Lecture 3: Bagging, Boosting, and Tree-Based Models

Isaiah Hull[1,2]

[1]BI Norwegian Business School
[2]CogniFrame

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Introduction

Lecture 3: Overview

1. Introduction to Tree-Based Models.
2. Applications.

1. Introduction to Tree-Based Models

Introduction to Tree-Based Models

Overview

- Based on James et al. (2023) and Hull (2021).
  - https://hastie.su.domains/ISLP/ISLP_website.pdf.viewingoogle.html
  - https://link.springer.com/chapter/10.1007/978-1-4842-6373-0_4

Introduction to Tree-Based Models

Tree-Based Methods Overview

- Tree-based methods used for regression and classification.
- Segment the predictor space into simple regions.
- Make predictions based on mean/mode response value for the region.
- Splitting rules summarized in a tree: known as decision tree methods.

Introduction to Tree-Based Models

Advantages and Disadvantages

1. Advantages: Simple and useful for interpretation.

2. Limitations: Not as accurate as some other supervised learning approaches.

3. Solutions for better accuracy: Bagging, random forests, boosting, Bayesian additive regression trees.

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Basics of Decision Trees

- Applicable to both regression and classification.
- Start with classification example.

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Understanding Decision Trees

- A decision tree consists of branches and three types of nodes: roots, internal nodes, and leaves.
- The root is where the first sample split occurs.
- Each split is associated with a branch.
- Internal nodes further split the sample.
- The tree terminates at the leaves, which yield predictions or probability distributions.

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HMDA Mortgage Data: An Example

- Objective: Predict mortgage acceptance based on applicant income.
- Simple tree model uses one feature: Applicant income.
- Focus: How the model splits the sample based on income.

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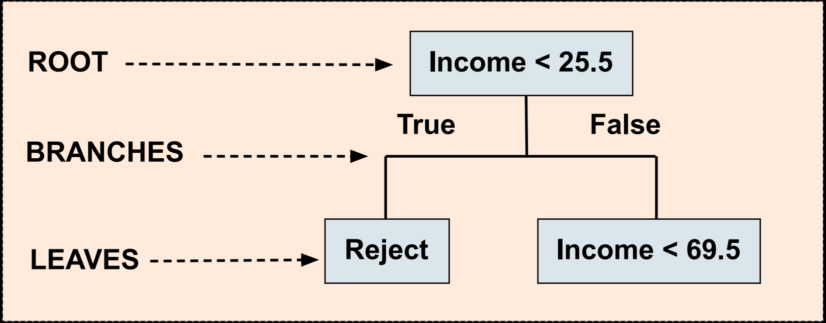
HMDA Mortgage Data: An Example



Source: Hull (2021)

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Decision Trees: Depth and Complexity

- Depth of a tree is measured by the number of branches from the root to the most distant leaf.
- A depth of one results in a “decision stump."
- Example: applicants with incomes below $25,500 are rejected.

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Extended Decision Tree Model

- Model extended by increasing tree depth to three.
- Added feature: ratio of census tract income to metropolitan statistical income (multiplied by 100).

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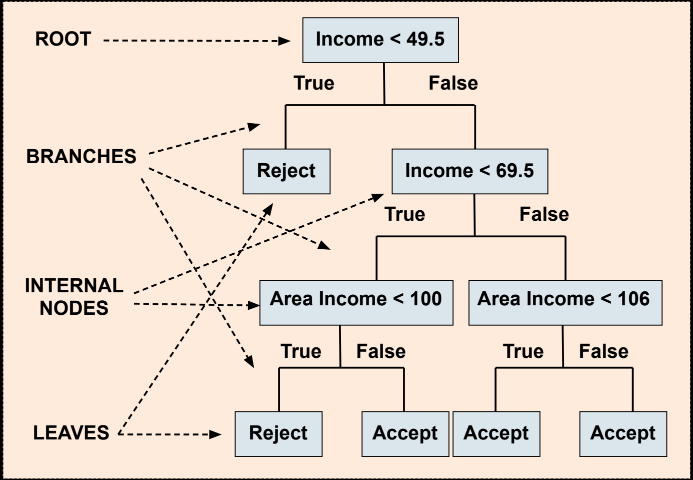

Source: Hull (2021)

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Observations from the Model

- Starting from root, the tree first partitions by applicant income.
- Presence of “internal nodes," which are neither roots nor leaves.
- Not all pairs of leaves contain both “accept" and “reject" classes.
- Class of a leaf depends on the empirical distribution associated with the leaf.

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Why Use Trees?

