GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 10: DECISION TREE CLASSIFIERS

LAST TIME:

- PROBABILITY
- NAIVE BAYES
- WORD COUNT MATRICES

QUESTIONS?

I. DECISION TREES
II. BUILDING DECISION TREES
III. OPTIMIZATION FUNCTIONS
IV. PREVENTING OVERFITTING

EXERCISE:
V. IMPLEMENTING DECISION TREES WITH SCIKIT-LEARN

I. DECISION TREES

Q: What is a decision tree?

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non-parametric: *no parameters, no distribution assumptions*

hierarchical: *consists of a sequence of questions which yield a class label when applied to any record*

Q: How is a decision tree represented?

EXAMPLE – DECISION TREE

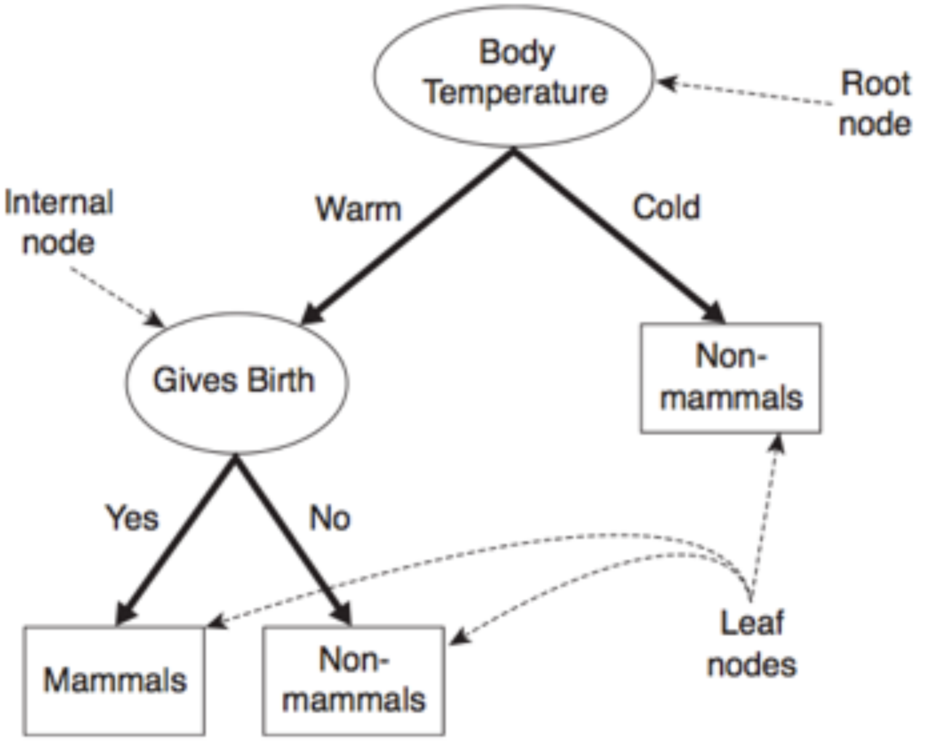

Figure 4.4. A decision tree for the mammal classification problem.

source: http://www-users.cs.umn.edu/~kumar/dmbook/ch4.pdf

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A: Using a configuration of **nodes** *and* **edges.**

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More concretely, as a multiway tree, which is a type of (directed acyclic) **graph**.

*In a decision tree, the nodes represent questions (***test conditions***) and the edges are the answers to these questions.*

The top node of the tree is called the **root node**. *This node has 0 incoming edges, and 2+ outgoing edges.*

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NOTE

The nodes in our tree are connected by *directed edges*.

These directed edges lead from *parent nodes* to *child nodes*.

EXAMPLE – DATA

Table 4.1. The vertebrate data set.

