

# Machine Learning for Economists and Business Analysts

## Trees and Forests

Anthony Strittmatter

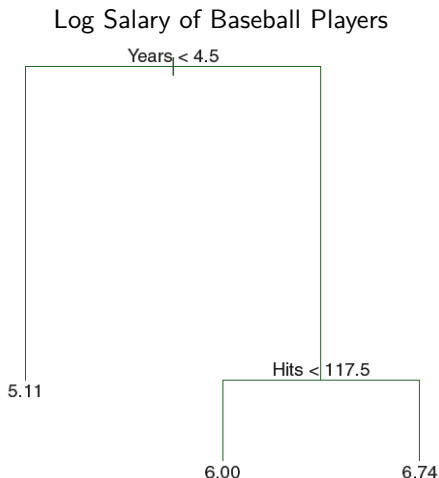
# Literature

- ▶ James, Witten, Hastie, and Tibshirani (2023): "An Introduction to Statistical Learning", Springer, [download](#),  
**Chapters 8.1-8.2.**
- ▶ Hastie, Tibshirani, and Friedman (2009): "Elements of Statistical Learning", 2nd ed., Springer, [download](#),  
**Chapter 9.2.**

# Tree

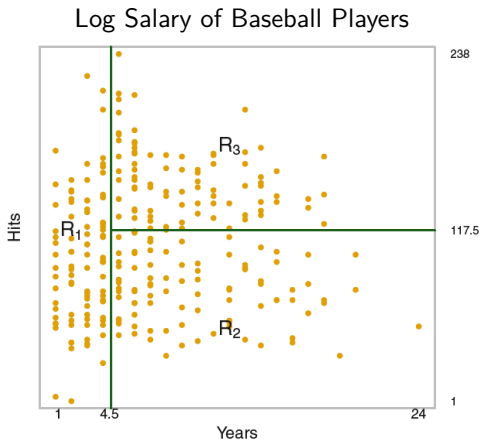
- ▶ Trees partition the sample into mutually exclusive groups  $l_j$ , which are called leaves.
- ▶ Let  $\pi = \{l_1, \dots, l_{\#(\pi)}\}$  be the terminal leaves of a specific tree or sample partition.
- ▶ Let  $l_j \equiv l_j(x, \pi)$  be the respective leaf (for  $j = 1, \dots, \#(\pi)$ ).
- ▶ The leaf  $l_j(x, \pi)$  of tree  $\pi$  is a function of the covariates  $X$  such that  $x \in l_j$ .
- ▶ Let  $\#(\pi)$  be the number of terminal leaves in tree  $\pi$ .

# Example: Shallow Tree



Source: James, Witten, Hastie, Tibshirani (2013)

## Example: Shallow Tree (cont.)



Source: James, Witten, Hastie, Tibshirani (2013)

# Recursive Partitioning

- ▶ Trees select the leaves with a top-down, greedy algorithm, which is called *recursive partitioning*.
- ▶ *Top-down* because we start with a root (tree without leaves) and successively add splits.
- ▶ *Greedy* because at each step of the tree building we add the split that improves the prediction power best (instead of looking ahead).

# Tree Building Algorithm

- (1) Start with the entire sample (root).
- (2) For each predictor  $X_j$  and cut-point  $s$  define the pair of half-planes

$$I_1^{(j,s)} = \{X | X_j < s\} \text{ and } I_2^{(j,s)} = \{X | X_j \geq s\}.$$

- ▶ Calculate the mean outcomes  $\bar{Y}_1$  and  $\bar{Y}_2$  in each half-plane, respectively.
- ▶ Seek the covariate  $X_{j_1}^*$  and the cut-point  $s_1^*$  that minimise

$$\sum_{i: X_i \in I_1^{(j,s)}} (Y_i - \bar{Y}_1)^2 + \sum_{i: X_i \in I_2^{(j,s)}} (Y_i - \bar{Y}_2)^2.$$

