GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LESSON 8: DECISION TREES & RANDOM FORESTS

I. NAIVE BAYES AND BAYESIAN ESTIMATORS

II. INSULT ESTIMATOR COMPETITION

QUESTIONS?

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

LAB:
VI. IMPLEMENTING DECISION TREES WITH SCIKIT-

I. DECISION TREES

What is a decision tree?

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A non-parametric hierarchical classification technique

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A **non-parametric** hierarchical classification technique

Non-parametric: no parameters, no distribution assumptions

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A non-parametric **hierarchical** classification technique

Non-parametric: no parameters, no distribution assumptions

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

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Using a configuration of **nodes** and **edges**

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

DECISION TREES

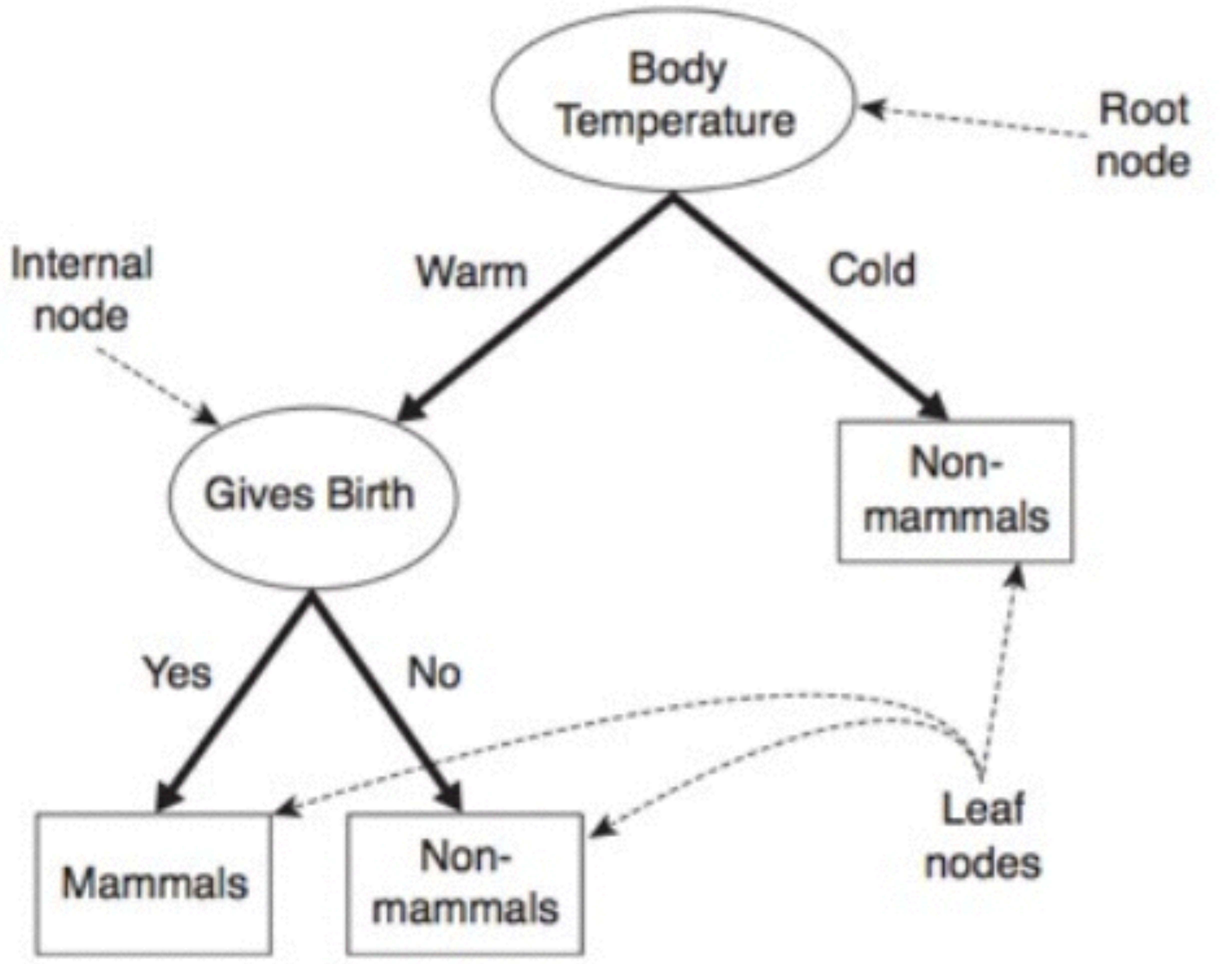

Figure 4.4. A decision tree for the mammal classification problem.

