

# Chapter 8:

# Tree-based Models

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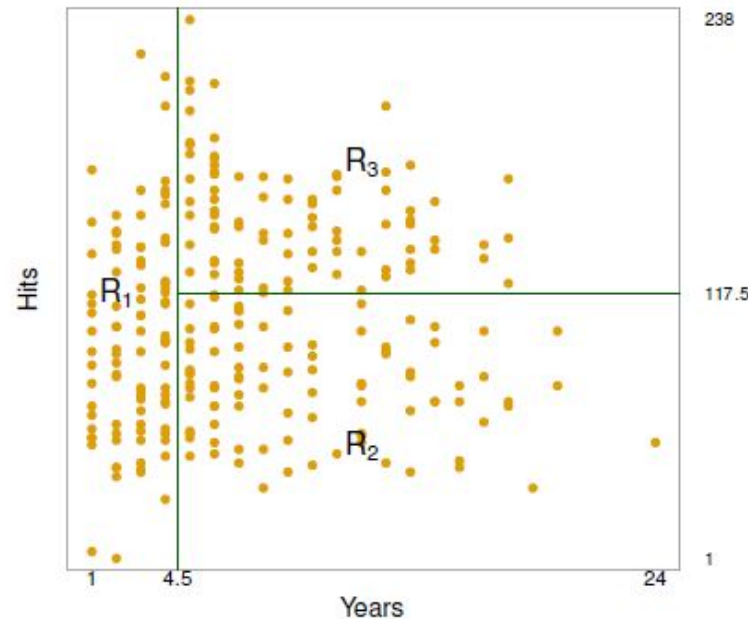
# Introduction

This chapter introduces tree-based methods for regression and classification

- Decision Trees
- Bagging
- Random Forest
- Boosting
- Bayesian Additive Regression Trees

## 8.1.1 Regression Trees

1. Divide the predictor space — that is, the set of possible values for  $X_1, X_2, \dots, X_p$  — into  $J$  distinct and **non-overlapping** regions,  $R_1, R_2, \dots, R_J$ .
2. For every observation that falls into the region  $R_j$ , where  $1 \leq j \leq J$ , take the **mean** of the response values for the training observations in  $R_j$ .



**FIGURE 8.2.** The three-region partition for the **Hitters** data set from the regression tree illustrated in Figure 8.1.

## 8.1.1 Regression Trees

The goal is to find boxes  $R_1, \dots, R_J$  that minimize the  $RSS$ , given by

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

where  $\hat{y}_{R_j}$  is the mean response for the training observations within the  $j$ th box.

Unfortunately, it is **computationally infeasible** to consider every possible partition of the feature space into  $J$  boxes.

## 8.1.1 Regression Trees

One way is given all predictors  $X_1, X_2, \dots, X_p$ , find the best cut off point  $s$  for a given predictor  $X_k$ , where  $1 \leq k \leq p$  such that the resulting two regions

$$R_1(k, s) = \{X | X_k < s\} \text{ and } R_2(k, s) = \{X | X_k \geq s\}$$

have the least  $RSS$  for all predictors

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

where  $\hat{y}_{R_1}$  is the mean response for the training observations in  $R_1(k, s)$ , and  $\hat{y}_{R_2}$  is the mean response for the training observations in  $R_2(k, s)$ .

Repeat the process until no region contains more than five observations.

See [https://bookdown.org/tpinto\\_home/Beyond-Additivity/regression-and-classification-trees.html](https://bookdown.org/tpinto_home/Beyond-Additivity/regression-and-classification-trees.html) and <https://www.youtube.com/watch?v=g9c66TUylZ4> for animation.

## 8.1.1 Regression Trees

However, the previous method may result in a tree that overfits the data.

A better strategy is to

1. grow a very large tree  $T_0$  as before
2. tune  $\alpha$  in the cost complexity pruning formula to prune/penalise  $T_0$  to give a sequence of sub trees.
3. apply cross validation or validation set on those sub trees and pick  $\alpha$  that gives the best sub tree (smallest  $RSS$ ).

The cost complexity pruning formula is

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

where  $\alpha \geq 0$ ,  $|T|$  is the number of terminal nodes the sub tree  $T$  holds.  $R_m$  is the box/region corresponding to the  $m$ th terminal node and  $y_i - \hat{y}_{R_m}$  is the mean response for the training observation in  $R_m$

## 8.1.1 Regression Trees

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

When  $\alpha = 0$ , the sub tree =  $T_0$  as the cost complexity pruning formula equals to the  $RSS$ .

