Introduction

Decision trees form a simple, easily-interpretable, hypothesis

- Interpretability useful in independent validation and explanation

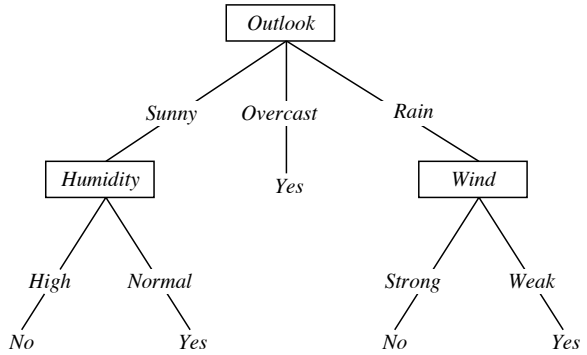
Quick to train

Quick to evaluate new instances

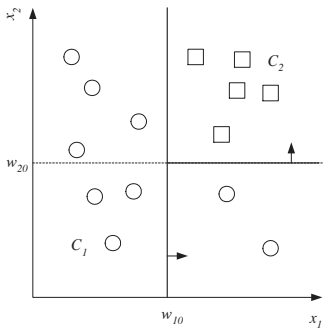
Effective "off-the-shelf" learning method

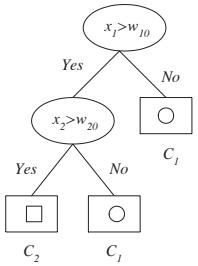
Can be combined with boosting, including using "stumps"

Decision Tree for *PlayTennis* (Mitchell)



With Numeric Attributes





Decision Tree Representation

- Each internal node tests an attribute
- Each branch corresponds to attribute value
- Each leaf node assigns a classification

How would we represent:

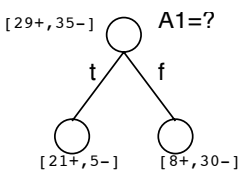
- $\wedge, \vee$, XOR
- $(A \wedge B) \vee (C \wedge \neg D \wedge E)$

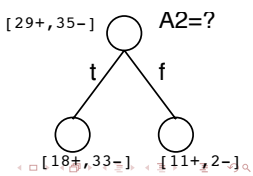
High-Level Learning Algorithm
(ID3, C4.5, CART)

Main loop:

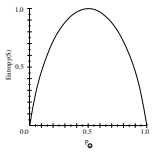
1. $A \leftarrow$ the "best" decision attribute for next node m
2. Assign A as decision attribute for m
3. For each value of A, create new descendant of m
4. Sort (*partition*) training examples over children based on A's value
5. If training examples perfectly classified, Then STOP, Else recursively iterate over new child nodes

Which attribute is best?





Entropy



- $\mathcal{X}_m$ is a sample of training examples reaching node m
- $p_m^{\oplus}$ is the proportion of positive examples in $\mathcal{X}_m$
- $p_m^{\ominus}$ is the proportion of negative examples in $\mathcal{X}_m$
- *Entropy* $\mathcal{I}_m$ measures the impurity of $\mathcal{X}_m$

$$\mathcal{I}_m \equiv -p_m^{\oplus} \log_2 p_m^{\oplus} - p_m^{\ominus} \log_2 p_m^{\ominus}$$

or for K classes,

$$\mathcal{I}_m \equiv -\sum_{i=1}^{K} p_m^i \log_2 p_m^i \qquad (9.3)$$

Total Impurity

- Now can look for an attribute A, when used to partition $\mathcal{X}_m$ by value, produces the most pure (lowest-entropy) subsets
  - Weight each subset by relative size
  - E.g., size-3 subsets should carry less influence than size-300 ones
- Let $N_m = |\mathcal{X}_m|$ = number of instances reaching node m
- Let N_{mj} = number of these instances with value $j \in \{1, \ldots, n\}$ for attribute A
- Let N^i_{mj} = number of these instances with label $i \in \{1, \ldots, K\}$
- Let $p^i_{mj} = N^i_{mj}/N_{mj}$
- Then the *total impurity* is

$$\mathcal{I}'_m(A) \equiv -\sum_{j=1}^{n} \frac{N_{mj}}{N_m} \sum_{i=1}^{K} p^i_{mj} \log_2 p^i_{mj} \tag{9.8}$$

