IDS 702: Module 8.4

Classification and regression trees

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Tree-based methods

- The regression approaches we have covered so far in this course are all parametric.
- Parametric means that we need to assume an underlying probability distribution to explain the randomness.
- For example, for linear regression,

$$y_i = \beta_0 + \beta_1 x_{i1} + \epsilon_i; \quad \epsilon_i \overset{iid}{\sim} N(0, \sigma^2),$$

  we assume a normal distribution.
- For logistic regression,

$$y_i | x_i \sim \text{Bernoulli}(\pi_i); \quad \log\left(\frac{\pi_i}{1-\pi_i}\right) = \beta_0 + \beta_1 x_i,$$

  we assume a Bernoulli distribution.

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Tree-based methods

- All the models we have covered requires specifying function for the mean or odds, and specifying distribution for randomness.
- We may not want to run the risk of mis-specifying those.
- As an alternative one can turn to nonparametric models that optimize certain criteria rather than specify models.
  - Classification and regression trees (CART)
  - Random forests
  - Boosting
  - Other machine learning methods
- Over the next few modules, we will briefly discuss a few of those methods.

CART

- Goal: predict outcome variable from several predictors.
- Can be used for categorical outcomes (classification trees) or continuous outcomes (regression trees).
- Let Y represent the outcome and X represent the predictors.
- CART recursively partitions the predictor space in a way that can be effectively represented by a tree structure, with leaves corresponding to the subsets of units.

CART FOR CATEGORICAL OUTCOMES

- Partition X space so that subsets of individuals formed by partitions have relatively homogeneous Y.
- Partitions from recursive binary splits of X.
- Grow tree until it reaches pre-determined maximum size (minimum number of points in leaves).
- Various ways to prune tree based on cross validation.
- Making predictions:
  - For any new X, trace down tree until you reach the appropriate leaf.
  - Use value of Y that occurs most frequently in leaf as the prediction.

CART

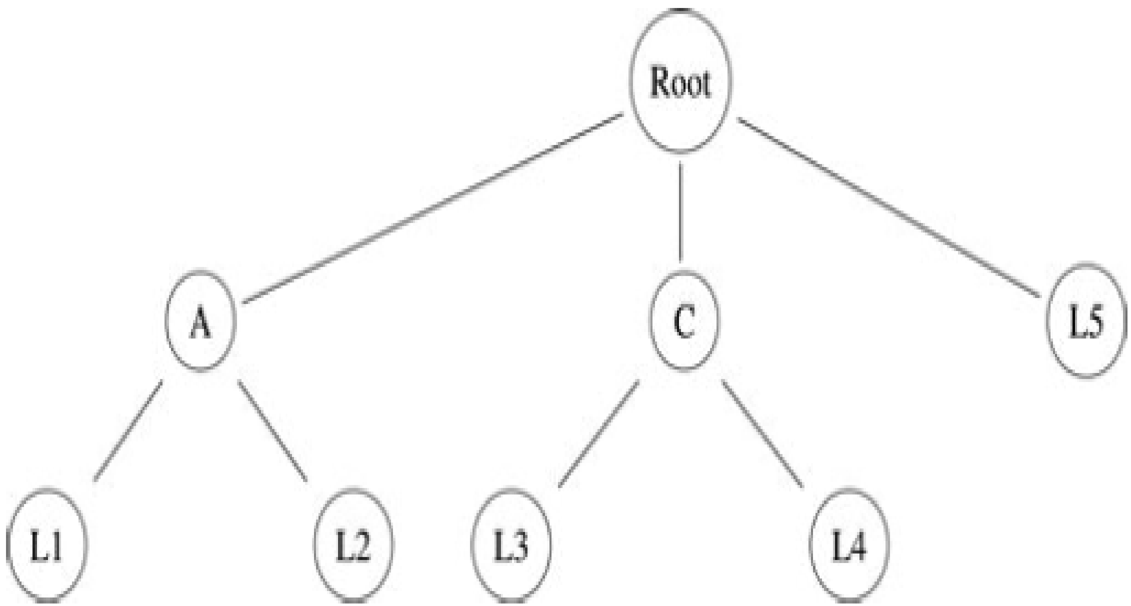

Figure 1. Illustration of the tree structure in CART. A: African-Americans; C: Caucasian; H: Hispanic; M: male; F: female. Leaf L1 contains female African-Americans; leaf L2 contains male African-Americans; leaf L3 contains female Caucasians; leaf L4 contains male Caucasians; and leaf L5 contains Hispanics of both genders.

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CART FOR CATEGORICAL OUTCOMES

- To illustrate, Figure 1 displays a fictional regression tree for
  - an outcome variable.
  - two predictors, gender (male or female) and race/ethnicity (African-American, Caucasian, or Hispanic).
- To approximate the conditional distribution of Y for a particular gender and race/ethnicity combination, one uses the values in the corresponding leaf.
- For example, to predict a Y value for for female Caucasians, one uses the Y value that occurs most frequently in leaf $L3$.

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CART FOR CONTINUOUS OUTCOMES

- Same idea as for categorical outcomes: grow tree by recursive partitions on X.
- Use the variance of the Y values as a splitting criterion: choose the split that makes the sum of the variances of the Y values in the leaves as small as possible.
- When making predictions for new X, use the average value of Y in the leaf for that X.

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Model diagnostics

- Can look at residuals, but...
  - No parametric model, so for continuous outcomes we can't check for linearity, non constant variance, normality, etc.
  - Big residuals identify X values for which the predictions are not close to the actual Y values. But...what should we do with them?
  - Could use binned residuals for logistic regression, but they only tell you where model does not give good predictions.
- Transforming the X values is irrelevant for trees (as long as transformation is monotonic, like logs)
- Can still do model validation, that is, compute and compare RMSEs, AUC, accuracy, and so on.

CART VS. PARAMETRIC REGRESSION: BENEFITS

- No parametric assumptions.
- Automatic model selection.
- Multi-collinearity not problematic.
- Useful exploratory tool to find important interactions.
- In R, use `tree` or `rpart`.

CART VS. PARAMETRIC REGRESSION: LIMITATIONS

- Regression predictions forced to range of observed Y values. May or may not be a limitation depending on the context.
- Bins continuous predictors, so fine grained relationships lost.
- Finds one tree, making it hard to interpret chance error for that tree.
- No obvious ways to assess variable importance.
- Harder to interpret effects of individual predictors.

Also, One big tree is limiting, but, we need different datasets or variables to grow more than one tree...

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What's next?

Move on to the readings for the next module!