Similar to lasso, as  $\alpha$  increase, some terminal nodes will not be used.

See <https://www.youtube.com/watch?v=D0efHEJsHfHo> for animation.

## 8.1.2 Classification Trees

In the case of classification, instead of taking the mean of a given region, we take the most commonly occurring class (or mode) of training observations in the region to which it belongs.

For the measurement of error, instead of  $RSS$ , one way is to use the fraction of the training observations in that region that do not belong to the most common class.

$$E = 1 - \max_k(\hat{p}_{mk})$$

where  $\hat{p}_{mk}$  the proportion of training observations in the  $m$ th region that are from the  $k$ th class. Hence,

$$0 \leq \hat{p}_{mk} \leq 1$$

However, this error rate is unsuited for tree-based classification.



## 8.1.2 Classification Trees

Instead, the Gini index or the entropy. Both are very similar measures, where small values indicate that the node contains large number of observations from a single class.

The Gini index is defined by

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

The entropy is defined by

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

Both Gini index and Entropy are small when all of the  $\hat{p}_{mk}$ 's are close to zero or one.

When building the classification tree, these classification error measurements can be used to evaluate the sub trees.

## 8.1.2 Classification Trees

See [https://bookdown.org/tpinto\\_home/Beyond-Additivity/regression-and-classification-trees.html](https://bookdown.org/tpinto_home/Beyond-Additivity/regression-and-classification-trees.html)

*Gini index:*  $1 - \sum_{k=1}^K p_k^2$

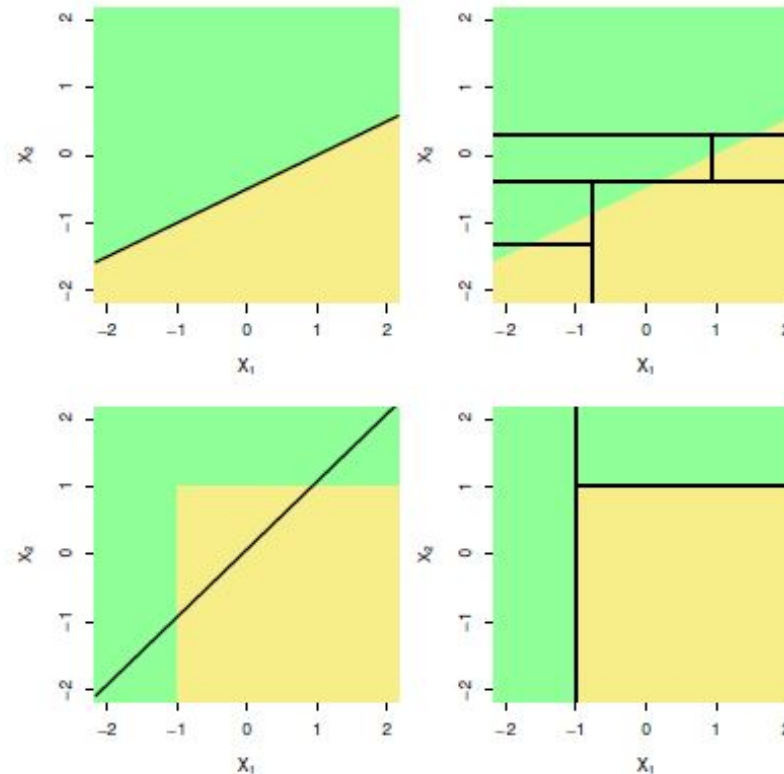
- Favours larger partitions.
- Perfectly classified, Gini Index would be zero.
- Evenly distributed would be  $1 - (1/\# \text{ Classes})$ .

*Information gain (entropy):*  $\sum_{k=1}^K -p_k \log_2 p_k$

- Favours splits with small counts but many unique values
- Weights probability of class by log2 of the class probability
- Information Gain is the entropy of the parent node minus the entropy of the child nodes.

## 8.1.3 Trees Versus Linear Models

In terms of prediction accuracy, ... it depends



**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).

## 8.1.3 Trees Versus Linear Models

Compared to linear models, decision trees are easier to explain to others because they mirror human decision-making. They can be displayed graphically and easily interpreted by non-experts.

