Trees: pruning and ensembles

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Slides on the course GitLab/at https://github.com/tedinburgh/ads2023

Today: Pruning and ensembles

- Tree sizes
- Pruning
- Boosting
- Bagging
- Random forests

Questions: halfway through, at the end, or by email (te269)

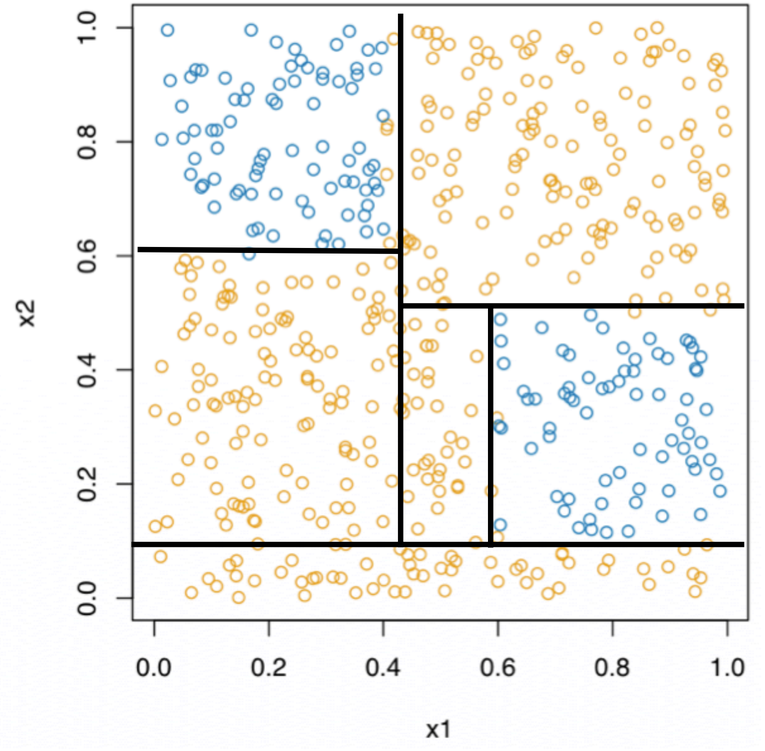
Resources

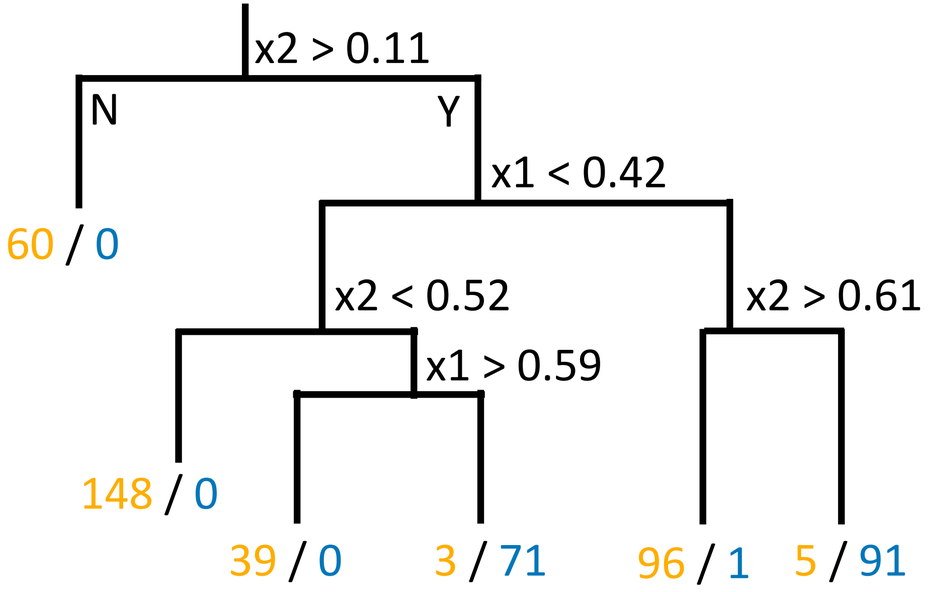
- An Introduction to Statistical Learning with Applications in R/Python (James, Witten, Hastie, Tibshirani, Taylor; 2013/2023)

- Slides adapted from:
  - Prof Alexandra Chouldechova, Carnegie Mellon
  - Prof Stephen Eglen, Cambridge

Recap: Overview

- Tree-based methods **segment** the feature space into simple regions (e.g. high-dimensional rectangles)
- **Predict** using the average (mean, mode), **classify** using the most common class





Recap: How to grow the tree?

