

Classification and Regression Trees

Julia Kempe & David S. Rosenberg

CDS, NYU

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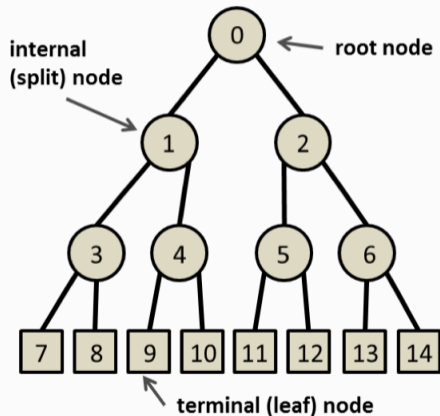
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Trees

Tree Terminology

A general tree structure



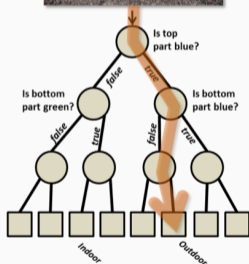
From Criminisi et al. MSR-TR-2011-114, 28 October 2011.

A Binary Decision Tree

binary tree: each node has either 2 children or 0 children



A decision tree

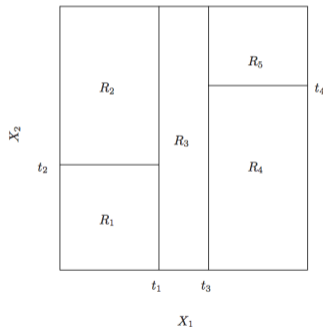
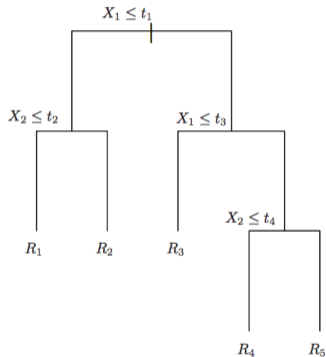


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From Criminisi et al. MSR-TR-2011-114, 28 October 2011.

Binary Decision Tree on \mathbf{R}^2

- Consider a binary tree on $\{(X_1, X_2) \mid X_1, X_2 \in \mathbf{R}\}$



From *An Introduction to Statistical Learning, with applications in R* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

Types of Decision Trees

- We'll only consider
 - **binary trees** (vs multiway trees where nodes can have more than 2 children)
 - decisions at each node involve only a single feature (i.e. input coordinate)
 - for continuous variables, splits always of the form

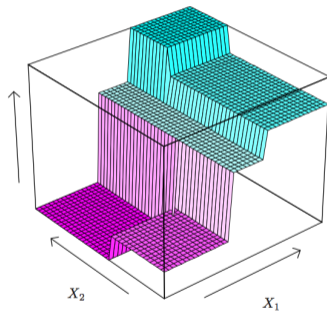
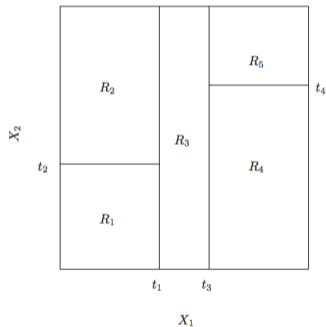
$$x_i \leq t$$

- for discrete variables, partitions values into two groups
- Other types of splitting rules
 - **oblique decision trees** or **binary space partition trees** (BSP trees) have a linear split at each node
 - **sphere trees** – space is partitioned by a sphere of a certain radius around a fixed point

Regression Trees

Binary Regression Tree on \mathbf{R}^2

- Consider a binary tree on $\{(X_1, X_2) \mid X_1, X_2 \in \mathbf{R}\}$



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Fitting a Regression Tree

- The decision tree gives the partition of \mathcal{X} into regions:

$$\{R_1, \dots, R_M\}.$$

- Recall that a partition is a **disjoint union**, that is:

$$\mathcal{X} = R_1 \cup R_2 \cup \dots \cup R_M$$

and

$$R_i \cap R_j = \emptyset \quad \forall i \neq j$$

Fitting a Regression Tree

- Given the partition $\{R_1, \dots, R_M\}$, final prediction is

$$f(x) = \sum_{m=1}^M c_m 1(x \in R_m)$$

- How to choose c_1, \dots, c_M ?
- For loss function $\ell(\hat{y}, y) = (\hat{y} - y)^2$, best is

$$\hat{c}_m = \text{ave}(y_i \mid x_i \in R_m).$$

Trees and Overfitting

- If we do enough splitting, every unique x value will be in its own partition.
- This very likely overfits.
- As usual, we need to control the complexity of our hypothesis space.
- CART (Breiman et al. 1984) uses **number of terminal nodes**.
- Tree depth is also common.

