GENERAL ASSEMBLY

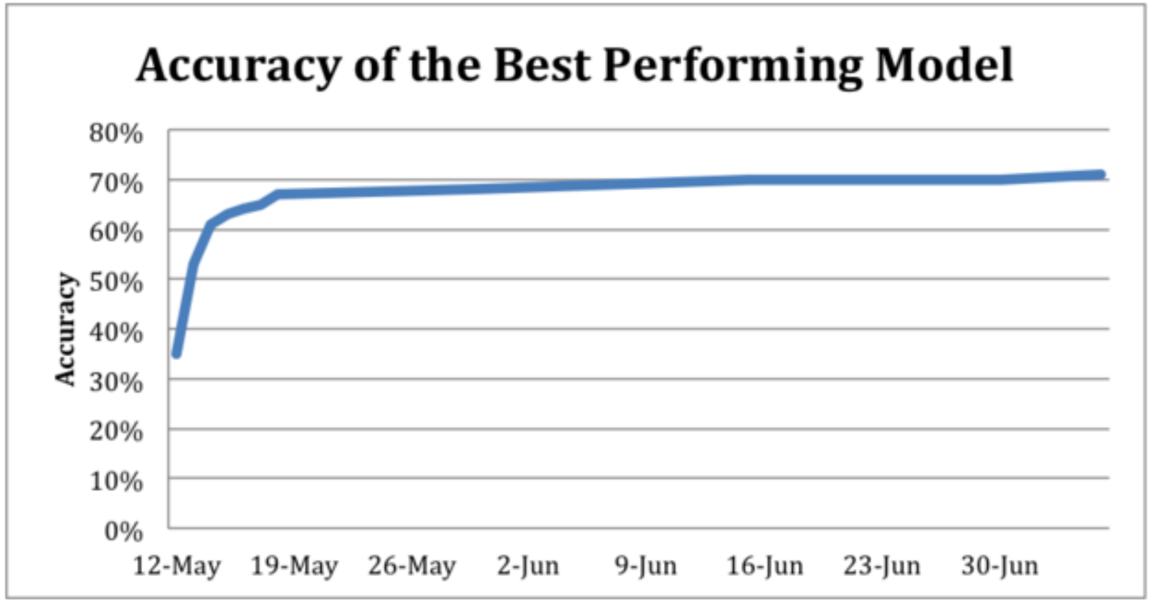
DECISION TREES

Brian Chung

QUESTIONS FROM LAST TIME - SUPPORT VECTOR MACHINES

- **RBF!?!? What the hell is that?**
- **Tradeoff between slack and misclassified samples?**
- **Applying SVM to classify N classes**
- **More data preparation techniques**

WHAT CAN YOU DO WITH AN 80% ALGORITHM?



A few months ago, my company, CrowdFlower, ran a machine learning competition on Kaggle. It perfectly highlighted the biggest opportunity (and challenge) with machine learning: What do you do with an 80% accurate algorithm?

We uploaded data collected on our platform and Kaggle sent it out to over 1,000 data scientists, who competed to see who could build the best search model.

The simplest approach gave a baseline accuracy of 32%. Within hours a team beat that with a 35% accurate model. By the next morning, one team already had a 53% accurate model.

With Microsoft's Azure ML and IBM's investment in Watson, making models is easier than ever. Companies no longer need a Google-size R&D budget to make machine learning applicable to their business. These models aren't perfect, but they're useful. The new challenge for businesses is how to integrate an imperfect machine-learning algorithm into their existing workflow.

http://www.computerworld.com/article/3023708/data-analytics/the-machine-learning-problem-of-the-next-decade.html

DECISION TREE AGENDA

I. DECISION TREES
II. FITTING DECISION TREES
III. OBJECTIVE FUNCTIONS
IV. REGULARIZATION
V. PROS/CONS & USAGE
VI. DECISION TREE LAB
VII. RANDOM FOREST (TIME PERMITTING)

DECISION TREE LEARNING OBJECTIVES

1. Understand how decision trees function for classification problems
2. Learn the objective functions used in building decision trees
3. Learn the regularization process in decision tree building

I. DECISION TREES

TYPES OF ML SOLUTIONS

	Continuous	Categorical
Supervised	Regression	Classification
Unsupervised	Dimension Reduction	Clustering

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The features can be both continuous and categorical and do not require any scaling or preprocessing

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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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*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