- General process:

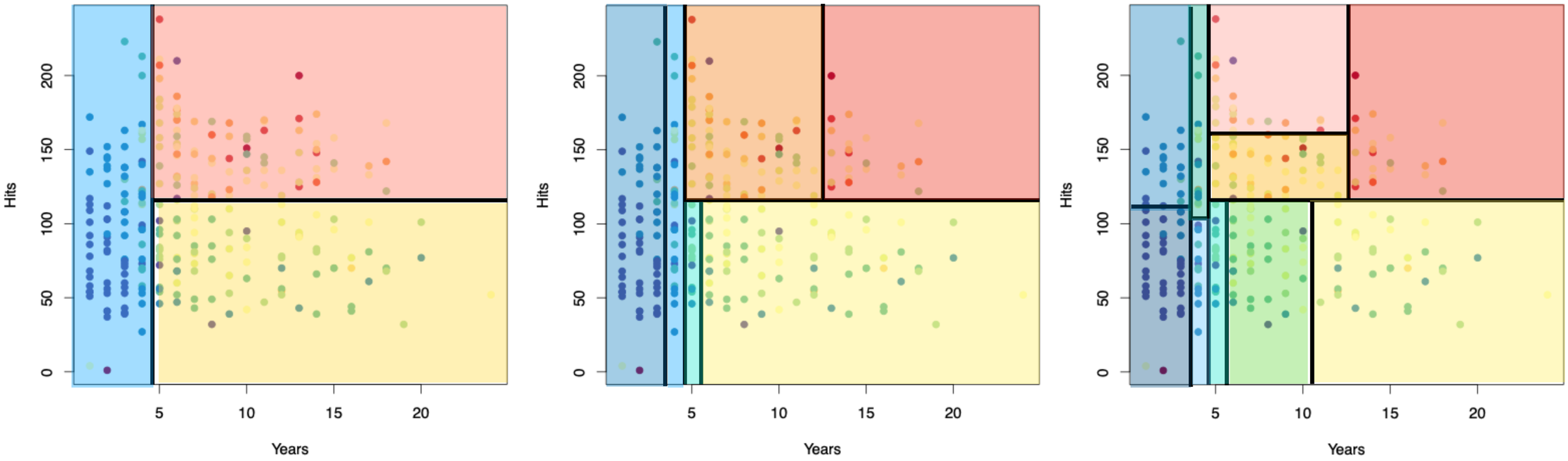
  1. Partition the predictor space (i.e. all possible values of $X_1, X_2, \ldots, X_p$) into J distinct, non-overlapping regions, labelled $R_1, \ldots, R_J$

  2. Each observation in a given region R_j is given the same predicted value (or class), which is the mean (or mode) of all response variables in that region

Recap: When do we stop growing the tree?

- Which is better: small trees or big trees?

Example: baseball salaries



Small trees vs large trees

- Small trees: generalise well but poor prediction, i.e. **underfitting**
- Large trees: good performance on training data but do not generalise well, i.e. **overfitting**
- There's a bias-variance tradeoff between the number of leaves and generalisation to unseen data

	Small	**Large**
Bias	High	Low
Variance	Low	High

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Bias comes from simplifying assumptions made by the model

Variance is the amount that the model estimate changes if we use slightly different training data

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The bias error comes from wrong assumptions (e.g. the problem is more complex than the assumption)

Variance error is error from sensitivity to fluctuations in the training data

	Small tree	**Large tree**
Bias	High	Low
Variance	Low	High

Small trees vs large trees

- We could stop adding new nodes if the decrease in RSS or Gini index is less than a fixed pre-specified threshold
- The problem is that the recursive binary partition algorithm is **greedy**
- We don’t know if a poor partition will be followed immediately a very good one