1. Advantages over other models:
   - Easier to interpret.
   - Graphically intuitive.

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Prediction via Stratification of the Feature Space

- Divide predictor space into J distinct and non-overlapping regions, $R_1, R_2, ..., R_J$.
- Predict with the mean response value of training observations in each region.

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How to Construct the Regions

- Regions can theoretically have any shape.
- Opt for high-dimensional rectangles for simplicity.
- Aim: Minimize the RSS, given by:

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

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Recursive Binary Splitting

- A top-down, greedy approach.
- Starts at top (all observations in a single region).
- Best split is made at each step without looking ahead.
- Split predictor space into regions: $X|X_j < s$ and $X|X_j \geq s$.

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Splitting Process

- For any j and s, define:

$$R_1(j, s) = \{X | X_j < s\}$$

$$R_2(j, s) = \{X | X_j \geq s\}$$

- Minimize equation:

$$\sum_{i: x_i \in R_1(j,s)} (y - \hat{y}_{R_1})^2 + \sum_{i: x_i \in R_2(j,s)} (y - \hat{y}_{R_2})^2$$

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Further Splitting

- Repeat the process to minimize RSS in resulting regions.
- Instead of entire predictor space, split one of the previous regions.
- Continue until a stopping criterion is met.

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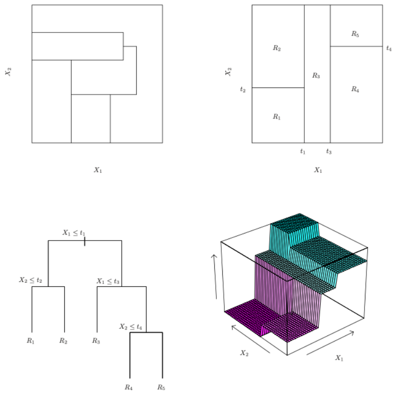

FIGURE 8.3. Top Left: *A partition of two-dimensional feature space that could not result from recursive binary splitting.* Top Right: *The output of recursive binary splitting on a two-dimensional example.* Bottom Left: *A tree corresponding to the partition in the top right panel.* Bottom Right: *A perspective plot of the prediction surface corresponding to that tree.*

Source: James et al. (2023)

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Tree Pruning

- Large trees may overfit data.
- Aim for a smaller tree to reduce variance and increase interpretability.
- One approach: grow a large tree and then prune it back.
- Use cost complexity pruning to achieve this.

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Cost Complexity Pruning

- Also known as weakest link pruning.
- Consider a sequence of trees indexed by tuning parameter α.
- α controls a trade-off between the subtree's complexity and its fit.
- Use validation or cross-validation to select α.

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Subtree Selection with α

Given a value of α:

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

- $|T|$: number of terminal nodes in tree T.
- R_m: rectangle of the m-th terminal node.
- $\hat{y}_{Rm}$: mean of training observations in R_m.
- $\alpha = 0$ implies $T = T_0$. As α increases, smaller subtrees are preferred.

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Analogy with the Lasso

- Akin to the lasso in linear models.
- Controls the complexity of a model.
- As α increases from 0, branches get pruned predictably.
- Obtain entire sequence of subtrees for varying α.
- Select α through validation or cross-validation.

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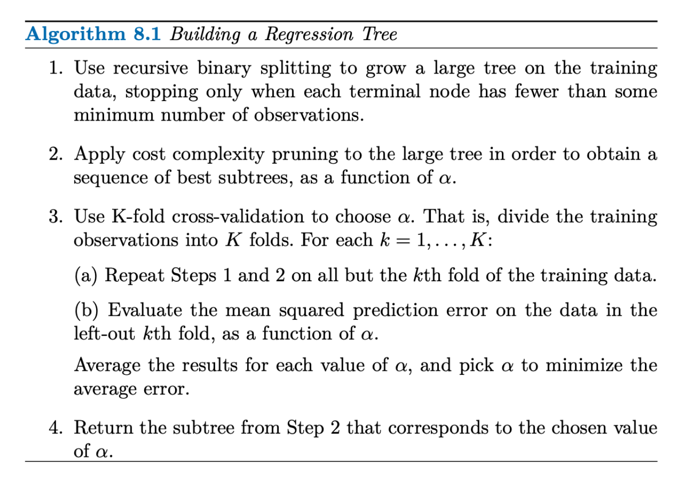

Algorithm 8.1 *Building a Regression Tree*

1. Use recursive binary splitting to grow a large tree on the training data, stopping only when each terminal node has fewer than some minimum number of observations.