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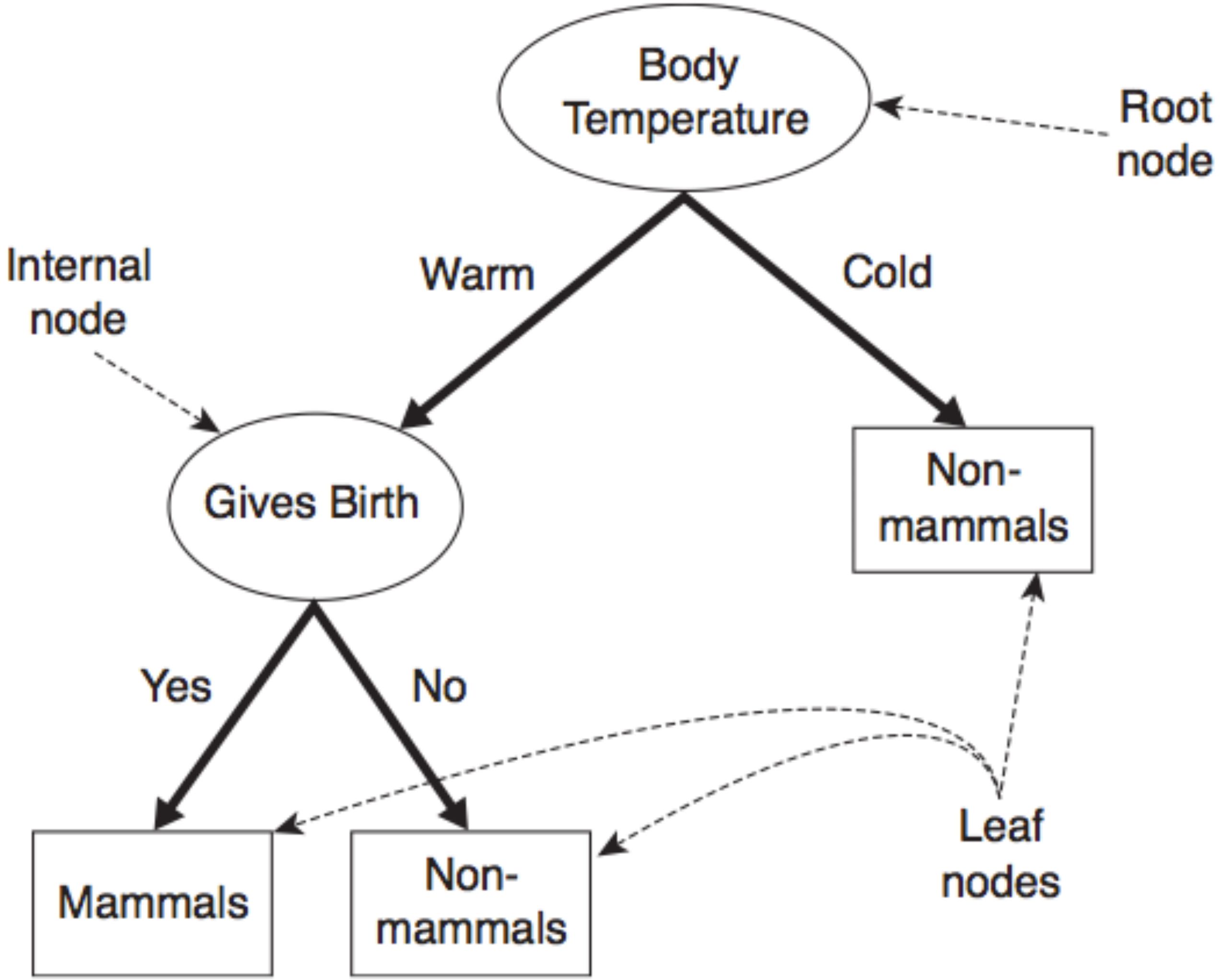
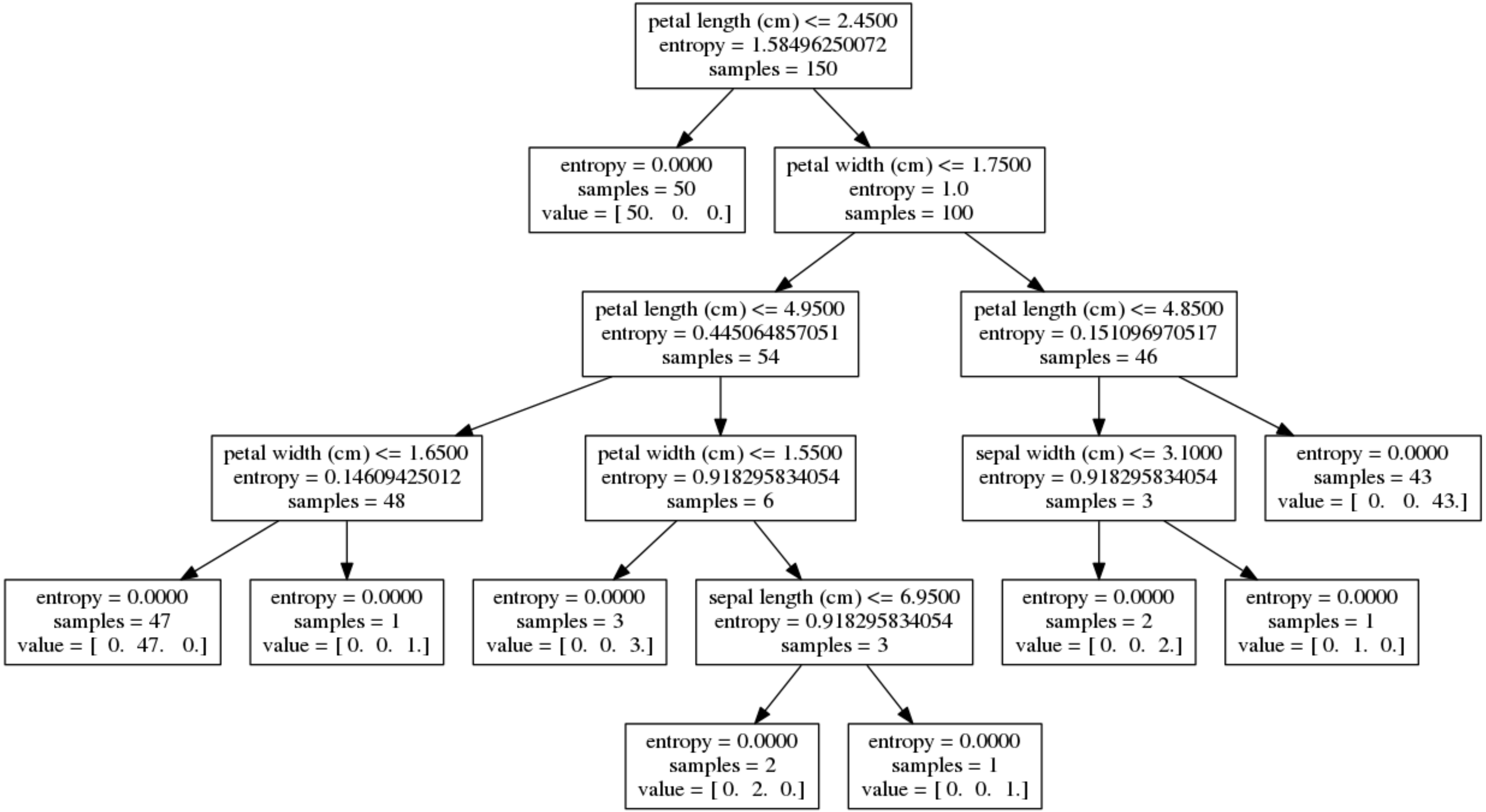


Figure 4.4. A decision tree for the mammal classification problem.

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

EXAMPLE - DECISION TREE WITH IRIS DATASET



II. BUILDING DECISION TREES

LET'S GO OVER OUR OWN

Let's go over an example of how one might be built with binary classes in R^2 space (i.e. two features).

- Our goal will be to split the space into **regions**.
- Inside each region, we'll classify any point in that space as the **max voted class** within that region
- We will only consider constant splits (no linear splits based on more than one feature)
- We can finish when either every leaf is pure, we have reached a max depth, or when there are less than x amount of data points at a node

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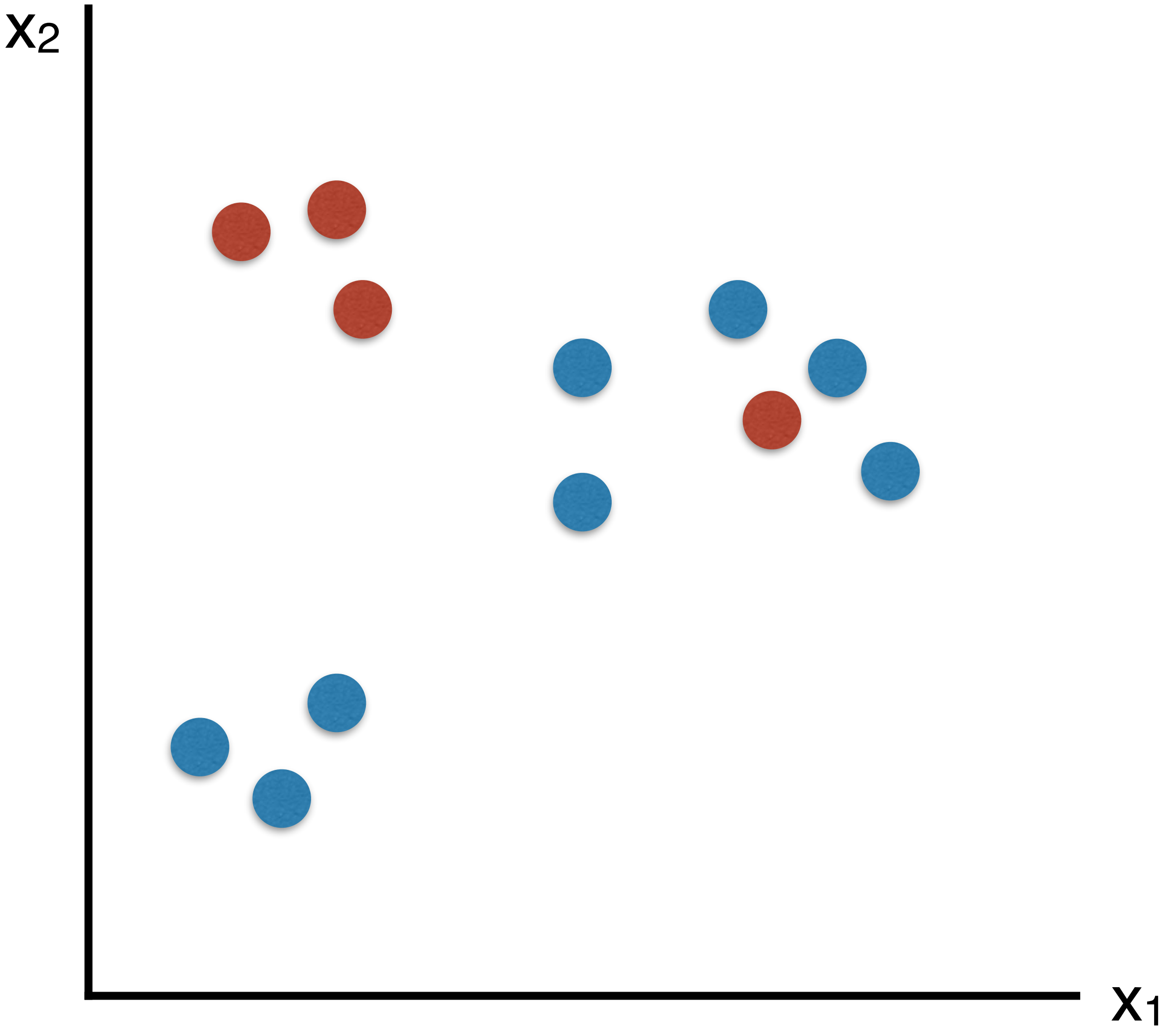