Pruning

- The solution is to grow a very large tree (lots of leaves), then prune some of the branches

- Start with a large tree T_0 and with complexity hyperparameter α. Find the subtree $T \subset T_0$ that minimises

$$\sum_{m=1}^{|T|} \sum_{i:\ x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$

  where $|T|$ is the number of leaves in tree T and R_m is the region associated with the mth leaf

- The two components are the model error term and a penalty on model complexity, similar to penalised regression e.g. Lasso regression

Pruning

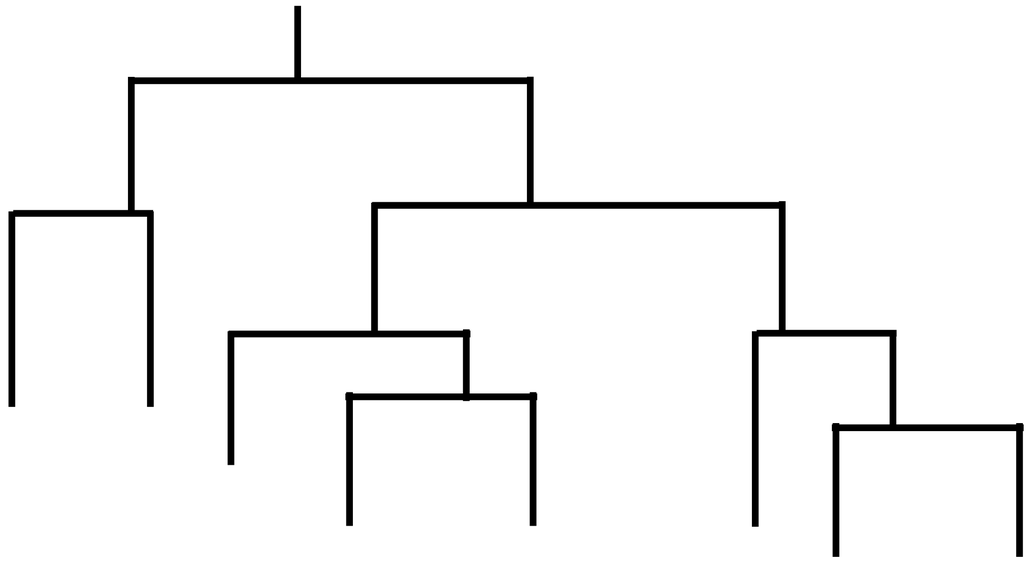
- There may be a lot of subtrees, which will make the computation difficult!
- **Bottom up** vs **top down**

- If we slowly increase α, then the optimal trees are nested (this is useful for computation!)
- If we start with $\alpha = 0$, then the optimal tree is just the full tree T_0
- As $\alpha \to \infty$, the penalty term will mean that the optimal tree only has one leaf
- This is known as **weakest link pruning** or **cost complexity pruning**

Pruning in practice

$$\sum_{m=1}^{|T|} \sum_{i:\ x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$