# Tree Building Algorithm (cont.)

(2) For each predictor  $X_j$  and cut-point  $s$  define the triple of half-planes

$$l_1^{(j,s)} = \{X | X_{j1}^* < s_1^*, X_j < s\}, l_2^{(j,s)} = \{X | X_{j1}^* < s_1^*, X_j \geq s\}, \text{ and} \\ l_3^{(j,s)} = \{X | X_{j1}^* \geq s_1^*\}$$

and

$$l_1^{(j,s)} = \{X | X_{j1}^* \geq s_1^*, X_j < s\}, l_2^{(j,s)} = \{X | X_{j1}^* \geq s_1^*, X_j \geq s\}, \text{ and} \\ l_3^{(j,s)} = \{X | X_{j1}^* < s_1^*\}.$$

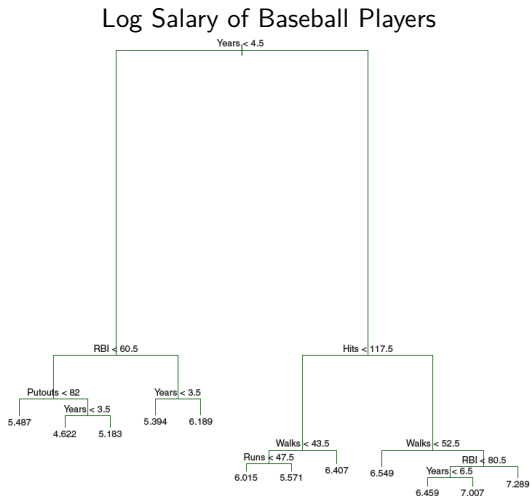
- Calculate the mean outcomes  $\bar{Y}_1$ ,  $\bar{Y}_2$ , and  $\bar{Y}_3$  in each half-plane, respectively.
- Seek the covariate  $X_{j2}^*$  and the cut-point  $s_2^*$  that minimise

$$\sum_{i: X_i \in l_1^{(j,s)}} (Y_i - \bar{Y}_1)^2 + \sum_{i: X_i \in l_2^{(j,s)}} (Y_i - \bar{Y}_2)^2 + \sum_{i: X_i \in l_3^{(j,s)}} (Y_i - \bar{Y}_3)^2.$$

(3) Continue until some stopping rule is reached (e.g., max. tree size, min. terminal leave size, min. MSE gain) .

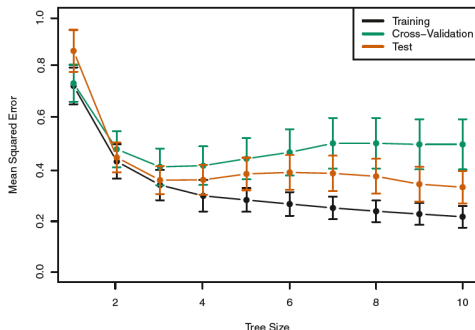


# "Deep" Tree



Source: James, Witten, Hastie, Tibshirani (2013)

# Selecting Optimal Tree Size



- Pruning the complexity of trees can improve out-of-sample prediction power.
- Select optimal tree size  $\pi$  with cross-validation.

Source: James, Witten, Hastie, Tibshirani (2013)

# Complexity Pruning

- (A) Use recursive partitioning to grow the deep tree  $\pi_0$  in the training data.
- (B) For each value of  $\alpha$  a subtree  $\pi \subseteq \pi_0$  minimises

$$\sum_{j=1}^{\#(\pi)} \sum_{i: X_i \in I_j} (Y_i - \bar{Y}_j)^2 + \alpha \#(\pi). \quad (1)$$

Obtain a sequence of best subtrees.

- (C) Use cross-validation to choose  $\alpha$ . Partition the sample in  $k$  folds. For each fold:
  - (a) Repeat steps (A) and (B) excluding the  $k$ th-fold.
  - (b) Evaluate the MSE using equation (1) in the  $k$ th-fold.
  - (c) Average the MSE across the  $k$  folds for each value of  $\alpha$  and select the  $\alpha$  that minimises the average MSE.
- (D) Return to the subtree from (B) with the selected value of  $\alpha$ .