Name	Body Temperature	Skin Cover	Gives Birth	Aquatic Creature	Aerial Creature	Has Legs	Hiber-nates	Class Label
human	warm-blooded	hair	yes	no	no	yes	no	mammal
python	cold-blooded	scales	no	no	no	no	yes	reptile
salmon	cold-blooded	scales	no	yes	no	no	no	fish
whale	warm-blooded	hair	yes	yes	no	no	no	mammal
frog	cold-blooded	none	no	semi	no	yes	yes	amphibian
komodo dragon	cold-blooded	scales	no	no	no	yes	no	reptile
bat	warm-blooded	hair	yes	no	yes	yes	yes	mammal
pigeon	warm-blooded	feathers	no	no	yes	yes	no	bird
cat	warm-blooded	fur	yes	no	no	yes	no	mammal
leopard shark	cold-blooded	scales	yes	yes	no	no	no	fish
turtle	cold-blooded	scales	no	semi	no	yes	no	reptile
penguin	warm-blooded	feathers	no	semi	no	yes	no	bird
porcupine	warm-blooded	quills	yes	no	no	yes	yes	mammal
eel	cold-blooded	scales	no	yes	no	no	no	fish
salamander	cold-blooded	none	no	semi	no	yes	yes	amphibian

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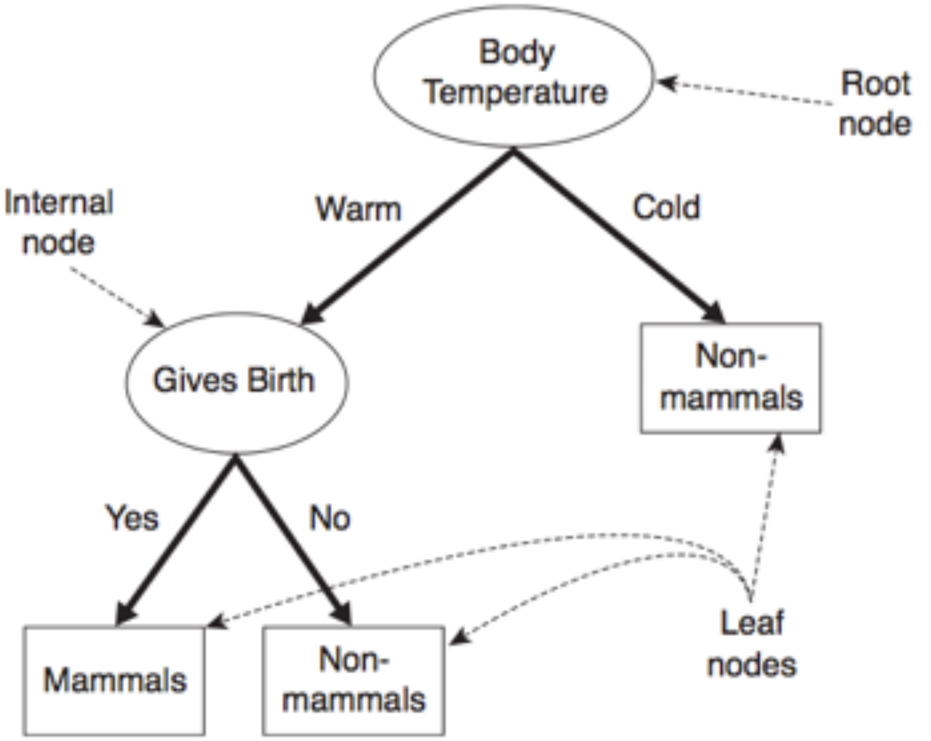
EXAMPLE – DECISION TREE



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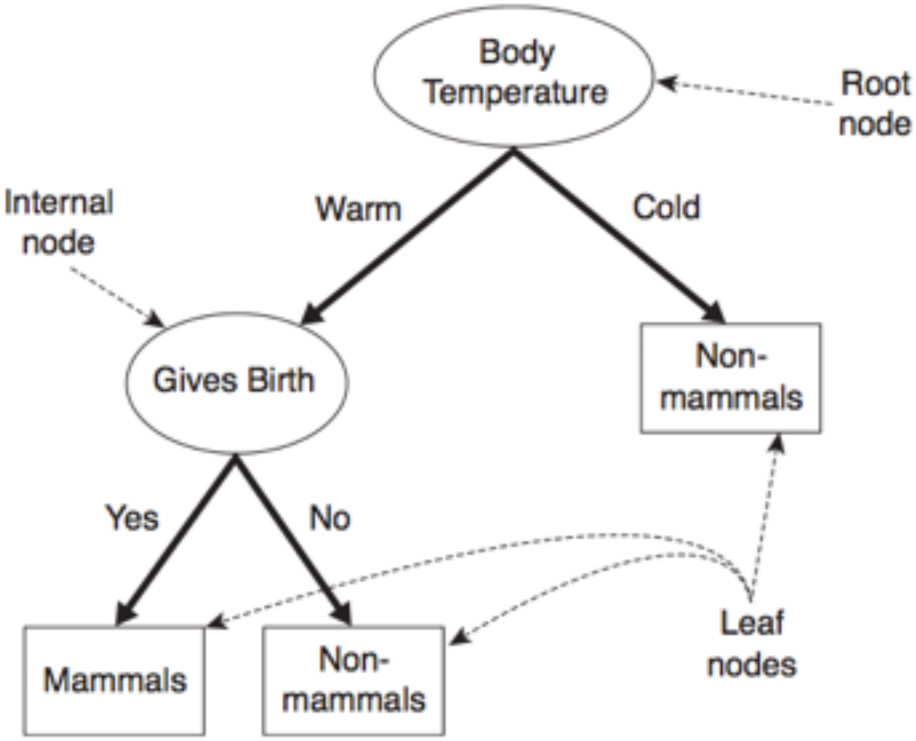