However, it is less robust than the linear models. A small change in the data set can cause a large change to the decision tree. This may hurt the decision trees performance in prediction.

To improve its performance, methods like bagging, random forests, and boosting are used (sometimes at the cost of interpretability).

## 8.2.1 Bagging

Bagging is an approach that tries to “stabilise”(make it more robust to change of data) the predictions from trees

The idea is to generate  $B$  different bootstrapped training datasets to create  $B$  different regression trees  $\hat{f}^{*b}$  respectively for  $1 \leq b \leq B$ . Given a new observation to predict called  $x$ , we use the  $B$  regression trees to create  $B$  predictions. The final prediction value is calculated by averaging all the predictions.

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

In the case of classification, we record the class predicted by each of the  $B$  trees, and take a majority vote.

What is missing is how do we estimate the test error rate (without using the test data) to pick the best  $B$  value or number of bagged trees ?

## 8.2.1 Bagging

Each bagged tree is trained using two-thirds of the training data. The other one-third of the training data, known as out-of-bag or *OOB* observations are then used.

Given an *OOB* observation, we first predict its response using only bagged trees that do not use this *OOB* observation in its training. An *OOB* prediction is made by averaging the predicted response (regression) or a majority vote (classification) among these specific bagged trees.

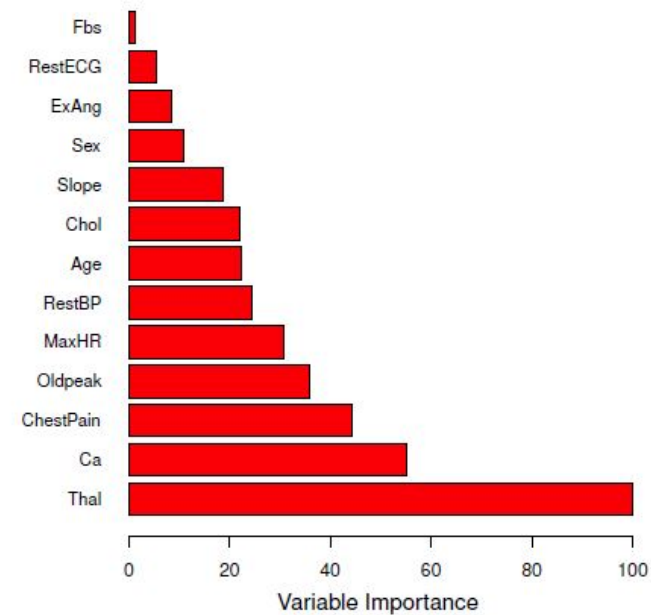
As each *OOB* observation has an *OOB* prediction and a true response, the *OOB* error can be computed via the overall *OOB RSS* (regression) or classification error like Gini index. The  $B$  value that gives the least *OOB* error will be taken.

## 8.2.1 Bagging

Bagging usually improves prediction accuracy at the expense of interpretability.

It is no longer clear which predictors are more important as we now have more than one tree (which may give differing views on the importance of a given predictor).

An overall summary of the importance of each predictor can be achieved by recording how much the average  $RSS$  or Gini index improves (or decreases) when each tree is splitted over a given predictor.



**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.

## 8.2.2 Random Forests

One problem with bagging is that each bagged tree may be highly similar to one another.

This happens if there is a strong predictor in the data set. By the greedy principle, most of the bagged trees will use this strong predictor in the top split, regardless of changes in the training set led by bootstrapping.

This may cause the tree model to be less robust to changes in the data over time.

To further improve the robustness of the model, a change is made during the creation of a split in a given bagged tree on bootstrapped training samples.

