GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

DECISION TREE CLASSIFIERS

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

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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.

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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

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

EXAMPLE – DECISION TREE

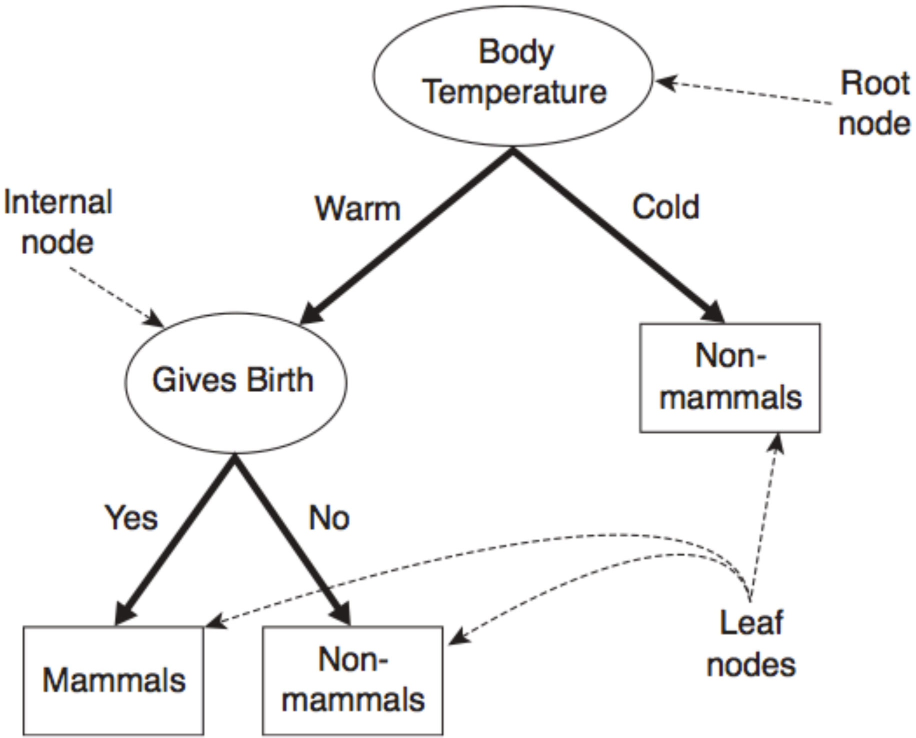

Figure 4.4. A decision tree for the mammal classification problem.

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

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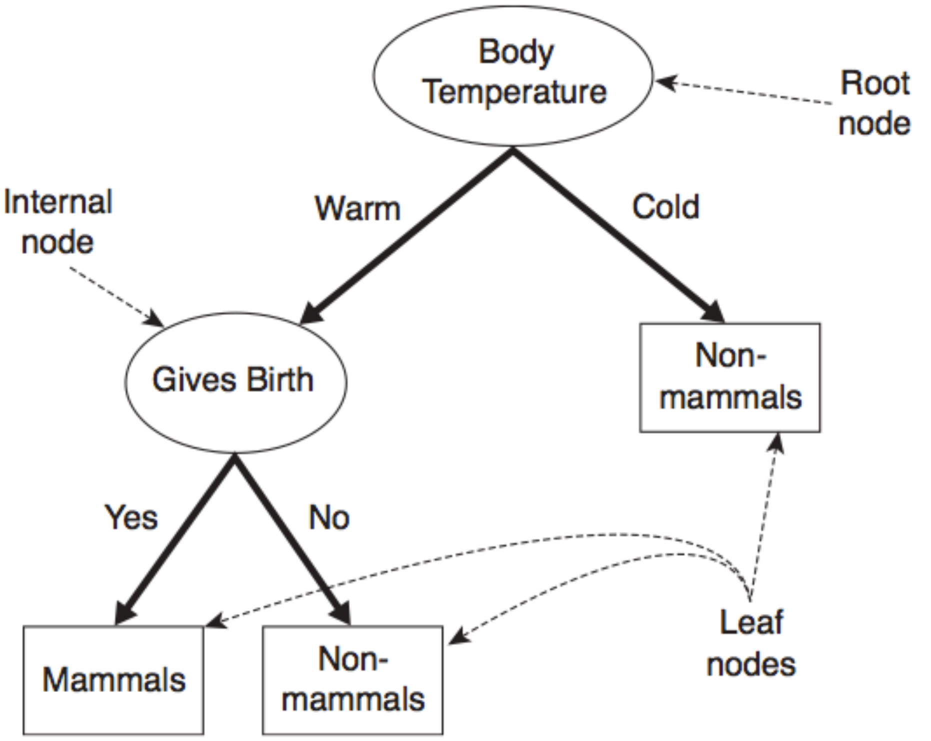