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

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

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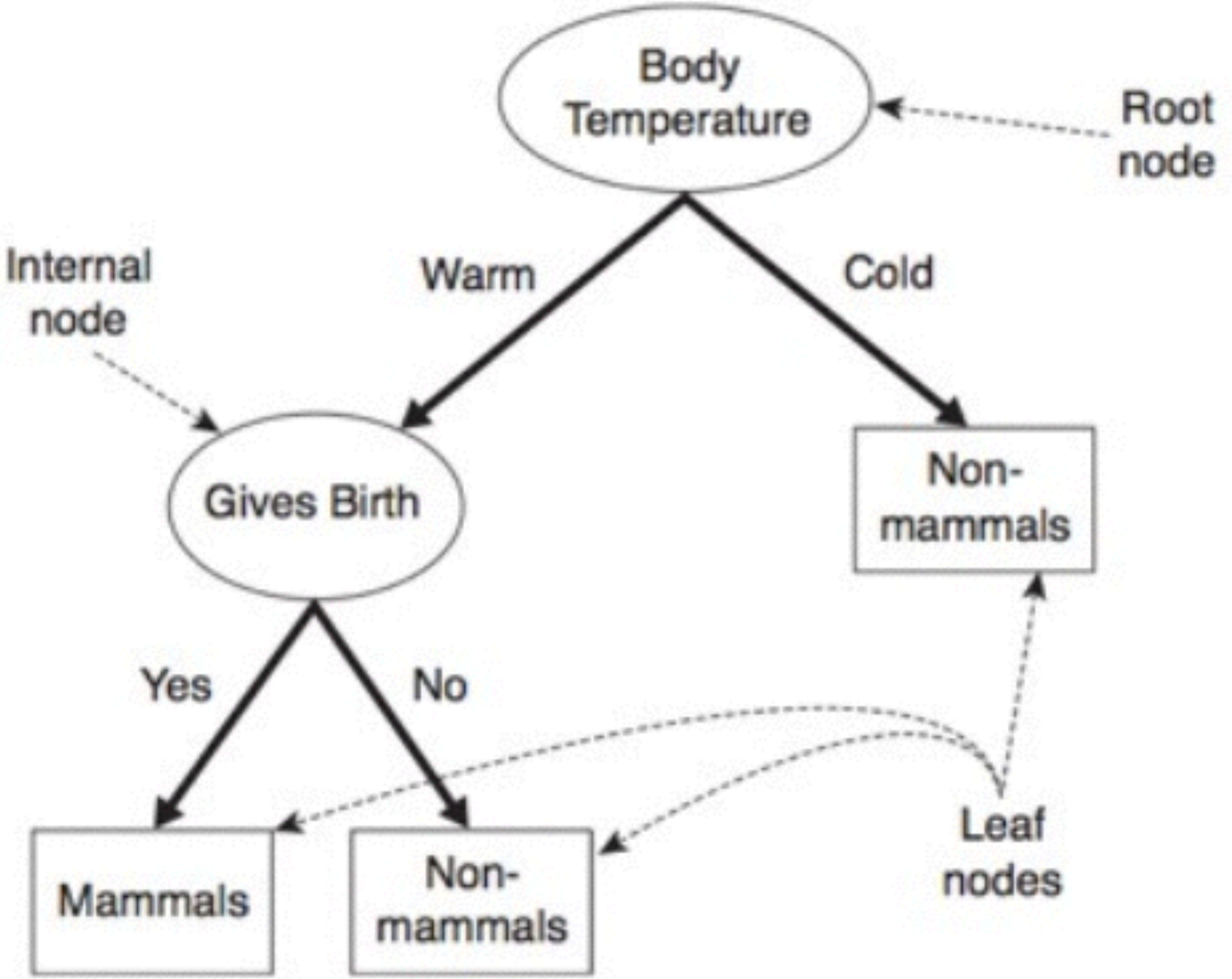
An **internal node** has 1 incoming edge and 2+ outgoing edges

A **leaf node** has 1 incoming edge and 0 outgoing edges. Leaf nodes correspond to class labels

DECISION TREES



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REVIEW

Questions?

