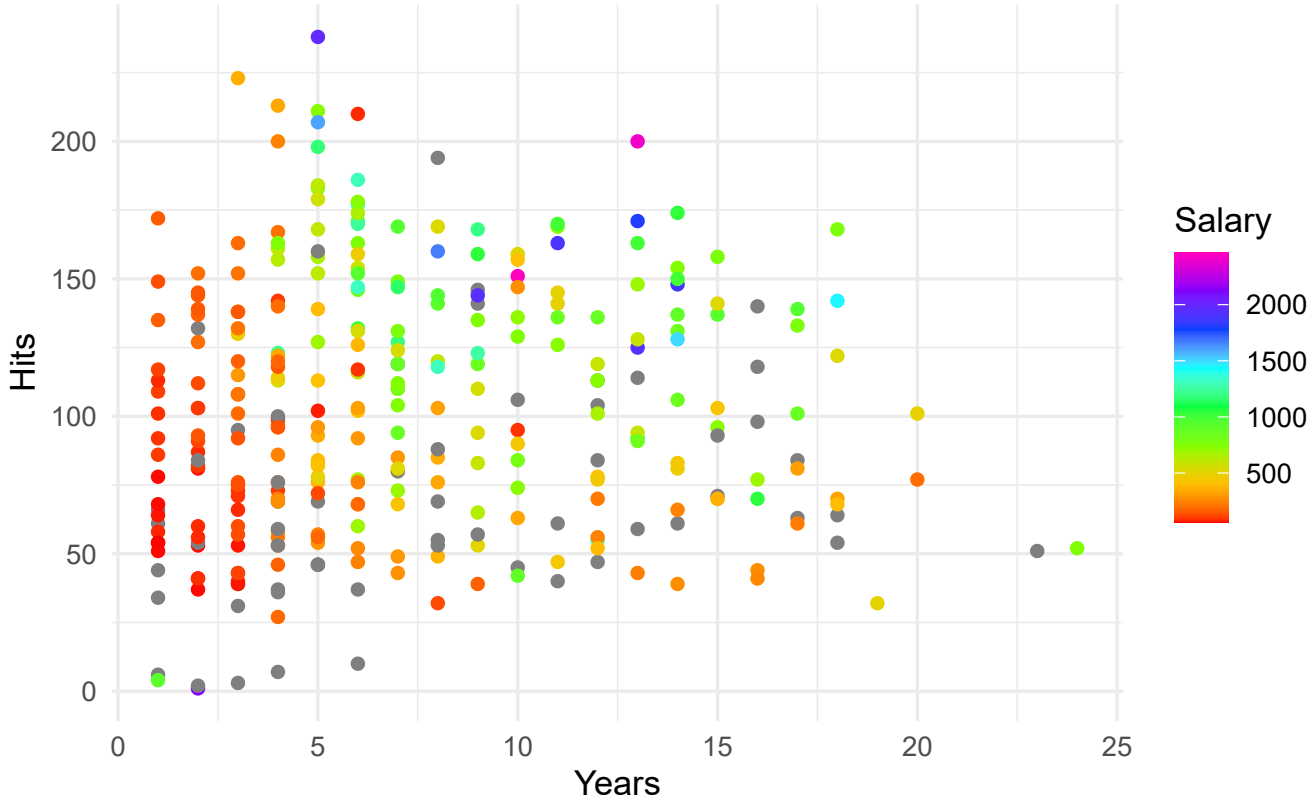
- 🏛 readings
  - Tree methods covered in Chapter 8 in James, Witten, Hastie, and Tibshirani (2013)
- Ⓡ functions
  - `tree::tree` (Create Regression and Decision trees)
  - `base::sample` (Bagging)
  - `ranger::ranger` (construct random forests)
  - `gbm::gbm` (Gradient boosting machines)

