Decision Trees
An Early Classifier

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Introduction to Non-Metric Methods

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  - For example (DHS), some teeth are small and fine (as in baleen whales) for straining tiny prey from the sea; others (as in sharks) come in multiple rows; other sea creatures have tusks (as in walruses), yet others lack teeth altogether (as in squid). There is no clear notion of similarity for this information about teeth.

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- Most of the other methods we study will involve real-valued feature vectors with clear metrics.
- We may also consider problems involving data tuples and data strings. And for recognition of these, decision trees and string grammars, respectively.

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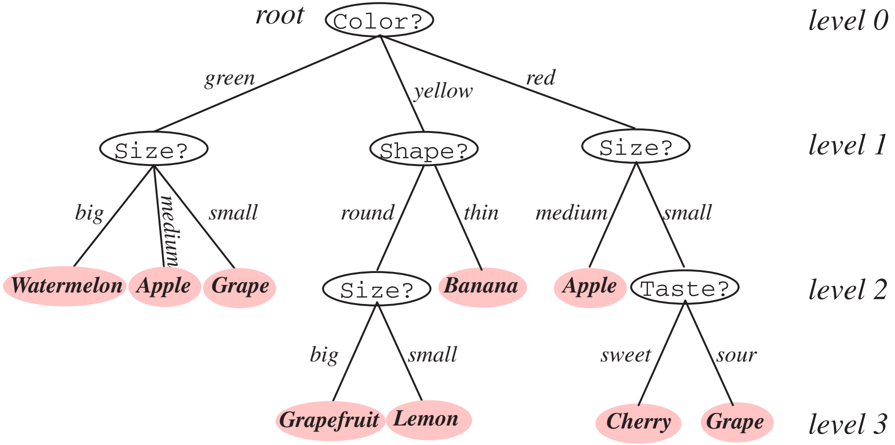
- How did you ask the questions?
- What underlying measure led you the questions, if any?
- Most importantly, iterative yes/no questions of this sort require no metric and are well suited for nominal data.

These sequence of questions are a decision tree...



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- We follow the link corresponding to the appropriate value of the pattern and continue to a new node, at which we check the next property. And so on.
- Decision trees have a particularly high degree of interpretability.

When to Consider Decision Trees

- Instances are wholly or partly described by attribute-value pairs.
- Target function is discrete valued.
- Disjunctive hypothesis may be required.
- Possibly noisy training data.
- Examples
  - Equipment or medical diagnosis.
  - Credit risk analysis.
  - Modeling calendar scheduling preferences.

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- Any decision tree will progressively split the data into subsets.
- If at any point all of the elements of a particular subset are of the same category, then we say this node is **pure** and we can stop splitting.
- Unfortunately, this rarely happens and we have to decide between whether to stop splitting and accept an imperfect decision or instead to select another property and grow the tree further.

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  6. How should missing data be handled?

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- So, DHS focuses on only binary tree learning.
- But, we note that in certain circumstances for learning and inference, the selection of a test at a node or its inference may be computationally expensive and a 3- or 4-way split may be more desirable for computational reasons.

Query Selection and Node Impurity

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- In all cases, we want $i(N)$ to be 0 if all of the patterns that reach the node bear the same category, and to be large if the categories are equally represented.
- **Entropy impurity** is the most popular measure:

$$i(N) = -\sum_{j} P(\omega_j) \log P(\omega_j) \quad . \tag{1}$$

It will be minimized for a node that has elements of only one class (pure).