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NOTE

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

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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The partitioning decision is made at each node according to a purity metric.

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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1) If all records in D_t belong to class *X*, then *t* is a leaf node corresponding to class *X*.

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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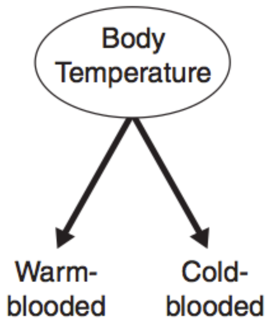
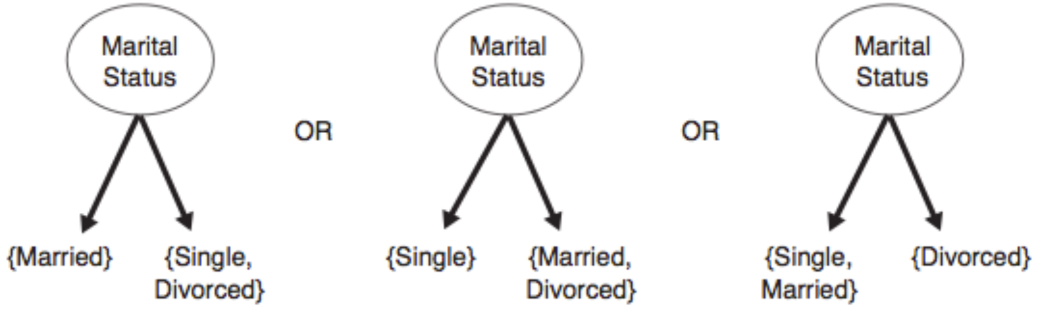


Figure 4.8. Test condition for binary attributes.

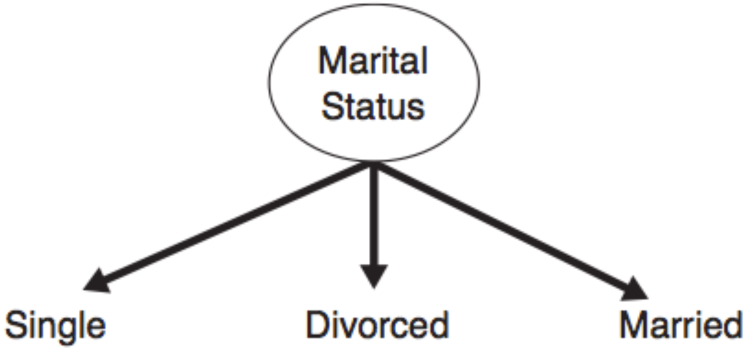


(b) Binary split {by grouping attribute values}

Q: How do we partition the training records?

A: There are a few ways to do this.