Regression/Decision Trees

THE UNIVERSITY OF SYDNEY

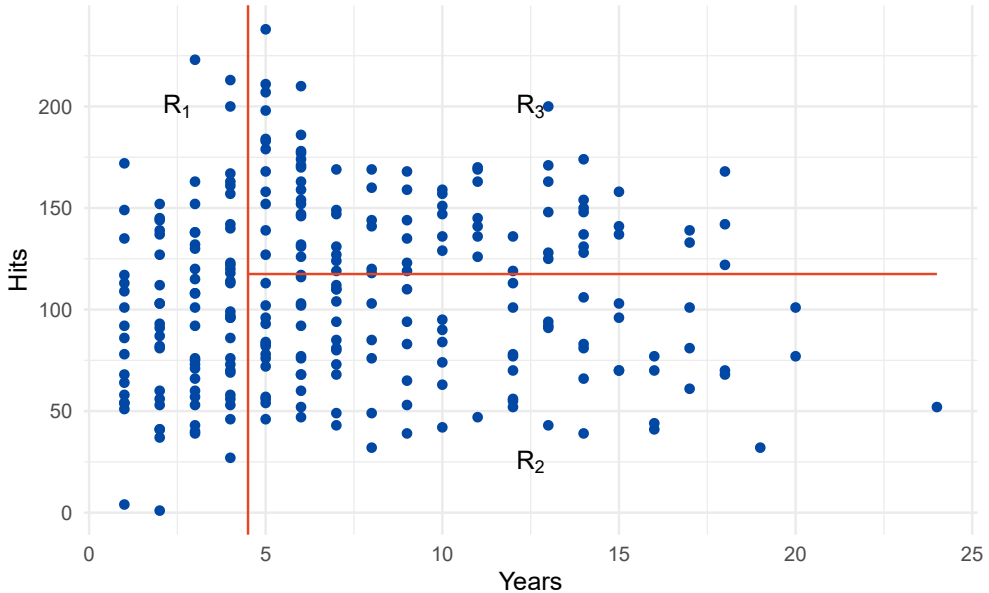
Decision tree for regression

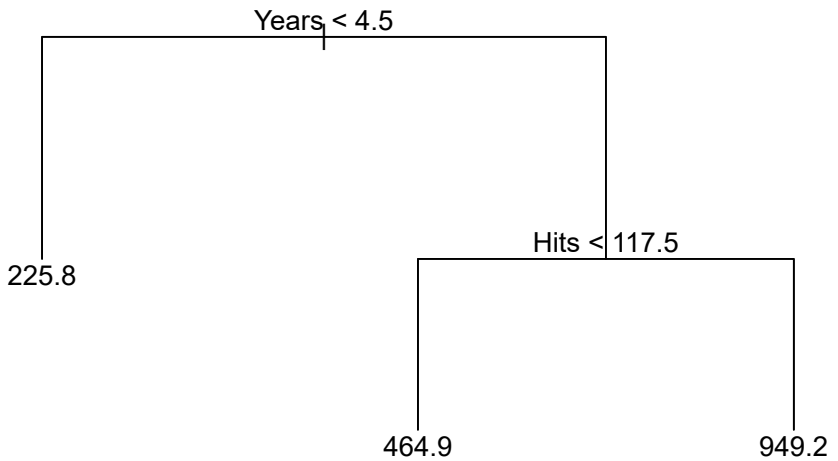
- Baseball player salary data: how would you stratify it?
  - **Salary** is colour-coded (`NA` values coded grey).



Decision tree

- Overall, the tree segments the players into three regions of predictor space:
  - $R_1 = \{X \mid \text{Years} < 4.5\}$
  - $R_2 = \{X \mid \text{Years} \geq 4.5,\ \text{Hits} < 117.5\}$
  - $R_3 = \{X \mid \text{Years} \geq 4.5,\ \text{Hits} \geq 117.5\}$





Terminology for trees

- In keeping with the tree analogy:
  - The regions R_1, R_2, and R_3 are known as terminal nodes.
  - Decision trees are typically drawn upside down, in the sense that the leaves are at the bottom of the tree.
  - The points along the tree where the predictor space is split are referred to as internal nodes.
- In the Baseball player salary tree, the two internal nodes are indicated by the text Years < 4.5 and Hits > 117.5.

Interpretation of Results

- **Years** is the most important factor in determining **Salary**:
  - Players with less experience earn lower salaries than more experienced players.
- Given that a player is less experienced:
  - The number of **Hits** that he made in the previous year seems to play little role in his **Salary**.
- Among players who have been in the major leagues for five or more years:
  - The number of Hits made in the previous year does affect Salary.
  - Players who made more Hits last year tend to have higher salaries.
- Obviously an over-simplification:
  - Compared to some other classification models (such as a regression model), it is easy to display, interpret, and explain.
  - Even easier than linear regression; you can interpret the decision tree to your grandparents :P

Details on tree building process

- In theory, the decision regions could have any shape.
- However, we choose to divide the predictor space into high-dimensional rectangles, or boxes, for simplicity and for ease of interpretation of the resulting predictive model
- The goal is to find boxes $R_1, \ldots, R_J$ that minimizes the residual sum of squares (RSS), given by:

$$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$

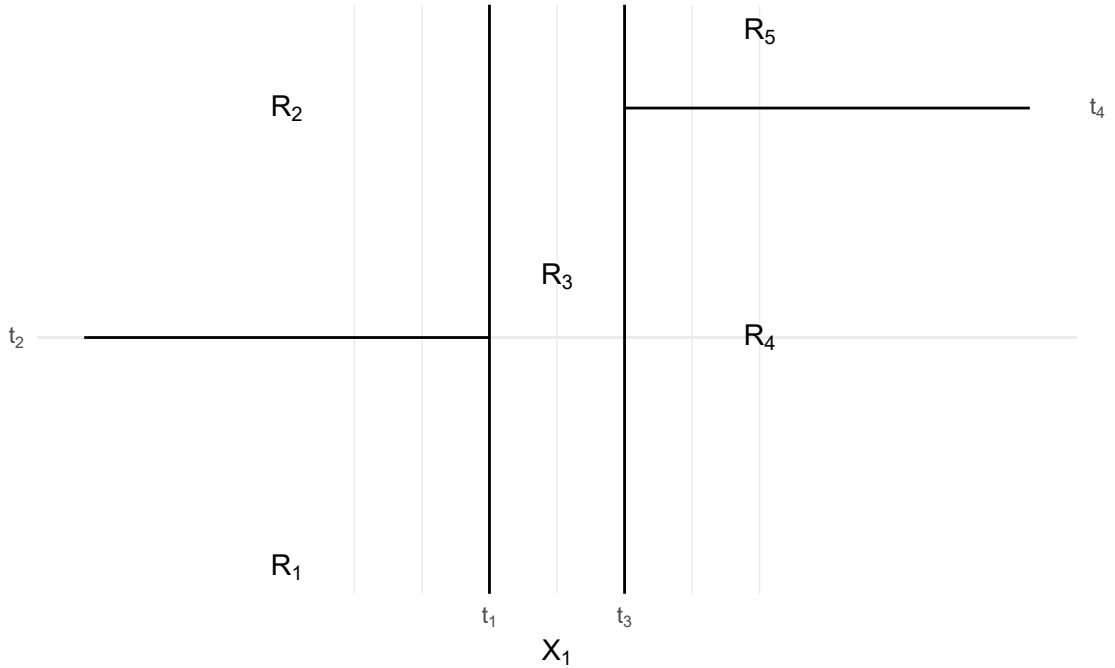
  - $\hat{y}_{R_j}$ is the mean response for the training observations within the j^{th} box

Tree building with recursive binary splitting

- It is computationally **infeasible** to consider every possible partition of the feature space into J boxes
- Take a top-down, **greedy** approach that is known as **recursive binary splitting**
- The approach is **top-down** because it begins at the top of the tree and then successively splits the predictor space
  - Each split is indicated via two new branches further down on the tree
- It is **greedy** because at each step of the tree-building process, the best split is made at that particular step, rather than looking ahead and picking a split that will lead to a better tree in some future step

Using Decision Trees for prediction

- We divide the predictor space:
  - That is, the set of possible values for $X_1, X_2, \ldots, X_p$, into J distinct and non-overlapping regions, $R_1, R_2, \ldots, R_J$.
- For every observation that falls into the region R_j, we make the same prediction, which is simply the mean of the response values for the training observations in R_j.



Decision trees for classification

- Very similar to a regression tree
  - Exception being the prediction of a qualitative response rather than a quantitative one.
- For a classification tree
  - Inspect the region that the observation belongs and predict the most commonly occurring class in that region.

Gini index

- Just as in the regression setting, we use recursive binary splitting to grow a classification tree.
- In the classification setting, RSS cannot be used as a criterion for making the binary splits.
- Alternative measure such as Gini index is used instead.
- The Gini index is defined by

$$G = \sum_{j=1}^{J} \sum_{k=1}^{K} \hat{p}_{jk}(1 - \hat{p}_{jk}).$$

  - $\hat{p}_{jk}$ represents the proportion of training observations in the j^{th} region that are from the k^{th} class.

Gini index

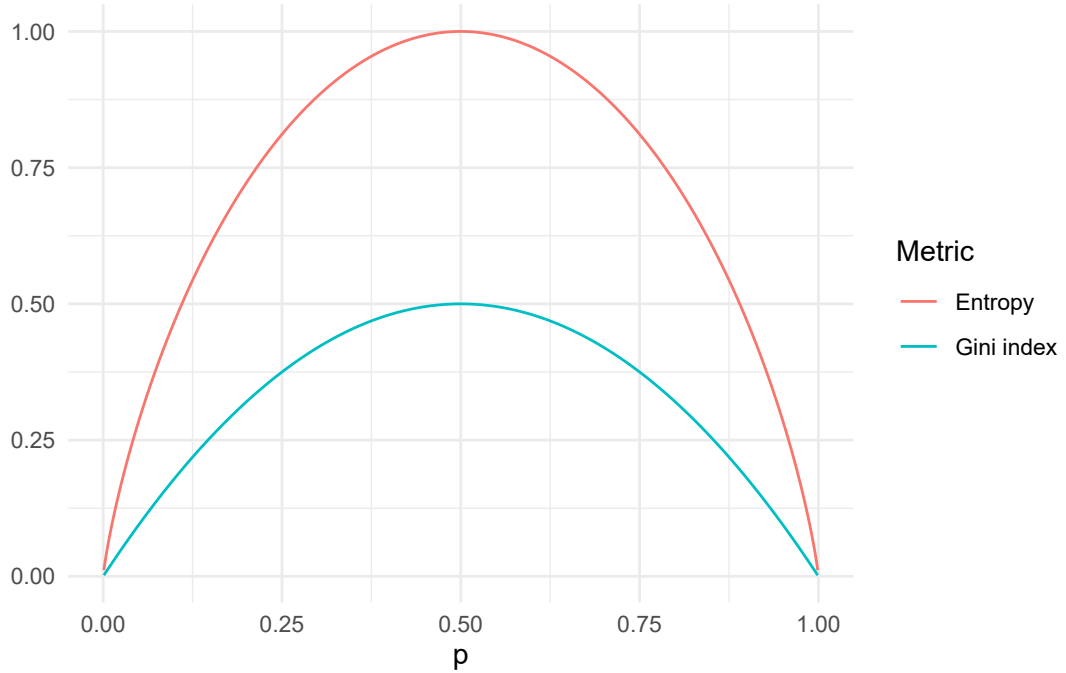
- The Gini index is a measure of total variance across the K classes.
  - It takes on a small value if all of the $\hat{p}_{jk}$ values are close to zero or one.
  - This occurs when there is a clear majority class!
- For this reason the Gini index is referred to as a measure of node **purity**.
  - A small value indicates that a node contains predominantly observations from a single class.