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NOTE

Internal nodes represent test conditions which *partition the records* at that node.

REVIEW:

1. *HOW DOES A DECISION TREE CLASSIFY DATA?*

2. *WHAT IS THE DIFFERENCE BETWEEN A ROOT, INTERNAL, AND TREE NOTE?*

II. BUILDING DECISION TREES

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A: Use a **heuristic** *algorithm.*

The basic method used to build (or "grow") a decision tree is **Hunt's algorithm**.

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greedy *– algorithm makes locally optimal decision at each step*
recursive *– splits task into subtasks, solves each the same way*
local optimum *– solution for a given neighborhood of points*

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A partition is 100% pure when all of its records belong to a single class.

Consider a binary classification problem with classes X, Y. Given a set of records D_t at node t, Hunt's algorithm proceeds as follows:

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NOTE

This is the *base case* for the recursive algorithm.

Consider a binary classification problem with classes X, Y. Given a set of records D_t at node t, Hunt's algorithm proceeds as follows:

2) If D_t contains records from both classes, then a test condition is created to partition the records further. In this case, t is an internal node whose outgoing edges correspond to the possible outcomes of this test condition.

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2) If D_t contains records from both classes, then a test condition is created to partition the records further. In this case, t is an internal node whose outgoing edges correspond to the possible outcomes of this test condition.

These outgoing edges terminate in **child nodes**. *A record d in D_t is assigned to one of these child nodes based on the outcome of the test condition applied to d.*

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NOTE

Decision trees are easy to interpret, but the algorithms to create them are a bit complicated.

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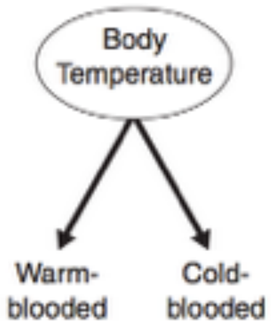
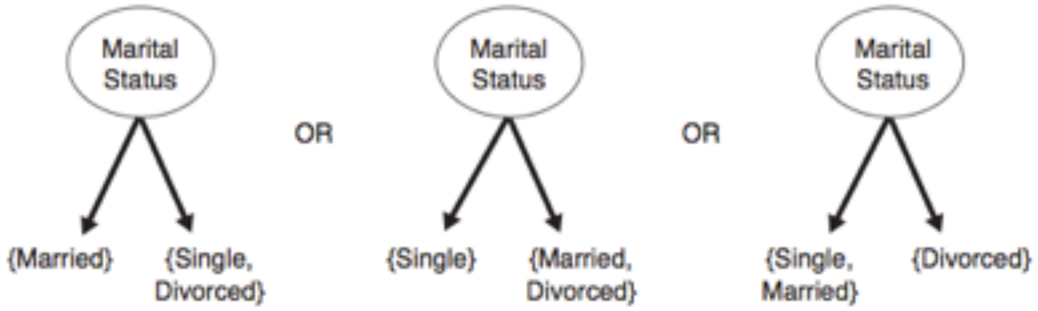


Figure 4.8. Test condition for binary attributes.