II. BUILDING DECISION TREES

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But this is generally too complex to be practical → $O(2^n)$.

Q: How do we find a practical solution that works?

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

BUILDING DECISION TREES

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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.

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NOTE

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

BUILDING DECISION TREES

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.

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.*

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:

3) *These steps are then recursively applied to each child node.*

NOTE

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

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Test conditions can create **binary splits***:*

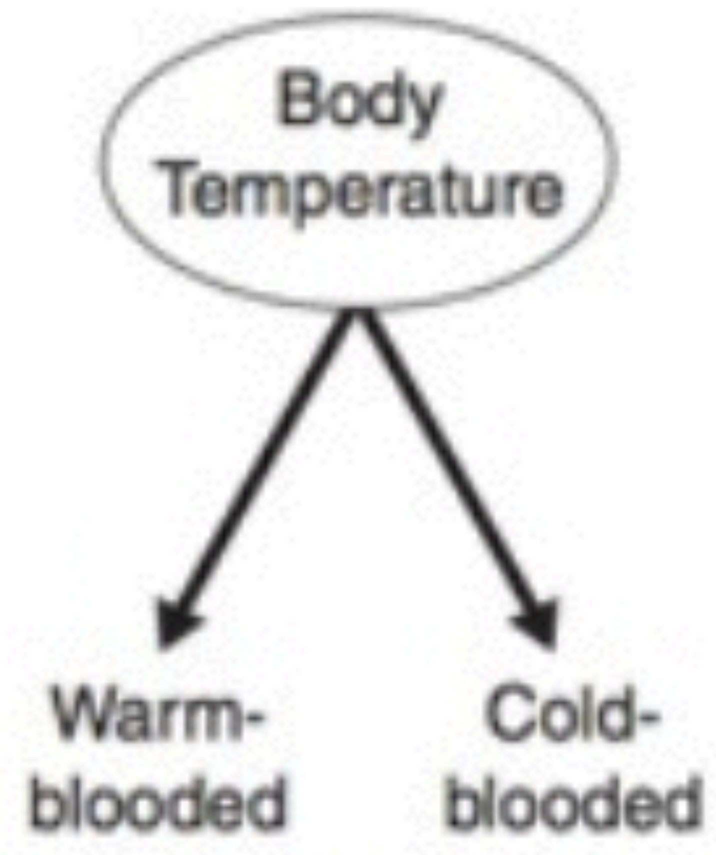
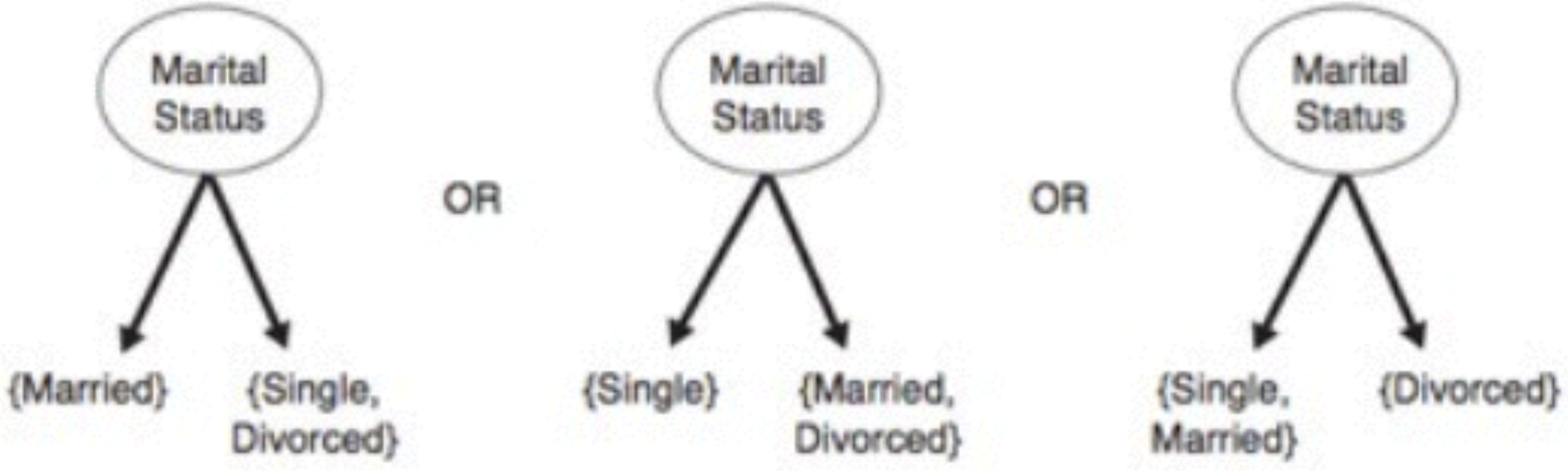