Within a region:

Prediction: Most common class label

Error: Fraction of misclassified labels

In the entire space:
N = 12 points
Prediction = Blue
Error = 4 / 12 = 33% misclassification error

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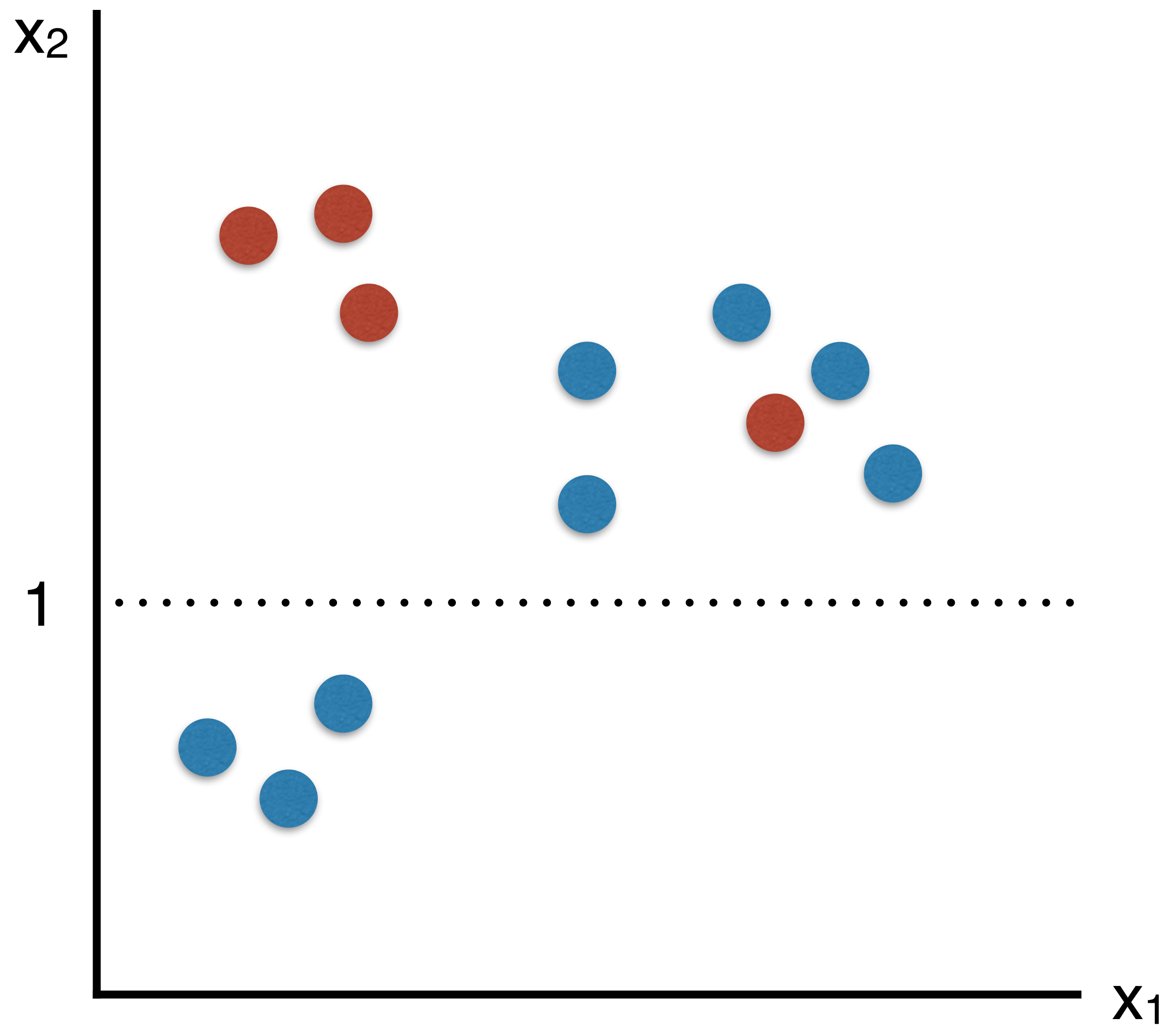

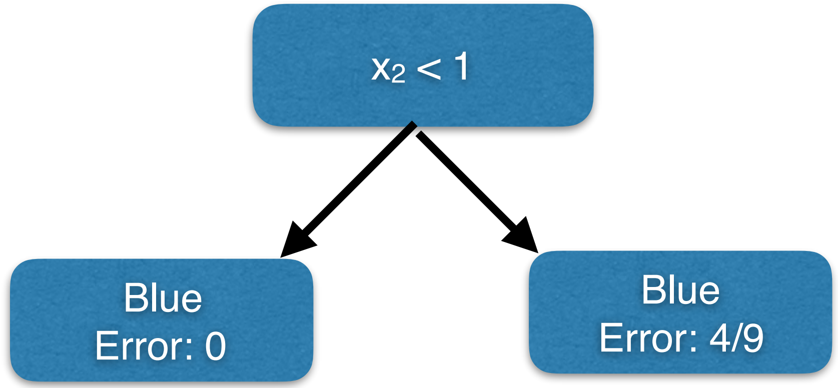

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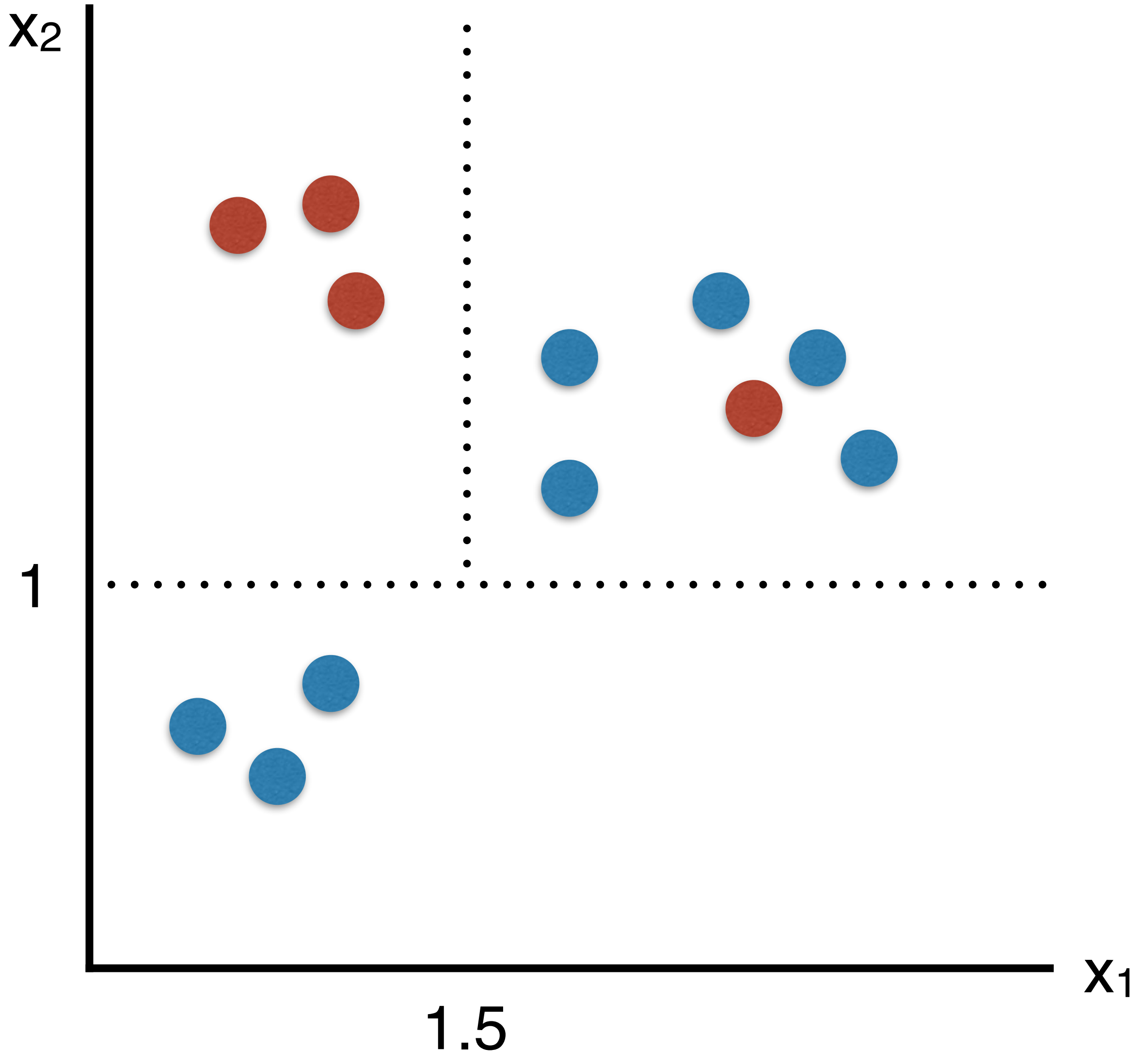