(b) Binary split {by grouping attribute values}

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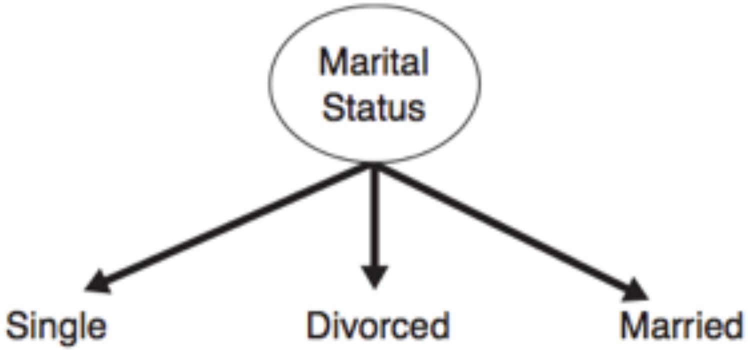
A: There are a few ways to do this.

Alternatively, we can create **multiway splits***:*



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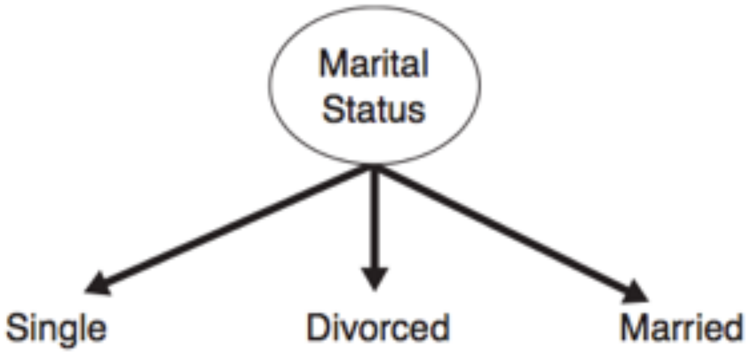

(a) Multiway split

NOTE

Multiway splits can produce purer subsets, but may lead to overfitting!

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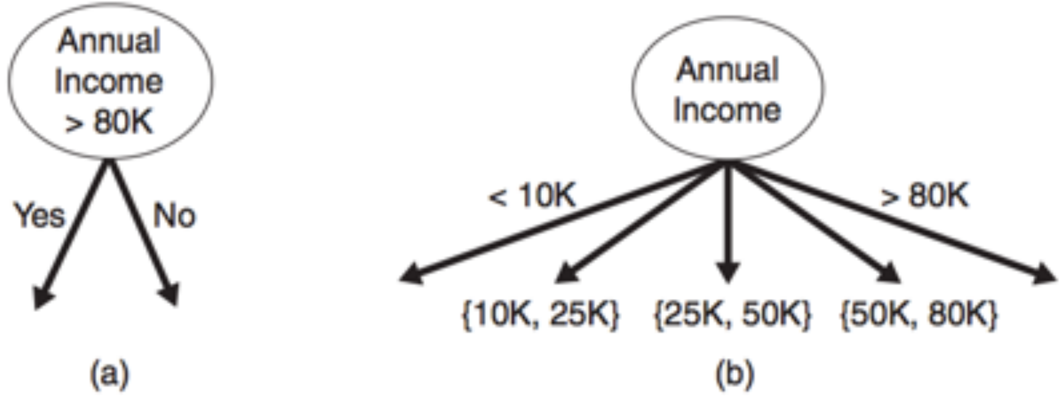
A: There are a few ways to do this.

For continuous features, we can use either method:



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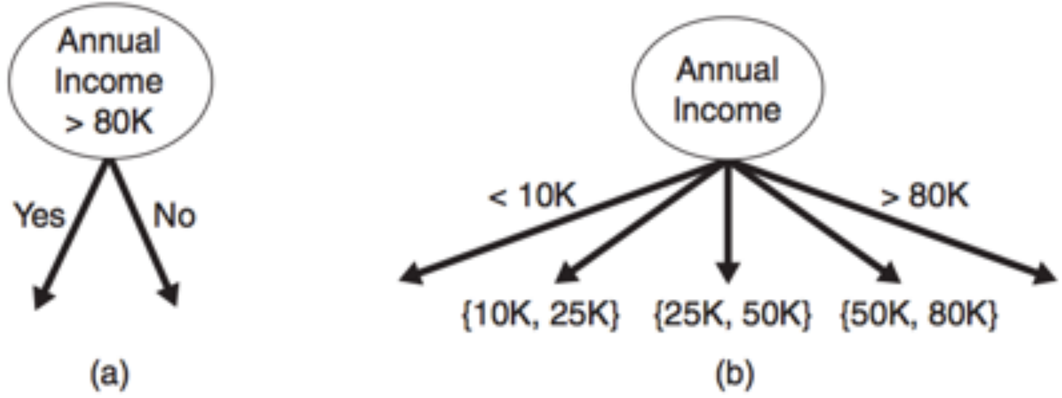

Figure 4.11. Test condition for continuous attributes.