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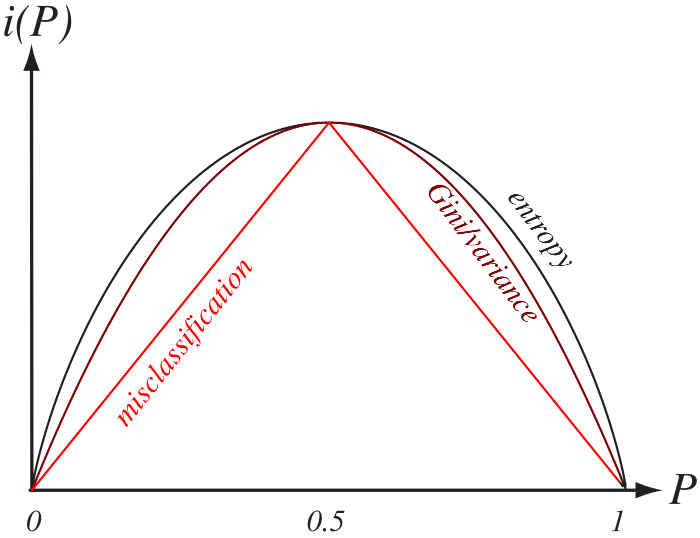
- The **misclassification impurity** measures the minimum probability that a training pattern would be misclassified at N:

$$i(N) = 1 - \max_j P(\omega_j) \tag{4}$$



For the two-category case, the impurity functions peak at equal class frequencies.

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- If the **entropy impurity** is used, this corresponds to choosing the feature that yields the highest **information gain**.

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  - In multi-class binary tree creation, we would want to use the **twoing criterion**. The goal is to find the split that best separates groups of the c categories. A candidate "supercategory" C_1 consists of all patterns in some subset of the categories and C_2 has the remainder. When searching for the feature s, we also need to search over possible category groupings.

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- This is a local, greedy optimization strategy.
- Hence, there is no guarantee that we have either the global optimum (in classification accuracy) or the smallest tree.
- In practice, it has been observed that the particular choice of impurity function rarely affects the final classifier and its accuracy.

A Note About Multiway Splits

- In the case of selecting a multiway split with branching factor B, the following is the direct generalization of the impurity gradient function:

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    - To see this, consider the uniform splitting case.
- So, we need to normalize each:

$$\Delta i_B(s) = \frac{\Delta i(s)}{-\sum_{k=1}^{B} P_k \log P_k} \quad . \tag{7}$$

And then we can again choose the feature that maximizes this normalized criterion.

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- So, how to stop splitting?

1. Cross-validation...
2. Threshold on the impurity gradient.
3. Incorporate a tree-complexity term and minimize.
4. Statistical significance of the impurity gradient.

Stopping by Thresholding the Impurity Gradient

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- Drawback: But, how do we set the value of the threshold β?

Stopping with a Complexity Term

- Define a new global criterion function

$$\alpha \cdot \text{size} + \sum_{\text{leaf nodes}} i(N) \ . \qquad (9)$$

which trades complexity for accuracy. Here, size could represent the number of nodes or links and α is some positive constant.

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- But, again, how do we set the constant α?

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- More generally, we can consider a hypothesis testing approach to stopping: we seek to determine whether a candidate split differs significantly from a random split.
- Suppose we have n samples at node N. A particular split s sends Pn patterns to the left branch and $(1-P)n$ patterns to the right branch. A random split would place P_{n_1} of the ω_1 samples to the left, P_{n_2} of the ω_2 samples to the left and corresponding amounts to the right.

- The chi-squared statistic calculates the deviation of a particular split s from this random one:

$$\chi^2 = \sum_{i=1}^{2} \frac{(n_{iL} - n_{ie})^2}{n_{ie}} \tag{10}$$

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- When it is greater than a critical value (based on desired significance bounds), we reject the null hypothesis (the random split) and proceed with s.

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- Unbalanced trees often result from this style of pruning/merging.

