Non-Metric Methods – Decision Trees

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However, there are instances in which some of the data may not possess such desirable characteristics.

We cover such problems involving nominal data in this chapter—that is, data that are discrete and without any natural notion of similarity or even ordering.

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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We will consider problems involving data tuples and data strings. And for recognition of these, decision trees and string grammars, respectively.
20 Questions

- I am thinking of a person. Ask me up to 20 yes/no questions to determine who this person is that I am thinking about.
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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...

FIGURE 8.1. Classification in a basic decision tree proceeds from top to bottom. The questions asked at each node concern a particular property of the pattern, and the downward links correspond to the possible values. Successive nodes are visited until a terminal or leaf node is reached, where the category label is read.

Note that the same question, Size?, appears in different places in the tree and that different questions can have different numbers of branches. Moreover, different leaf nodes, shown in pink, can be labeled by the same category (e.g., Apple).

From: Richard O. Duda, Peter E. Hart, and David G. Stork, Pattern Classification. Copyright © 2001 by John Wiley & Sons, Inc.
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- The links off of the root node correspond to different possible values of the property.
- 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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CART for Decision Tree Learning

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- Now, we want to learn how to organize these properties into a decision tree to maximize accuracy.
- Any decision tree will progressively split and split the data into subsets.
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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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1. How many branches will be selected from a node?
2. Which property should be tested at a node?
3. When should a node be declared a leaf?
4. How can we prune a tree once it has become too large?
5. If a leaf node is impure, how should the category be assigned?
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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- We seek a property query $T$ at each node $N$ that makes the data reaching the immediate descendant nodes as “pure” as possible.

Entropy impurity is the most popular measure:

$$i(N) = -\sum \omega_j \log \omega_j.$$  

It will be minimized for a node that has elements of only one class (pure).
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Its generalization to the multi-class is the **Gini impurity**:

\[ i(N) = \sum_{i \neq j} P(\omega_i)P(\omega_j) = 1 - \sum_j P^2(\omega_j) \]  

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which is the expected error rate at node \( N \) if the category is selected randomly from the class distribution present at the node.
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The **misclassification impurity** measures the minimum probability that a training pattern would be misclassified at \( N \):

\[ i(N) = 1 - \max_j P(\omega_j) \tag{4} \]
FIGURE 8.4. For the two-category case, the impurity functions peak at equal class frequencies and the variance and the Gini impurity functions are identical. The entropy, variance, Gini, and misclassification impurities (given by Eqs. 1–4, respectively) have been adjusted in scale and offset to facilitate comparison here; such scale and offset do not directly affect learning or classification. From: Richard O. Duda, Peter E. Hart, and David G. Stork, Pattern Classification. Copyright c⃝ 2001 by John Wiley & Sons, Inc.
Query Selection

- Key Question: **Given a partial tree down to node \( N \), what feature \( s \) should we choose for the property test \( T \)?

The obvious heuristic is to choose the feature that yields as big a decrease in the impurity as possible. The impurity gradient is

\[
\Delta_i(N) = i(N) - P_L i(N_L) - (1 - P_L) i(N_R),
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where \( N_L \) and \( N_R \) are the left and right descendants, respectively, \( P_L \) is the fraction of data that will go to the left sub-tree when property \( T \) is used. The strategy is then to choose the feature that maximizes \( \Delta_i(N) \).

If the entropy impurity is used, this corresponds to choosing the feature that yields the highest information gain.
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- In the higher branching factor case, it would yield a higher-dimensional optimization problem.
  - 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:

$$\Delta i(s) = i(N) - \sum_{k=1}^{B} P_k i(N_k)$$  \hspace{1cm} (6)
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- To see this, consider the uniform splitting case.

- So, we need to normalize each:

$$\Delta i_B(s) = \frac{\Delta i(s)}{-\sum_{k=1}^{B} P_k \log P_k}.$$  \hspace{1cm} (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.
Splitting is stopped if the best candidate split at a node reduces the impurity by less than the preset amount, $\beta$:

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- Drawback: But, how do we set the value of the threshold $\beta$?
Stopping with a Complexity Term

- Define a new global criterion function

\[ \alpha \cdot \text{size} + \sum_{\text{leaf nodes}} i(N) \]  \hspace{1cm} (9)

which trades complexity for accuracy. Here, size could represent the number of nodes or links and \( \alpha \) is some positive constant.
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But, again, how do we set the constant \( \alpha \)?
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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 $Pn_1$ of the $\omega_1$ samples to the left, $Pn_2$ of the $\omega_2$ 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:

$$\chi^2 = \sum_{i=1}^{2} \frac{(n_{iL} - n_{ie})^2}{n_{ie}}$$  \hspace{1cm} (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 $s$. 