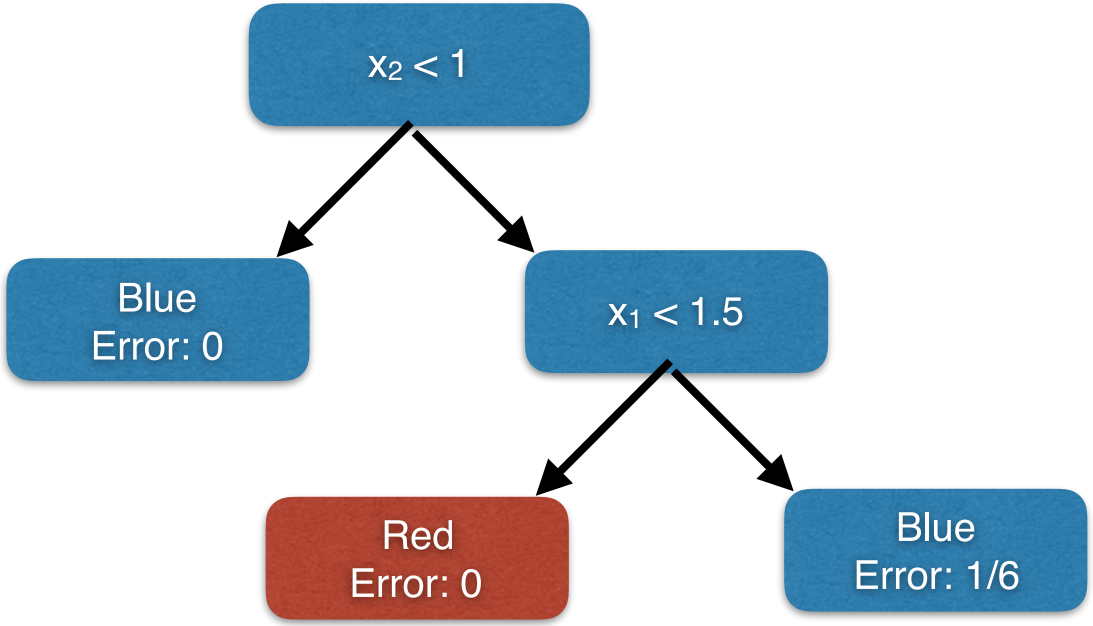

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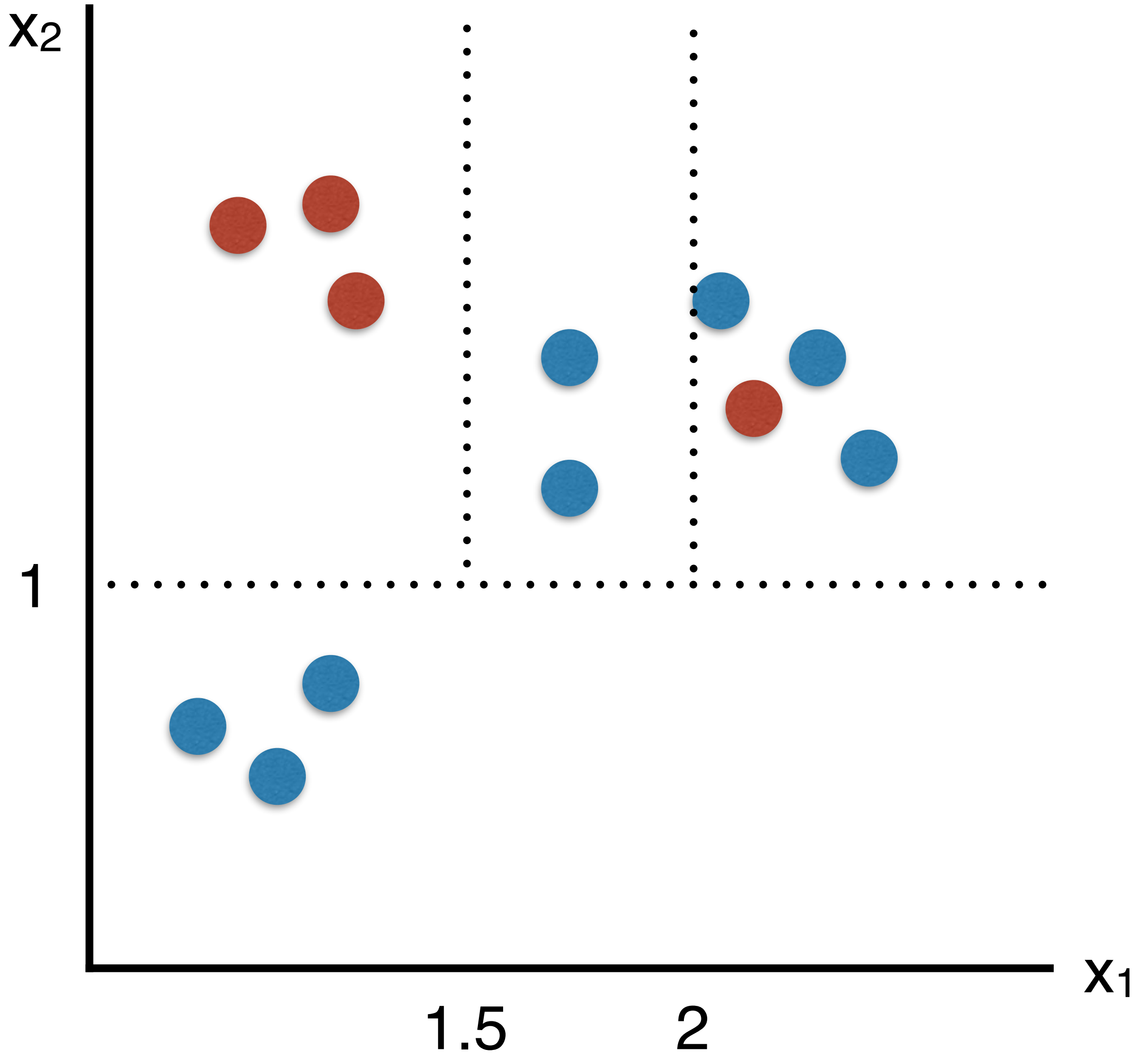

