Classification and Regression Trees

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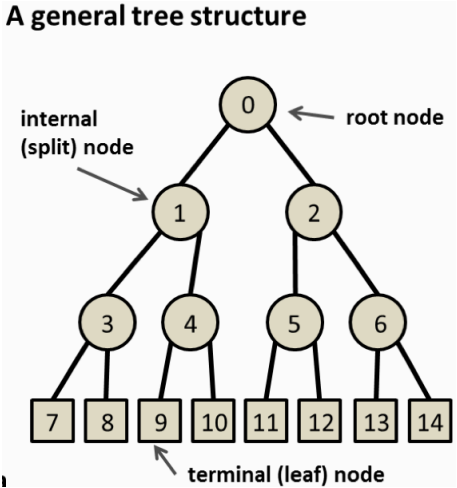
Contents

Trees

Tree Terminology



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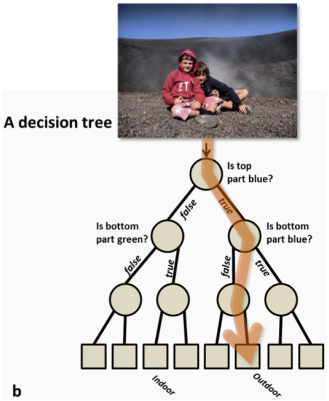
A Binary Decision Tree

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



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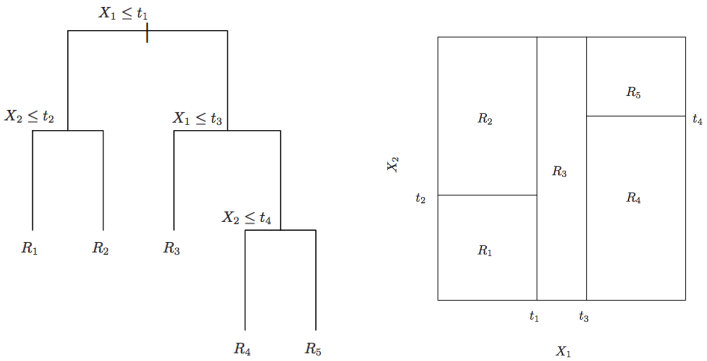
Binary Decision Tree on $\mathbf{R}^2$

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



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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

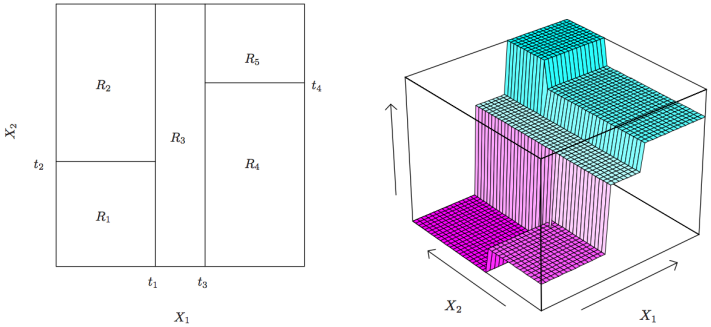
$$x_i \leqslant t$$

  - 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:

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

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

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

and

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

Fitting a Regression Tree

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

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

- How to choose $c_1, \ldots, c_M$?
- 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 $x = (x_1, \ldots, x_d) \in \mathbf{R}^d$. ($d$ features)
- **Splitting variable** $j \in \{1, \ldots, d\}$.
- **Split point** $s \in \mathbf{R}$.
- Partition based on j and s:

$$R_1(j, s) = \{x \mid x_j \leqslant s\}$$
$$R_2(j, s) = \{x \mid x_j > s\}$$

Root Node, Continuous Variables

- For each splitting variable j and split point s,

$$\begin{aligned} \hat{c}_1(j,s) &= \text{ave}(y_i \mid x_i \in R_1(j,s)) \\ \hat{c}_2(j,s) &= \text{ave}(y_i \mid x_i \in R_2(j,s)) \end{aligned}$$

- 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 $x_{j(1)}, \ldots, x_{j(n)}$ 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:

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

- 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 $\leqslant 5$ points).
  2. **"Prune"** the tree back greedily all the way to the root, assessing performance on validation.