T_0



$\alpha = 0$

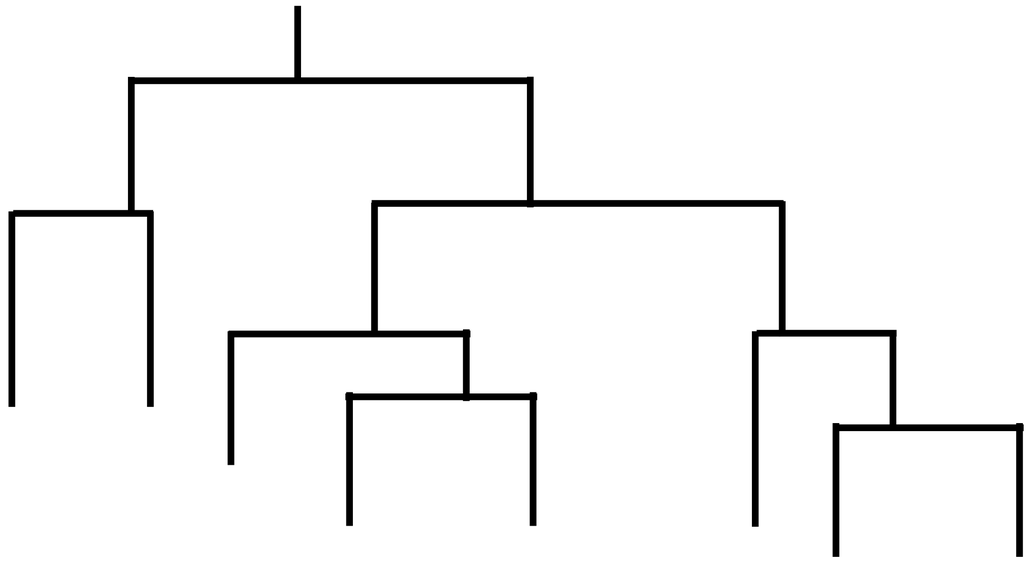
T_∞

$\alpha \to \infty$

Pruning in practice

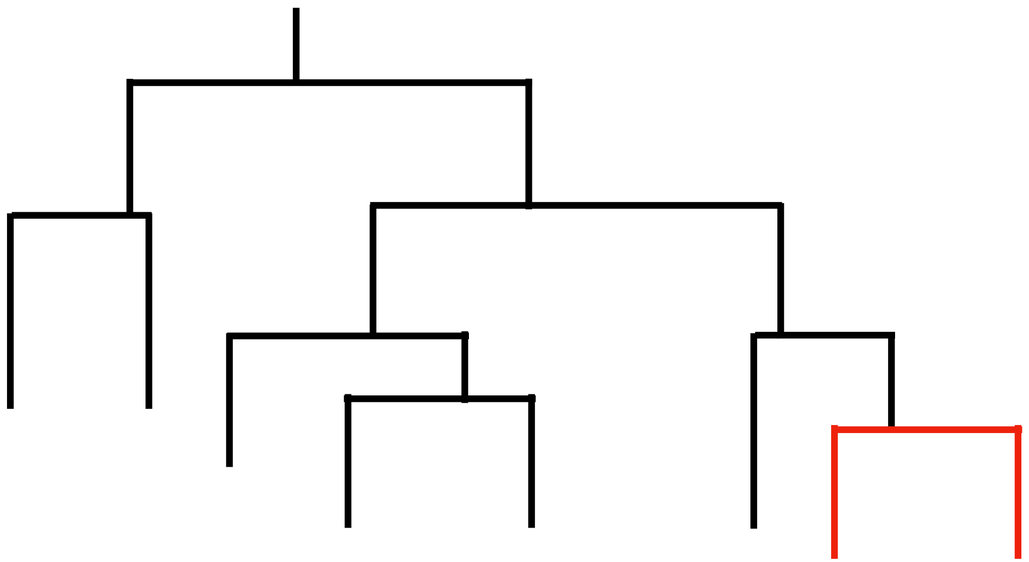
$$\sum_{m=1}^{|T|} \sum_{i:\ x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$