# Prediction

- For the selected tree  $\pi^*$  use the estimation sample to predict

$$\hat{Y}_i = \frac{1}{\sum_{j=1}^{\#(\pi^*)} \sum_{i=1}^N 1\{X_i \in I_j(x, \pi^*)\}} \sum_{j=1}^{\#(\pi^*)} \sum_{i=1}^N 1\{X_i \in I_j(x, \pi^*)\} \cdot Y_i.$$

- This is equivalent to the linear regression

$$\min_{\beta} \sum_{i=1}^N \left( Y_i - \sum_{j=1}^{\#(\pi^*)} 1\{X_i \in I_j(x, \pi^*)\} \beta_j \right)^2.$$

# Advantages and Disadvantages of Trees

## Advantages:

- ▶ Shallow trees are very easy to understand.
- ▶ Shallow trees can be displayed graphically in a nice way.
- ▶ Trees automatically handle interactions between covariates.
- ▶ It is not necessary to transform covariates as long as they have an order.

## Disadvantages:

- ▶ Often trees are unstable and have a high variance.

# Bootstrap Sampling

- ▶ We observe a sample  $\{Y_i, X_i\}_{i=1}^N$  with size  $N$
- ▶ Bootstrap algorithm:
  1. Draw randomly  $N$  observations with replacement from the original sample
  2. Estimate  $\hat{Y}_i^b$  in the “bootstrapped” sample  $b$  with a tree
  3. Repeat 1. and 2.  $B$  times
- ▶ We obtain  $B$  estimates  $\hat{Y}_i^1, \hat{Y}_i^2, \dots, \hat{Y}_i^B$

# Subsampling

- ▶ We observe a sample  $\{Y_i, X_i\}_{i=1}^N$  with size  $N$
- ▶ Subsampling algorithm:
  1. Draw randomly  $M < N$  observations without replacement from the original sample
  2. Estimate  $\hat{Y}_i^s$  in the subsample  $s$  with a tree
  3. Repeat 1. and 2.  $S$  times
- ▶ We obtain  $S$  estimates  $\hat{Y}_i^1, \hat{Y}_i^2, \dots, \hat{Y}_i^S$

# Random Forests

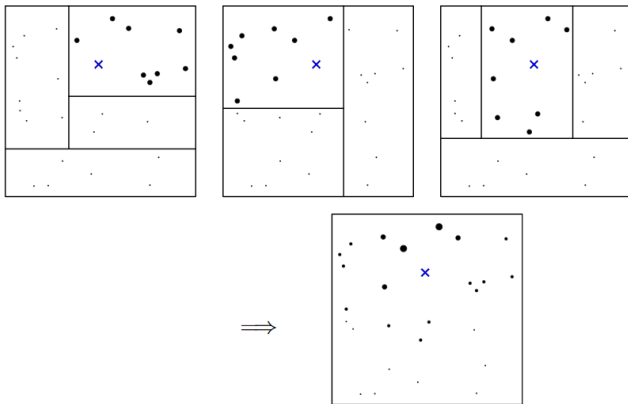
- ▶ Build  $G$  deep trees  $\pi_g$  on different subsets of the data (subsampling or bootstrapping) and covariates.
  - decorrelated trees
- ▶ These trees are overfitted in the sample and will have a high out-of-sample variance.
- ▶ To overcome this problem, we aggregate the trees

$$\hat{Y}_i^{RF} = \frac{1}{G} \sum_{g=1}^G \hat{Y}_i^{\pi_g}.$$

- ▶ This procedure is often called bootstrap-aggregation ("bagging").
- ▶ We lose interpretability but gain prediction power compared to (shallow) trees.
- ▶ Tuning parameters: Forest size, subsample selection, covariate selection, tree size, honest inference, etc.