Figure 4.8. Test condition for binary attributes.

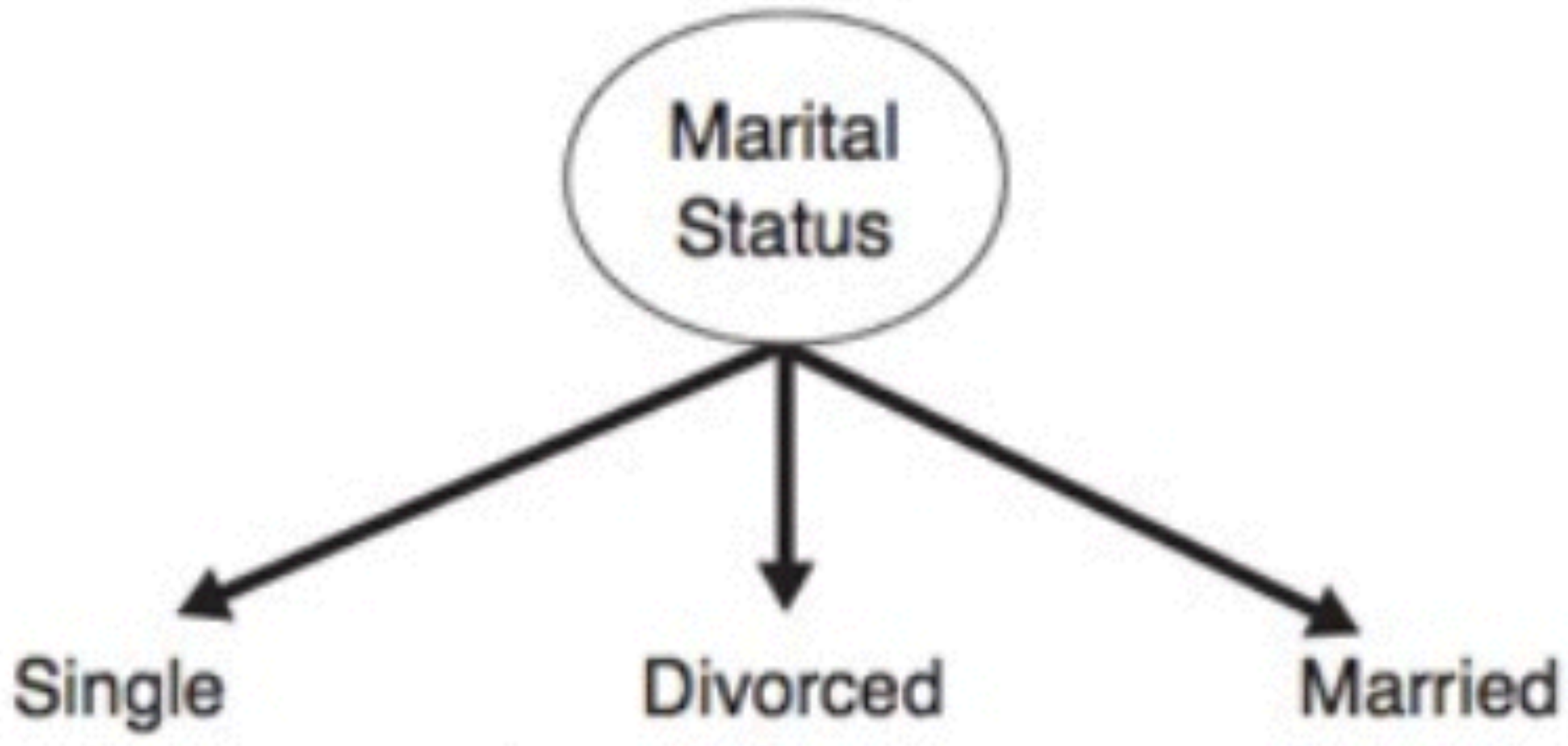


(b) Binary split {by grouping attribute values}

Q: How do we partition the training records?

A: There are a few ways to do this.

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



(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:

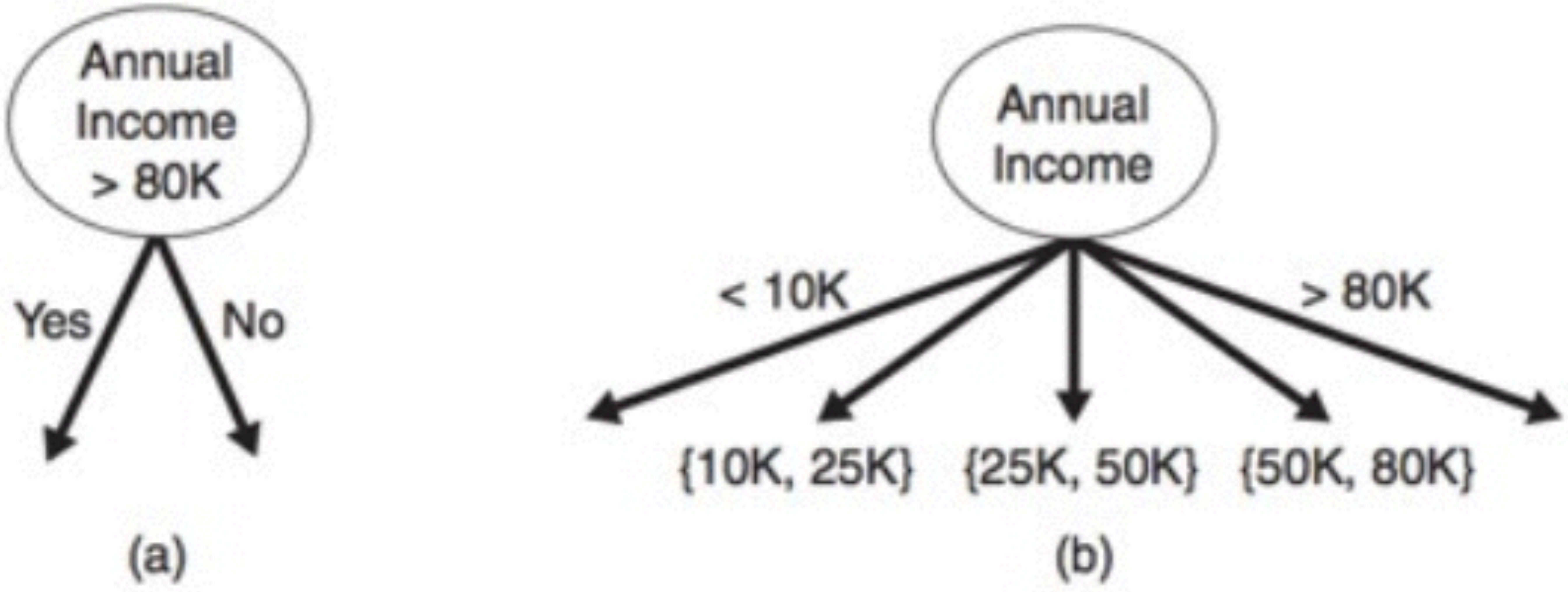


Figure 4.11. Test condition for continuous attributes.

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

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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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E.G. the fraction of records labeled i at node t

Then for a binary (0/1) classification problem,

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The minimum purity partition is given by the distribution:

$$p(0|t) = p(1|t) = 0.5$$

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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.