Learning Algorithm

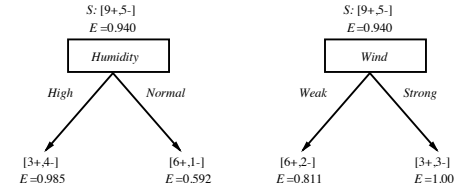
```
GenerateTree(X)
    If NodeEntropy(X)< θ_I /* equation 9.3 */
      Create leaf labelled by majority class in X
      Return
    i ← SplitAttribute(X)
    For each branch of x_i
      Find X_i falling in branch
      GenerateTree(X_i)

SplitAttribute(X)
    MinEnt← MAX
    For all attributes i = 1,...,d
      If x_i is discrete with n values
        Split X into X_1,...,X_n by x_i
        e ← SplitEntropy(X_1,...,X_n) /* equation 9.8 */
        If e<MinEnt MinEnt ← e; bestf ← i
      Else /* x_i is numeric */
        For all possible splits
          Split X into X_1, X_2 on x_i
          e←SplitEntropy(X_1, X_2)
          If e<MinEnt MinEnt ← e; bestf ← i
    Return bestf
```


Example Run
Training Examples

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

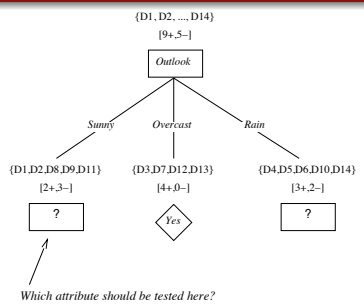
Example Run
Selecting the First Attribute

Comparing *Humidity* to *Wind*:



$$\mathcal{I}'_m(Humidity) = (7/14)0.985 + (7/14)0.592 = 0.789$$
$$\mathcal{I}'_m(Wind) = (8/14)0.811 + (6/14)1.000 = 0.892$$
$$\mathcal{I}'_m(Outlook) = (5/14)0.971 + (4/14)0.0 + (5/14)0.971 = 0.694$$
$$\mathcal{I}'_m(Temp) = (4/14)1.000 + (6/14)0.918 + (4/14)0.811 = 0.911$$

Example Run
Selecting the Next Attribute



$\mathcal{X}_m = \{D_1, D_2, D_8, D_9, D_{11}\}$
$\mathcal{I}'_m(Humidity) = (3/5)0.0 + (2/14)0.0 = 0.0$
$\mathcal{I}'_m(Wind) = (2/5)1.0 + (3/5)0.918 = 0.951$
$\mathcal{I}'_m(Temp) = (2/5)0.0 + (2/5)1.0 + (1/5)0.0 = 0.400$

Regression Trees

- A *regression tree* is similar to a decision tree, but with real-valued labels at the leaves
- To measure impurity at a node m, replace entropy with variance of labels:

$$E_m \equiv \frac{1}{N_m} \sum_{(\mathbf{x}^t, r^t) \in \mathcal{X}_m} (r^t - g_m)^2 \ ,$$

where g_m is the mean (or median) label in $\mathcal{X}_m$

Regression Trees (cont'd)

- Now can adapt Eq. (9.8) from classification to regression:

$$E'_m(A) \equiv \sum_{j=1}^{n} \frac{N_{mj}}{N_m} \left(\frac{1}{N_{mj}} \sum_{(\mathbf{x}^t, r^t) \in \mathcal{X}_{mj}} (r^t - g_{mj})^2 \right)$$

$$= \frac{1}{N_m} \sum_{j=1}^{n} \sum_{(\mathbf{x}^t, r^t) \in \mathcal{X}_{mj}} (r^t - g_{mj})^2 \quad , \tag{9.14}$$

  where j iterates over the values of attribute A
- When variance of a subset is sufficiently low, insert leaf with mean or median label as constant value

Continuous-Valued Attributes

Use threshold to map continuous to boolean, e.g. $(Temperature > 72.3) \in \{t, f\}$

Temperature:	40	48	60	72	80	90
PlayTennis:	No	No	Yes	Yes	Yes	No

- Can show that threshold minimizing impurity must lie between two adjacent attribute values in $\mathcal{X}$ such that label changed, so try all such values, e.g., $(48 + 60)/2 = 54$ and $(80 + 90)/2 = 85$
- Now (dynamically) replace continuous attribute with boolean attributes $Temperature_{>54}$ and $Temperature_{>85}$ and run algorithm normally
- Other options: Split into multiple intervals rather than two; use thresholded linear combinations of continuous attributes (Sec 9.6)

Attributes with Many Values

Problem:

- If attribute A has many values, it might artificially minimize $\mathcal{I}'_m(A)$
- E.g., if $Date$ is attribute, $\mathcal{I}'_m(A)$ will be low because several very small subsets will be created

One approach: penalize A with a measure of *split information*, which measures how broadly and uniformly attribute A splits data:

$$\mathcal{S}(A) \equiv -\sum_{j=1}^{n} \frac{N_{mj}}{N_m} \log_2 \frac{N_{mj}}{N_m} \quad \in [0, \log_2 n]$$

Unknown Attribute Values

What if a training example is missing a value of A?