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



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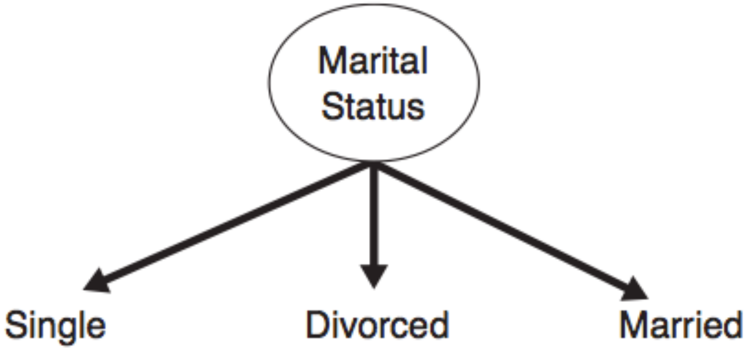


(a) Multiway split

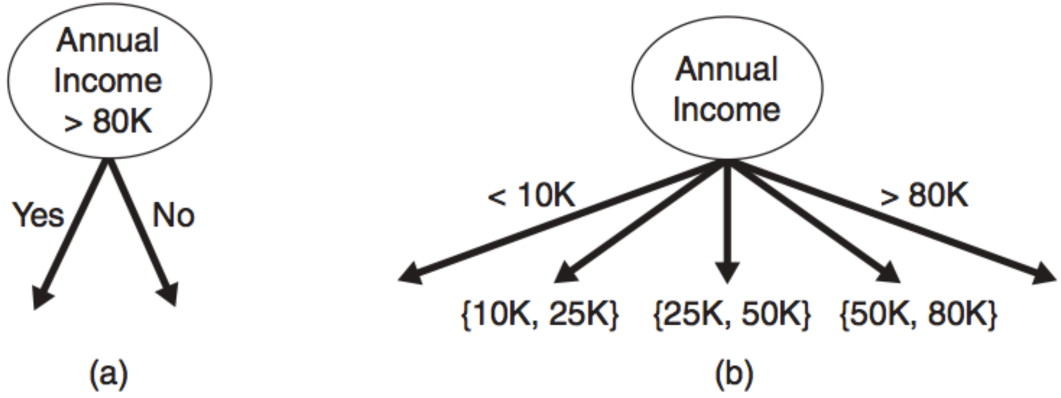
NOTE

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

Q: How do we partition the training records?

A: There are a few ways to do this.

For continuous features, we can use either method:



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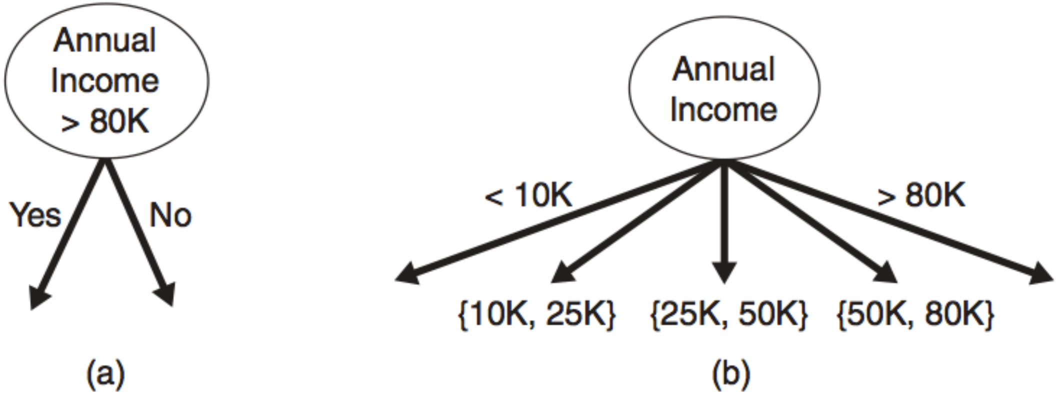

Figure 4.11. Test condition for continuous attributes.

NOTE

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

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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 $p(i|t)$ be the probability of class i at node t (eg, the fraction of records labeled i at node t).

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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:

$$p(0|t) = 1 - p(1|t) = 1$$

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.