Entropy

- An alternative to the Gini index is entropy, given by

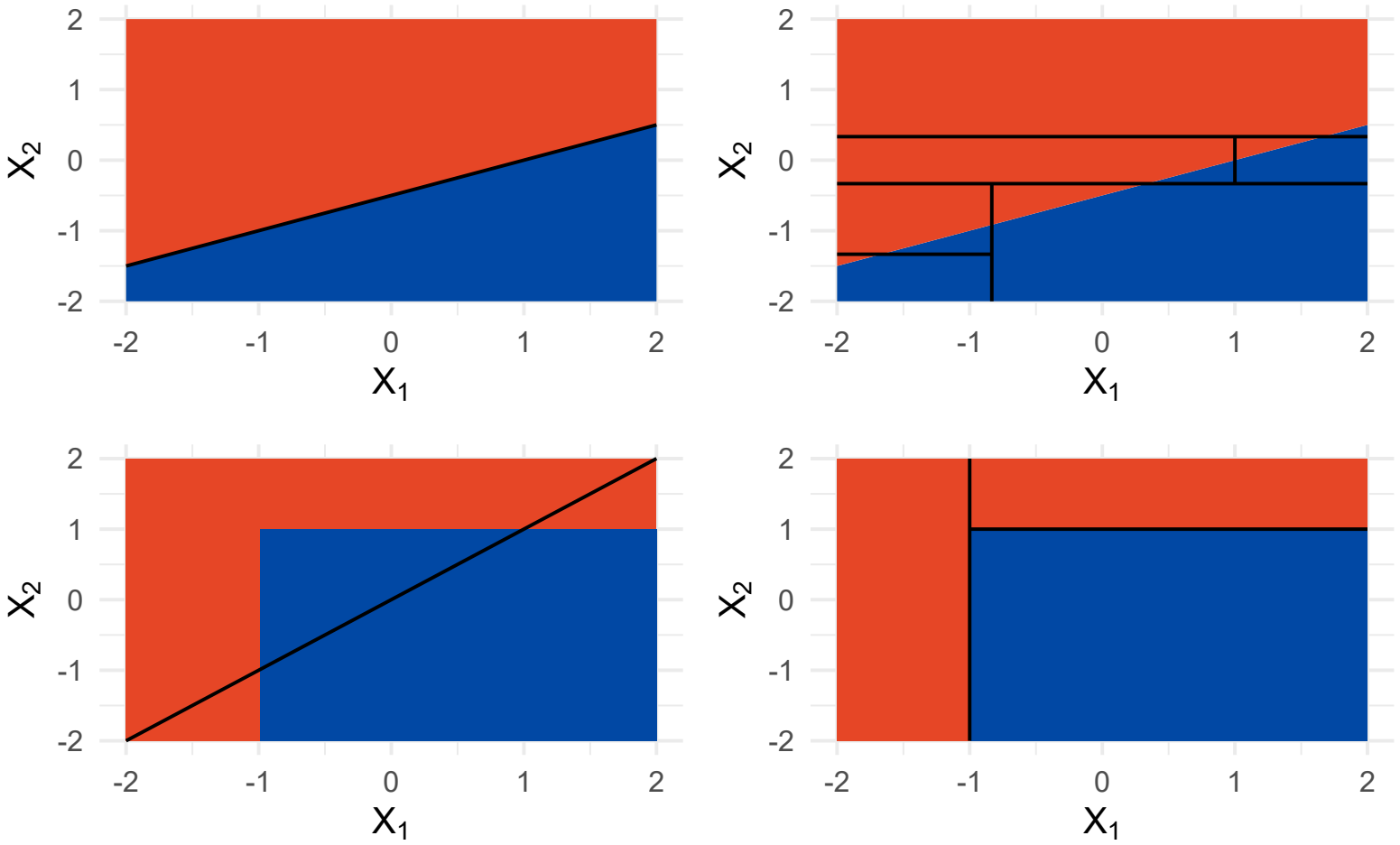
$$D = -\sum_{j=1}^{J}\sum_{k=1}^{K}\hat{p}_{jk}\log\hat{p}_{jk}$$

- It turns out that the Gini index and the Entropy are very similar numerically



Tree vs linear model

```
## Warning: Using `size` aesthetic for lines was deprecated in ggplot2 3.4.0.
## i Please use `linewidth` instead.
```