Use it anyway (sift it through tree)

- If node m tests A, assign most common value of A among other training examples sifted to m
- Assign most common value of A among other examples with same target value (either overall or at m)
- Assign probability p_j to each possible value v_j of A
  - Assign fraction p_j of example to each descendant in tree

Classify new examples in same fashion

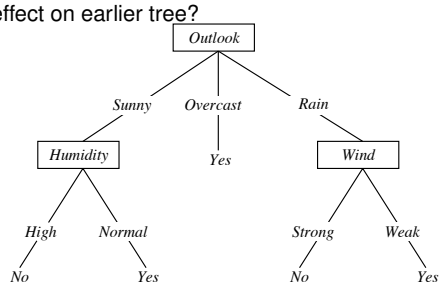
Inductive Bias of Learning Algorithm

- Hypothesis space $\mathcal{H}$ is complete, in that *any* function can be represented
- Thus inductive bias does not come from restricting $\mathcal{H}$, but from *preferring* some trees over others
  - Tends to prefer shorter trees
  - Computationally intractable to find a guaranteed shortest tree, so heuristically apply greedy approach to locally minimize impurity

Overfitting

- Consider adding noisy training example #15:

  $Sunny, Hot, Normal, Strong, PlayTennis = No$
- What effect on earlier tree?



- Expect old tree to generalize better since new one fits noisy example

Overfitting (cont'd)

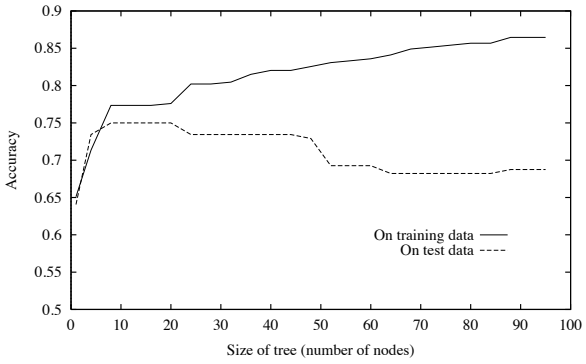
- Consider error of hypothesis h over
  - training data (empirical error): $error_{train}(h)$
  - entire distribution $\mathcal{D}$ of data (generalization error): $error_{\mathcal{D}}(h)$
- Hypothesis $h \in \mathcal{H}$ *overfits* training data if there is an alternative hypothesis $h' \in \mathcal{H}$ such that

$$error_{train}(h) < error_{train}(h')$$

and

$$error_{\mathcal{D}}(h) > error_{\mathcal{D}}(h')$$

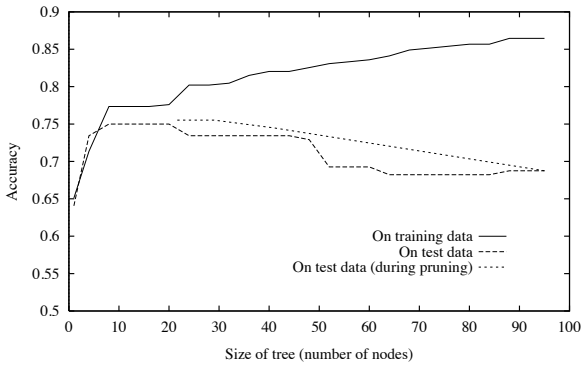
Overfitting (cont'd)



Pruning to Avoid Overfitting

- To prevent trees from growing too much and overfitting the data, we can *prune* them
  - In spirit of Occam's Razor, minimum description length
- In *prepruning,* we allow skipping a recursive call on set $\mathcal{X}_m$ and instead insert a leaf, even if $\mathcal{X}_m$ is not pure
  - Can do this when entropy (or variance) is below a threshold (θ_I in pseudocode)
  - Can do this when $|\mathcal{X}_m|$ is below a threshold, e.g., 5
- In *postpruning*, we grow the tree until it has zero error on training set and then prune it back afterwards
  - First, set aside a *pruning set* not used in initial training
  - Then repeat until pruning is harmful:
    1. Evaluate impact on validation set of pruning each possible node (plus those below it)
    2. Greedily remove the one that most improves validation set accuracy

Pruning Example

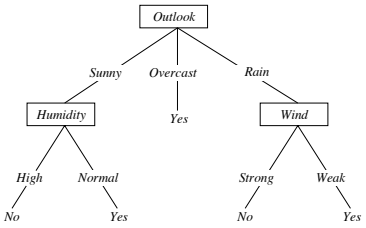


Rule Postpruning

- Convert tree to equivalent set of rules
- Prune each rule independently of others by removing selected preconditions (the ones that improve accuracy the most)
- Sort final rules into desired sequence for use

Perhaps most frequently used method (e.g. C4.5)

Converting A Tree to Rules



IF $(Outlook = Sunny) \wedge (Humidity = High)$
THEN $PlayTennis = No$

IF $(Outlook = Sunny) \wedge (Humidity = Normal)$
THEN $PlayTennis = Yes$
...