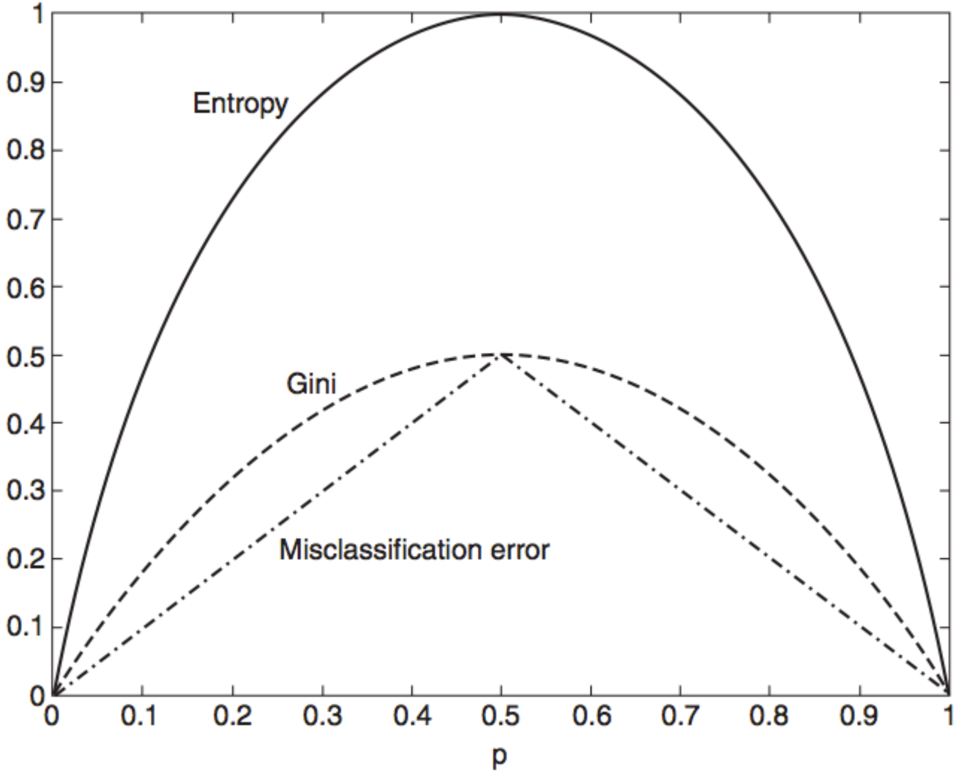

Figure 4.13. Comparison among the impurity measures for binary classification problems.

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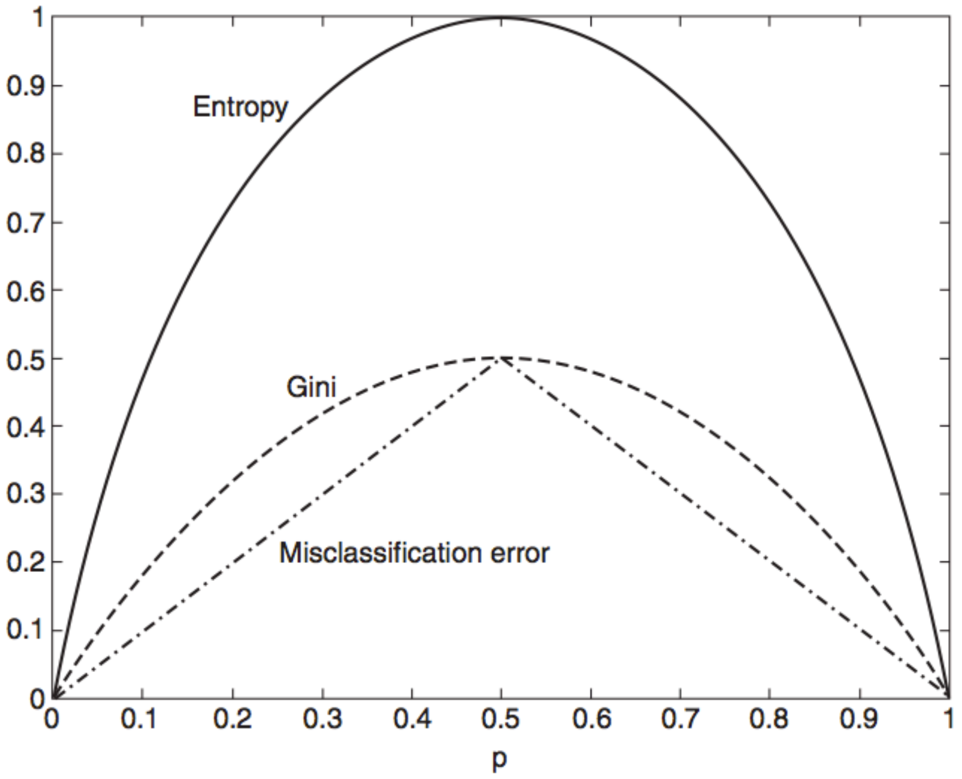
NOTE

