# Classification and Regression Trees

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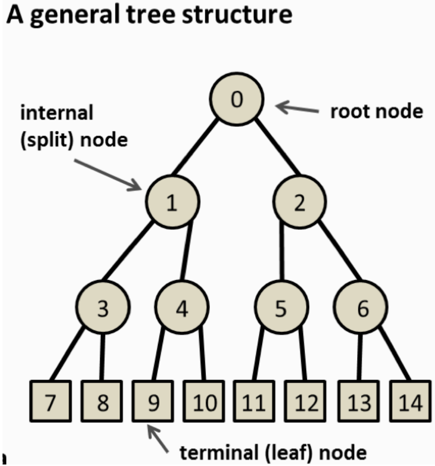
# Trees

# Tree Terminology

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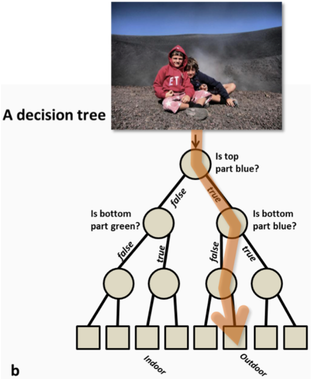
# A Binary Decision Tree

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

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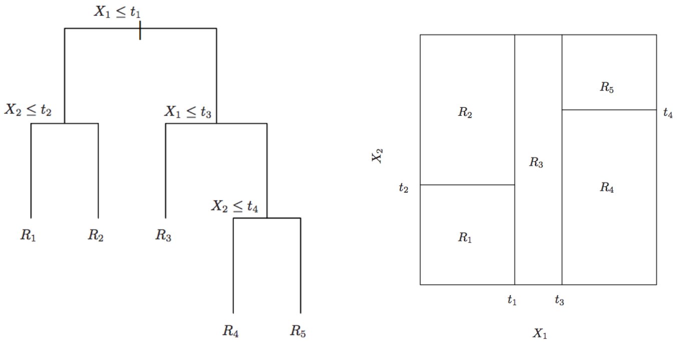
# Binary Decision Tree on $\mathbf{R}^2$

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

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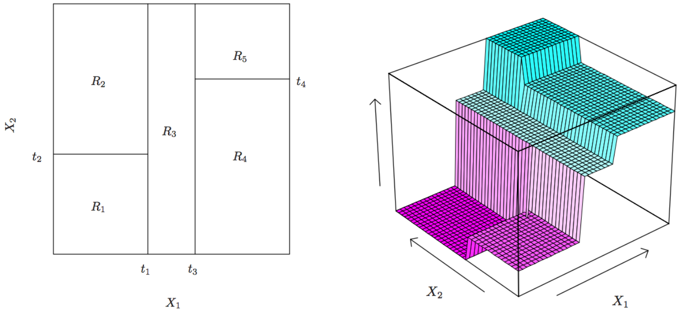
# Types of Decision Trees

- 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)
  - splits always of the form
$$x_i \leqslant t$$
- 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 in its own partition.
- This very likely overfits.

- As usual, we need to control the complexity of our hypothesis space.
- In Lecture 2, our tree complexity measure was **tree depth**.

- This lecture we'll use **number of terminal nodes**.
- This is the complexity measure used by CART.

# 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 $s$:

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

# 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?

# Finding the Split Point

- Consider splitting on the $j$'th feature $x_j$.
- As we change the split point $s$,
  - the performance on training data changes at most $n-1$.
- 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).
- 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.

# Stopping Conditions for Building the Big Tree

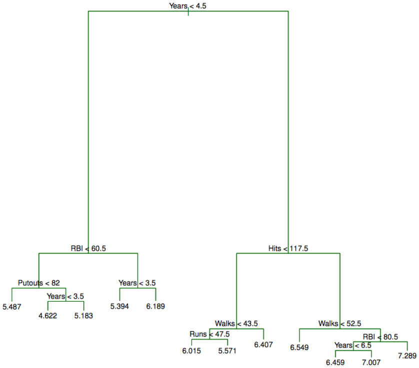
- First step is to build the "big tree".
- Keep splitting nodes until every node either has
  - Zero error OR
  - Node has $C$ or fewer examples (typically $C = 5$ or $C = 1$)

# 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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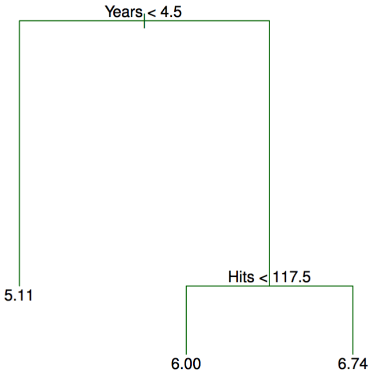
# Tree Pruning

- 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 $\alpha$ is

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

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

# Do we need to search over all subtrees?

- The **cost complexity criterion** with parameter $\alpha$ 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 $T \subset T_0$

- Amazingly, we only need to try $N$, where $N$ is the number of vertices of $T_0$.