NOTE

There are optimizations that can improve the naïve quadratic complexity of determining the optimum split point for continuous atrributes.

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A: Recall that no split is necessary (at a given node) when all records belong to the same class.

Therefore we want each step to create the partition with the highest possible purity.

We need an objective function to optimize!

III. OPTIMIZATION FUNCTIONS

We want our objective function to measure the gain in purity from a particular split.

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For example, let $p(i \mid t)$ be the probability of class i at node t (eg, the fraction of records labeled i at node t).

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NOTE

We are using the *frequentist* definition of probability here!

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The minimum purity partition is given by the distribution:

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The maximum purity partition is given (eg) by the distribution:

$$p(0 \mid t) = 1 - p(1 \mid t) = 1$$

Some measures of impurity include:

$$\begin{aligned}
\text{Entropy}(t) &= -\sum_{i=0}^{c-1} p(i|t) \log_2 p(i|t), \\
\text{Gini}(t) &= 1 - \sum_{i=0}^{c-1} [p(i|t)]^2, \\
\text{Classification error}(t) &= 1 - \max_i [p(i|t)],
\end{aligned}$$

Note that each measure achieves its max at 0.5, min at 0 & 1.

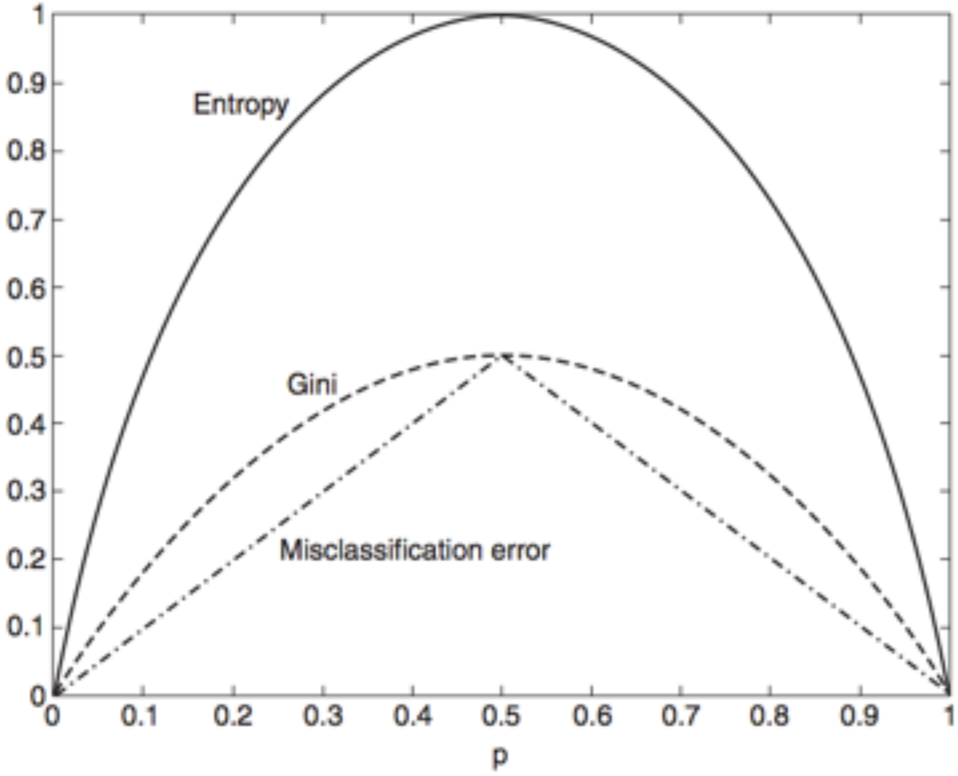

Figure 4.13. Comparison among the impurity measures for binary classification problems.

