

Classification and Regression Trees

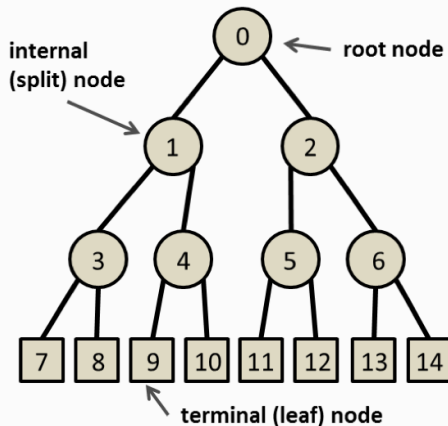
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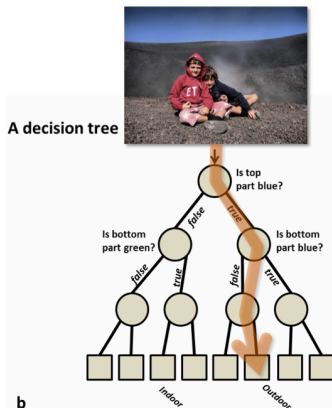
General Tree Structure

A general tree structure



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

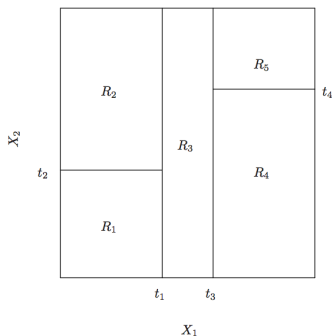
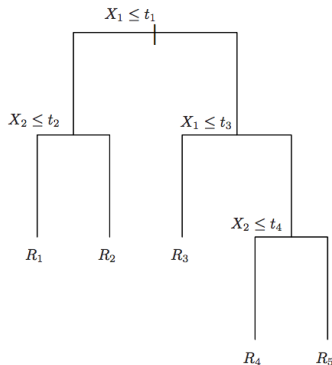
Decision Tree



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

Binary Decision Tree on \mathbf{R}^2

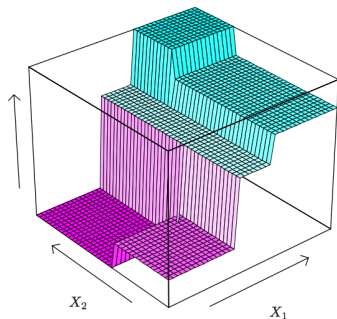
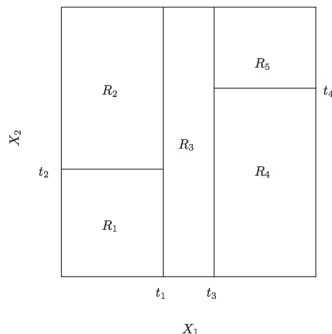
- Consider a binary tree on $\{(X_1, X_2) \mid X_1, X_2 \in \mathbf{R}\}$



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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:

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

- 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

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

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 $x = (x_1, \dots, x_d) \in \mathbb{R}^d$.
- **Splitting variable** $j \in \{1, \dots, d\}$.
- **Split point** $s \in \mathbb{R}$.
- 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 ,

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

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

- Find j, s minimizing

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

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

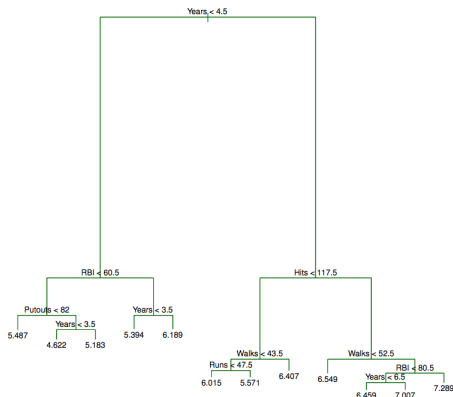
- If the tree is too big, we may overfit.
- If too small, we may miss patterns in the data (underfit).
- Typical approach:
 - 1 Build a really big tree (e.g. until all regions have ≤ 5 points).
 - 2 Prune the tree.

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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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 $T \subset T_0$, $\hat{R}(T) \geq \hat{R}(T_0)$.
- 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 tree $T \subset T_0$ minimizing $C_{\alpha}(T)$.
 - Use cross validation to find the right choice of α .

Greedy Pruning is Sufficient

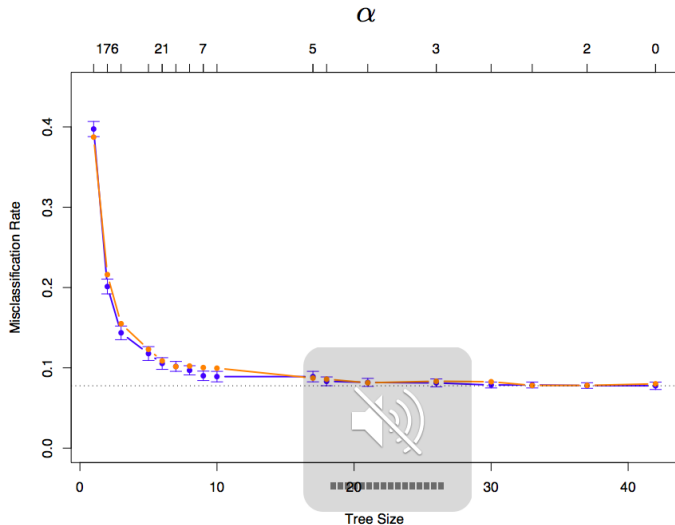
- Find subtree $T_1 \subset T_0$ that minimizes $\hat{R}(T_1) - \hat{R}(T_0)$.
- Then find $T_2 \subset T_1$.
- Repeat until we have just a single node.
- If N is the number of nodes of T_0 (terminal and internal nodes), then we end up with a set of trees:

$$\mathcal{T} = \{ T_0 \supset T_1 \supset T_2 \supset \dots \supset T_{|N|} \}$$