Complexity of a Tree

- Let $|T| = M$ denote the number of terminal nodes in T .
- We will use $|T|$ to measure the complexity of a tree.
- For any given complexity,
 - we want the tree minimizing square error on training set.
- Finding the optimal binary tree of a given complexity is computationally intractable.
- We proceed with a **greedy algorithm**
 - Means build the tree one node at a time, without any planning ahead.

Root Node, Continuous Variables

- Let $x = (x_1, \dots, x_d) \in \mathbf{R}^d$. (d features)
- **Splitting variable** $j \in \{1, \dots, d\}$.
- **Split point** $s \in \mathbf{R}$.
- Partition based on j and s :

$$R_1(j, s) = \{x \mid x_j \leq s\}$$

$$R_2(j, s) = \{x \mid x_j > s\}$$

Root Node, Continuous Variables

- For each splitting variable j and split point s ,

$$\hat{c}_1(j, s) = \text{ave}(y_i \mid x_i \in R_1(j, s))$$

$$\hat{c}_2(j, s) = \text{ave}(y_i \mid x_i \in R_2(j, s))$$

- Find j, s minimizing loss

$$L(j, s) = \sum_{i: x_i \in R_1(j, s)} (y_i - \hat{c}_1(j, s))^2 + \sum_{i: x_i \in R_2(j, s)} (y_i - \hat{c}_2(j, s))^2$$

- How?

Finding the Split Point

- Consider splitting on the j 'th feature x_j .
- If $x_{j(1)}, \dots, x_{j(n)}$ are the sorted values of the j 'th feature,
 - we only need to check split points between adjacent values
 - traditionally take split points halfway between adjacent values:

$$s_j \in \left\{ \frac{1}{2} (x_{j(r)} + x_{j(r+1)}) \mid r = 1, \dots, n-1 \right\}.$$

- So only need to check performance of $n-1$ splits.

Then Proceed Recursively

- ① We have determined R_1 and R_2
 - ② Find best split for points in R_1
 - ③ Find best split for points in R_2
 - ④ Continue...
- When do we stop?

Complexity Control Strategy

- If the tree is too big, we may overfit.
- If too small, we may miss patterns in the data (underfit).
- Can limit max depth of tree.
- Can require all leaf nodes contain a minimum number of points.
- Can require a node have at least a certain number of data points to split.
- Can do **backward pruning** – the approach of **CART** (Breiman et al 1984):
 - 1 Build a really big tree (e.g. until all regions have ≤ 5 points).
 - 2 “**Prune**” the tree back greedily all the way to the root, assessing performance on validation.

Classification Trees

Classification Trees

- Consider classification case: $\mathcal{Y} = \{1, 2, \dots, K\}$.
- We need to modify
 - criteria for splitting nodes

Classification Trees

- Let node m represent region R_m , with N_m observations
- Denote proportion of observations in R_m with class k by

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{\{i: x_i \in R_m\}} 1(y_i = k).$$

- **Predicted classification** for node m is

$$k(m) = \arg \max_k \hat{p}_{mk}.$$

- **Predicted class probability distribution** is $(\hat{p}_{m1}, \dots, \hat{p}_{mK})$.

Misclassification Error

- Consider node m representing region R_m , with N_m observations
- Suppose we predict

$$k(m) = \arg \max_k \hat{p}_{mk}$$

as the class for all inputs in region R_m .

- What is the misclassification rate on the training data?
- It's just

$$1 - \hat{p}_{mk(m)}.$$

What loss function to use for node splitting?

- Natural loss function for classification is 0/1 loss.
- Is this tractable for finding the best split? Yes!
- Should we use it? Maybe not!
- If we're only splitting once, then make sense to split using ultimate loss function (say 0/1).
- But we can split nodes repeatedly – don't have to get it right all at once.

