MATH 637: Mathematical Techniques in Data Science
Decision trees

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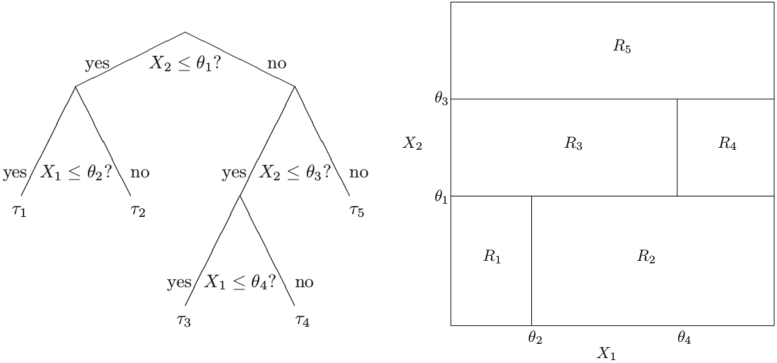
Tree-based methods:

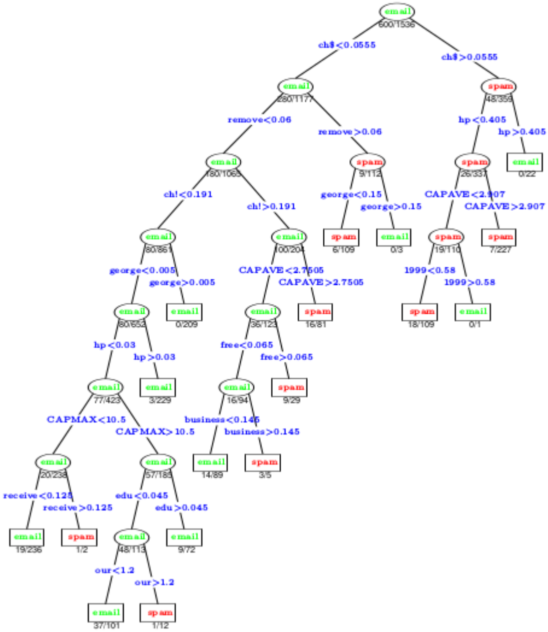
- Partition the feature space into a set of rectangles.
- Fit a simple model (e.g. a constant) in each rectangle.
- Conceptually simple yet powerful.



Izenman, 2013, Figure 9.1.

Example: spam data

ESL, Figure 9.5.



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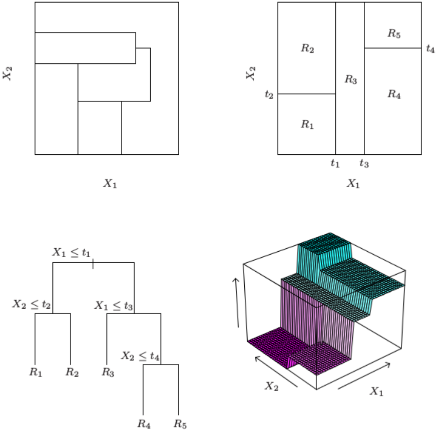
- However, by **aggregating many decision trees** and using other variants, one can improve the performance significantly.
- Such techniques lead to state-of-the-art models.
- However, in doing so, one loses the easy **interpretability** of decision trees.

Binary decision trees

To simplify, we will only consider **binary** decision trees.



ESL, Figure 9.2.

Top Left: Not binary. Top Right: binary.

Bottom Left: Tree corresponding to Top Right partition. Bottom Right: Prediction surface.

How to grow a decision tree?

Regression tree:

- Data: $y \in \mathbb{R}^n$, $X \in \mathbb{R}^{n \times p}$.
- Each observation: $(y_i, x_i) \in \mathbb{R}^{p+1}$, $i = 1, \ldots, n$.

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We need to decide:

1. Which variable to split.
2. Where to split that variable.

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Define the two half-planes:

$$R_1(j,s) := \{x \in \mathbb{R}^p : x_j \leq s\}, \qquad R_2(j,s) := \{x \in \mathbb{R}^p : x_j > s\}.$$

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We choose j, s to minimize

$$\min_{j,s} \left[\min_{c_1 \in \mathbb{R}} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2 \in \mathbb{R}} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2 \right].$$

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- The determination of the splitting point s can be done very quickly.
- Hence, determining the best pair (j, s) is **feasible**.

Repeat the same process to each block.

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(a.k.a cost complexity pruning)
Let $T \subset T_0$ be a **subtree** of T_0 with $|T|$ **terminal nodes**. For $\alpha > 0$, define:

$$C_\alpha(T) := \sum_{m=1}^{|T|} \sum_{i:x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha \cdot |T|.$$

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Once α has been chosen by CV, use whole dataset to find the tree corresponding to that value.