2. Apply cost complexity pruning to the large tree in order to obtain a sequence of best subtrees, as a function of α.

3. Use K-fold cross-validation to choose α. That is, divide the training observations into K folds. For each $k = 1, \ldots, K$:

   (a) Repeat Steps 1 and 2 on all but the kth fold of the training data.

   (b) Evaluate the mean squared prediction error on the data in the left-out kth fold, as a function of α.

   Average the results for each value of α, and pick α to minimize the average error.

4. Return the subtree from Step 2 that corresponds to the chosen value of α.

Source: James et al. (2023)

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Classification Trees

Distinction from Regression Trees:

- Predicts a qualitative response, not quantitative.
- Predicted response: most commonly occurring class in a region.
- Also, interested in class proportions for each region.

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Growing a Classification Tree

Similarities and Differences:

- Growth similar to regression trees.
- Recursive binary splitting is used.
- RSS not applicable.

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Classification Error Rate

- Error rate definition:

$$E = 1 - \max_{k}(\hat{p}_{mk}) \tag{2}$$

- Where $\hat{p}_{mk}$ is the proportion of training observations in the m^{th} region from the k^{th} class.
- Classification error isn't sufficiently sensitive for tree-growing.

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Gini Index

- Defined as:

$$G = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk}) \tag{3}$$

- Measures total variance across classes.
- Small if all $\hat{p}_{mk}$'s are near 0 or 1.
- Indicates node purity.

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Entropy as an Alternative

- Entropy is given by:

$$D = -\sum_{k=1}^{K} \hat{p}_{mk} \log(\hat{p}_{mk}) \tag{4}$$

- Used as an alternative to the Gini Index.

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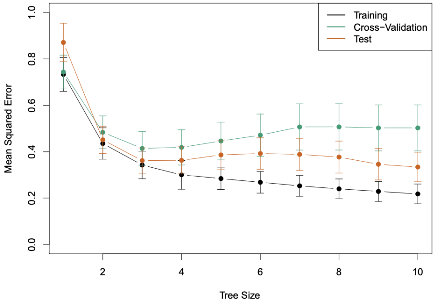

FIGURE 8.5. *Regression tree analysis for the* Hitters *data. The training, cross-validation, and test MSE are shown as a function of the number of terminal nodes in the pruned tree. Standard error bands are displayed. The minimum cross-validation error occurs at a tree size of three.*

Source: James et al. (2023)

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Understanding Entropy

- $0 \leq \hat{p}_{mk} \leq 1$ implies $0 \leq -\hat{p}_{mk} \log(\hat{p}_{mk})$.
- Value near zero if $\hat{p}_{mk}$'s are near 0 or 1.
- Indicates node purity, similar to Gini index.

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Choosing Between Metrics

- Gini index and entropy evaluate split quality for classification trees.
- Preferable over classification error rate for building.
- For pruning: classification error rate prioritized for prediction accuracy.

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The Heart Dataset Example

- Binary outcome HD for 303 patients.
- Yes/No represents presence/absence of heart disease.
- 13 predictors (e.g., Age, Sex, Chol).
- Resultant tree has six terminal nodes.

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Qualitative Predictor Variables

- Decision trees can handle qualitative predictors.
- Splits assign certain qualitative values to branches.
- Example: Splits on “Thal" and “ChestPain."

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Interesting Tree Characteristics

- Some splits yield terminal nodes with identical predictions.
- Example: Split “xwRestECG<1."
- The objective is to increase node purity.
- Node purity improves Gini index and entropy, enhancing certainty.

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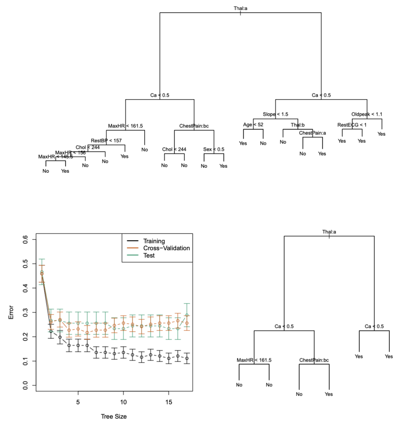

FIGURE 8.6. `Heart` *data.* Top: *The unpruned tree.* Bottom Left: *Cross-validation error, training, and test error, for different sizes of the pruned tree.* Bottom Right: *The pruned tree corresponding to the minimal cross-validation error.*

Source: James et al. (2023)

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Trees Versus Linear Models

- Linear regression assumes:$f(X) = X\beta$
- Regression trees assume: $f(X) = \sum_{m=1}^{M} c_m \cdot 1(X \in R_m)$
- $R_1, \ldots, R_M$ partition the feature space.