[1] As many as $2^{N-1} + N - 1$ for trees with $N$ vertices. 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 $T_1$ be removing a single pair of leaf nodes.
  - This $T_1$ will have 1 fewer node than $T_0$.
- Then find proper subtree $T_2 \subset T_1$ that minimizes minimizes $\hat{R}(T_2) - \hat{R}(T_1)$.
- 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:

$$\mathcal{T} = \left\{ T_0 \supset T_1 \supset T_2 \supset \cdots \supset T_{|N|-1} \right\}$$

[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:

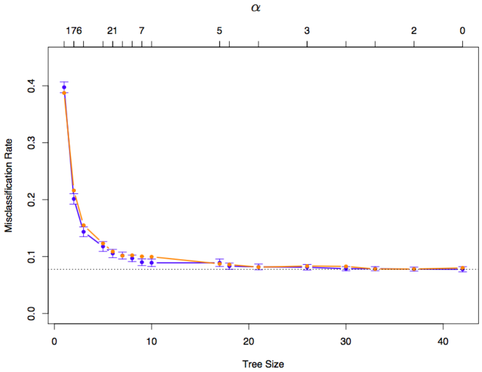
$$\mathcal{T} = \left\{ T_0 \supset T_1 \supset T_2 \supset \cdots \supset T_{|N|-1} \right\}$$

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

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

- Only need to evaluate $N$ trees rather than $O(2^N)$.

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




For each $\alpha$, we find optimal tree $T_\alpha$ 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.

# Classification Trees

# Classification Trees

- Consider classification case: $\mathcal{Y} = \{1, 2, \ldots, K\}$.
- 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

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

- **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

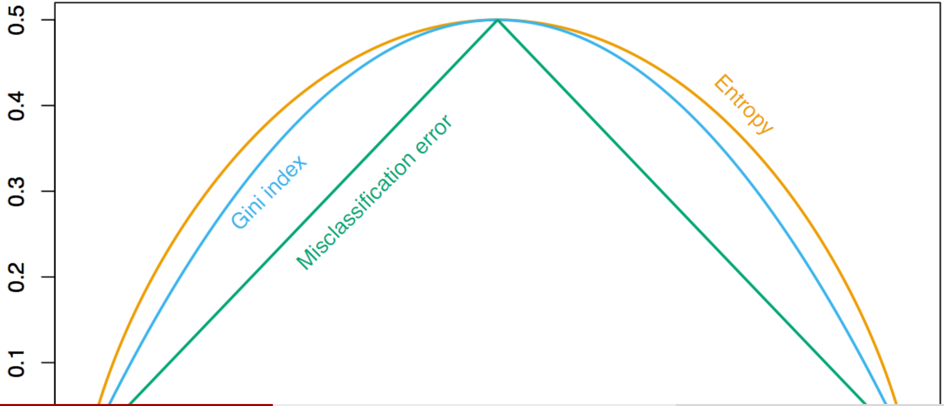
$$1 - \hat{p}_{mk(m)}.$$

# 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

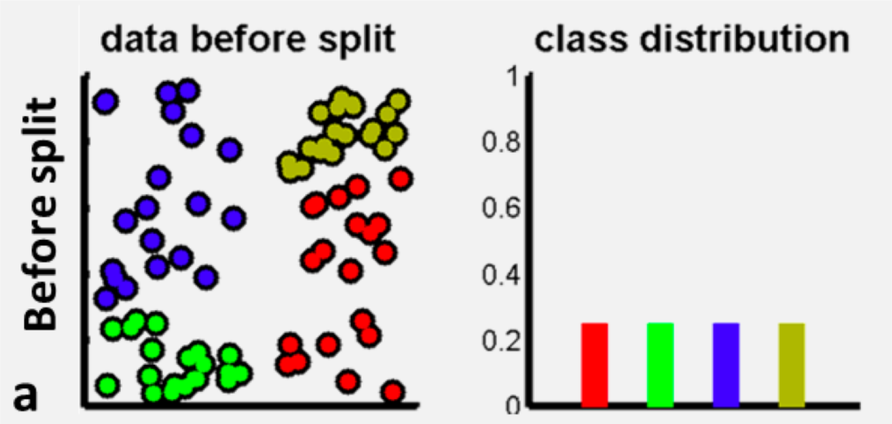
- Consider binary classification
- Let $p$ be the relative frequency of class 1.
- Here are three node impurity measures as a function of $p$



# 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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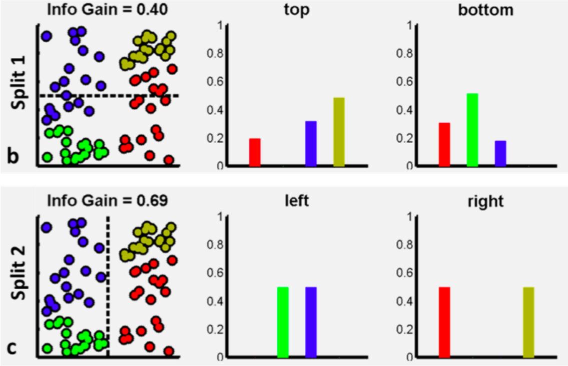
# Class Distributions: Split Search




(Maximizing information gain is equivalent to minimizing entropy.)

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

# 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
- 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 rergion 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.
- For pruning the tree, use misclassification error – closer to risk estimate.

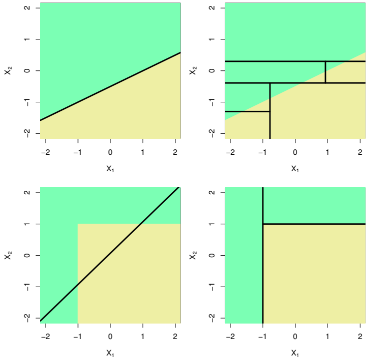
# Trees in General

# 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** (e.g. in lasso regression).
- This is called **rule fit** by Friedman.
- 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