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

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

Regularization Path for Trees



Classification Trees

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

Classification Trees

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

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

- 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

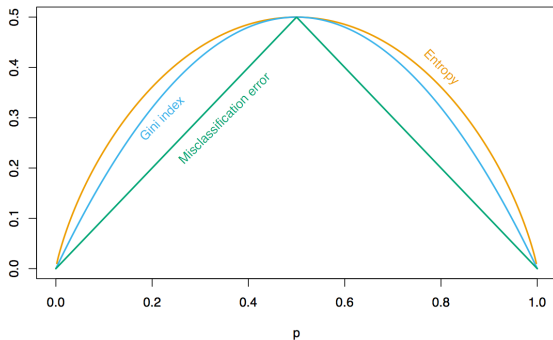
$$1 - \hat{p}_{mk(m)}.$$

Classification Trees: Node Impurity Measures

- Consider node m representing region R_m , with N_m observations
- How can we generalize from squared error to classification?
- We will introduce some different measures of **node impurity**.
 - We want **pure** leaf nodes (i.e. as close to a single class as possible)
- We'll find splitting variables and split point **minimizing node impurity**.

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:

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

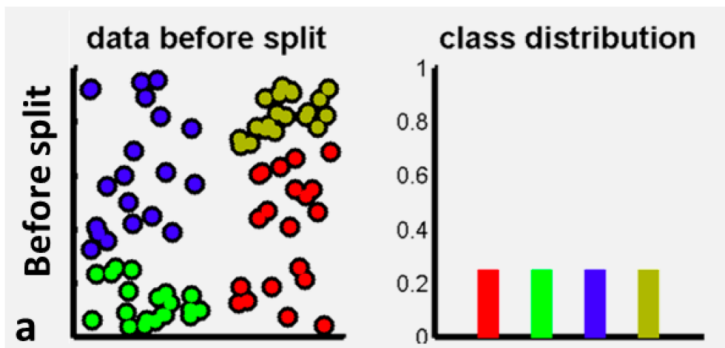
- Gini index:

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

- Entropy or deviance:

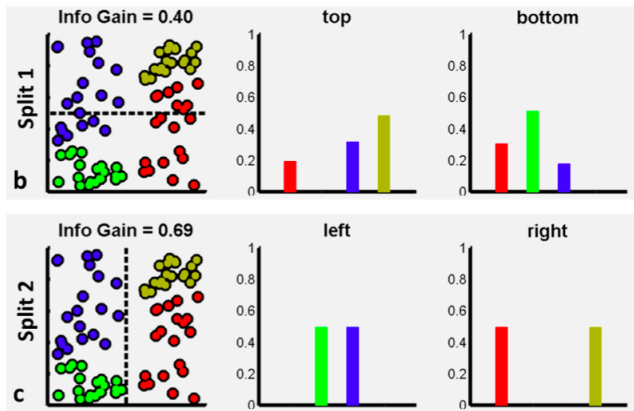
$$-\sum_{k=1}^K \hat{p}_{mk} \log \hat{p}_{mk}.$$

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)

Classification Trees: 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.
- The we search for a split that minimizes

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

Classification Trees: Node Impurity Measures

- For building the tree, Gini and Entropy are more effective.
 - They push for more pure nodes, not just misclassification rate
- For pruning the tree, use misclassification error – closer to risk estimate.

Missing Features (or “Predictors”)

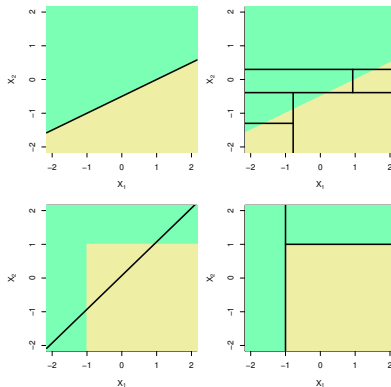
- Features are also called **covariates** or **predictors**.
- What to do about missing features?
 - Throw out inputs with missing features
 - Impute missing values with feature means
 - If a categorical feature, let “missing” be a new category.
- For trees, can use **surrogate splits**
 - For every 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.

Categorical Features

- Suppose we have feature with q possible values (unordered).
- We want to find the best split into 2 groups
- There are $2^q - 1$ possible partitions.
- Search time?
 - For binary classification ($K = 2$), there is an efficient algorithm. (Breiman 1984)
 - Otherwise, can use approximations.
- Statistical issue?
 - 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, \dots, 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.

Instability / High Variance of Trees

- Trees are **high variance**:
 - If we randomly split the data, we may get quite different trees from each part
- By contrast, linear models have low variance (at least when well-regularized)
- Later we investigate several ways to reduce this variance

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