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Choosing the Right Model

- Linear model works best if relationship is linear.
- Regression trees work for non-linear, complex relationships.
- Performance can be assessed using test error.
- Methods: cross-validation or validation set approach.

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Other Considerations

- Beyond test error, interpretability and visualization are vital.
- Tree-based models offer clear visualization paths.
- Choice depends on problem specifics and desired outcomes.

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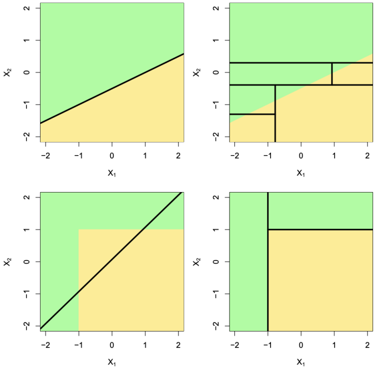

FIGURE 8.7. Top Row: *A two-dimensional classification example in which the true decision boundary is linear, and is indicated by the shaded regions. A classical approach that assumes a linear boundary (left) will outperform a decision tree that performs splits parallel to the axes (right).* Bottom Row: *Here the true decision boundary is non-linear. Here a linear model is unable to capture the true decision boundary (left), whereas a decision tree is successful (right).*

Source: James et al. (2023)

Introduction to Tree-Based Models

Advantages and Disadvantages of Trees

- Trees are easy to explain, often simpler than linear regression.
- Trees mirror human decision-making.
- Graphically displayed and easily interpreted.
- Handle qualitative predictors without dummy variables.

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Challenges with Trees

- Lower predictive accuracy compared to other models.
- Non-robustness: small data changes can affect outcomes.

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Improving Tree Predictions

- Aggregate many decision trees for better performance.
- Methods: bagging, random forests, boosting.

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Ensemble Methods and Their Importance

- An ensemble method combines many “building block” models to create a powerful singular model.
- Building blocks often referred to as *weak learners*.
- Focus: Bagging, random forests, boosting, and Bayesian additive regression trees.
- Building blocks for these methods are regression or classification trees.

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Bagging: Introduction and Motivation

- Bootstrap: A powerful concept, often used to compute hard-to-determine standard deviations.
- Decision trees have high variance.
- Bagging (Bootstrap Aggregation): Reduces variance of statistical methods, especially useful for decision trees.

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Bagging: Conceptual Overview

- High variance means different results for different data splits.
- Averaging observations reduces variance.
- Goal: Build prediction models on many training sets and average predictions.
- Challenge: Generally, only one training set is available.
- Solution: Bootstrap – take repeated samples from the single training data set.

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Bagging: Mathematical Insight

- Averaging B models:

$$f_{avg}(x) = \frac{1}{B}\sum_{b=1}^{B} \hat{f}_b(x) \tag{5}$$

- Using bootstrap for B training sets, the bagged estimator is:

$$\hat{f}_{bag}(x) = \frac{1}{B}\sum_{b=1}^{B} \hat{f}^{*}_{b}(x) \tag{6}$$

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Bagging: An Overview

- Bagging improves predictions for many regression methods, especially for decision trees.
- Procedure: Construct B regression trees using B bootstrapped training sets and average the predictions.
- Individual trees: High variance, low bias.
- Averaging B trees helps in reducing the variance.

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Bagging in Regression vs Classification

- Described procedure suits regression (quantitative outcome).
- For classification (qualitative outcome):
  - Predict class using each of the B trees.
  - Take a majority vote to determine the overall prediction.

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Bagging: Performance Insights

- Bagging test error rate is often lower than the error rate from a single tree.
- Number of trees, B, isn't critical; very large B doesn't lead to overfitting.
- Practical tip: Choose B large enough for error stabilization (e.g., B = 100 in the example).

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Out-of-Bag Error Estimation

- Bagging uses bootstrapped subsets of observations. On average, each tree uses about two-thirds of the observations.
- The remaining one-third are the out-of-bag (OOB) observations.
- For each observation, around $B/3$ OOB predictions are made.
- OOB error is a valid estimate of the test error.
- OOB error is roughly equivalent to leave-one-out cross-validation error with sufficiently large B.

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Variable Importance Measures

- Bagging improves accuracy but reduces interpretability.
- One advantage of trees is their easily interpreted diagram.
- Measure importance with RSS (regression trees) or Gini index (classification trees).
- For regression, track total RSS decrease due to splits over a predictor, averaged over all B trees.
- For classification, sum the total decrease in Gini index by splits over a predictor, averaged over all B trees.