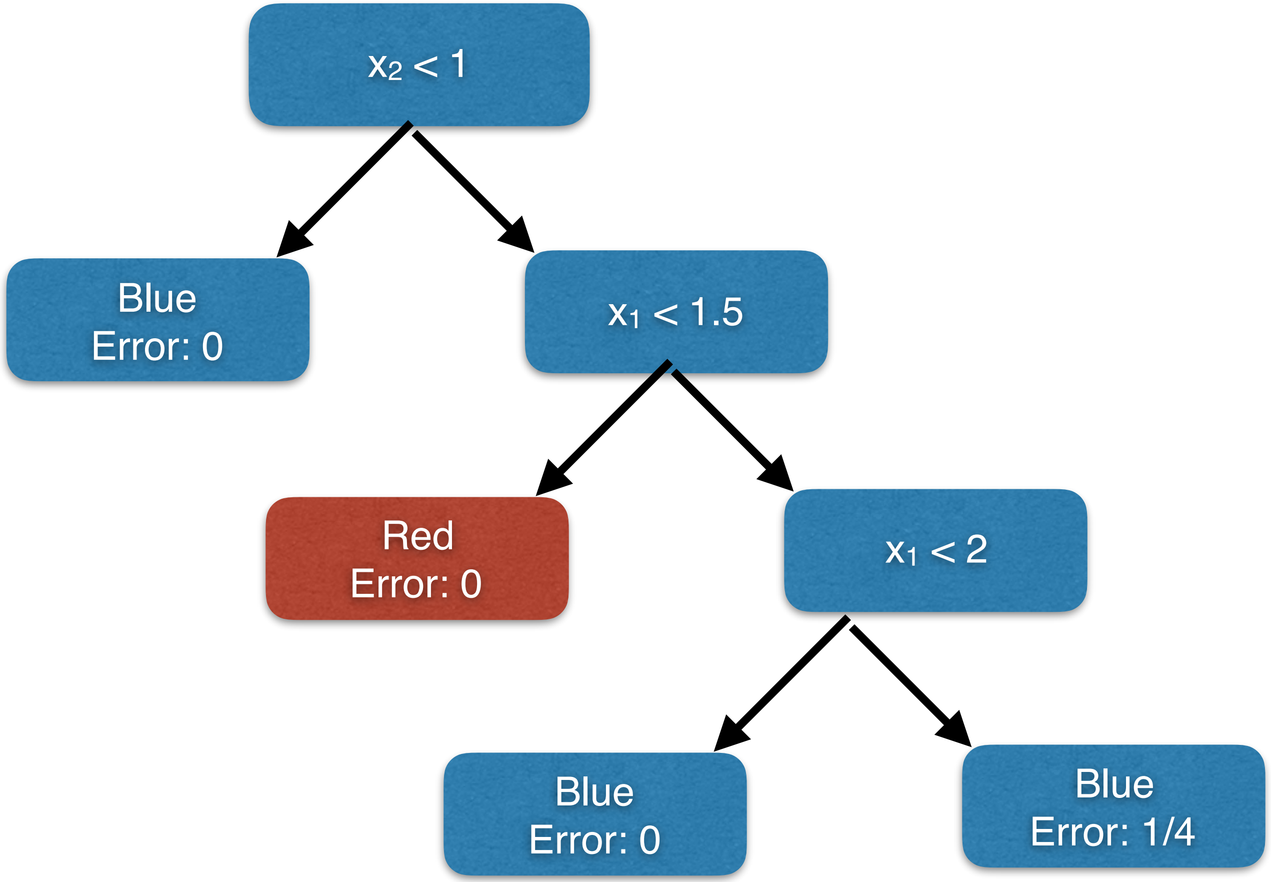

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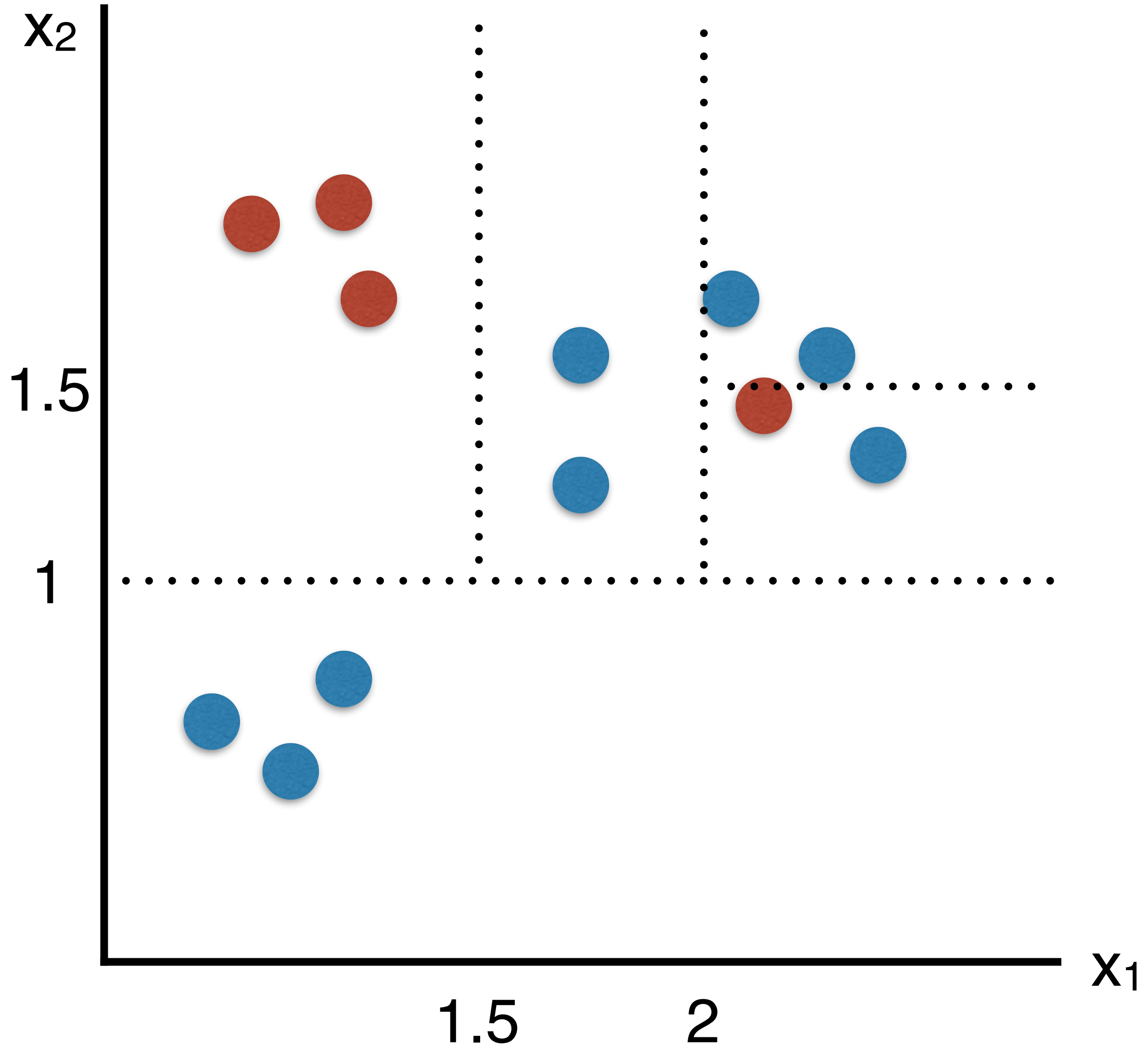