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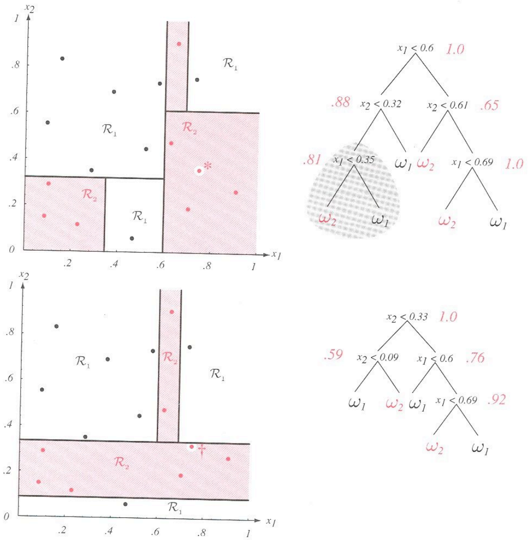
- Tree construction based on "when to stop splitting" biases the learning algorithm toward trees in which the greatest impurity reduction occurs near the root. It makes no attempt to *look ahead* at what splits may occur in the leaf and beyond.
- **Pruning** is the principal alternative strategy for tree construction.
- In pruning, we exhaustively build the tree. Then, all pairs of neighboring leafs nodes are considered for elimination.
- Any pair that yields a satisfactory increase in impurity (a small one) is eliminated and the common ancestor node is declared a leaf.
- Unbalanced trees often result from this style of pruning/merging.
- Pruning avoids the "local"-ness of the earlier methods and uses all of the training data, but it does so at added computational cost during the tree construction.

Assignment of Leaf Node Labels

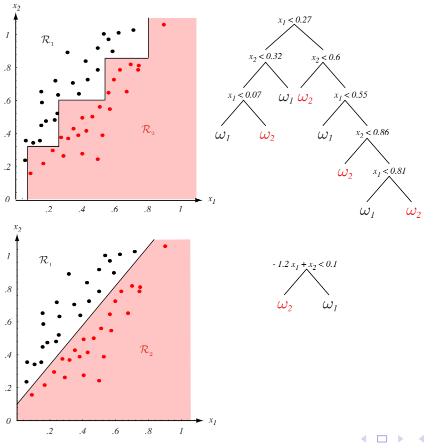
- This part is easy...a particular leaf node should make the label assignment based on the distribution of samples in it during training. Take the label of the maximally represented class.
- We will see clear justification for this in the next chapter on Decision Theory.

Instability of the Tree Construction

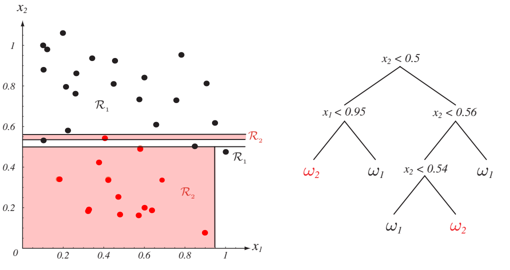


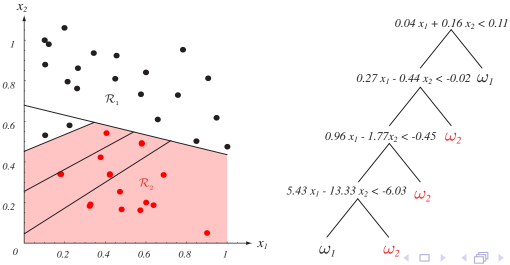
Importance of Feature Choice

- The selection of features will ultimately play a major role in accuracy, generalization, and complexity.
- This is an instance of the Ugly Duckling principle.



- Furthermore, the use of multiple variables in selecting a decision rule may greatly improve the accuracy and generalization.





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- One can follow this by pruning.

C4.5 Method (in brief)

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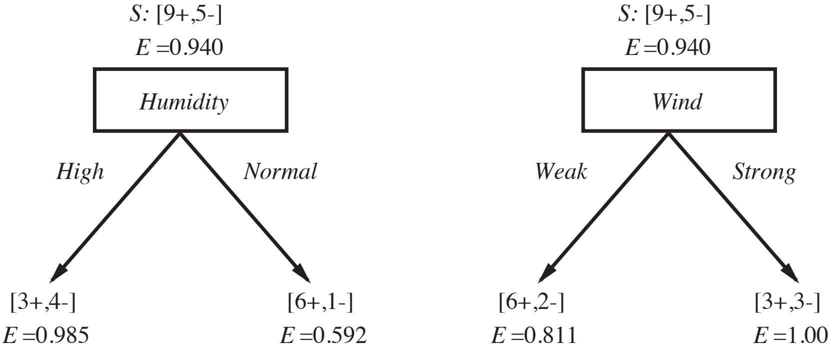
- Pruning is performed based on statistical significance tests.