Pruning

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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.
Instability of the Tree Construction
Importance of Feature Choice

- As we know from Ugly Duckling and various empirical evidence, the selection of features will ultimately play a major role in accuracy, generalization, and complexity.
Furthermore, the use of multiple variables in selecting a decision rule may greatly improve the accuracy and generalization.
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- The algorithm continues until all nodes are pure or there are no more variables on which to split.
- One can follow this by pruning.
C4.5 Method (in brief)

- This is a successor to the ID3 method.
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- It handles real valued variables like CART and uses the ID3 multiway splits for nominal data.
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- It handles real valued variables like CART and uses the ID3 multiway splits for nominal data.
- Pruning is performed based on statistical significance tests.
### Example from T. Mitchell Book: PlayTennis

<table>
<thead>
<tr>
<th>Day</th>
<th>Outlook</th>
<th>Temperature</th>
<th>Humidity</th>
<th>Wind</th>
<th>PlayTennis</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1</td>
<td>Sunny</td>
<td>Hot</td>
<td>High</td>
<td>Weak</td>
<td>No</td>
</tr>
<tr>
<td>D2</td>
<td>Sunny</td>
<td>Hot</td>
<td>High</td>
<td>Strong</td>
<td>No</td>
</tr>
<tr>
<td>D3</td>
<td>Overcast</td>
<td>Hot</td>
<td>High</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>D4</td>
<td>Rain</td>
<td>Mild</td>
<td>High</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>D5</td>
<td>Rain</td>
<td>Cool</td>
<td>Normal</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>D6</td>
<td>Rain</td>
<td>Cool</td>
<td>Normal</td>
<td>Strong</td>
<td>No</td>
</tr>
<tr>
<td>D7</td>
<td>Overcast</td>
<td>Cool</td>
<td>Normal</td>
<td>Strong</td>
<td>Yes</td>
</tr>
<tr>
<td>D8</td>
<td>Sunny</td>
<td>Mild</td>
<td>High</td>
<td>Weak</td>
<td>No</td>
</tr>
<tr>
<td>D9</td>
<td>Sunny</td>
<td>Cool</td>
<td>Normal</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>D10</td>
<td>Rain</td>
<td>Mild</td>
<td>Normal</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>D11</td>
<td>Sunny</td>
<td>Mild</td>
<td>Normal</td>
<td>Strong</td>
<td>Yes</td>
</tr>
<tr>
<td>D12</td>
<td>Overcast</td>
<td>Mild</td>
<td>High</td>
<td>Strong</td>
<td>Yes</td>
</tr>
<tr>
<td>D13</td>
<td>Overcast</td>
<td>Hot</td>
<td>Normal</td>
<td>Weak</td>
<td>Yes</td>
</tr>
<tr>
<td>D14</td>
<td>Rain</td>
<td>Mild</td>
<td>High</td>
<td>Strong</td>
<td>No</td>
</tr>
</tbody>
</table>
Which attribute is the best classifier?

\[ S: [9+,5-] \]
\[ E = 0.940 \]

**Humidity**

- High: \[ [3+,4-] \]
  - \[ E = 0.985 \]
- Normal: \[ [6+,1-] \]
  - \[ E = 0.592 \]

\[ \text{Gain} (S, \text{Humidity}) = 0.940 - (7/14) \cdot 0.985 - (7/14) \cdot 0.592 = 0.151 \]

\[ S: [9+,5-] \]
\[ E = 0.940 \]

**Wind**

- Weak: \[ [6+,2-] \]
  - \[ E = 0.811 \]
- Strong: \[ [3+,3-] \]
  - \[ E = 1.00 \]

\[ \text{Gain} (S, \text{Wind}) = 0.940 - (8/14) \cdot 0.811 - (6/14) \cdot 1.0 = 0.048 \]
Which attribute should be tested here?

\[ S_{\text{sunny}} = \{D1, D2, D8, D9, D11\} \]

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

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

\[
\text{Gain} (S_{\text{sunny}}, \text{Wind}) = .970 - (2/5) 1.0 - (3/5) .918 = .019
\]
Hypothesis Space Search by ID3
Learned Tree

```
Outlook
  Sunny
    Humidity
      High
        No
        Yes
    Normal
  Overcast
    Yes
  Rain
    Wind
      Strong
        No
      Weak
        Yes
```
Overfitting Instance

- Consider adding a new, noisy training example #15:
  
  \[\text{Sunny, Hot, Normal, Strong, PlayTennis} = \text{No}\]

- What effect would it have on the earlier tree?
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