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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One way of dealing with this is to restrict the algorithm to binary splits only (CART).

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

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**.

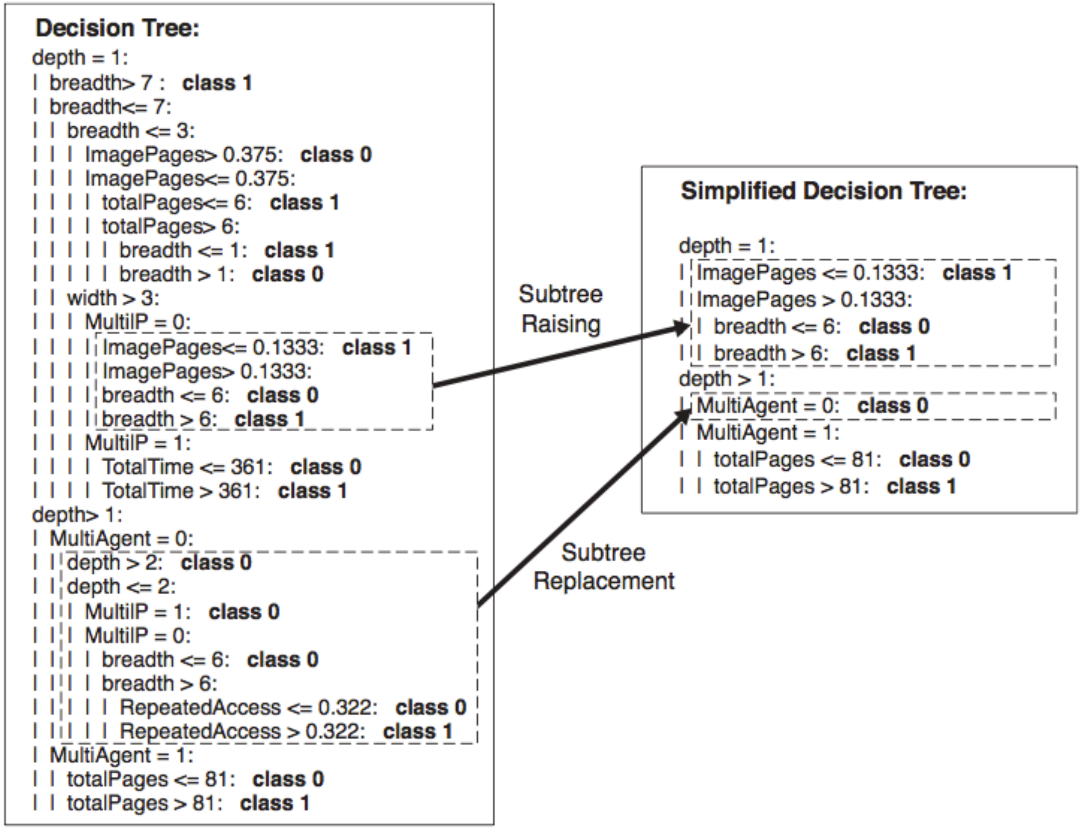

Figure 4.29. Post-pruning of the decision tree for Web robot detection.

In practice it’s easier to set a stopping condition for growing trees, such as:

- Max depth
- Min samples split
- Min samples leaf
- Max leaf nodes

These correspond to options in scikit-learn.

EX: DECISION TREES IN PYTHON