NOTE

Despite consistency, different measures may create different splits.

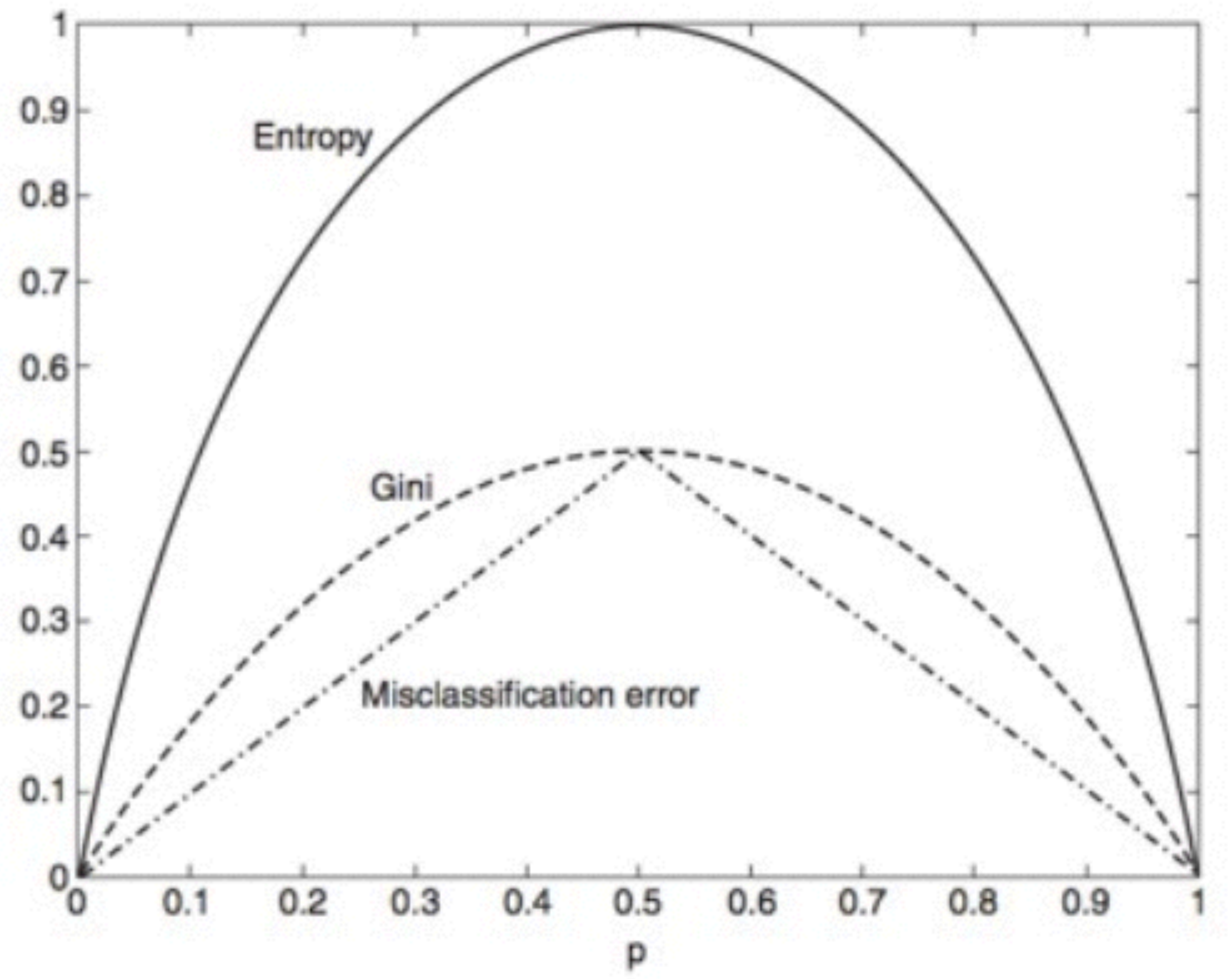

Figure 4.13. Comparison among the impurity measures for binary classification problems.

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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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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)

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

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

NOTE

This is a form of regularization!

