Regression Trees

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Motivation

- Linear regression performs poorly on many kinds of data.
- E.g. data with non-linear relationships and interaction effects.
- What might be a better approach for these situations?
- Regression Trees can be useful in many situations.

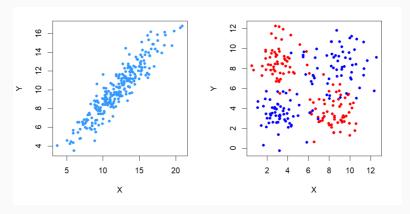


Figure 1: Can you guess where regression trees and where linear regression will perform better?

1

Outline of the Talk

- 1. Motivation
- 2. Basics of Regression Trees
- 3. Comparing regression Trees and Linear Regression
- 4. Overfitting and Pruning
- 5. Ensemble methods and BART
- 6. Conclusion
- 7. References

Basics of Regression Trees

• Regression trees split the predictor space into regions that minimize the RSS given by

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

- In each region \hat{y} simply takes on the mean of all observations in that region.
- Typically we can't find the optimal regions.
- Instead we use a greedy algorithm Recursive binary splitting to find the optimal split to minimize prediction error at each stage.

- Main differences between linear regression and trees
 - Regression trees do not assume a linear relationship between predictors and the response.
 - Trees capture interaction effects naturally.

Simulation: Linear Data

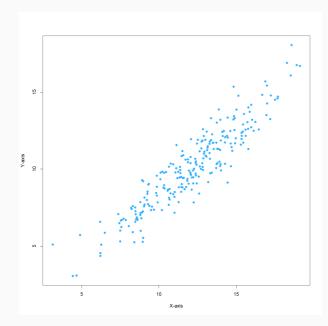


Figure 2: Linear Relation between Variables

- We will run all simulations 400 times.
- For now the regression trees will have 4 terminal Nodes.
- And we will always compare the Mean Squared Error (MSE).
- Data generated as: $Y = \beta_0 + \beta_1 X + \epsilon$
- Where $\epsilon \sim N(0, \sigma^2)$

Simulation: Linear Data

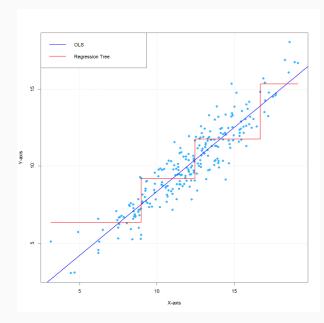


Figure 3: Linear Relation between Variables

- We will run all simulations 400 times.
- For now the regression trees will have 4 terminal Nodes.
- And we will always compare the Mean Squared Error (MSE).

- Results:
- MSE for OLS model: 0.9917
- MSE for regression tree model: 1.4935

Simulation: Non-linear Data

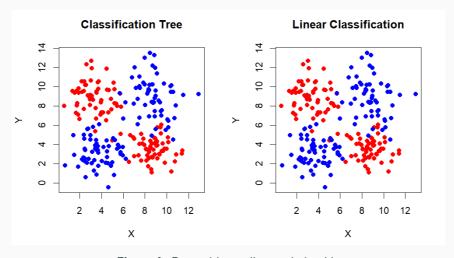


Figure 4: Data with non-linear relationship

- Non-Linear Data generated using 4 normal distributions
- $\bullet \ \mathsf{NW} \ \& \ \mathsf{SE} = \mathsf{red}, \ \mathsf{NE} \ \& \ \mathsf{SW} = \mathsf{blue}$

Simulation: Non-linear Data

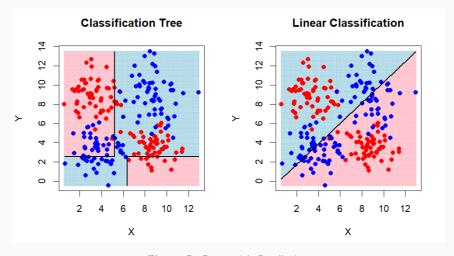


Figure 5: Data with Prediction

- Classification Tree MSE: 0.3757
 Linear Classification MSE: 0.5103
- Trees capture interaction: e.g. Large Y is only indicative of red if X is small.

Two Problems with Regression Trees

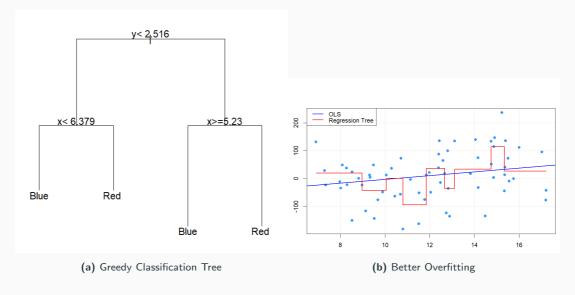


Figure 6: Two Problems that can arise with Trees

• Overfitting and non-Optimal Splitting

Pruning

- Cost complexity pruning counteracts overfitting by removing non-essential splits.
- Lets us grow a large Tree and then

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

- Select a parameter α .
- For each α , find the subtree that minimizes the cost.
- Use cross-validation to select the best α .
- Instead of evaluating a Model on the data we trained it on we evaluate it on a separate set.
- Objective: Achieve a good tradeoff between bias and variance.
- Large α results in very small trees, small α in larger trees.

Simulation: Finding the optimal Tree size

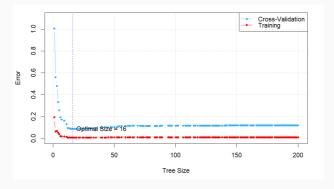


Figure 7: Training and Cross-Validation Error

- Pruning helps against overfitting and improves overall performance
- Original Tree MSE on Test set = 198.2861
- Pruned Tree MSE on Test set = 173.861
- Sweet spot balances variance and bias, minimizing overfitting.
- Training set used to build model, test set to evaluate performance

Ensemble methods

- Even with pruning trees often perform worse than linear other ML methods
- Ensemble methods improve results by combining many regression trees. Each one contributes a small part to the overall prediction.
- Each tree can be independent of previous trees (e.g. Random Forests)
- Or can be grown on the residuals of the current fit (e.g. Bayesian Additive Regression Trees (BART))

- BART models the response as a sum of many tree-based models plus noise.
- Model:

$$Y_i = \sum_{j=1}^m g(X_i; T_j, M_j) + \epsilon_i.$$
 (1)

- BART calculates the residuals of the current sum of Trees.
- Then modifies one Tree to decrease the residuals.
- Then take the average over all but the burn-in iterations.
- Unlike single trees, BART avoids overfitting by averaging the predictions of many trees.
- BART provides a probabilistic prediction, giving a measure of uncertainty.

Conclusion and Discussion

- Regression trees are powerful for non-linear and interactive effects.
 - Will often outperform linear regression.
- They are also very easy to interpret.
- Trees require pruning to combat overfitting.
- By averaging independent Trees or fitting trees on the residuals ensemble methods can improve results.
- BART is a sophisticated method offering good results in many scenarios.

References

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- All images were made using R.
- Also thanks to Claude and ChatGPT for making LATEX a lot nicer to use.