T_0



$\alpha = 0$

T_1

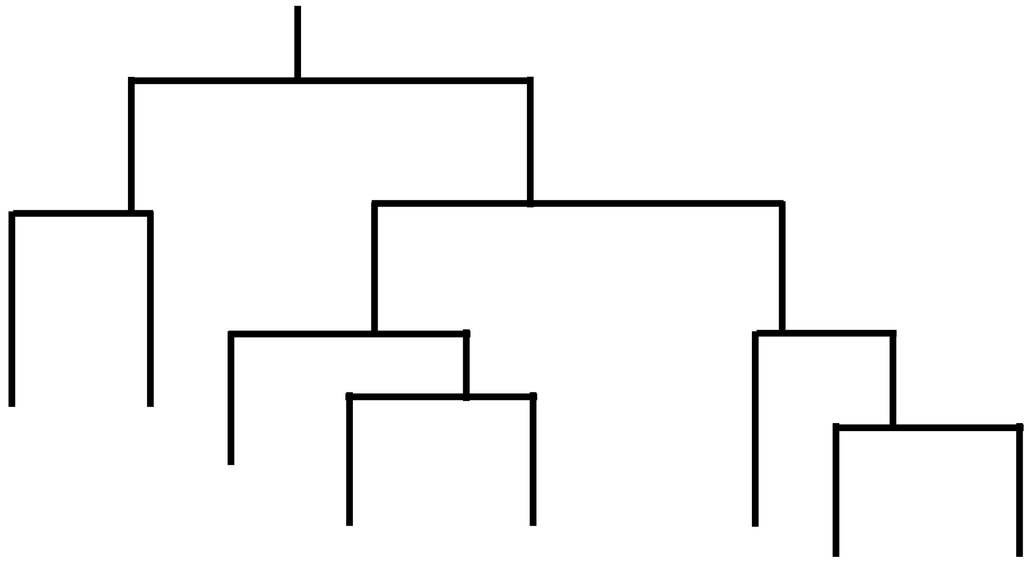


$0 < \alpha < \alpha_1$

Pruning in practice

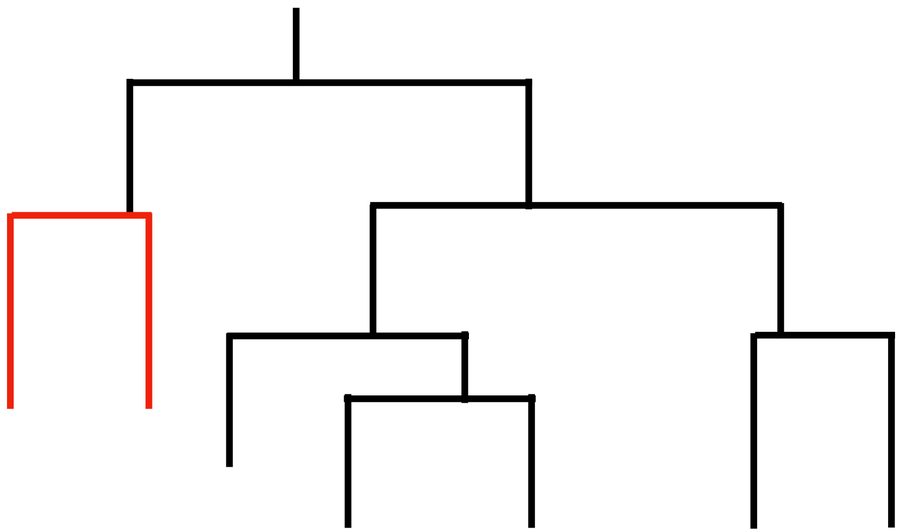
$$\sum_{m=1}^{|T|} \sum_{i:\ x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$