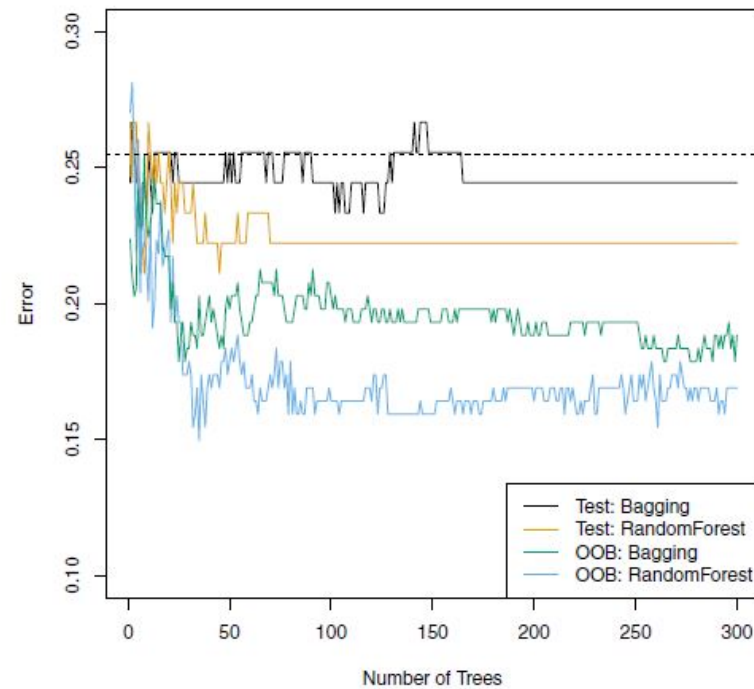
Instead of using the full set of  $p$  predictors as split candidates, only a random sample of  $m \approx \sqrt{p}$  predictors are used instead.

This reduces the odds of the strong predictor being selected during the split and provide other predictors a chance.

See [https://www.youtube.com/watch?v=J4Wdy0Wc\\_xQ](https://www.youtube.com/watch?v=J4Wdy0Wc_xQ) for animation.



## 8.2.2 Random Forests



**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.

## 8.2.3 Boosting

Recall in bagging, each tree is built on a bootstrap training data set.

On the other hand, in boosting, each tree is built on information that the previous trees are unable to catch. That is, we fit a tree using the current residuals, rather than the response.

This is similar to the partial least square components in which each component is build based on the response's residual left by the model created from the previous partial least square components.

The key is to make each tree small (with a few terminal nodes) but still "different" from one another.

For simplicity, only boosting regression trees are described in the book.

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## 8.2.3 Boosting

Boosting has three tuning parameters.

1. The number of trees  $B$
2. The maximum number of splits/depth  $d$  each tree is allow to have. (to make each tree small)
3. A shrinkage parameter or learning rate  $\lambda$  (to make each tree "different" from one another)

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**Algorithm 8.2** *Boosting for Regression Trees*

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1. Set  $\hat{f}(x) = 0$  and  $r_i = y_i$  for all  $i$  in the training set.
2. For  $b = 1, 2, \dots, B$ , 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 shrunk version of the new tree:

$$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x). \quad (8.10)$$

- (c) Update the residuals,

$$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i). \quad (8.11)$$

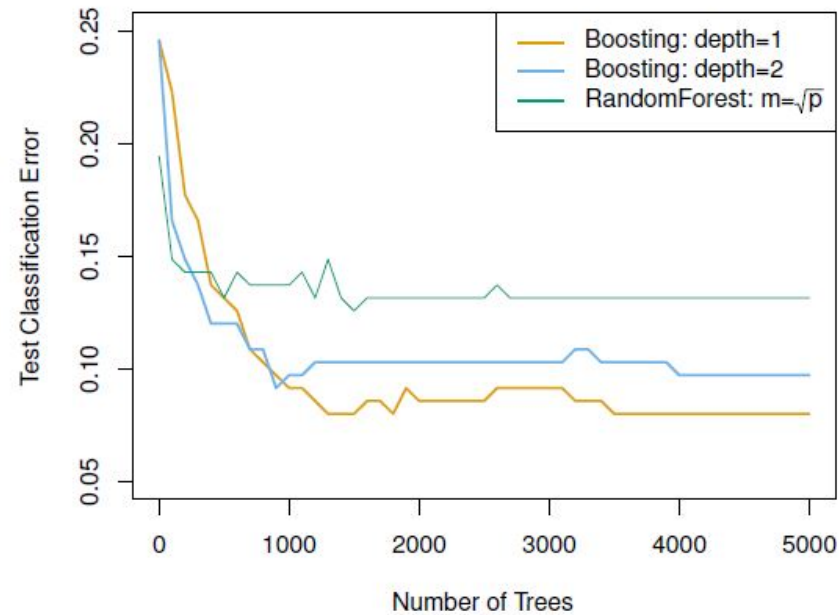
3. Output the boosted model,

$$\hat{f}(x) = \sum_{b=1}^B \lambda \hat{f}^b(x). \quad (8.12)$$

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See <https://www.youtube.com/watch?v=3CC4N4z3GJc> for animation.