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Graphical Representation of Variable Importances

- The variable importances can be visually represented.
- It shows the mean decrease in Gini index for each variable.
- Variables with the most significant mean decrease in Gini index are Thal, Ca, and ChestPain.

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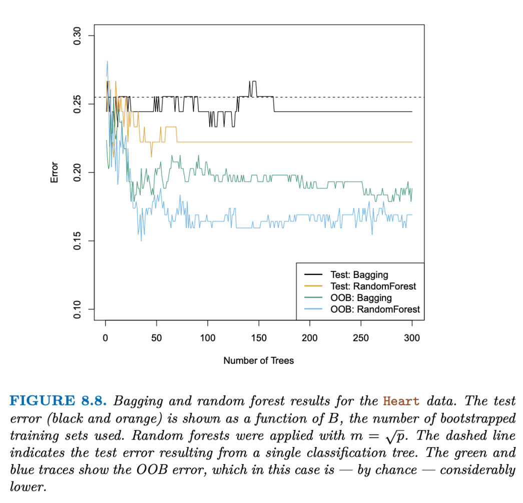

FIGURE 8.8. *Bagging and random forest results for the* Heart *data. The test error (black and orange) is shown as a function of B, the number of bootstrapped training sets used. Random forests were applied with $m = \sqrt{p}$. The dashed line indicates the test error resulting from a single classification tree. The green and blue traces show the OOB error, which in this case is — by chance — considerably lower.*

Source: James et al. (2023)

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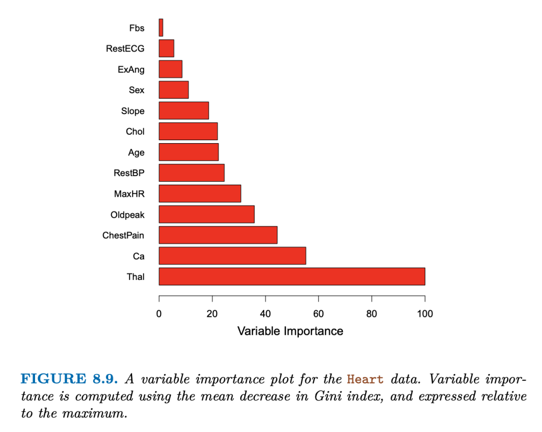

FIGURE 8.9. *A variable importance plot for the* `Heart` *data. Variable importance is computed using the mean decrease in Gini index, and expressed relative to the maximum.*

Source: James et al. (2023)

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Random Forests

- Improvement over bagged trees by decorrelating trees.
- Build decision trees on bootstrapped training samples.
- At each tree split, a random sample of m predictors is chosen out of p.
- Typically, $m \approx \sqrt{p}$.

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Rationale Behind Random Forests

- If one strong predictor dominates, all bagged trees will look similar.
- Predictions from similar trees are highly correlated.
- Averaging many correlated predictions doesn’t reduce variance much.

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Rationale Behind Random Forests

- Random forests limit the predictors considered at each split.
- Decorrelates the trees, making their average more reliable.

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Differences: Bagging vs. Random Forests

- Main difference is the choice of predictor subset size m.
- For $m = p$, random forests are equivalent to bagging.
- Random forests reduce both test error and OOB error.
- Using small m values helps when predictors are correlated.

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Application on Biological Data

- Data: Expression measurements of 4,718 genes from 349 patients.
- Goal: Predict cancer type based on 500 genes with highest variance.
- Randomly split data into training and test sets.

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Application on Biological Data

- Applied random forests with different values of m.
- Using 400 trees is sufficient for good performance.
- Choice of $m = \sqrt{p}$ gave a small improvement over bagging.

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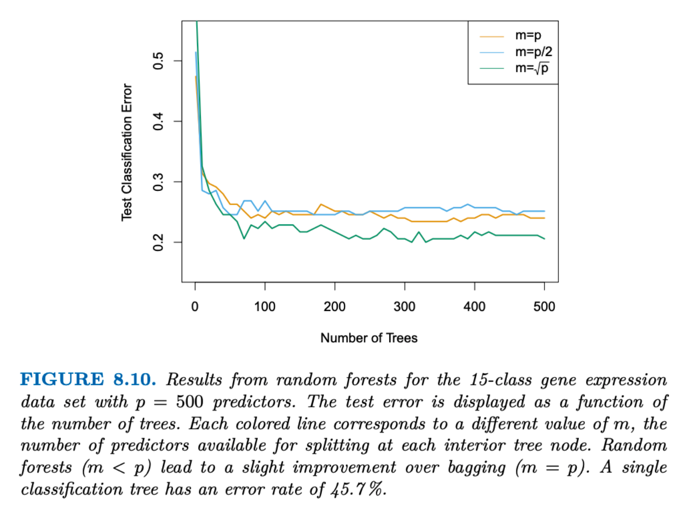