Advantages and disadvantages of trees

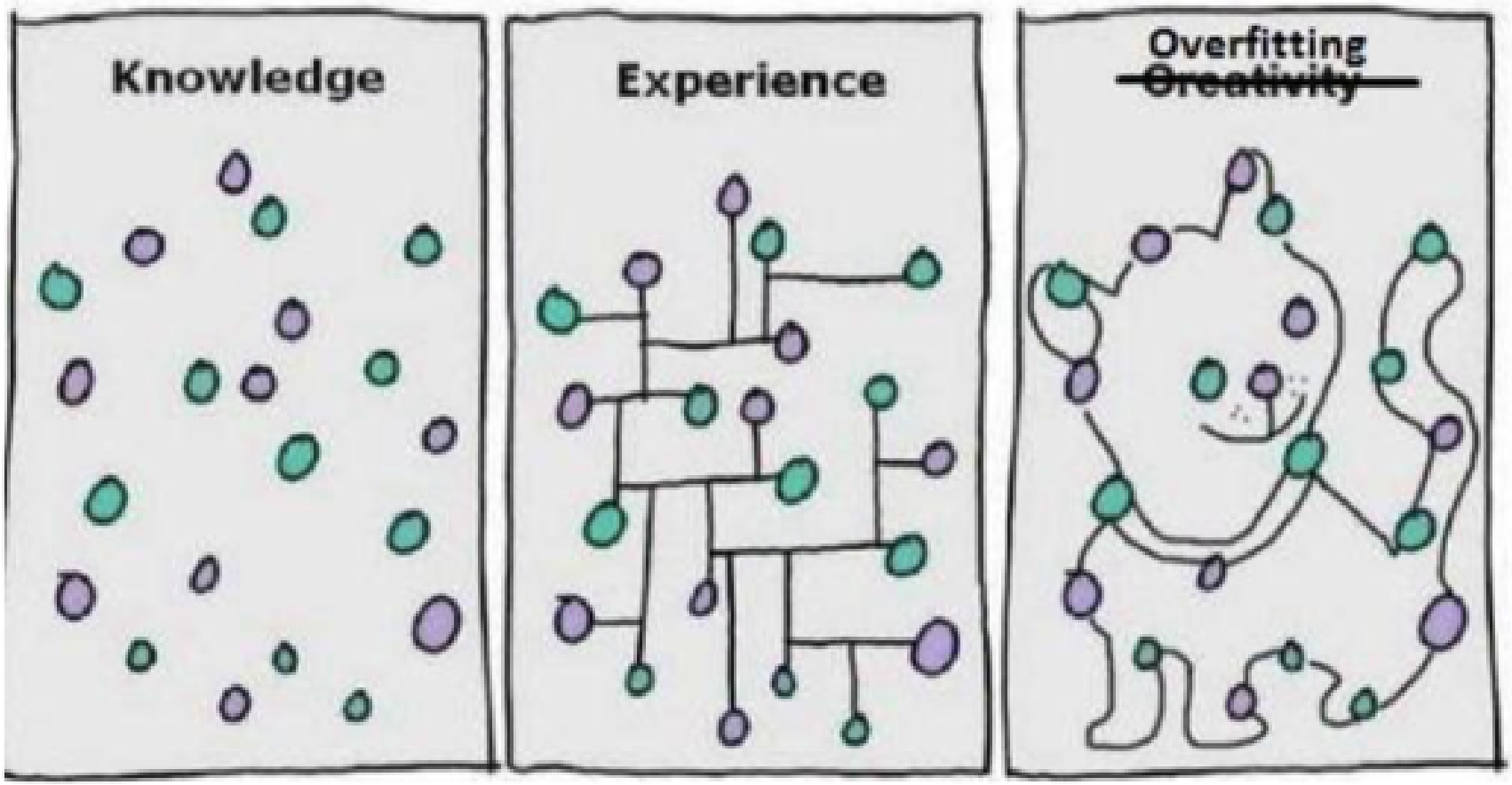
Advantages:

- Trees are very easy to explain to people
- Some people believe that decision trees closely relate to human decision-making
- Trees can be displayed graphically
- Can handle different data types and doesn't require scaling

Disadvantages:

- Trees do not have the same level of predictive accuracy as some of the other regression and classification approaches we have discussed

A single decision tree is prone to over-fitting



Ensemble methods via bootstrapping

THE UNIVERSITY OF SYDNEY

Ensemble of trees

- An alternative is available than just relying on one tree and hope we make the right decision at each split

Ensemble Methods

- Take a sample of Decision Trees into account
- Calculate which features to use at each split
- Make final prediction model using the **aggregated** result from an **ensemble** of trees

Bagging (Bootstrap Aggregating)

- Bootstrap aggregating, or bagging, is a general purpose procedure for reducing the variance of a statistical learning method.
  - It is particularly useful and frequently used in the context of decision trees.
- Recall that given a set of n independent observations $Z_1, \ldots, Z_n$ each with a variance of σ^2:
  - The variance of the mean $\overline{Z}$ is given by σ^2/n.
- In other words, averaging a set of observations reduces variance.
- Since it is typically not possible to have access to multiple training sets:
  - We can use **bootstrapping** to create multiple training sets.