T_0



$\alpha = 0$

T_2

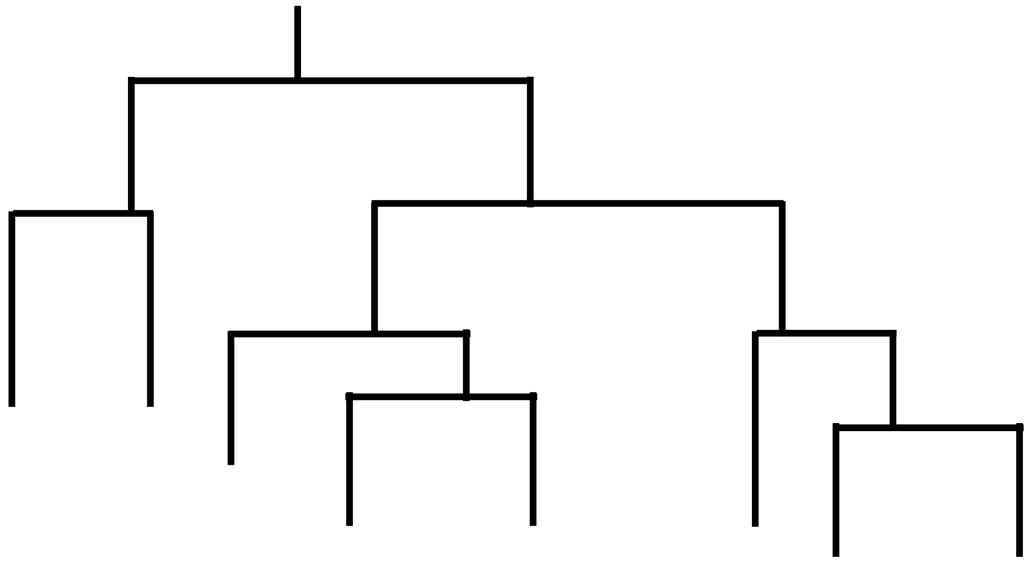


$\alpha_1 < \alpha < \alpha_2$

Pruning in practice

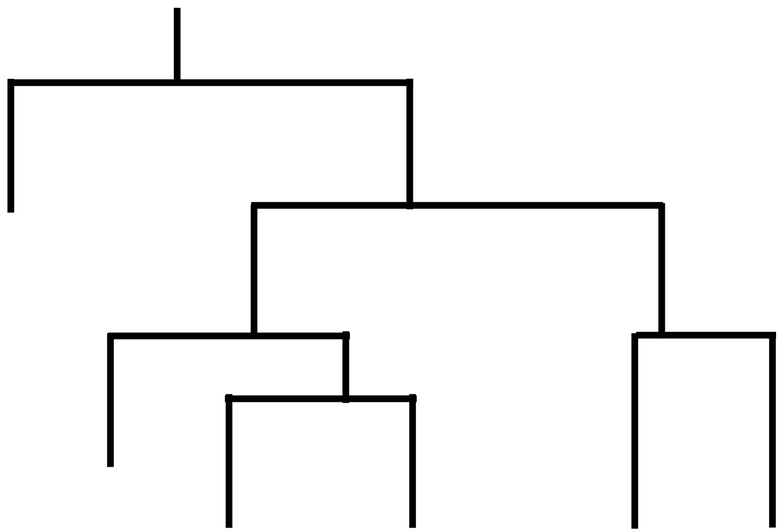
$$\sum_{m=1}^{|T|} \sum_{i:\ x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$

T_0

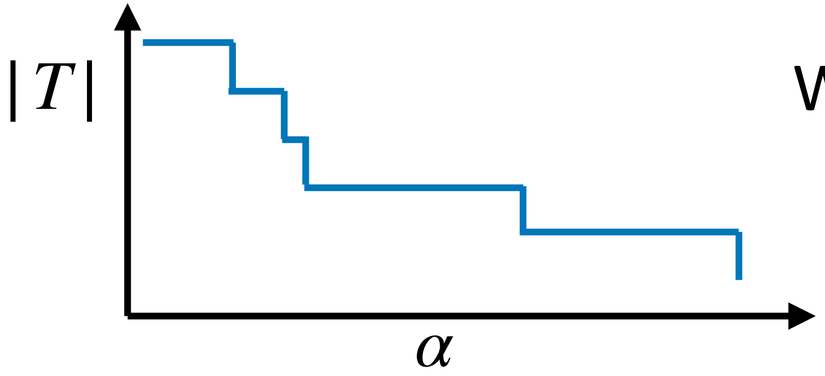


$\alpha = 0$

T_3



$\alpha_2 < \alpha$



What is a good value of α?

Pruning steps

1. Construct a very large tree T_0 using recursive binary partition
2. Apply weakest link pruning to T_0 to create nested sequence of trees as a function of α
3. Use k-fold cross-validation to select the hyper parameter α
   - Split the training data into K folds of equal size
   - For $k = 1, \ldots, K$, repeat steps 1. and 2. on all training data except the kth fold, and evaluate the mean squared prediction error on the kth fold
   - Average the result, then choose α that minimises the average error
4. The optimal tree is the subtree from 2. corresponding to that value of α

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     MSPE is similar to RSS (there are subtle differences between errors and residuals)

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Pruning: code

- Jupyter notebook about regression trees
- (On GitHub https://github.com/tedinburgh/ads2023 and the course GitLab)

Questions?

Decision trees: pros and cons

- Trees are very interpretable! You can easily read off why the model gave a particular prediction. ✓
- Trees handle mixed data types (both predictors and response variables) ✓
- Trees can handle missing data (e.g. using surrogate variables) ✓
- Trees are not very robust. Small changes to the input data can completely change the (unpruned) tree structure. ✘
- Most of the time, trees aren't particularly good at prediction. ✘
- Does this mirror human intuition better than other methods for prediction or classification?