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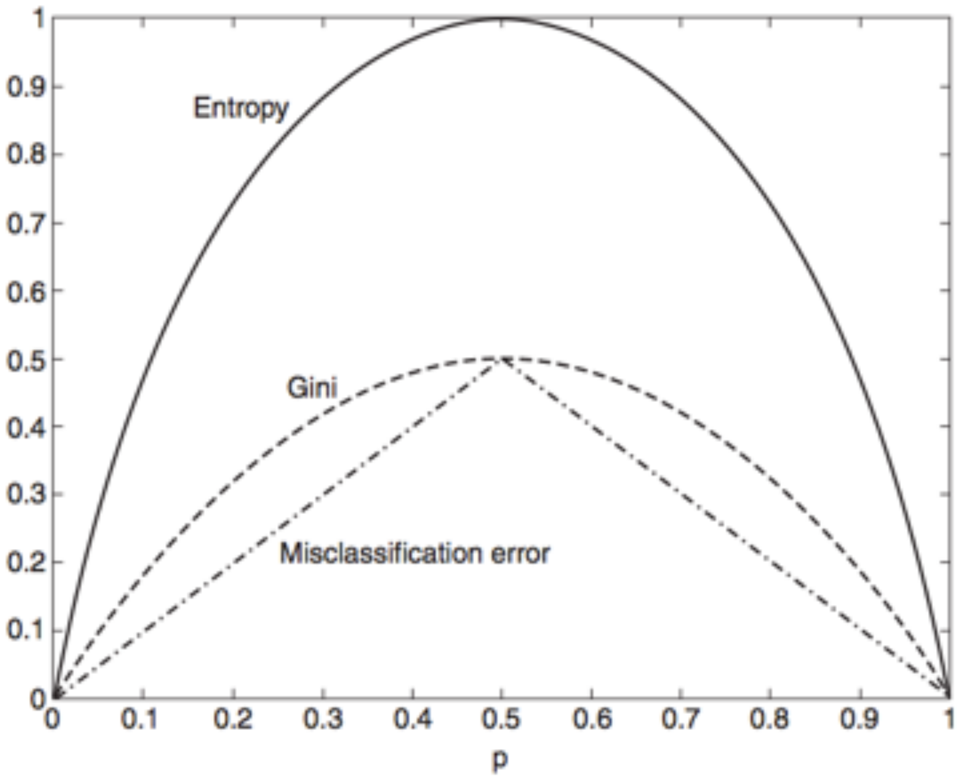
NOTE

Despite consistency, different measures may create different splits.



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Q: Why is this true?

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Q: Why is this true?
A: We still need to look at impurity before & after the split.

We can make this comparison using the **gain***:*

$$\Delta = I(\text{parent}) - \sum_{\text{children } j} \frac{N_j}{N} I(\text{child } j)$$

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(Here I is the impurity measure, N_j denotes the number of records at child node j, and N denotes the number of records at the parent node.)

When I is the entropy, this quantity is called the **information gain***.*

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Another way is to use a splitting criterion which explicitly penalizes the number of outcomes (C4.5)

We can use a function of the information gain called the **gain ratio** *to explicitly penalize high numbers of outcomes:*

$$\text{gain ratio} = \frac{\Delta_{info}}{-\sum p(v_i) log_2 p(v_i)}$$

(Where $p(v_i)$ refers to the probability of label i at node v)

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NOTE

This is a form of regularization!

(Where $p(v_i)$ refers to the probability of label i at node v)

IV. PREVENTING OVERFITTING

In addition to determining splits, we also need a stopping criterion to tell us when we’re done.

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This is correct in principle, but would likely lead to overfitting.

One possibility is **pre-pruning**, *which involves setting a minimum threshold on the gain, and stopping when no split achieves a gain above this threshold.*

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This prevents overfitting, but is difficult to calibrate in practice (may preserve bias!)

Alternatively we could build the full tree, and then perform **pruning** *as a post-processing step.*

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To prune a tree, we examine the nodes from the bottom-up and simplify pieces of the tree (according to some criteria).

Complicated subtrees can be replaced either with a single node, or with a simpler (child) subtree.

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The first approach is called **subtree replacement**, *and the second is* **subtree raising**.

