Machine Learning Crash Course

Trees and Forests

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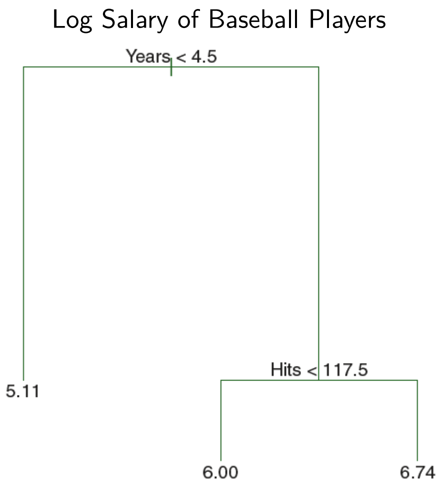
Literature

- James, Witten, Hastie, and Tibshirani (2013): "An Introduction to Statistical Learning", Springer, download, **Chapters 4.1-4.2 and 8**.
- 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 $\pi = \{l_1, ..., l_{\#(\pi)}\}$ be the terminal leaves of a specific tree or sample partition.
- Let $l_j \equiv l_j(x, \pi)$ be the respective leaf (for $j = 1, ..., \#(\pi)$).
- The leaf $l_j(x, \pi)$ of tree π is a function of the covariates X such that $x \in l_j$.
- Let $\#(\pi)$ be the number of terminal leaves in tree π.

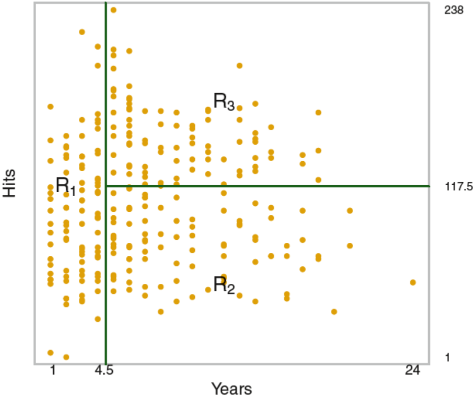
Example: Shallow Tree



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

Example: Shallow Tree (cont.)

Log Salary of Baseball Players



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_{j1}^* 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

$I_1^{(j,s)} = \{X | X_{j1}^* < s_1^*, X_j < s\}$, $I_2^{(j,s)} = \{X | X_{j1}^* < s_1^*, X_j \geq s\}$, and $I_3^{(j,s)} = \{X | X_{j1}^* \geq s_1^*\}$

and

$I_1^{(j,s)} = \{X | X_{j1}^* \geq s_1^*, X_j < s\}$, $I_2^{(j,s)} = \{X | X_{j1}^* \geq s_1^*, X_j \geq s\}$, and $I_3^{(j,s)} = \{X | X_{j1}^* < s_1^*\}$.

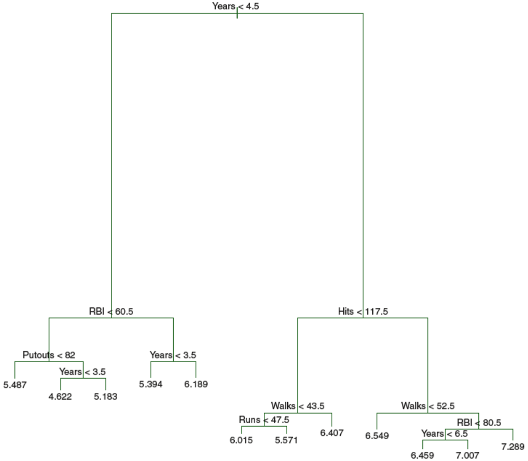
- Calculate the mean outcomes $\bar{Y}_1$, $\bar{Y}_2$, and $\bar{Y}_3$ in each half-plane, respectively.
- Seek the covariate X_{j2}^* and the cut-point s_2^* that minimise

$$\sum_{i:X_i \in I_1^{(j,s)}} (Y_i - \bar{Y}_1)^2 + \sum_{i:X_i \in I_2^{(j,s)}} (Y_i - \bar{Y}_2)^2 + \sum_{i:X_i \in I_3^{(j,s)}} (Y_i - \bar{Y}_3)^2.$$

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

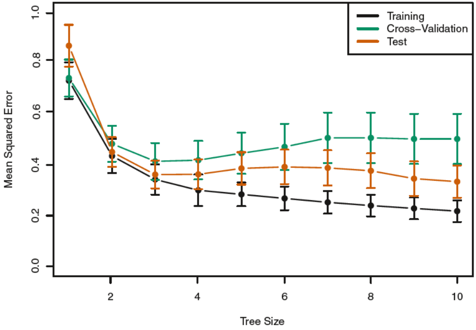
"Deep" Tree

Log Salary of Baseball Players



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 π with cross-validation.

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

Complexity Pruning

(A) Use recursive partitioning to grow the deep tree π_0 in the training data.

(B) For each value of α a subtree $\pi \subseteq \pi_0$ minimises

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

Obtain a sequence of best subtrees.

(C) Use cross-validation to choose α. Partition the sample in k folds. For each fold:

  (a) Repeat steps (A) and (B) excluding the kth-fold.
  (b) Evaluate the MSE using equation (1) in the kth-fold.
  (c) Average the MSE across the k folds for each value of α and select the α that minimises the average MSE.

(D) Return to the subtree from (B) with the selected value of α.

Prediction

- For the selected tree π^* use the estimation sample to predict

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

- This is equivalent to the linear regression

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

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 $\widehat{Y}_i^b$ in the "bootstrapped" sample b with a tree
  3. Repeat 1. and 2. B times
- We obtain B estimates $\widehat{Y}_i^1, \widehat{Y}_i^2, ..., \widehat{Y}_i^B$

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 $\widehat{Y}_i^s$ in the subsample s with a tree
  3. Repeat 1. and 2. S times
- We obtain S estimates $\widehat{Y}_i^1, \widehat{Y}_i^2, ..., \widehat{Y}_i^S$

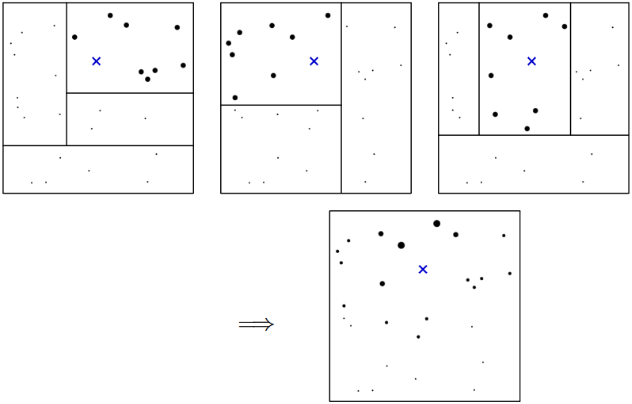
Random Forests

- Build G deep trees π_g on different subsets of the data (subsampling or bootstrapping) and covariates.
  - $\rightarrow$ 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

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

- This procedure is often called bootstrap-aggregation ("bagging").
- We loose 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)