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

IV. PREVENTING OVERFITTING

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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.*

PREVENTING 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.*

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**.

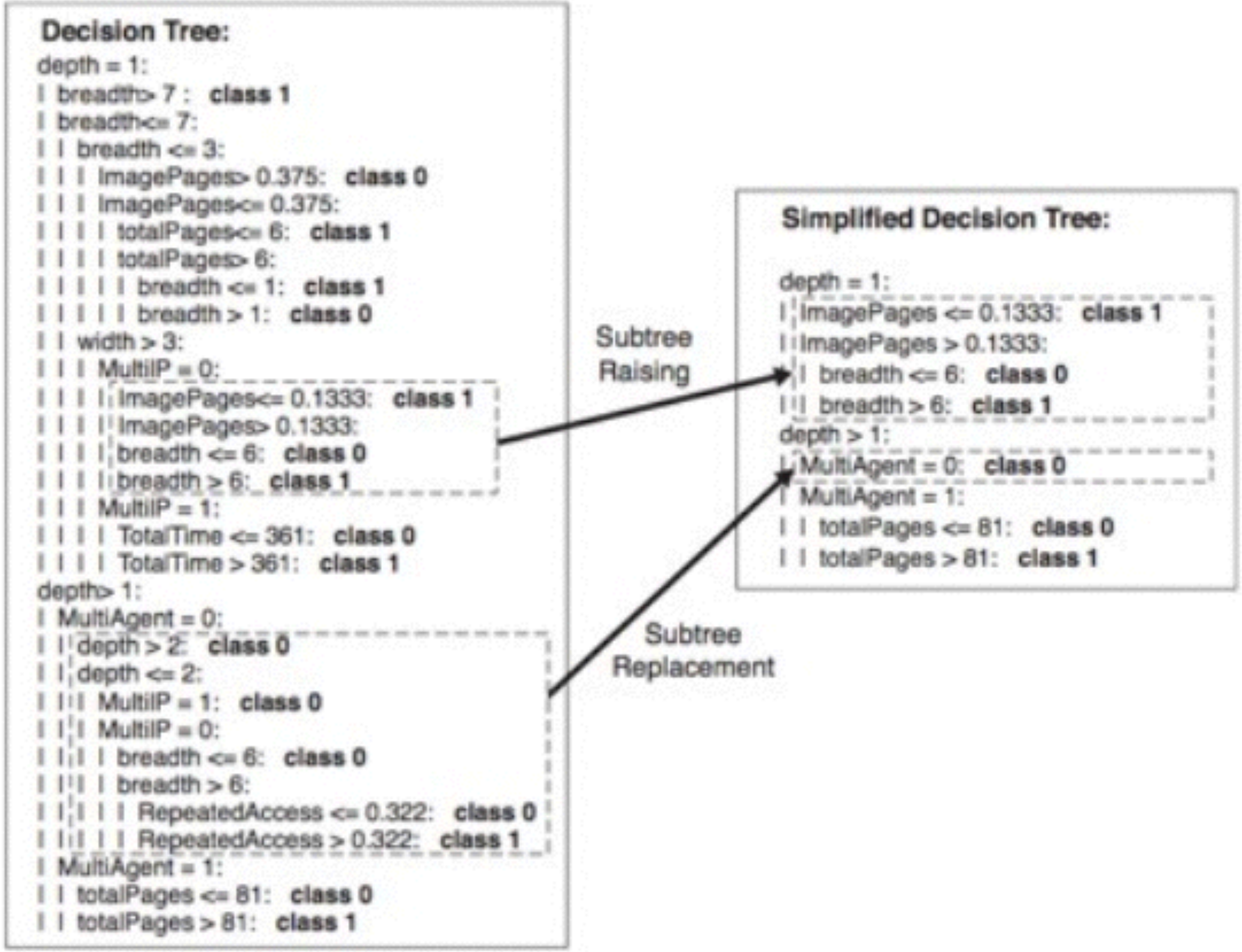

Figure 4.29. Post-pruning of the decision tree for Web robot detection.

V. RANDOM FORESTS

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2) *Repeat (1) for N iterations*
3) *Predict based on majority vote of N trees*

VI. DECISION TREES AND RANDOM FORESTS LAB