ACTL3142 Week 9 - Tree-based Methods

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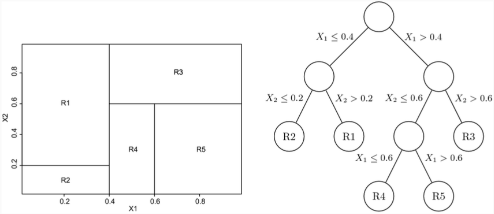
Decision Trees

A decision tree partitions the predictor space into *terminal nodes* or *leaves* to make predictions.

Given a new observation lies in a particular node:

- In a regression, the average of all training observations in that node is the prediction;
- In a classification, the majority class of all training observations in that node is the prediction.



Training a Decision Tree

Recursive Binary Splitting

1. Considering all p predictors, find the additional split that leads to the largest reduction in some score;
   - In regression, this could be MSE;
   - In classification, this could be Gini index or entropy.
2. Repeat the above, finding more splits in the data until some stopping criterion is reached (nodes have ≤ 5 observations, maximum depth reached, etc.).

Controlling Flexibility

Intuitively, more nodes $\implies$ more flexibility...

Cost-Complexity Pruning

The cost-complexity criterion has the form,

$$\text{Total cost} = \text{Measure of fit} + \text{Measure of complexity}.$$

For example,

$$C_\alpha(T) = \sum_{m=1}^{|T|} \sum_{i \in R_m} (y_i - \hat{y}_m)^2 + \alpha |T|,$$

where $|T|$ is the number of terminal nodes.

With the above, we can train a 'big' tree, 'prune' it by finding the a solution to $C_\alpha(T)$ by working backwards, and then cross-validate all the solutions to pick the best one.

Ensemble Methods

Trees are typically rubbish by themselves! But, there is strength in numbers...

Ensemble Methods

An **ensemble method** is a prediction method that combines several models together to make predictions. Say we train d models;

- In a regression problem, we would make predictions with all d models and then take the average;
- In a classification problem, we would make predictions with all d models and then take the majority class.

Bagging

A shortfall of trees is they tend to fit to noise very easily and mistake random patterns for trends we want to capture.

Bagging

1. Re-sample the original dataset repeatedly with replacement (bootstrap), obtaining B different training data sets.
2. Train a deep decision tree on all B training sets (no need to prune - why?).
3. Make a prediction using all B models as usual with an ensemble method.

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No !! It's simply a variance reduction method.

Random Forests

An issue with bagging is that across all B samples, the models tend to be very similar, where the top splits are the same strong predictors. This leads to the predictions being highly correlated and leading to a lesser variance reduction, An issue with bagging is that across all B samples, the models tend to be very similar, where the top splits are the same strong predictors. This leads to the predictions being highly correlated and leading to a lesser variance reduction,

Random Forest

A random forest is very similar to boosting, but when training each tree at each split only a random subset of size $m < p$ of the predictors is considered.

This adds variability to the trees, which decorrelates them and leads to a better variance reduction !

Boosted Trees

Boosted models **sequentially** train on an updated training set with changing residuals based on previous models.

Boosted Trees

1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all i.
2. For $b = 1, 2, \ldots, B$:
   a. Fit a tree $\hat{f}^b$ with d splits $(d+1)$ terminal nodes to the training data (X, r).
   b. Update $\hat{f}$ by adding a shrunken version of the new tree,
   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda f^b(x).$$
   c. Update the residuals,
   $$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i).$$
3. The final model is the last iteration of $\hat{f}(x)$.

Notes on Boosted Trees

The idea of training on updated residuals and in a sequential manner is to learn off the mistakes of the past models - if there are big residuals in some predictions from past models, future models will aim to rectify this.

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There are lots of hyperparameters here (and even more in other versions of boosted trees!) These are tuned in so many ways, but most commonly a grid-search.