## 8.2.3 Boosting



**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 %.

## 8.2.4 Bayesian Additive Regression Trees (BART)

For simplicity, only BART for regression are described in the book.

- In bagging, each tree is built on a random set of training data.
- In random forest, each tree also uses a random set of predictors.
- In boosting, each tree is built to capture signal that is not yet accounted for by the current set of trees

BART combines all these elements together.

## 8.2.4 Bayesian Additive Regression Trees (BART)

The book define some notation

- $K$  be the total number of regression trees used to create the model (later by adding them together)
- $B$  be the number of iterations the BART algorithm will run to improve the additive regression trees.
- $\hat{f}_k^b(x)$  be the prediction of an observation  $x$  for the  $k$ th regression tree used in the  $b$ th iteration of the BART algorithm, where  $1 \leq k \leq K$  and  $1 \leq b \leq B$
- $L$ , where  $L < B$  be the number of burn-in iterations.

Like boosting, the tree model is created by summing all regression trees at the end of each iteration.

$$\hat{f}^b(x) = \sum_{k=1}^K \hat{f}_k^b(x)$$

for  $b = 1, \dots, B$

## 8.2.4 Bayesian Additive Regression Trees (BART)

In the first iteration of the BART algorithm, all  $K$  trees are initialized to predict only one value:

$\hat{f}_k^1(x) = \frac{1}{nK} \sum_{i=1}^n y_i$ , the mean of the response values divided by the total number of trees. Thus

$$\hat{f}^1(x) = \sum_{k=1}^K \hat{f}_k^1(x) = \frac{1}{n} \sum_{i=1}^n y_i$$

## 8.2.4 Bayesian Additive Regression Trees (BART)

In subsequent  $b$  iteration, where  $2 \leq b \leq B$

Given the  $k$ th tree, we calculate for each observation  $i$  where,  $1 \leq i \leq n$ , a partial residual  $r_i$  is created by subtracting the response  $y_i$  with the predictions made from the other  $K - 1$  trees denoted as  $(k')$ . The other  $K - 1$  trees include those that have already been updated by BART and those that will be updated by BART later.

$$r_i = y_i - \sum_{k' < k} \hat{f}_{k'}^b(x_i) - \sum_{k' > k} \hat{f}_{k'}^{b-1}(x_i)$$



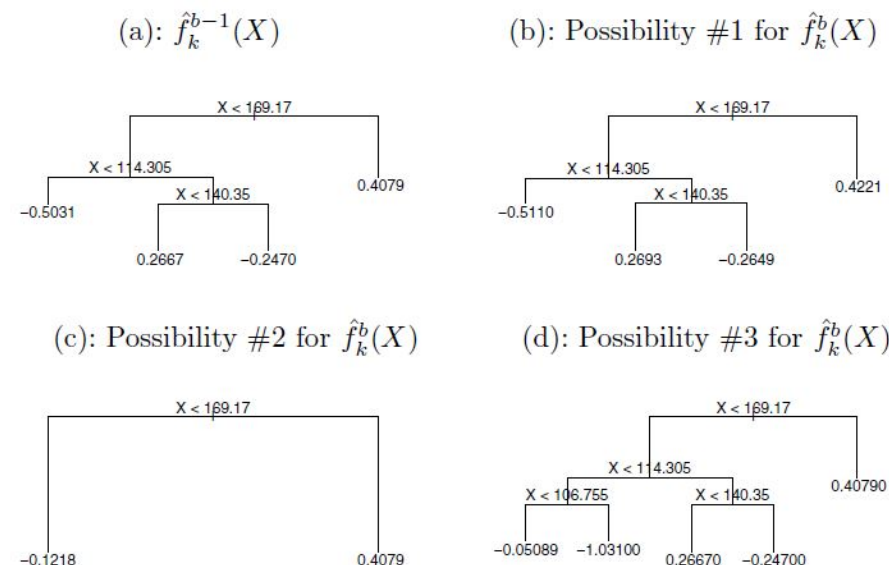
## 8.2.4 Bayesian Additive Regression Trees (BART)

Next, BART will create possible changes/perturbations on the  $k$ th tree and assign a probability calculated by Bayesian methods (given the current  $k$ th tree terminal nodes or  $\hat{f}_k^{b-1}(x)$ ).