FIGURE 8.10. *Results from random forests for the 15-class gene expression data set with $p = 500$ predictors. The test error is displayed as a function of the number of trees. Each colored line corresponds to a different value of m, the number of predictors available for splitting at each interior tree node. Random forests ($m < p$) lead to a slight improvement over bagging ($m = p$). A single classification tree has an error rate of 45.7%.*

Source: James et al. (2023)

Introduction to Tree-Based Models

Boosting Overview

- Boosting improves predictions from decision trees.
- Can be applied to many learning methods.
- Unlike bagging, trees in boosting are grown sequentially.
- Each tree improves on previous trees.
- Does not use bootstrap sampling.

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Boosting Mechanics

- Each tree is fit on a modified version of the original dataset.
- Boosting learns slowly: fits small trees to residuals.
- Shrinkage parameter λ slows the learning.
- Each tree depends on prior trees (unlike bagging).

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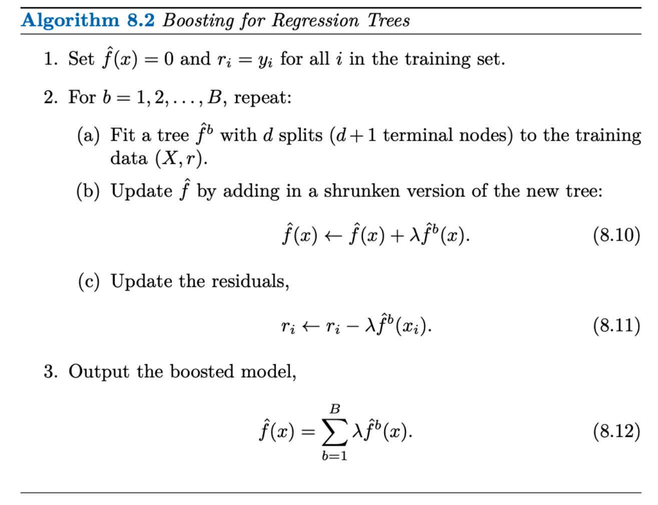

Algorithm 8.2 *Boosting for Regression Trees*

```
1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all $i$ in the training set.
2. For $b = 1, 2, \ldots, B$, repeat:
    (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 in a shrunken version of the new tree:
            $\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x).$    (8.10)
    (c) Update the residuals,
            $r_i \leftarrow r_i - \lambda \hat{f}^b(x_i).$    (8.11)
3. Output the boosted model,
            $\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x).$    (8.12)
```

Source: James et al. (2023)

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Parameters in Boosting

- Number of trees B: Boosting can overfit with a large B.
- Shrinkage parameter λ: Controls learning rate.
- Number of splits d: Controls tree complexity.
- $d = 1$ (a stump) often works well.
- d is the interaction depth of the boosted model.

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Boosting vs Random Forests

- Boosting considers other trees while growing a tree.
- Often, smaller trees are sufficient in boosting.
- Using stumps leads to an additive model.
- Boosted stumps can outperform more complex models.

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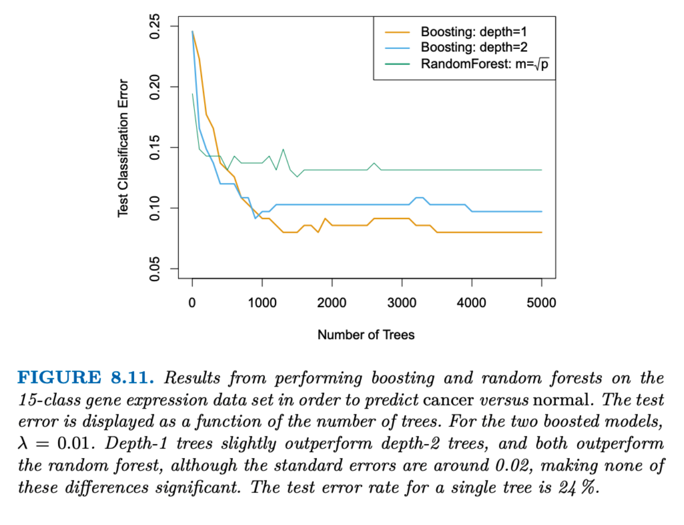

