Decision trees

COMS 4771 Fall 2019

Overview

- Decision tree learning
- Comparison to NN

Example of decision tree

```
if age ≥ 40 then
    if genre = western then
        return 4.3
    else if release date > 1998 then
        return 2.5
    else
        ⋮
    end if
else if ··· then
    ⋮
end if
```


General structure of decision trees

- *Decision tree*: nested if-then-else rules
- Family of possible if-clauses is pre-determined
  - Typically very simple predicates (e.g., "age is at least 40?")
- *Axis-aligned / coordinate splits* for numerical features
  - For input $\boldsymbol{x} = (x_1, \dots, x_d) \in \mathbb{R}^d$, splits are of the form

$$\mathbb{1}_{\{x_i > \theta\}} = \begin{cases} 1 & \text{if } x_i > \theta \\ 0 & \text{if } x_i \leq \theta \end{cases}$$

  - (Other types of splits are possible.)

Example: iris classification

- Three classes of irises $\{1, 2, 3\}$ (red, green, blue)
- Each input $x = (x_1, x_2)$ represented by two numerical features
  - $x_1 =$ sepal length-to-width ratio
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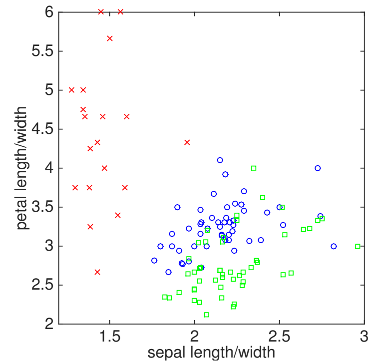

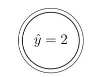

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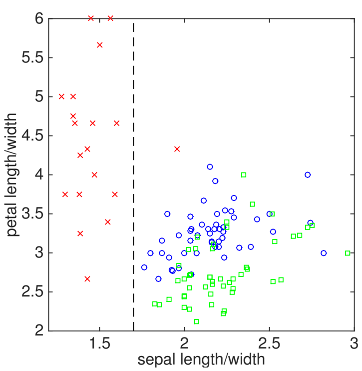

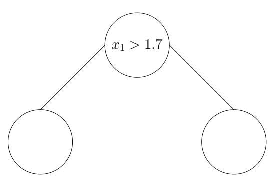

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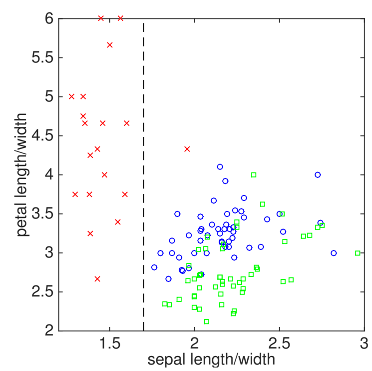

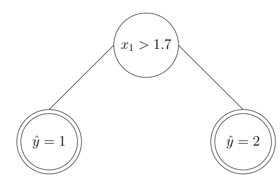

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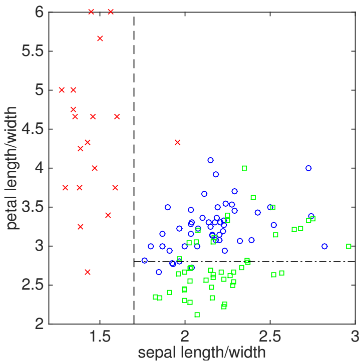

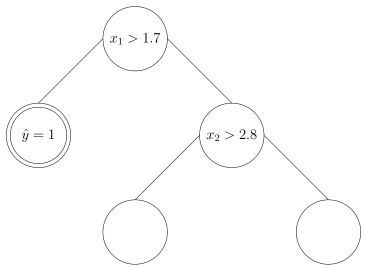

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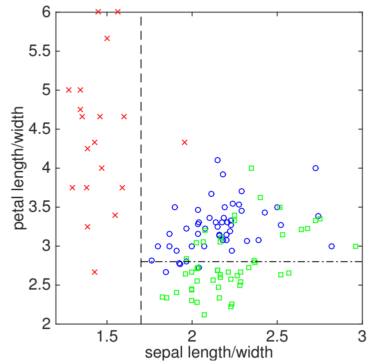
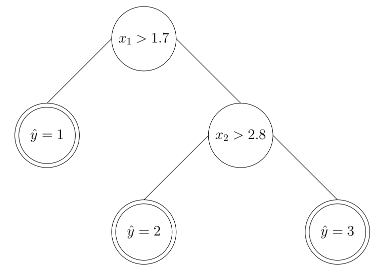
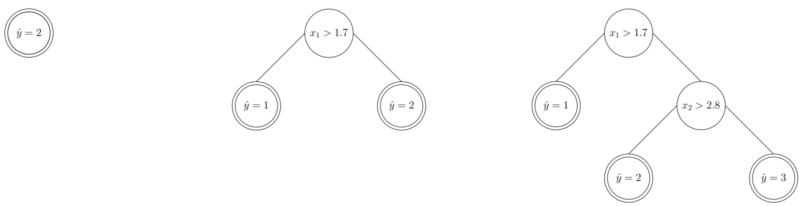




Growing a decision tree



- Leaf nodes form a *partitioning* of the input space
  - Prediction to use at each leaf node: plurality label
- *Greedy algorithm for decision trees*:
  - Start with a single leaf node
  - Repeat: pick a leaf node and split into two new leaf nodes
  - Rule for picking leaf + split: choose leaf and splitting rule to maximally reduce "uncertainty"