- Adding branches
- Pruning branches
- Change the prediction on terminal nodes
- Remain as they are

Changes that greatly improve the fit to the partial residual will be given a higher probability. However, penalty scores will be given when adding new branches to prevent the tree from growing too deep.

Recall that unlike boosting, we do not have control on the depth.



**FIGURE 8.12.** A schematic of perturbed trees from the BART algorithm. (a): The  $k$ th 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  $\hat{f}_k^{b-1}(X)$ .

## 8.2.4 Bayesian Additive Regression Trees (BART)

BART will then "roll a dice" to choose a perturbation on the  $k$ th tree as  $\hat{f}_k^b(x)$ . High probability does not mean it will get chosen.

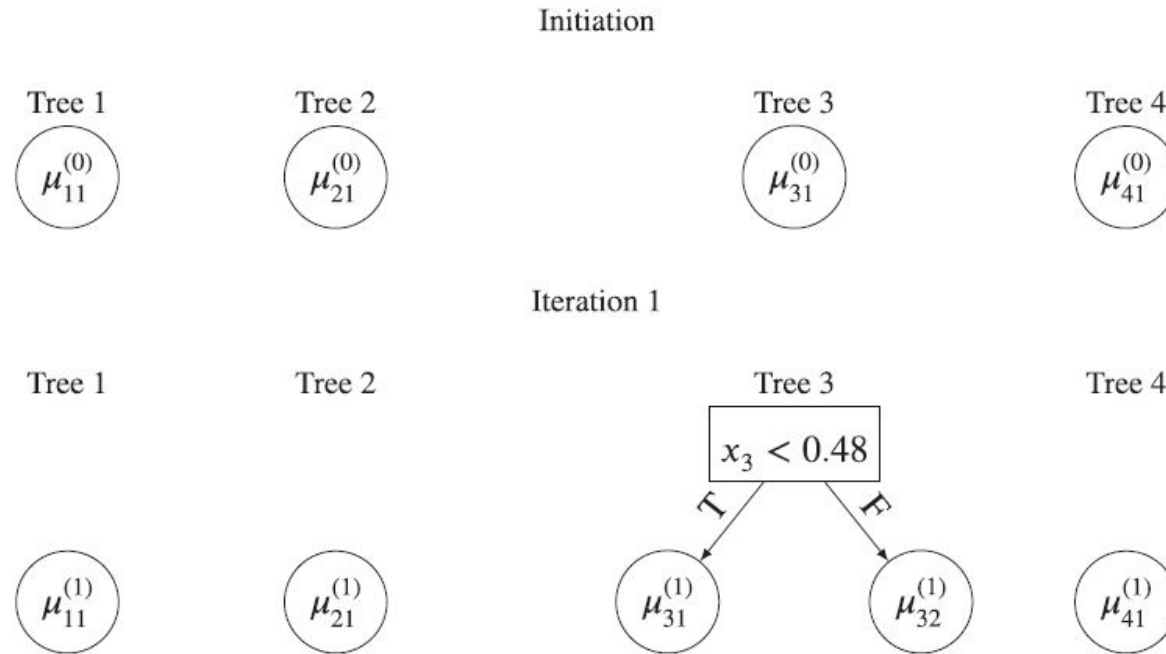
The selected tree  $\hat{f}_k^b(x)$  will then be used to fit the partial residual  $r_i$

This same process will be done for all  $K$  trees.

Adding up all the regression trees will give the new tree model as  $\hat{f}^b(x) = \sum_{k=1}^K \hat{f}_k^b(x)$  for the  $b$ th iteration.