Ensembles

- Predictions from one decision tree on its own may not be very good

- An ensemble method uses many individual decision trees (**weak learners**) as building blocks
- These building blocks can be combined together in a much more powerful model

Bagging and cross-validation

- **Bagging** (bootstrap aggregating) averages across lots of estimates in order to decrease the variance of a high-variance predictor
- Idea: averaging a set of observations reduces the variance (e.g. if $Z_1, \ldots, Z_n$ are independent observations each with variance σ^2, then the variance of the mean $\bar{Z} = 1/n \sum_n Z_n$ is σ^2/n)
- This is similar to cross-validation, which outperforms a single validation set
- A single validation set may give highly variable estimates (pick a different training-validation split and the estimate may change a lot)
- Averaging over multiple folds produces a more stable error

The bootstrap

- This is a very important resampling technique, and is used widely in statistics
- The idea is to use the empirical distribution of the data to estimate the true unknown data-generating distribution

- Sample from the observed data with replacement until you have a dataset of the same size (i.e. sample rows with replacement). This is a bootstrap sample.

$$X = \begin{pmatrix} X_1 & X_2 & \dots & X_p \end{pmatrix} = \begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix} \qquad y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

The bootstrap

- Not all of the observations will be in each bootstrap sample
- The probability that row i is in a particular bootstrap sample at least once is $p = 1 - (1 - 1/n)^n \approx 0.632$ (hint: what is the probability that it's not chosen as the first pick?)
- The observations not in the bootstrap sample (called out-of-bag observations) are useful later for validation!

Bagging (bootstrap aggregating)

- Generate B bootstrap samples (sometimes hundreds)
- Build deep trees (no pruning), each on a separate bootstrap sample
- Classification: use **majority voting** (overall prediction is the most common class among all B predictions)
- Regression: take the average, i.e. $\hat{f}_{bag}(x) = \frac{1}{B}\sum_b \hat{f}^{\star b}(x)$

Prediction from decision tree using the bth bootstrap sample

- Out-of-bag (OOB) error is similar to leave-one-out cross-validation error, so can be used model validation.

Probability bagging

- Classification in bagging usually uses **majority voting**

- An alternative is to calculate the bagging estimate of class probabilities

$$\hat{p}_k^{bag}(x) = \frac{1}{B} \sum_b \hat{p}_k^{\star b}(x)$$

- We can classify using $\hat{y}^{bag} = \arg\max_{k=1,\ldots,K} \hat{p}_k^{bag}(x)$

Interpretability

- We lose simple interpretability by aggregating lots of trees
- But we can calculate feature/variable importance as the total amount that the RSS (or Gini index) decreases due to partitions on that variable, averaged over all of the trees

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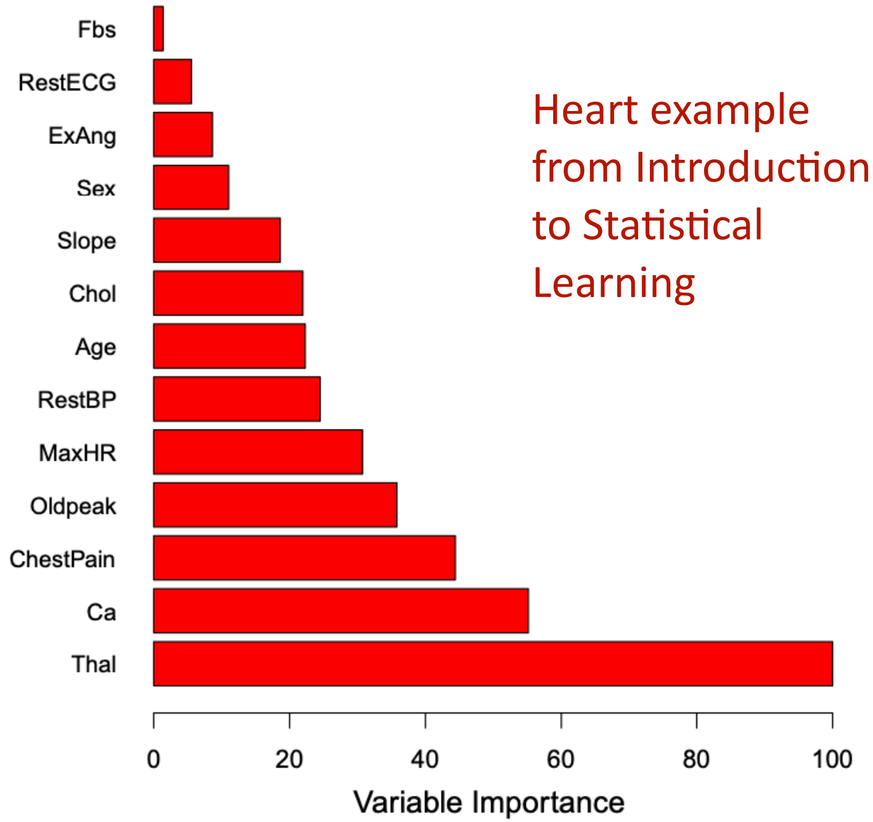