FIGURE 8.11. *Results from performing boosting and random forests on the 15-class gene expression data set in order to predict* cancer *versus* normal. *The test error is displayed as a function of the number of trees. For the two boosted models,* $\lambda = 0.01$. *Depth-1 trees slightly outperform depth-2 trees, and both outperform the random forest, although the standard errors are around 0.02, making none of these differences significant. The test error rate for a single tree is 24 %.*

Source: James et al. (2023)

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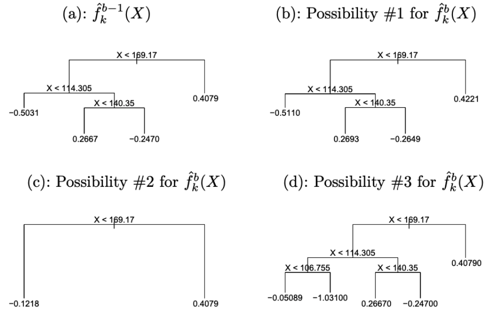

(a): $\hat{f}_k^{b-1}(X)$

(b): Possibility #1 for $\hat{f}_k^{b}(X)$

(c): Possibility #2 for $\hat{f}_k^{b}(X)$

(d): Possibility #3 for $\hat{f}_k^{b}(X)$

FIGURE 8.12. *A schematic of perturbed trees from the BART algorithm.* (a): *The kth tree at the* $(b-1)$*st iteration,* $\hat{f}_k^{b-1}(X)$*, is displayed. Panels (b)–(d) display three of many possibilities for* $\hat{f}_k^{b}(X)$*, given the form of* $\hat{f}_k^{b-1}(X)$*.* (b): *One possibility is that* $\hat{f}_k^{b}(X)$ *has the same structure as* $\hat{f}_k^{b-1}(X)$*, but with different predictions at the terminal nodes.* (c): *Another possibility is that* $\hat{f}_k^{b}(X)$ *results from pruning* $\hat{f}_k^{b-1}(X)$*.* (d): *Alternatively,* $\hat{f}_k^{b}(X)$ *may have more terminal nodes than* $\hat{f}_k^{b-1}(X)$*.*

Source: James et al. (2023)

Introduction to Bayesian Methods

Bayesian Additive Regression Trees (BART)

- Ensemble method using decision trees.
- Related to bagging, random forests, and boosting.
- Each tree captures unaccounted signal.
- Novelty lies in tree generation.

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Notations in BART

- K: Number of regression trees.
- B: Number of iterations in the BART algorithm.
- $f^b(x)$: Prediction at x for k^{th} tree in b^{th} iteration.
- After each iteration: $\hat{f}^b(x) = \sum_{k=1}^{K} \hat{f}^b(x)$ for $b = 1, ..., B$.

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BART Algorithm

- Initially: $\hat{f}^1(x) = \frac{1}{K} \sum_{i=1}^{n} y_i$.
- Each tree is updated in subsequent iterations.
- Partial residuals help decide perturbations.
- Perturbations can change tree structure or node predictions.

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Perturbations in BART

- Perturbations are chosen based on fit to the partial residual.
- Tree structure can be altered by adding/pruning branches.
- Terminal node predictions can be modified.

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BART Output

- Output: Collection of prediction models $\hat{f}(x)$.
- For every observation: $\hat{f}(x) = \hat{f}b(x),$ for $b = 1, 2, ..., B$.

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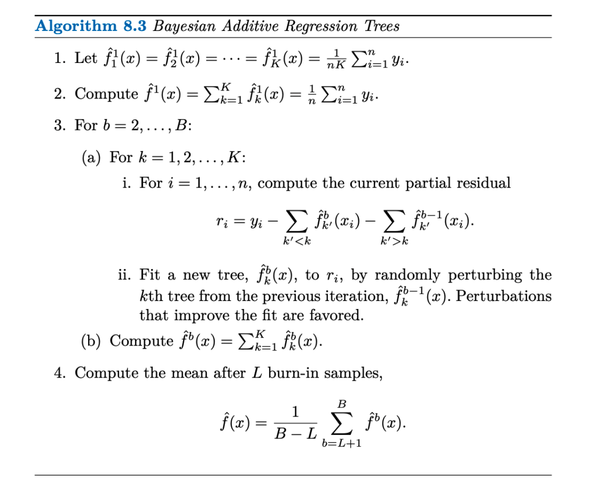