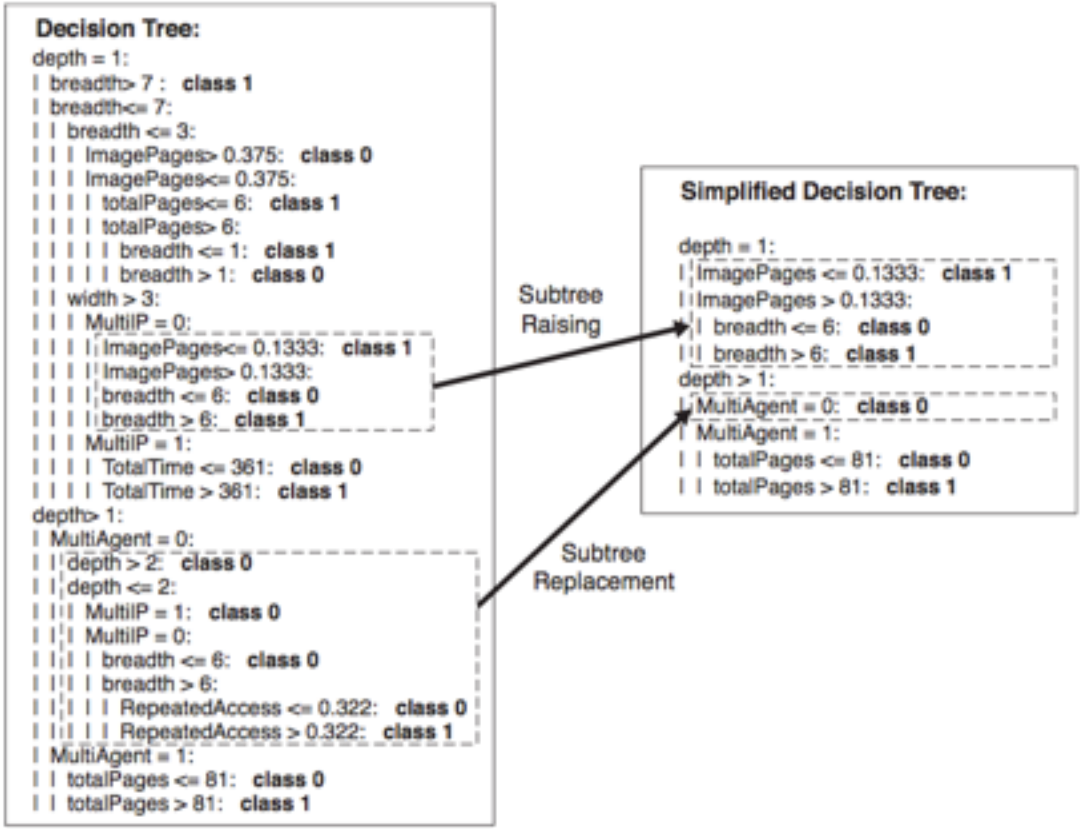

Figure 4.29. Post-pruning of the decision tree for Web robot detection.

Generally, (or at least depending on your data), it can be ***very easy*** *to overfit a model with decision trees.*

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Pay careful attention to what is going in and out of your model!

```
>>> X_test_features = X_test[features].values
>>> clf.score(X_train_features, X_train['IsBadBuy'].values)
0.99998042593172565
>>> clf.score(X_test_features, X_test['IsBadBuy'].values)
0.78131993605846084
```

PROS AND CONS

When will you want to use decision trees, and when should you not expect good performance?

Easy to understand why a classification was made.

Less data preparation necessary.

Easy to mix numerical, categorical data.

Fast to predict.

Susceptible to overfitting.

Possibly chaotic sensitivity to training data.

Typically, finding a globally optimal tree is intractable: must resort to heuristics to find local optima.

ENSEMBLE METHODS

Some of the dangers of decision trees can be mitigated by combining ensembles of individual trees trained on subsets of the data or feature space. Often, this means sacrificing the ability to interpret the steps leading to a classification.

Look out for random forests. Most Kaggle competitions are won with these.

Train several tree classifiers on small subsets of the feature space. Take the most common prediction among the trees as the final output.

Pros: fast to train, harder to overfit, typically very good classification performance

Cons: best possible fit is slightly worse, obfuscates the classification path.

DISCUSSION/LAB