Splitting Example

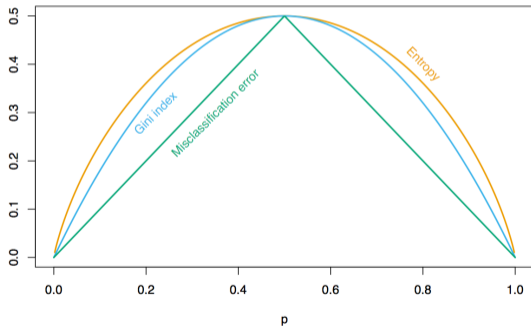
- Two class problem: 4 observations in each class.
- Split 1: (3,1) and (1,3) [each region has 3 of one class and 1 of other]
- Split 2: (2,4) and (2,0) [one region has 2 of one class and 4 of other, other region pure]
- Misclassification rate for the two splits are same. (2).
- In split 1, we'll want to split each node again, and
 - we'll end up with a leaf node with a single element.node .
- In split 2, we're already done with the node (2,0).

Splitting Criteria

- Eventually we want **pure** leaf nodes (i.e. as close to a single class as possible).
- We'll find splitting variables and split point minimizing some **node impurity** measure.

Two-Class Node Impurity Measures

- Consider binary classification
- Let p be the relative frequency of class 1.
- Here are three node impurity measures as a function of p



HTF Figure 9.3

Classification Trees: Node Impurity Measures

- Consider leaf node m representing region R_m , with N_m observations
- Three measures $Q_m(T)$ of **node impurity** for leaf node m :

- Misclassification error:

$$1 - \hat{p}_{mk(m)}.$$

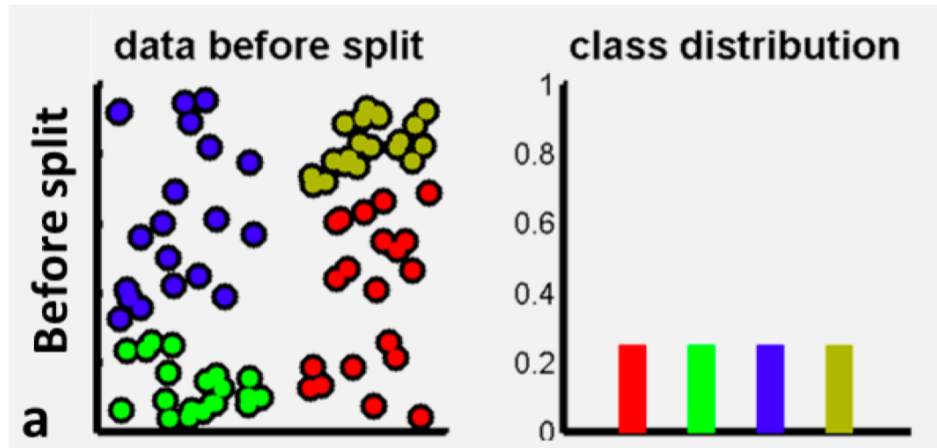
- Gini index:

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

- Entropy or deviance (equivalent to using information gain):

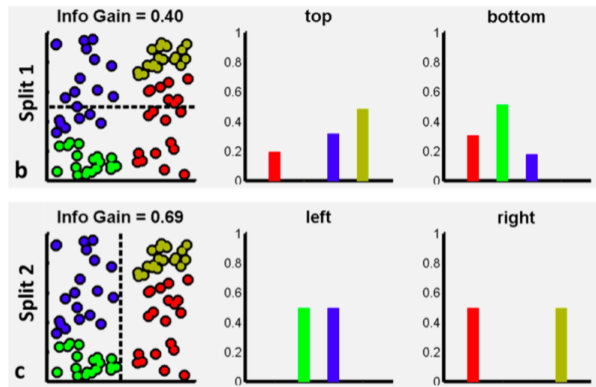
$$-\sum_{k=1}^K \hat{p}_{mk} \log \hat{p}_{mk}.$$

Class Distributions: Pre-split



From Criminisi et al. MSR-TR-2011-114, 28 October 2011.

Class Distributions: Split Search



(Maximizing information gain is equivalent to minimizing entropy.)

Splitting nodes: How exactly do we do this?

- Let R_L and R_R be regions corresponding to a potential node split.
- Suppose we have N_L points in R_L and N_R points in R_R .
- Let $Q(R_L)$ and $Q(R_R)$ be the node impurity measures.
- Then find split that minimizes the **weighted average of node impurities**:

$$N_L Q(R_L) + N_R Q(R_R)$$

Classification Trees: Node Impurity Measures

- For building the tree, Gini and Entropy seem to be more effective.
- They push for more pure nodes, not just misclassification rate
- A good split may not change misclassification rate at all!
- Two class problem: 4 observations in each class.
- Split 1: (3,1) and (1,3) [each region has 3 of one class and 1 of other]
- Split 2: (2,4) and (2,0) [one region has 2 of one class and 4 of other, other region pure]
- Misclassification rate for two splits are same.
- **Gini and entropy split prefer Split 2.**

Trees in General

Missing Features

- What to do about missing features?
 - Throw out inputs with missing features
 - Impute missing values with feature means
 - If a categorical feature, let “missing” be a new category.
- For trees we can do something else...