Example from T. Mitchell Book: PlayTennis

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

Which attribute is the best classifier?

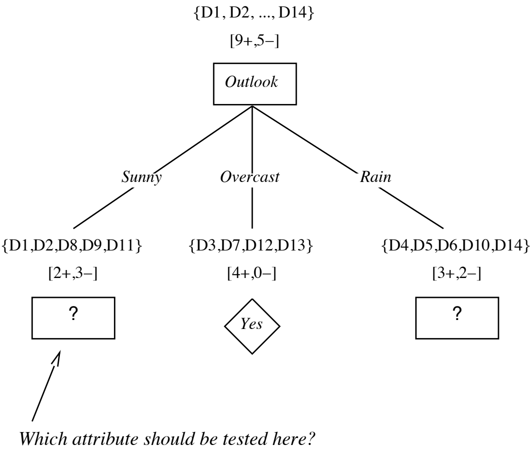


Gain (S, Humidity)

= .940 - (7/14).985 - (7/14).592
= .151

Gain (S, Wind)

= .940 - (8/14).811 - (6/14)1.0
= .048



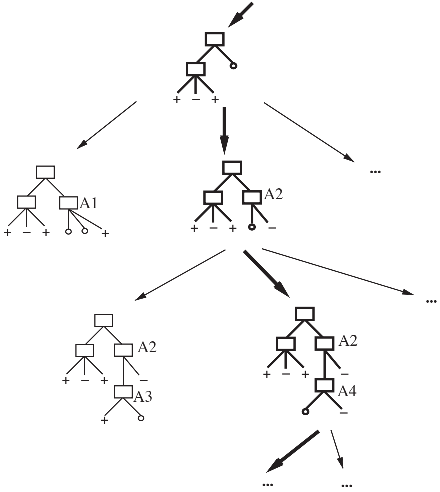
$S_{sunny} = \{D1, D2, D8, D9, D11\}$

$Gain(S_{sunny}, Humidity) = .970 - (3/5)\,0.0 - (2/5)\,0.0 = .970$

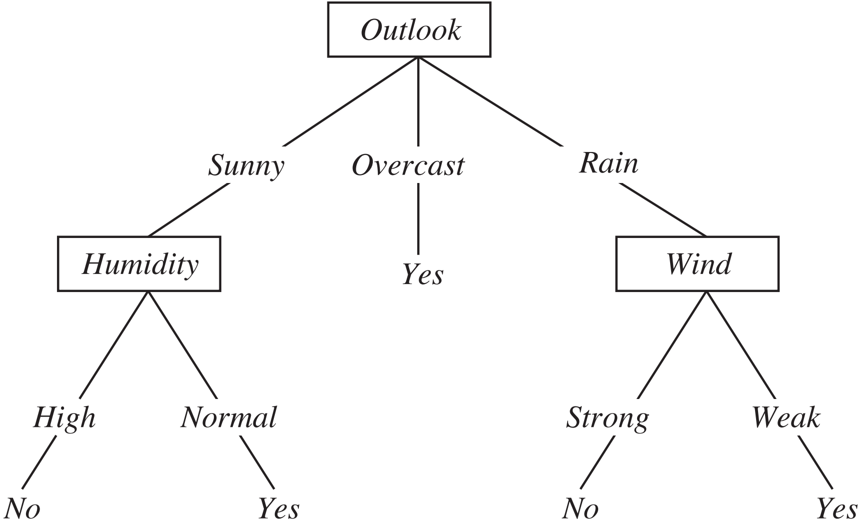
$Gain(S_{sunny}, Temperature) = .970 - (2/5)\,0.0 - (2/5)\,1.0 - (1/5)\,0.0 = .570$

$Gain(S_{sunny}, Wind) = .970 - (2/5)\,1.0 - (3/5)\,.918 = .019$

Hypothesis Space Search by ID3



Learned Tree



Overfitting Instance

- Consider adding a new, noisy training example #15:

$$Sunny,\ Hot,\ Normal,\ Strong,\ PlayTennis = No$$

- What effect would it have on the earlier tree?

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