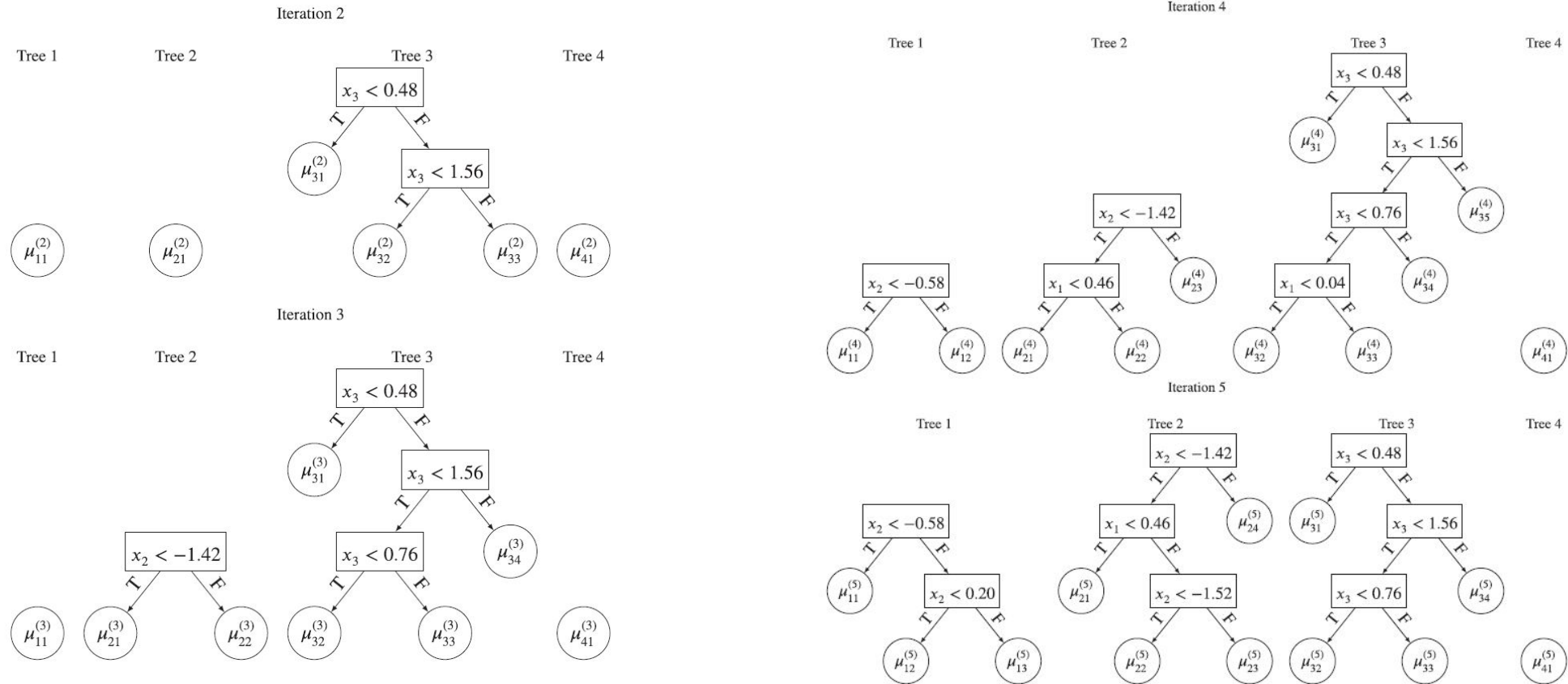
## 8.2.4 Bayesian Additive Regression Trees (BART)

Figures from <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6800811/>



## 8.2.4 Bayesian Additive Regression Trees (BART)

Figures from <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6800811/>



## 8.2.4 Bayesian Additive Regression Trees (BART)

In total there will be a total of  $B$  tree models

$$\hat{f}^1(x), \dots, \hat{f}^B(x)$$

However, the first few models usually gives a poor prediction. Hence it is better to get rid of the first few  $L$  models.

To obtain a single prediction, the final tree model involves taking the average predicted value of the remaining  $B - L$  tree models.

$$\hat{f}(x) = \frac{1}{B - L} \sum_{b=L+1}^B \hat{f}^b(x)$$

## 8.2.4 Bayesian Additive Regression Trees (BART)

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**Algorithm 8.3** *Bayesian Additive Regression Trees*

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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  $b = 2, \dots, B$ :
  - (a) For  $k = 1, 2, \dots, K$ :
    - i. For  $i = 1, \dots, n$ , 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,

$$\hat{f}(x) = \frac{1}{B-L} \sum_{b=L+1}^B \hat{f}^b(x).$$

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