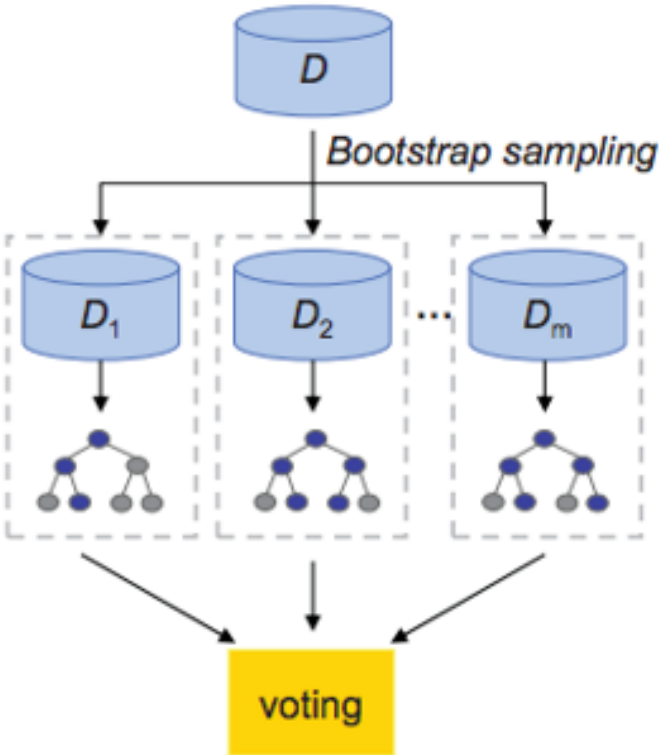
Bagging continued

- Use bootstrapping to take repeated samples from a (single) training data set.
- In this approach, we generate B different bootstrapped training data sets.
  - Train our method of the b^{th} bootstrapping set in order to obtain $\widehat{f}^*_b(x)$, the prediction at a point x.

- Average all the observations to obtain:

$$\widehat{f}(x) = \frac{1}{B}\sum_{b=1}^{B}\widehat{f}^*_b(x).$$

- This is called bagging.



Out of bag error estimation

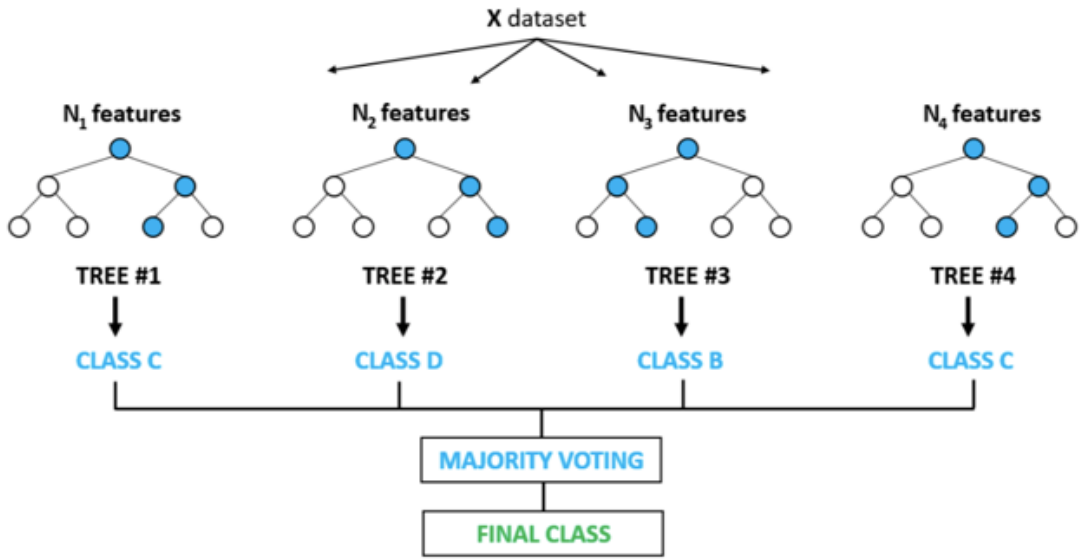
- It turns out that there is a very straightforward way to estimate the test error of a bagged model.
- Recall that the key to bagging is that trees are repeatedly fit to bootstrapped subsets of the observations.
  - One can show that on average, each bagged tree makes use of around $2/3$ of the observations when the sample size n is large.
- The remaining $1/3$ of the observations not used to fit a given bagged tree are referred to as the out-of-bag (OOB) observations.
- We can predict the response for the i^{th} observation using each of the trees in which that observation was OOB.
  - This will yield around $B/3$ predictions for the i^{th} observation, which we average.
  - This estimate is essentially the leave-one-out (LOO) cross-validation error for bagging, if B is large.