Heart example from Introduction to Statistical Learning

Random forests

- Random forests use the same general procedure as bagging, with a small adjustment to decrease correlation between individual trees (this reduces variance when averaging across trees
- This still uses B bootstrap samples (each building its own tree)
- But at every node, we can only partition on a randomly selected subset of m predictors (out of the p predictors) (a rule of thumb is $m \approx \sqrt{p}$)
- Suppose there's one very strong predictor, several reasonably strong predictors, and some not weak predictors - some of the trees will be forced to ignore the very strong predictor in the top split in favour of a reasonably strong predictor

Random forests

- It turns out that increasing the diversity of the trees improves performance!
- Random forests are less likely to get stuck in local optima and explore more of the model space

Boosting

- Boosting also involves combining trees, but there's no bootstrapping involved
- The idea is learn a sequence of **weak learners** (individual trees) that learn slowly
- Each small tree (sometimes just a stump) learns the residuals from the trees before it

- Use cross-validation to select the number of trees

Boosting

- The first tree predicts the response variable $\hat{y}_i = \hat{f}_1(x_i)$
- The next tree predicts the residuals $r_i^{(0)} = y_i - \hat{y}_i, \quad \hat{r}_i^{(0)} = \hat{f}_2(x_i)$
- The overall prediction becomes $\hat{y}_i^{(1)} = \hat{f}_1(x_i) + \lambda \hat{f}_2(x_i)$ (where λ is a small shrinkage parameter)
- The bth tree predicts the residuals $r_i^{(b)} = y_i - \hat{y}_i^{(b-1)}, \quad \hat{r}_i^{(b)} = \hat{f}_b(x_i)$
- The final prediction (after B trees) is $\hat{y}_i^{(B)} = \hat{f}_1(x_i) + \lambda \sum_{b=2}^{B} \hat{f}_b(x_i)$

Boosting: code

- Jupyter notebook about regression trees
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AdaBoost, gradient boosting, XGBoost

- Boosting corrects previous errors using mean squared error as loss function

- AdaBoost re-computes the weights of each tree at every iteration (works best for binary classification)
- Gradient boosting generalises the MSE to other loss functions
- XGBoost (eXtreme Gradient Boosting) became very popular in 2010s and was often used by winning teams in ML competitions
  - It uses Newton-Raphson method for optimisation, plus better regularisation and various tuned parameters, in order to improve the boosting

Format of the data

$$X = \begin{pmatrix} X_1 & X_2 & \dots & X_p \end{pmatrix} = \begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix} \qquad y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

- What if features are not independent?
- Rotation forest: for each tree, PCA on a random subset of features

Summary

- Decision trees segment the predictor space, they are interpretable but generally not brilliant at prediction
- Grow a large tree, then prune it back to avoid overfitting
- Ensembles combine lots of trees and are much better at prediction
- Bagging: independent trees from bootstrap samples
- Random forest: restrict the predictors available at each partition
- Boosting: grow successive trees using slow weak learners (shrinking)

Questions?

- Feel free to email me at te269@cam.ac.uk

Next time

- Unsupervised learning
  - Dimensionality reduction
    - Principal component analysis
    - Outliers/anomalies