#### Classification Trees

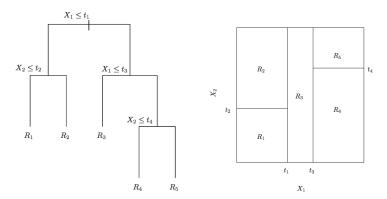
David Rosenberg

New York University

April 7, 2016

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

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



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.

### General Tree Building Procedure

- Choose a splitting variable and a split point
  - Splits input space X into  $R_1$  and  $R_2$
- We need to modify
  - criteria for splitting nodes
  - method for pruning tree

#### Classification Trees

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

# Root Node, Continuous Variables

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

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

#### 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

$$k(m) = \underset{k}{\operatorname{arg\,max}} \hat{p}_{mk}$$

as the class for all inputs in region  $R_m$ .

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

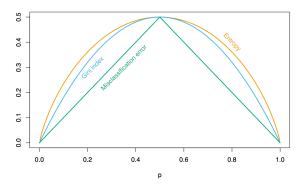
$$1-\hat{p}_{mk(m)}$$
.

### 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:

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

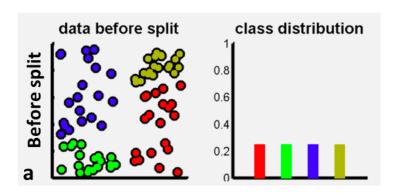
• Gini index:

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

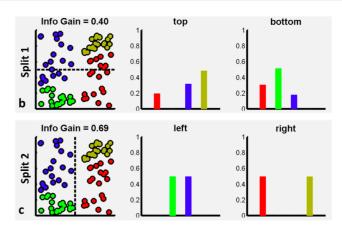
Entropy or deviance:

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

# Class Distributions: Pre-split



# 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.

#### 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