Classification Trees

Classification Trees

- Consider classification case: $\mathcal{Y} = \{1, 2, \ldots, K\}$.
- 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 $(\hat{p}_{m1}, \ldots, \hat{p}_{mK})$.

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

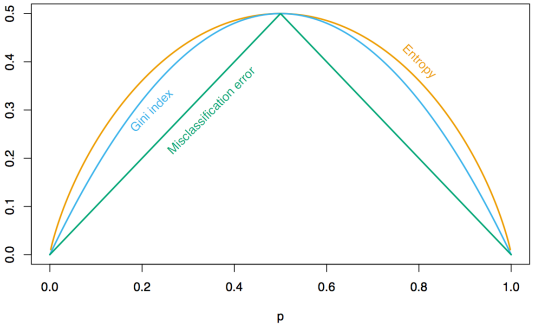
- Two class problem: 4 observations in each class.
- Split 1: (3,1) and (1,3) [each region has 3 of one class and 1 of other]
- Split 2: (2,4) and (2,0) [one region has 2 of one class and 4 of other, other region pure]
- Misclassification rate for the two splits are same. (2).
- In split 1, we'll want 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

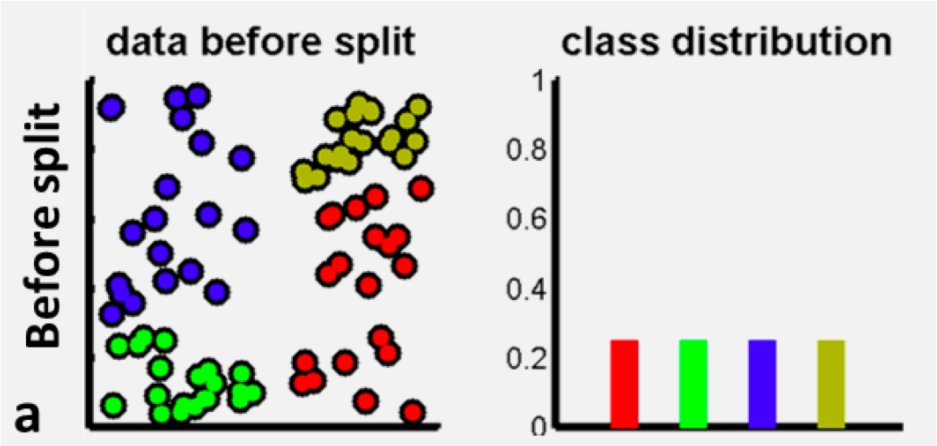


HTF Figure 9.3

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



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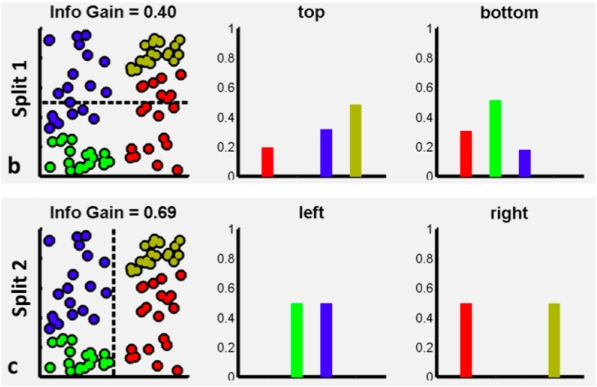
Class Distributions: Split Search



(Maximizing information gain is equivalent to minimizing entropy.)