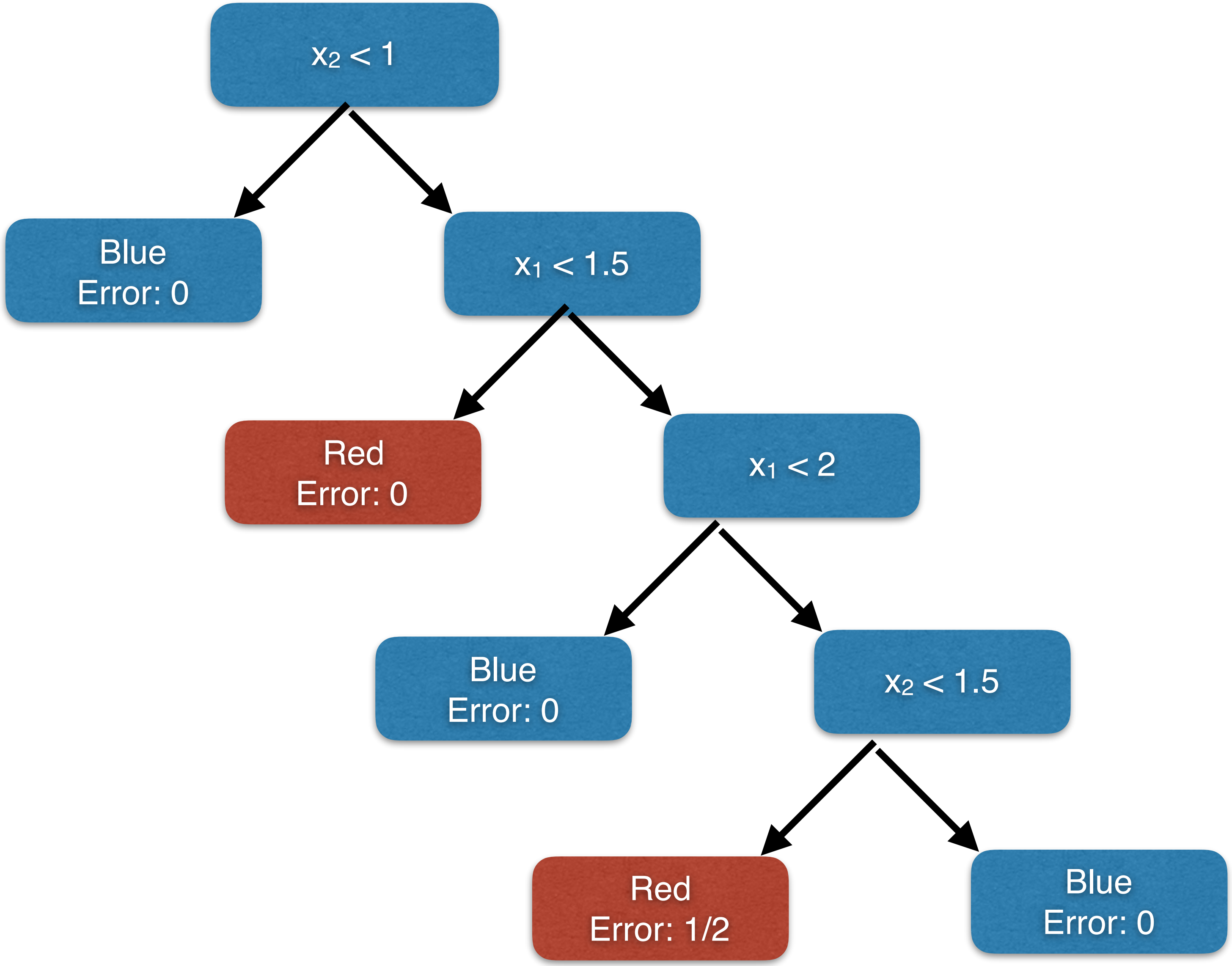

BUILDING A DECISION TREE

Okay, so we went over an example process of what the subdivision of the regions looked like. Let's formalize this more.

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

BUILDING A DECISION TREE

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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 A DECISION TREE

Consider a binary classification problem with classes Y_1, Y_2. 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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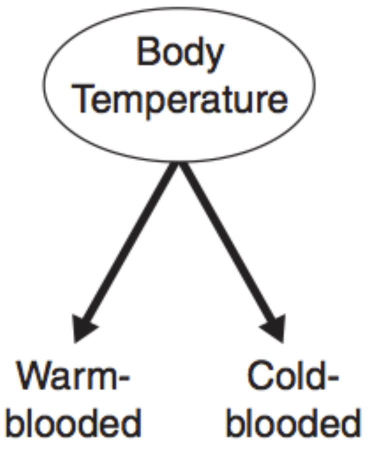
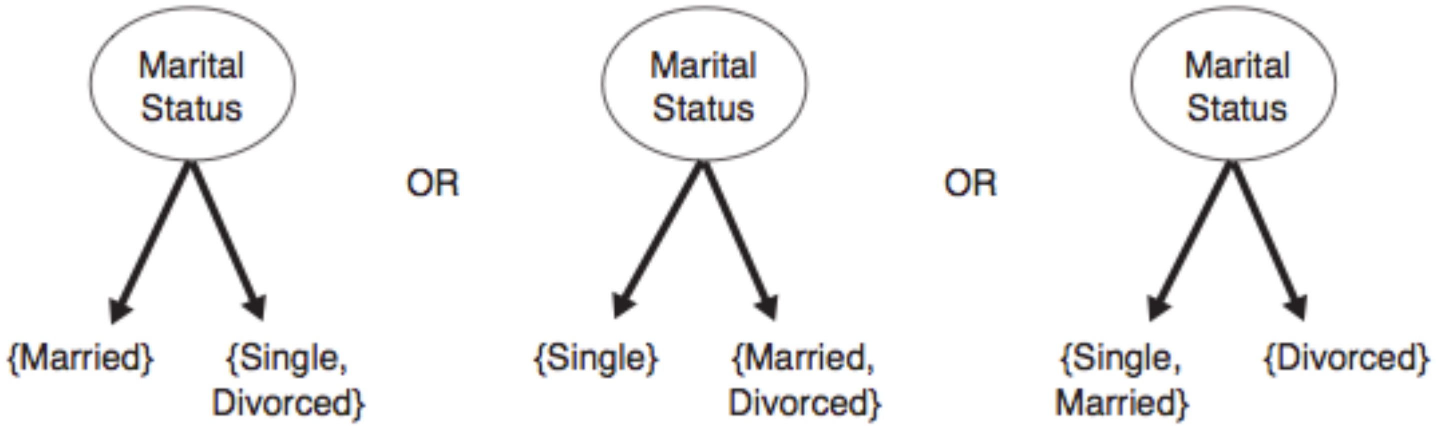


Figure 4.8. Test condition for binary attributes.



(b) Binary split {by grouping attribute values}

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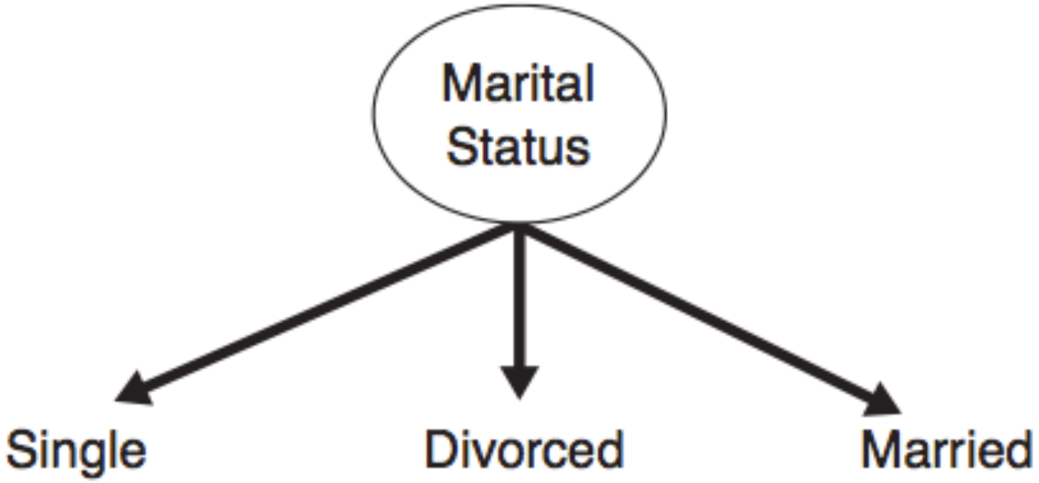
A: There are a few ways to do this.