Notions of uncertainty

- Fix attention to single leaf
  - Let p_k be the proportion of examples reaching a leaf with label k
  - Classification error rate: $1 - \max_k p_k$
  - Gini index: $1 - \sum_k p_k^2$
  - Entropy: $\sum_k p_k \ln \frac{1}{p_k}$
  - Each is maximized when labels are in equal proportion
  - Each is minimized when only a single label appears

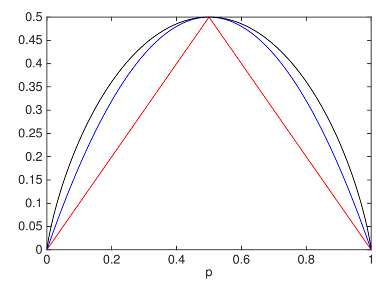


Figure 1: Uncertainty measures

Overall uncertainty

- (Overall) uncertainty:

$$\sum_{\text{leaf } \ell} (\text{\# training examples reaching } \ell) \cdot (\text{uncertainty at } \ell)$$

- In greedy algorithm, we consider reduction in uncertainty from splitting a leaf

Limits of uncertainty notions

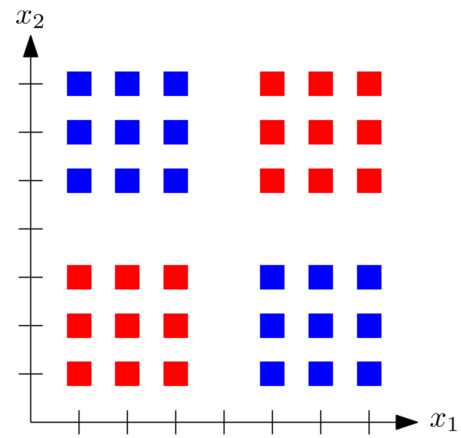


Figure 2: XOR example

Stopping criterion

- Option 1: Stop when tree reaches pre-specified size
  - Tree size is a hyperparameter
- Option 2: Stop when uncertainty is zero
  - Risk of over-fitting (since training error rate is zero)

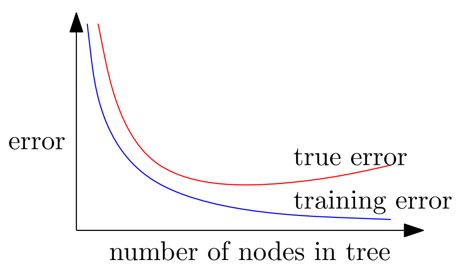


Figure 3: Typical error rate curves

Pruning a large tree

- An instantiation of the hold-out approach
- Split training data into G (grow) and P (prune)
  - Use G to grow the tree until zero uncertainty
  - Use P to choose a good pruning of the tree
- Pruning algorithm:
  - Repeat: replace any non-leaf node by leaf node if it improves error rate with respect to (*wrt*) P

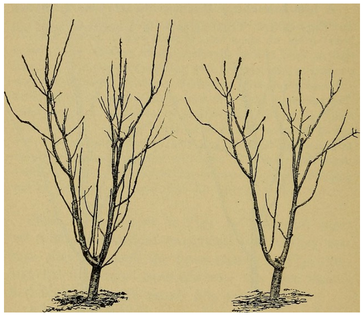
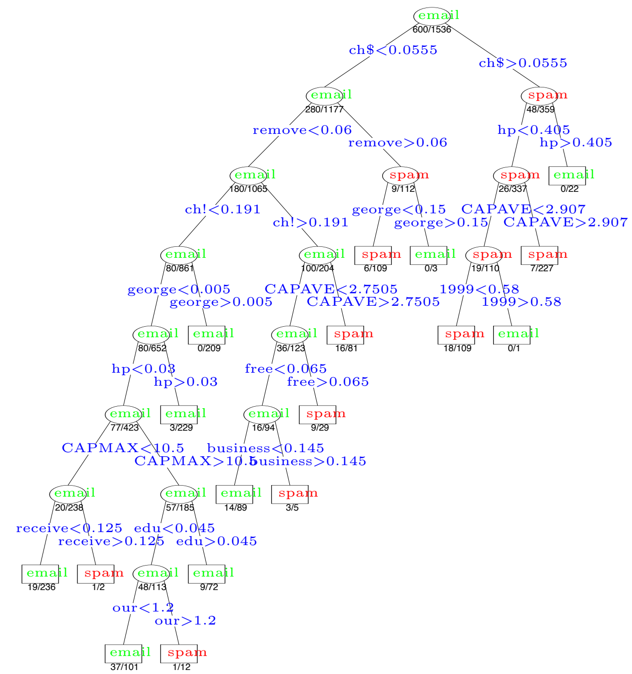


Figure 4: Pruning a tree

Example: spam filtering I

- Spam dataset
- 4601 email messages, about 39% are spam
- Classify message by spam and not-spam
- 57 features
  - 48 are of the form "percentage of email words that is (WORD)"
  - 6 are of the form "percentage of email characters is (CHAR)"
  - 3 other features (e.g., "longest sequence of all-caps")
- Final tree after pruning has 17 leaves, 9.3% test error rate

Example: spam filtering II



Comparing k-NN and decision trees

- k-NN
  - Training/fitting: memorize data set
  - Testing/predicting: find neighbors in memorized data set, output plurality label
- Decision tree
  - Training/fitting: greedily partition feature space to reduce "uncertainty"
  - Testing/prediction: traverse tree, output leaf label