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As a result, we choose:

$$\hat{c}_i = \frac{1}{N_i} \sum_{x_k \in R_i} y_k,$$

where N_i denotes the number of observations in R_i.

Classification trees (cont.)

Similarly, when the output is categorical, we can count the proportion of class k observations in node i:

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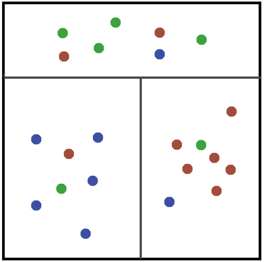
Different measures are commonly used to determine how good a given partition is (and how to split a given partition):

1. **Misclassification error:** $\frac{1}{N_i} \sum_{x_l \in R_i} \mathbf{1}_{y_l \neq k(i)} = 1 - \hat{p}_{i,k(i)}$.
2. **Gini index:** $\sum_{k=1}^{K} \hat{p}_{ik}(1 - \hat{p}_{ik}) = 1 - \sum_{k=1}^{K} \hat{p}_{ik}^2$.
   (Probability that a randomly chosen point is incorrectly classified.)
3. **Entropy:** $-\sum_{k=1}^{K} \hat{p}_{ik} \log \hat{p}_{ik}$.
   (Measure of "disorder" in a given category.)

Example



Let us focus on the **top** box.

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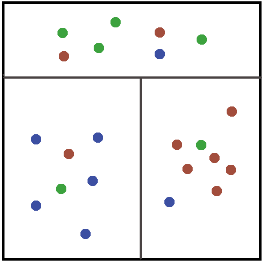

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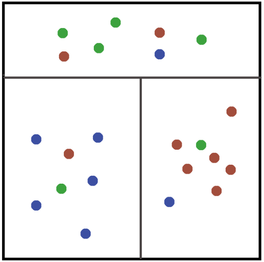

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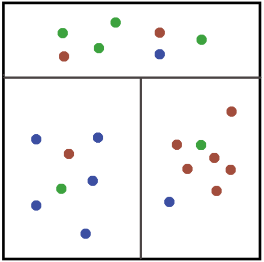

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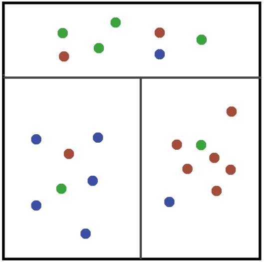

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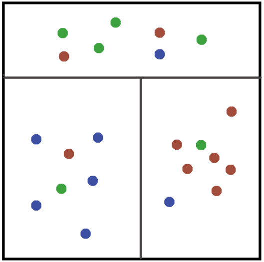

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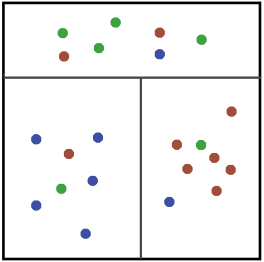

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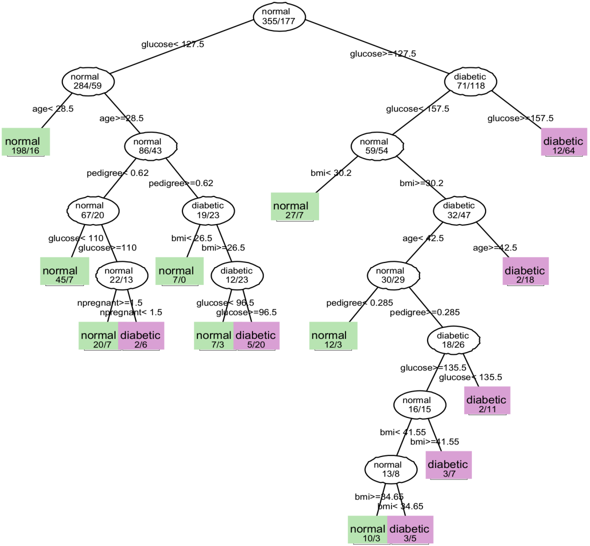
Best case possible: $(1,0,0),(0,1,0),(0,0,1)$. Entropy $= 0$.

Worst case possible $(1/3,1/3,1/3)$. Entropy $= 1.58$.

Case study: Pima Indians Diabetes (Izenman, 2013)

- Pima Indian (nativa American) population lives near Phoenix, Arizona.
- The diversion of the water and the introduction of non-native diet had devastating effects on the health of the people. They have the highest prevalence of type 2 diabetes in the world, much more than is observed in other U.S. populations. They have been the subject of intensive study of diabetes. [1]
- Patients listed in the dataset are females at least 21 years old of Pima Indian heritage.
- 8 input variables (e.g. number of times pregnant, body mass index, plasma glucose concentration, etc.).

[1] Wikipedia



Classification tree for the Pima indians diabetes data. Impurity measure = Gini index. (Izenman, Figure 9.5.)