Surrogate Splits for Missing Data

- For any non-terminal node that splits using feature f ,
- we can find a **surrogate split** using each of the other features.
- To make a surrogate using f' , we find the split using f' that best approximates the split using f .
 - Define “best” in term of 0/1 loss on the examples for which neither f nor f' is missing.
- If there are d features, we'll have $d - 1$ **surrogate splits** to approximate the split on f .
- We can rank these splits by how well they approximate the original split.
- We repeat the above process for every non-terminal node.
 - So each node has the primary split and $d - 1$ surrogate splits, where d is the number of features.
- If we're predicting on an example and the feature needed to evaluate a split is missing,
 - simply go down the list of surrogate splits until we get to one for which the feature is not missing.

I found the CART book a bit vague on this, so this is my best guess for what is intended. If somebody finds a clear statement, please let me know.

Categorical Features

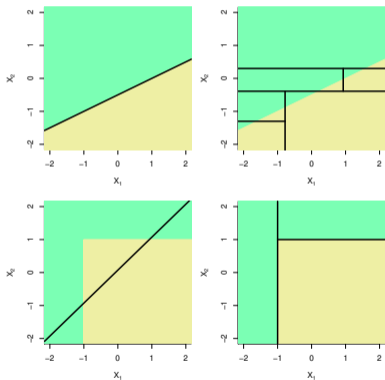
- Suppose we have a categorical feature with q possible values (unordered).
- We want to find the best split into 2 groups
- There are $2^{q-1} - 1$ distinct splits.
- Is this tractable? Maybe not in general. But...
- For binary classification $\mathcal{Y} = \{0, 1\}$, there is an efficient algorithm.

Categorical Features in Binary Classification

- Assign each category a number
 - the proportion of class 0 among training examples with that category.
- Then find optimal split as though it were a numeric feature.
- For binary classification, this is equivalent to searching over all splits
 - at least for certain for node impurity measures of a certain class, including square error, gini and entropy.
- (This trick doesn't work for multiclass – would have to use approximations...)
- Statistical issues with categorical features?
 - If a category has a very large number of categories, we can overfit.
 - Extreme example: Row Number could lead to perfect classification with a single split.

Trees vs Linear Models

- Trees have to work much harder to capture linear relations.



From *An Introduction to Statistical Learning, with applications in R* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

- Trees are certainly easy to explain.
- You can show a tree on a slide.
- Small trees seem interpretable.
- For large trees, maybe not so easy.

Trees for Nonlinear Feature Discovery

- Suppose tree T gives partition R_1, \dots, R_M .
- Predictions are

$$f(x) = \sum_{m=1}^M c_m 1(x \in R_m)$$

- Each region R_m can be viewed as giving a feature function $x \mapsto 1(x \in R_m)$.
- Can use these nonlinear features in e.g. lasso regression.

- Trees make no use of **geometry**
 - No inner products or distances
 - called a “nonmetric” method
 - **Feature scale irrelevant**
- Prediction functions are not continuous
 - not so bad for classification
 - may not be desirable for regression

Appendix: Tree Pruning

Stopping Conditions for Building the Big Tree

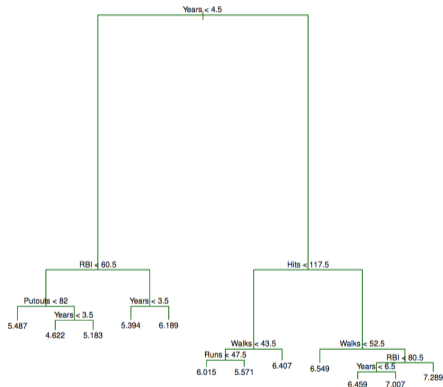
- First step is to build the “big tree”.
- Keep splitting nodes until every node either has
 - Zero error OR
 - Node has C or fewer examples (typically $C = 5$ or $C = 1$) OR
 - All inputs in node are identical (and thus we cannot split more)

Pruning the Tree

- Consider an internal node n .
- To prune the subtree rooted at n
 - eliminate all descendants of n
 - n becomes a terminal node