From bagging to Random Forest

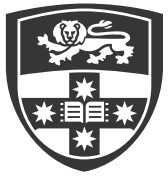
- Random forests (sometimes) provide an improvement over bagged trees by way of a small tweak that decorrelates the trees. This reduces the variance when we average the trees.
- As in bagging, we build a number of decision trees on bootstrapped training samples.
- But when building these decision trees, each time a split in a tree is considered, a random selection of m predictors is chosen as split candidates from the full set of p predictors.
  - The split is allowed to use only one of those m predictors.
- A fresh selection of m predictors is taken at each split, and typically we choose $m \approx \sqrt{p}$.
  - That is, the number of predictors considered at each split is approximately equal to the square root of the total number of predictors.

Random Forest algorithm pseudocode

```
Set number of models to build, B
for i = 1 to B
    Generate a boostrap sample of the original data
    Train a tree model on this sample where
    for each split
        Randomly select m (< p) of the original predictors
        select the best predictor among the m predictors and parition the data
    endfor
endfor
```



Ensemble methods via boosting



THE UNIVERSITY OF SYDNEY

Boosting

- Like bagging, boosting is a general approach that can be applied to many statistical learning methods for regression or classification. We only discuss boosting for decision trees.
- Recall that bagging involves creating multiple copies of the original training data set using the bootstrap, fitting a separate decision tree to each copy, and then combining all of the trees in order to create a single predictive model.
- Notably, each tree is built on a bootstrap data set, independent of other trees.
- Boosting works in a similar way, except that the trees are grown *sequentially*.
    - Each tree is grown using information from previously grown trees.

Idea behind boosting

- Unlike fitting a single large decision tree to the data, which amounts to *fitting the data hard* and potentially overfitting, the boosting approach instead *learns slowly*.
- Given the current model, we fit a decision tree to the residuals form the model. We then add this new decision tree into the fitted function in order to update the residuals.
- Each of these trees can be rather small which have just a few terminal nodes.
- By fitting small trees to the residuals, we slowly improve $\widehat{f}(x)$ in areas where it does not perform well.
- There is a shrinkage parameter λ that slows the process down even further, allowing more and different shaped trees to attack the residuals.

Boosting for regression trees

1. Set $\widehat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set
   - r_i denotes the i^{th} residual, and y_i is the outcome
2. For $b = 1, 2, \ldots, B$:
   - Fit a tree $\widehat{f}_b$ with d splits ($d + 1$ terminal nodes) to the new training data (X, r)
     - That is, r is the new response value
   - Update $\widehat{f}$ by adding in a shrunken version of the new tree
     - $\widehat{f}(x) \leftarrow \widehat{f}(x) + \lambda \widehat{f}_b(x)$
   - Update the residuals
     - $r_i \leftarrow r_i - \lambda \widehat{f}_b(x)$
3. Compute the final model

$$\widehat{f}(x) = \sum_{i=1}^{B} \lambda \widehat{f}_b(x)$$

Parameters to tune in boosting

- Number of trees B
- The shrinkage parameter λ: a small positive number
  - Typical values are between 0.01 and 0.001
- Number of split d in each tree
  - Controls the complexity of the boosted ensemble
  - If $d = 1$, then the tree is just a stump. This actually usually works quite well

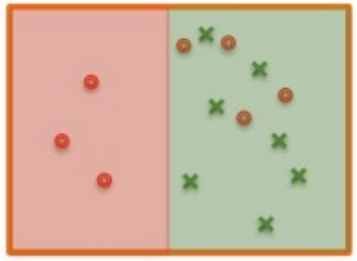
Other boosting algorithms

- AdaBoost
- Stochastic gradient boosting
- XGBoost

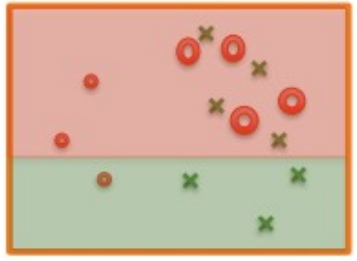
AdaBoost

- Short for Adaptive Boosting, one of the first boosting algorithms for classification
- Convert a set of weak classifiers into a strong one
- Basic idea
  - At each iteration, reweight the data to place more weight on data points that the classifier got wrong
- At the end, combine all the weak classifiers by taking a weighted combination
  - Put more weight on the weak classifiers with the higher accuracies

