Classification and Regression Trees

David Rosenberg

New York University

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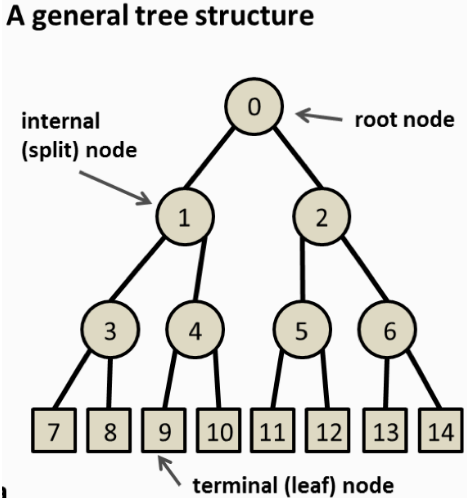
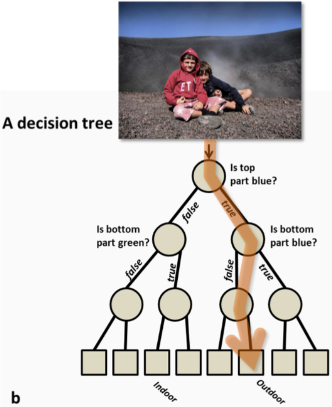
Trees

Tree Terminology



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

A Binary Decision Tree



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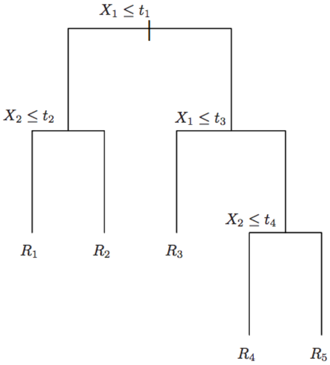
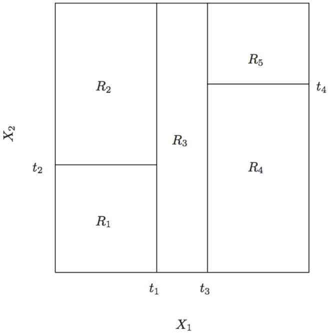
Binary Decision Tree on $\mathbf{R}^2$

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





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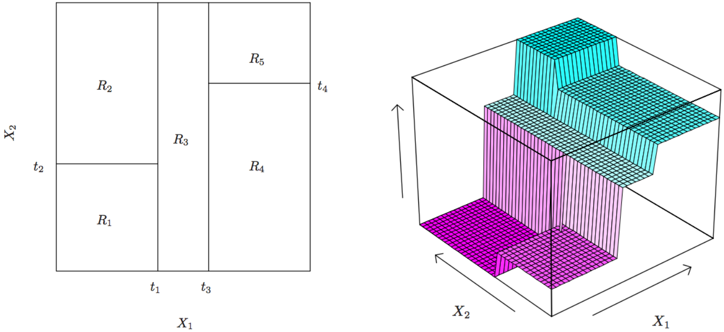
Binary Regression Tree on $\mathbf{R}^2$

- 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

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

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 $x = (x_1, \ldots, x_d) \in \mathbf{R}^d$.
- **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,

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

- Find j,s minimizing

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

- How?

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

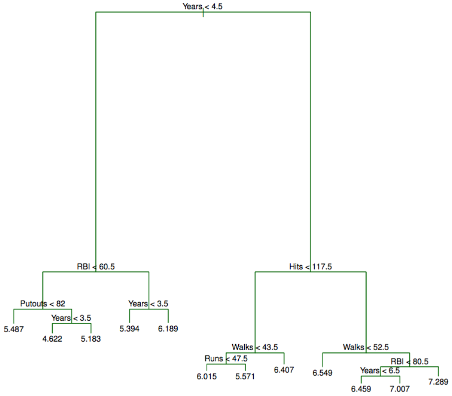
- If the tree is too big, we may overfit.
- If too small, we may miss patterns in the data (underfit).
- Typical approach:
    1. Build a really big tree (e.g. until all regions have $\leqslant 5$ points).
    2. Prune the tree.

Tree Terminology

- Each **internal node**
  - has a splitting variable and a split point
  - corresponds to binary partition of the space
- A **terminal node** or **leaf node**
  - corresponds to a region
  - corresponds to a particular prediction
- A **subtree** $T \subset T_0$ is any tree obtained by **pruning** T_0, which means collapsing any number of its internal nodes.

Tree Pruning

- Full Tree T_0



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Tree Pruning

- Subtree $T \subset T_0$

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Emprical 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 $T \subset T_0$, $\hat{R}(T) \geqslant \hat{R}(T_0)$.
- 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 tree $T \subset T_0$ minimizing $C_\alpha(T)$.
  - Use cross validation to find the right choice of α.
- $C_\alpha(T)$ has familiar regularized ERM form, but
  - Cannot take the gradient w.r.t. T.

Greedy Pruning is Sufficient

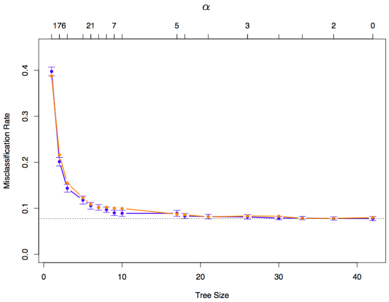
- Find subtree $T_1 \subset T_0$ that minimizes $\hat{R}(T_1) - \hat{R}(T_0)$.
- Then find $T_2 \subset T_1$.
- Repeat until we have just a single node.
- If N is the number of nodes of T_0 (terminal and internal nodes), then we end up with a set of trees:

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

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

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

Regularization Path for Trees



SPAM dataset: Blue curve is cross-validation estimate of misclassification rate as a function of tree size. Orange curve is test error. The cross-validation is indexed by values of α, shown above. The tree sizes shown below refer to $|T_\alpha|$, the size of the original tree indexed by α.

HTF Figure 9.4

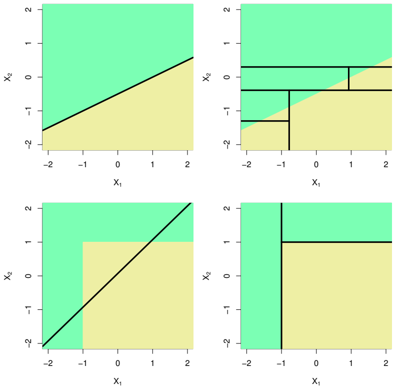
Trees in General

Missing Features (or "Predictors")

- Features are also called **covariates** or **predictors**.
- 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, 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.

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

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

- If we make a feature for every region R:

$$1(x \in R),$$

  we can view this as a **linear model**.
- Trees can be used to discover nonlinear features.

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