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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

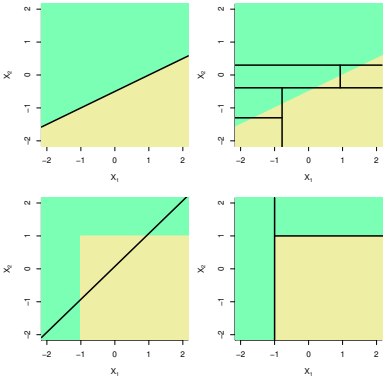
- What to do about missing features?
  - Throw out inputs with missing features
  - Impute missing values with feature means
  - If a categorical feature, let "missing" be a new category.
- For trees, we can use **surrogate splits**
  - For every internal node, form a list of surrogate features and split points
  - Goal is to approximate the original split as well as possible
  - Surrogates ordered by how well they approximate the original split.
    - In terms of how many examples are sent in the same direction by each split.

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.
  - Assign each category a number, the proportion of class 0.
  - Then find optimal split as though it were a numeric feature.
  - Proved to be equivalent to search over all splits in (Breiman et al. 1984).
- Otherwise, can use approximations..
- Statistical issues?
  - 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.



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Interpretability

- 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 $R_1, \ldots, R_m$.
- 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.

Comments about Trees

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

Tree Pruning

Stopping Conditions for Building the Big Tree

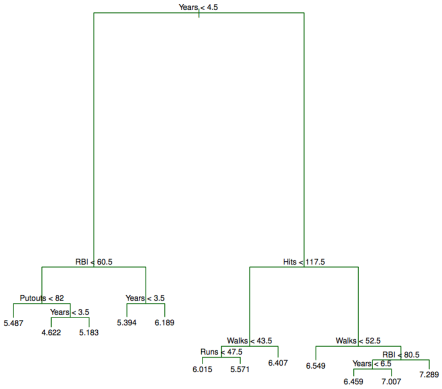
- First step is to build the "big tree".
- Keep splitting nodes until every node either has
  - Zero error OR
  - Node has C or fewer examples (typically $C = 5$ or $C = 1$)

Pruning the Tree

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

Tree Pruning

- Full Tree T_0



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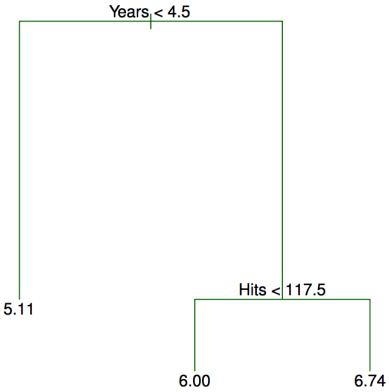
Tree Pruning

- 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 $T \subset T_0$, $\hat{R}(T) \geqslant \hat{R}(T_0)$.
- 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 many[1] 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.

[1] See On subtrees of trees.

Cost Complexity Greedy Pruning Algorithm

- Find a proper[2] 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 minimizes $\hat{R}(T_2) - \hat{R}(T_1)$.
- Repeat until we have removed all interal 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:

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

[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:

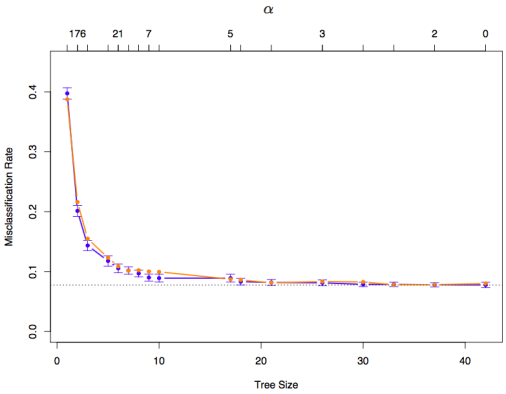
$$\mathcal{T} = \left\{ T_0 \supset T_1 \supset T_2 \supset \cdots \supset T_{|N_{\text{Int}}|} \right\}$$

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

$$\left\{ \operatorname*{arg\,min}_{T \subset T_0} C_\alpha(T) \mid \alpha \geqslant 0 \right\} \subset \mathcal{T}$$

- 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.