Algorithm 8.3 *Bayesian Additive Regression Trees*

```
1. Let $\hat{f}_1^1(x) = \hat{f}_2^1(x) = \cdots = \hat{f}_K^1(x) = \frac{1}{nK}\sum_{i=1}^n y_i$.
2. Compute $\hat{f}^1(x) = \sum_{k=1}^K \hat{f}_k^1(x) = \frac{1}{n}\sum_{i=1}^n y_i$.
3. For $b = 2, \ldots, B$:
   (a) For $k = 1, 2, \ldots, K$:
       i. For $i = 1, \ldots, n$, compute the current partial residual
            $r_i = y_i - \sum_{k'<k} \hat{f}_{k'}^b(x_i) - \sum_{k'>k} \hat{f}_{k'}^{b-1}(x_i).$
       ii. Fit a new tree, $\hat{f}_k^b(x)$, to $r_i$, by randomly perturbing the
           $k$th tree from the previous iteration, $\hat{f}_k^{b-1}(x)$. Perturbations
           that improve the fit are favored.
   (b) Compute $\hat{f}^b(x) = \sum_{k=1}^K \hat{f}_k^b(x)$.
4. Compute the mean after $L$ burn-in samples,
       $\hat{f}(x) = \frac{1}{B-L}\sum_{b=L+1}^{B} \hat{f}^b(x).$
```

Source: James et al. (2023)

Introduction to Tree-Based Models

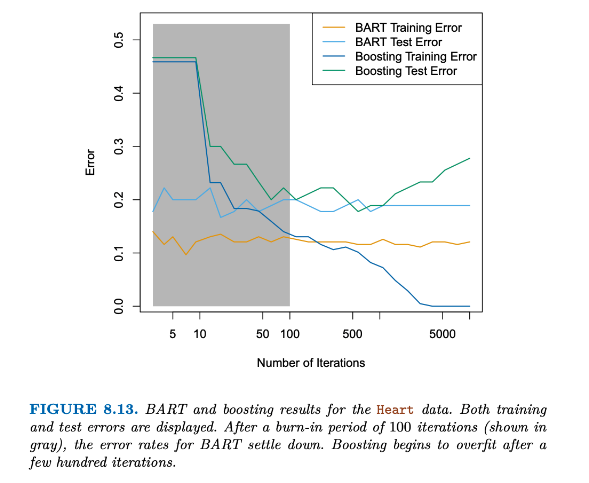

FIGURE 8.13. *BART and boosting results for the* `Heart` *data. Both training and test errors are displayed. After a burn-in period of* 100 *iterations (shown in gray), the error rates for BART settle down. Boosting begins to overfit after a few hundred iterations.*

Source: James et al. (2023)

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Burn-in Period in BART

- The first few models, called burn-in period, are discarded.
- Denoted by L, e.g., $L = 200$.
- Averages taken after burn-in: $f(x) = \frac{1}{B-L} \sum_{b=L+1}^{B} f^b(x)$.
- Beyond averages, percentiles can show prediction uncertainty.

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BART Tree Modifications

- Trees aren’t entirely refitted but slightly modified.
- Limits overfitting.
- Individual trees are generally small to avoid overfitting.

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BART Application on Heart Data

- Used $K = 200$ trees and increased iterations to 10,000.
- Initial iterations showed varying errors.
- Small difference between training and test errors.
- Indicates effective prevention of overfitting.

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Comparison with Boosting

- Boosting test error approaches BART, but then rises.
- Boosting overfits with increased iterations.
- BART seen as a Bayesian approach to ensemble trees.
- Applies a Markov chain Monte Carlo method.

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Parameter Choices in BART

- Must select: K (trees), B (iterations), L (burn-in iterations).
- Typical choices: $K = 200$, $B = 1,000$, $L = 100$.
- BART is known for impressive out-of-box performance.

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Importance of Trees in Ensemble Methods

- Flexible and can handle various predictor types.
- Suitable for both qualitative and quantitative predictors.

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Overview of Four Tree Ensemble Approaches

- Bagging
- Random Forests
- Boosting
- BART

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Bagging

- Trees grown independently on random observation samples.
- Trees tend to be very similar.
- Risks getting caught in local optima.

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Random Forests

- Like bagging, trees grown independently on random samples.
- Uses random subset of features for each split.
- Trees are decorrelated for better model space exploration.

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Boosting

- Utilizes original data without random samples.
- Trees grown successively and use a "slow" learning approach.
- Each tree fits the residual signal and is then shrunk.

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BART

- Uses original data and trees are grown successively.
- Each tree is perturbed for a more thorough model exploration.
- Avoids local minima challenges.

2. Applications

Introduction to TensorFlow

Colab Tutorial

- Tree-Based Models in Sklearn
- Tree-Based Models in TensorFlow
- Official CatBoost Tutorial

References I

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