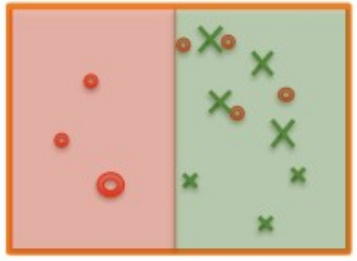
AdaBoost plot



Iteration 1



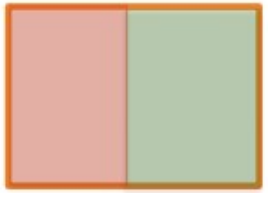
Iteration 2



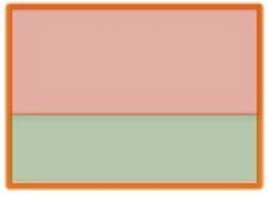
Iteration 3

Final Model

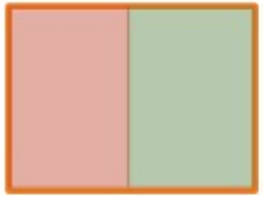
f(x) = 0.46



+ 0.29



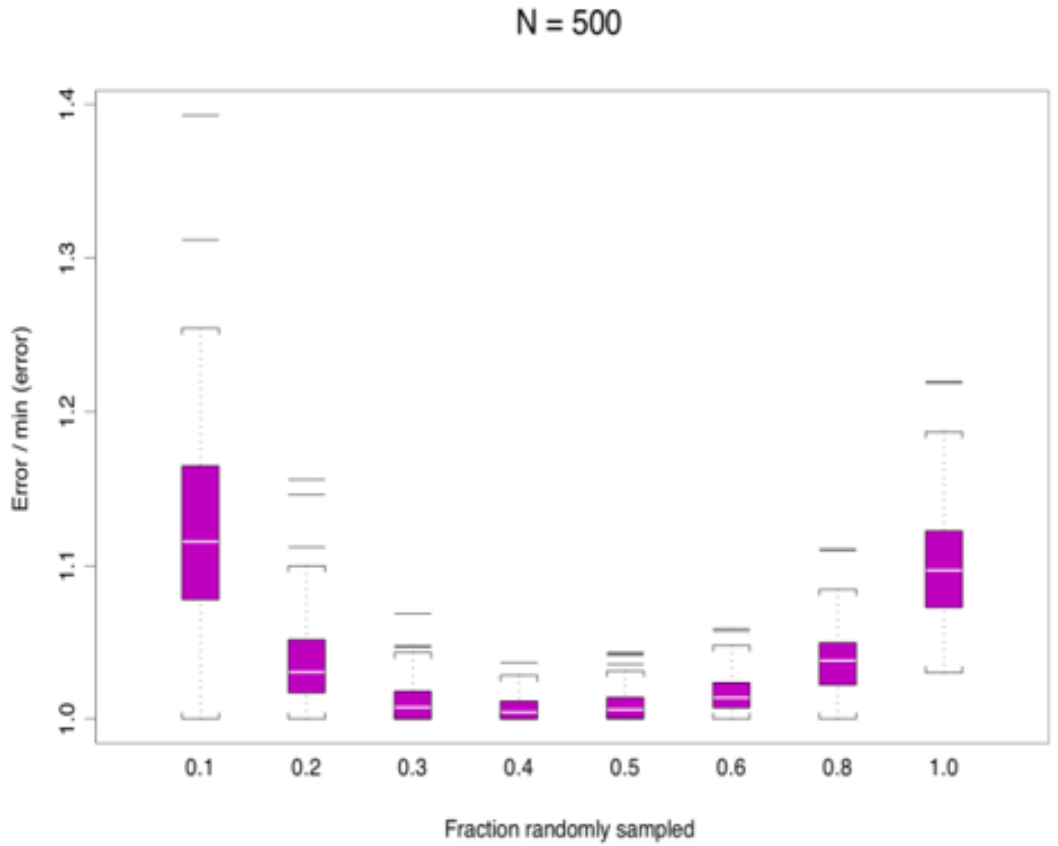
+ 0.46



Stochastic gradient boosting

- Use the idea behind bagging
- In each iteration of stochastic boosting, a sample of the training set instead of the full training set is used
- Instead of a bootstrap sample (with replacement), the algorithms samples a fraction of the training set
- This introduced randomness can improve performance
- Paper by Friedman (2002) covers this technique

Stochastic gradient boosting plot



- Taken from Friedman (2002)

XGBoost

- XGBoost is short for eXtreme Gradient Boosting
- It is a library for high performance gradient boosting models written in C++ with implementations in Python, R, and Julia
- Designed for speed: up to 10 times faster than the `gbm` package
- Has been very popular in recent years and has won a number of machine learning competitions (especially on tabular data)
- Supports regularization
- Can handle missing data

Bagging vs Boosting

- Both ensemble methods get N learners from 1 learner
  - Built independently for bagging
  - Built sequentially for boosting
- Trees built in boosting are weak learners (sometimes just a stump) while trees in Random Forest have higher complexity
- Fewer parameters to tune in Random Forest, many more in Boosting (depending on which variation you are using)
- Both combine outputs from N trees

Summary

- Decision trees are simple and interpretable models for regression and classification.
- However, they are often not competitive with other methods in terms of prediction accuracy.
- Bagging, random forests, and boosting are good methods for improving the prediction accuracy of trees.
  - They work by growing many trees on the training data and then combining the predictions of the resulting ensemble of trees.
- The latter two methods, random forests and boosting, are among the state-of-the-art methods for supervised learning.
  - Their results can be difficult to interpret.
  - But we can still get relative importance of each predictor (read the example code).

References

Friedman, J. H. (2002). "Stochastic gradient boosting". In: *Computational statistics & data analysis* 38.4, pp. 367-378.

James, G., D. Witten, T. Hastie, et al. (2013). *An introduction to statistical learning*. Vol. 112. Springer.