Tree Pruning

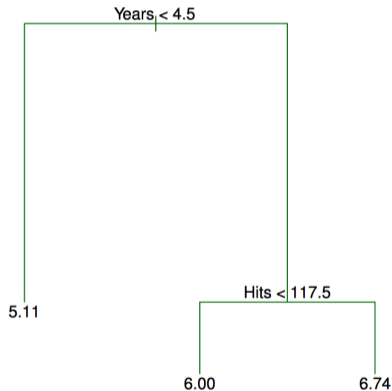
- Full Tree T_0



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Tree Pruning

- Subtree $T \subset T_0$



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Empirical Risk and Tree Complexity

- Suppose we want to prune a big tree T_0 .
- Let $\hat{R}(T)$ be the empirical risk of T (i.e. square error on training)
- Clearly, for any subtree $T \subset T_0$, $\hat{R}(T) \geq \hat{R}(T_0)$.
- Let $|T|$ be the number of terminal nodes in T .
- $|T|$ is our measure of complexity for a tree.

Cost Complexity (or Weakest Link) Pruning

Definitions

The **cost complexity criterion** with parameter α is

$$C_{\alpha}(T) = \hat{R}(T) + \alpha|T|$$

- Trades off between empirical risk and complexity of tree.
- Cost complexity pruning:
 - For each α , find the subtree $T \subset T_0$ minimizing $C_{\alpha}(T)$ (on training data).
 - Use cross validation to find the right choice of α .

Do we need to search over all subtrees?

- The **cost complexity criterion** with parameter α is

$$C_\alpha(T) = \hat{R}(T) + \alpha|T|$$

- $C_\alpha(T)$ has familiar regularized ERM form, but
- Cannot just differentiate w.r.t. parameters of a tree T .
- To minimize $C_\alpha(T)$ over subtrees $T \subset T_0$,
 - seems like we need to evaluate exponentially many¹ subtrees $T \subset T_0$.
 - (In particular, we can include or exclude any subset of internal nodes that are parents of leaf nodes.)
- Amazingly, we only need to try N_{Int} , where N_{Int} is the number of internal nodes of T_0 .

¹See [On subtrees of trees](#).

Cost Complexity Greedy Pruning Algorithm

- Find a proper² subtree $T_1 \subset T_0$ that minimizes $\hat{R}(T_1) - \hat{R}(T_0)$.
 - Can get T_1 by removing a single pair of leaf nodes, and their internal node parent becomes a leaf node.
 - This T_1 will have 1 fewer internal node than T_0 . (And 1 fewer leaf node.)
- Then find proper subtree $T_2 \subset T_1$ that minimizes $\hat{R}(T_2) - \hat{R}(T_1)$.
- Repeat until we have removed all internal nodes are left with just a single node (a leaf node).
- If N_{Int} is the number of internal nodes of T_0 , then we end up with a nested sequence of trees:

$$\mathcal{T} = \{T_0 \supset T_1 \supset T_2 \supset \cdots \supset T_{|N_{\text{Int}}|}\}$$

² T_1 is a proper subtree of T_0 if tree $T_1 \subset T_0$ and $T_1 \neq T_0$.

Greedy Pruning is Sufficient

- Cost complexity pruning algorithm gives us a set of nested trees:

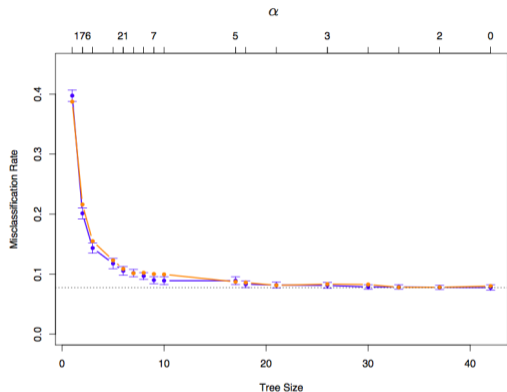
$$\mathcal{T} = \{T_0 \supset T_1 \supset T_2 \supset \cdots \supset T_{|N_{\text{Int}}|}\}$$

- Breiman et al. (1984) proved that this is all you need. That is:

$$\left\{ \arg \min_{T \subset T_0} C_\alpha(T) \mid \alpha \geq 0 \right\} \subset \mathcal{T}$$

- Only need to evaluate N_{Int} trees.

Regularization Path for Trees on SPAM dataset (HTF Figure 9.4)



For each α , we find optimal tree T_α on training set. Corresponding tree size $|T_\alpha|$ is shown on bottom. Blue curves gives error rate estimates from cross-validation (tree-size in each fold may be different from $|T_\alpha|$). Orange curve is test error.