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



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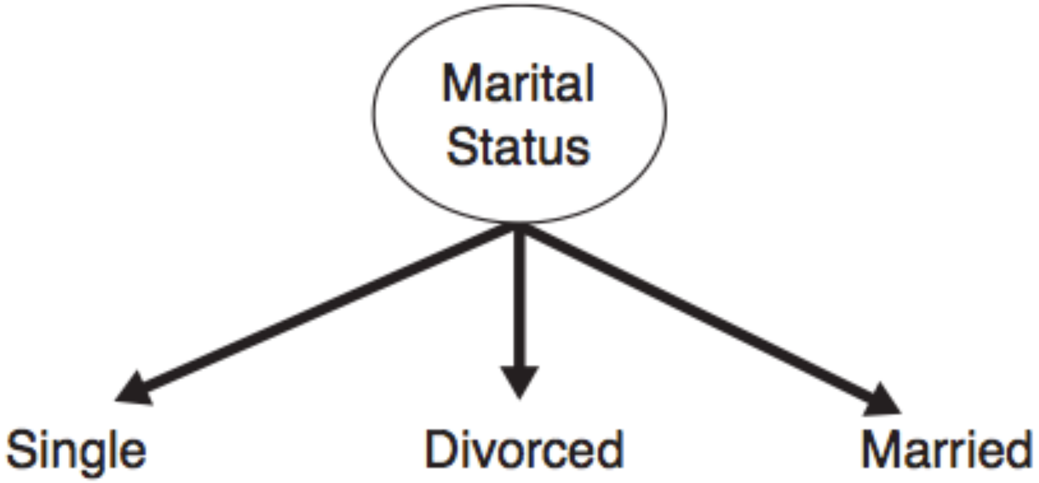

(a) Multiway split

NOTE

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

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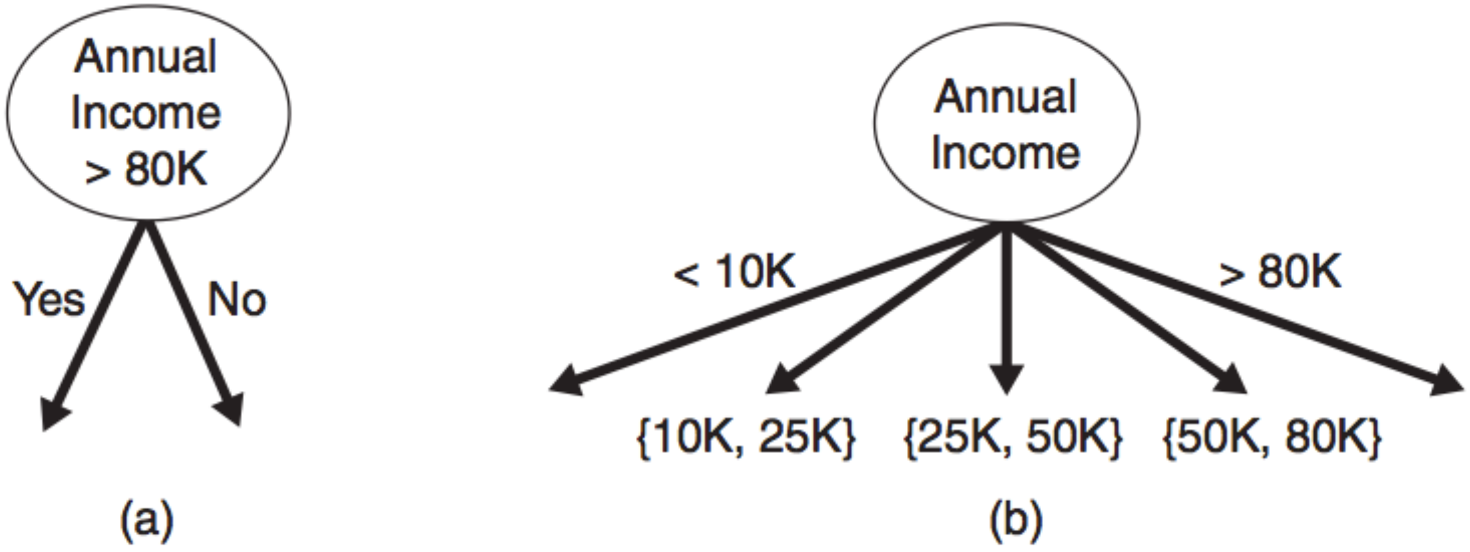
A: There are a few ways to do this.

For continuous features, we can use either method:



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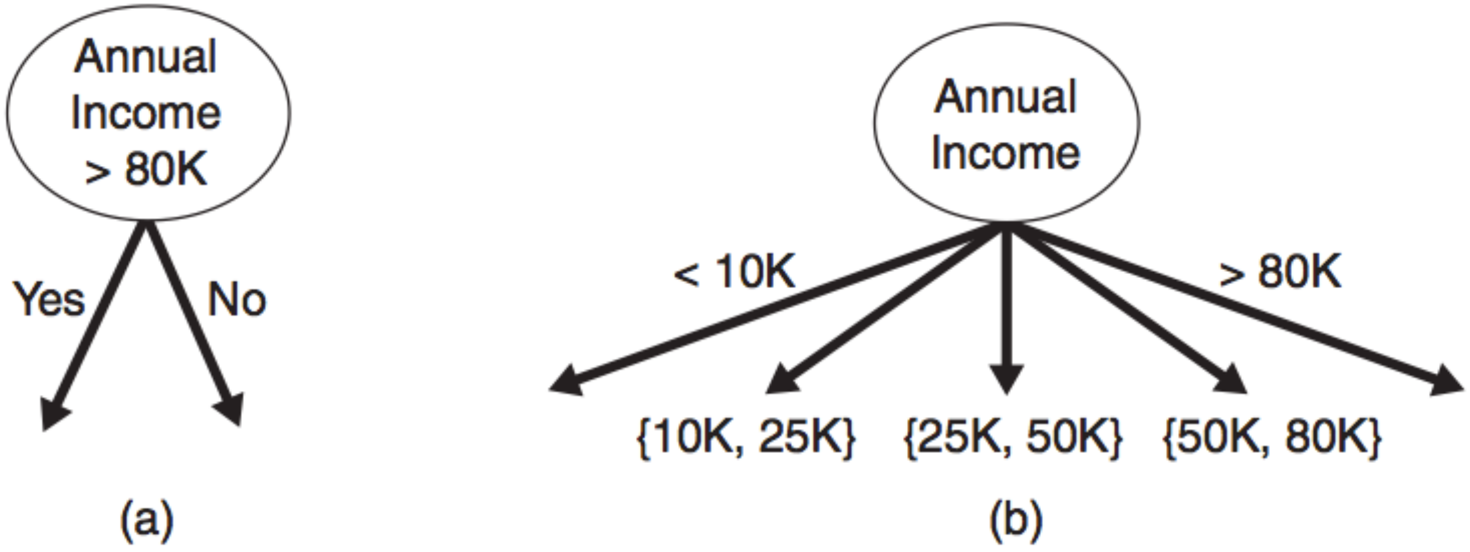

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NOTE

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. OBJECTIVE FUNCTIONS

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fraction of records labeled i at node t).