# Random Forest: Weighted Representation



Source: [Athey, Tibshirani, Wager \(2018\)](#)

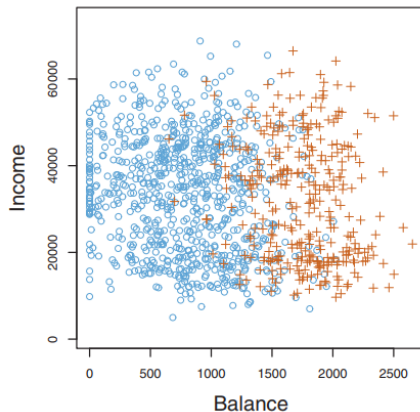
# Classification

## **Outcome variable is categorical:**

- ▶ School degrees (ordered)
- ▶ Occupations (unordered)
- ▶ Credit default (binary dummy)

→ In this lecture we consider binary dummies as outcome variable.

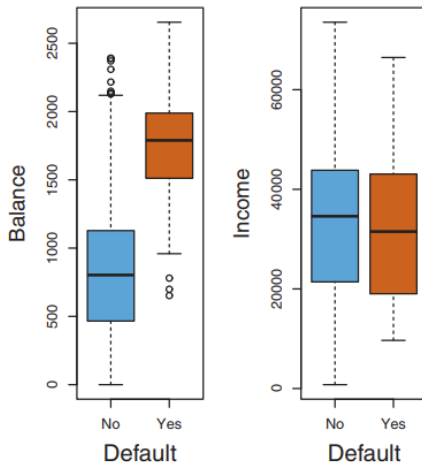
# Example: Credit Default Risk



→ defaulted (orange crosses) and not defaulted (blue circles)

Source: James, Witten, Hastie, Tibshirani (2013)

# Example: Credit Default Risk



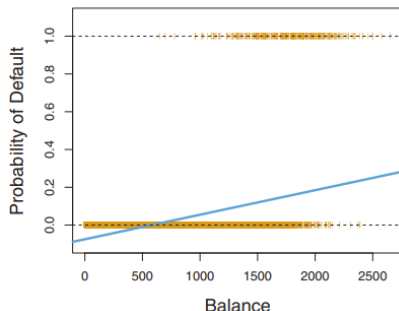
→ defaulted (orange) and not defaulted (blue)

Source: James, Witten, Hastie, Tibshirani (2013)

# Why not linear Regression?

Possible disadvantages of linear regression when outcome is binary:

- Predictions off-support:



- Linearity assumption violated by construction.
- Heteroskedasticity → there exist more efficient estimators.

# Why are Trees Suited for Binary Outcomes?

## Advantages:

- ▶ Trees allow for non-linearities.
- ▶ Group averages cannot lie outside of support  $[0, 1]$ .

## Disadvantages:

- ▶ MSE is not optimal to select optimal complexity of “classification” trees.

Y	Estimator 1		Estimator 2	
	$\widehat{Pr}(Y = 1)$	$(Y - \widehat{Pr}(Y = 1))^2$	$\widehat{Pr}(Y = 1)$	$(Y - \widehat{Pr}(Y = 1))^2$
1	0.51	0.2401	0.49	0.2601
0	0.49	0.2401	0.01	0.0001
1	0.51	0.2401	0.99	0.0001
MSE		0.2401		0.0868

# Alternatives to MSE

## Node Purity:

- ▶ Gini-Index:

$$G = \sum_{j=1}^{\#(\pi)} \hat{p}_j(1 - \hat{p}_j),$$

with  $\hat{p}_j = \widehat{Pr}(Y = 1|l_j)$  and  $l_j$  indicating the terminal leaves for  $j = 1, \dots, \#(\pi)$ .

- ▶ Cross-Entropy:

$$D = - \sum_{j=1}^{\#(\pi)} \hat{p}_j \log(\hat{p}_j).$$

- Both node purity measures are minimized when each terminal leave contains only observations with  $Y = 1$  or  $Y = 0$ .
- We use one node purity measure for complexity pruning ( $\alpha$ -pruning).

# Classification Tree