NOTE

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

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

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

OBJECTIVE FUNCTIONS

Some measures of impurity include:

$$\text{Entropy(r)} = -\sum_{c \in C} p(c \mid r) \log(c \mid r)$$

$$\text{Gini(r)} = \sum_{c \in C} p(c \mid r)(1 - p(c \mid r))$$

$$\text{ClassificationError(r)} = 1 - \max_{c}[p(c \mid r)]$$

OBJECTIVE FUNCTIONS

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

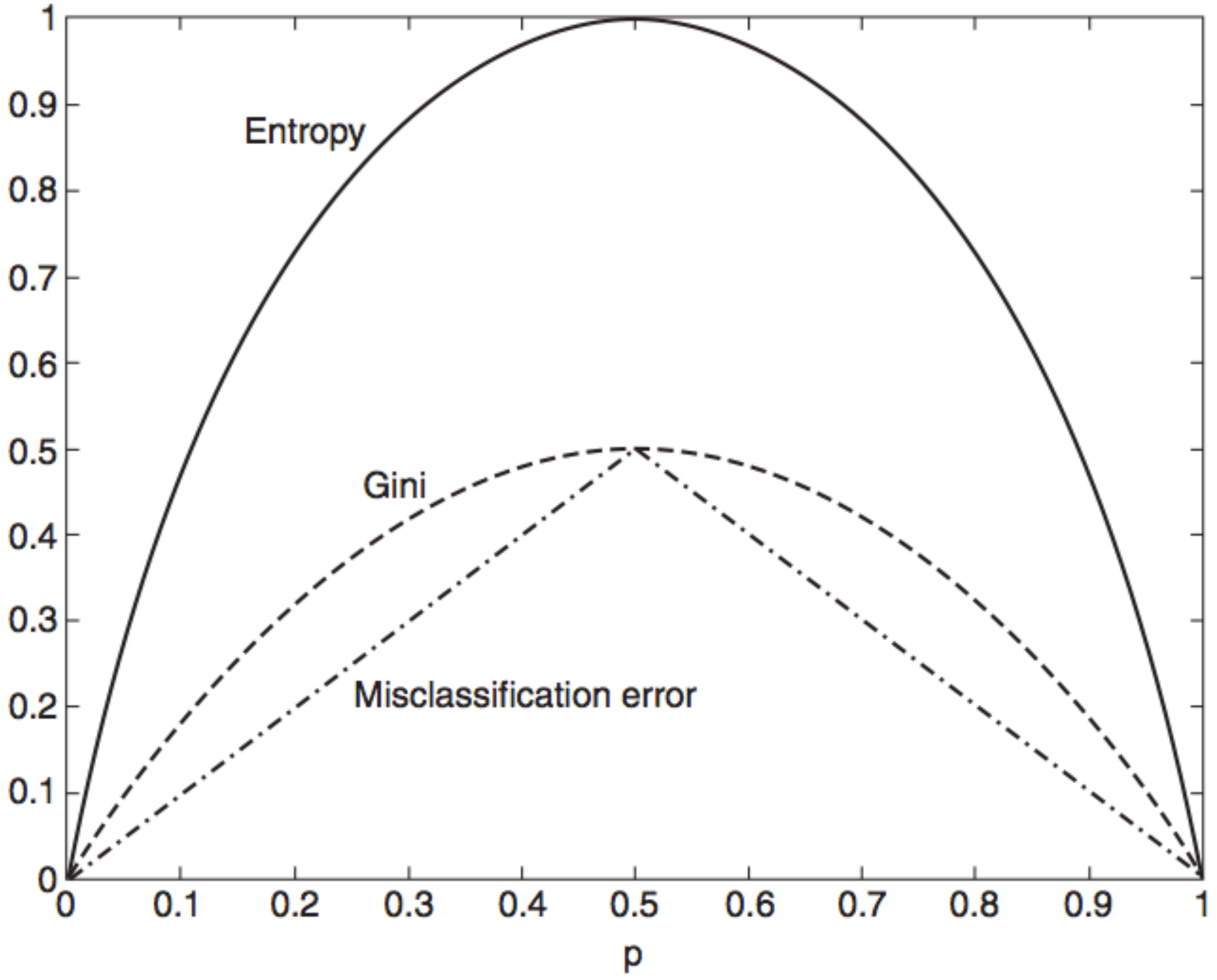

Figure 4.13. Comparison among the impurity measures for binary classification problems.

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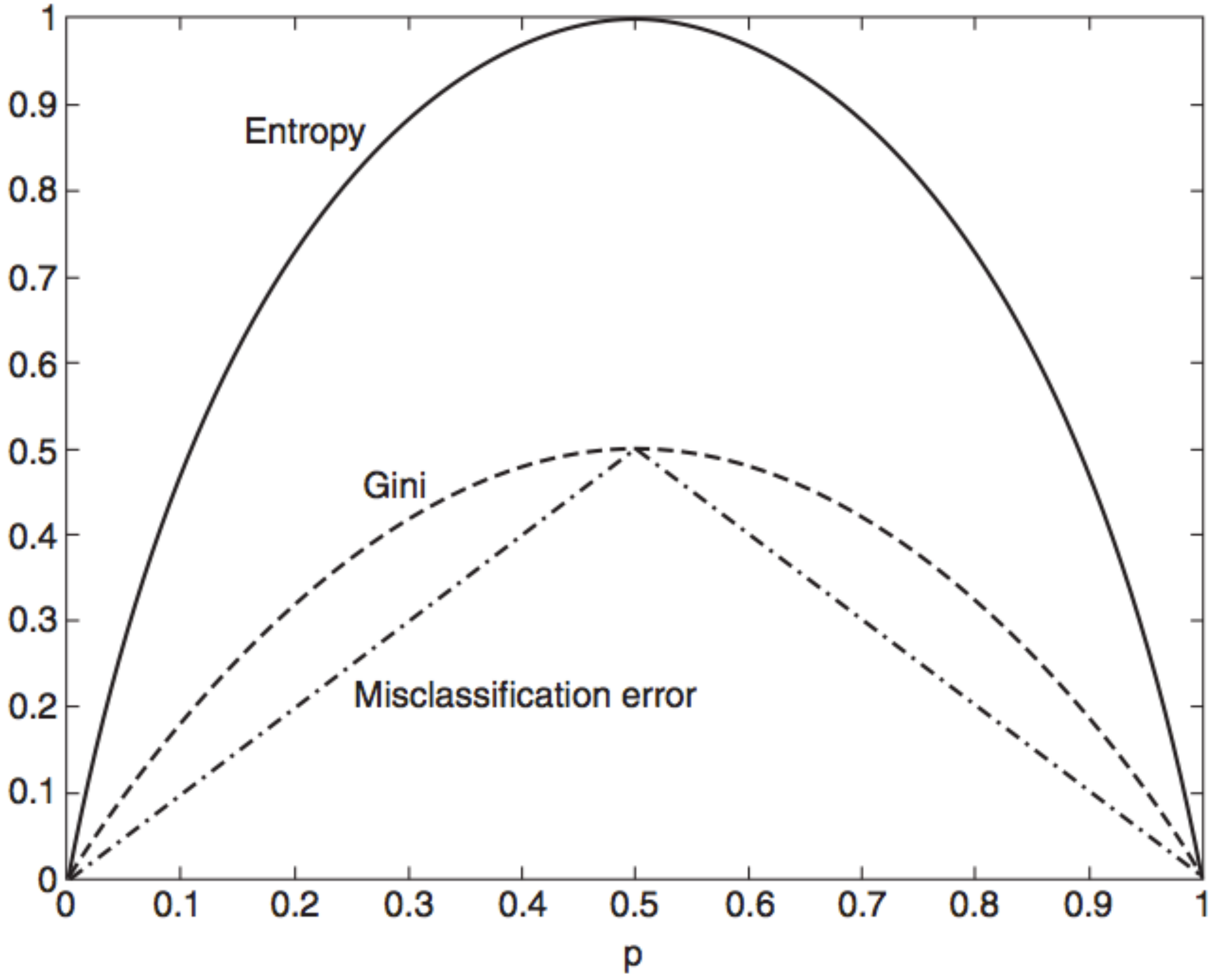
NOTE

Despite consistency, different measures may create different splits.



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Q: Why is this true?
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!

IV. REGULARIZATION

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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!)

REGULARIZATION

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**.

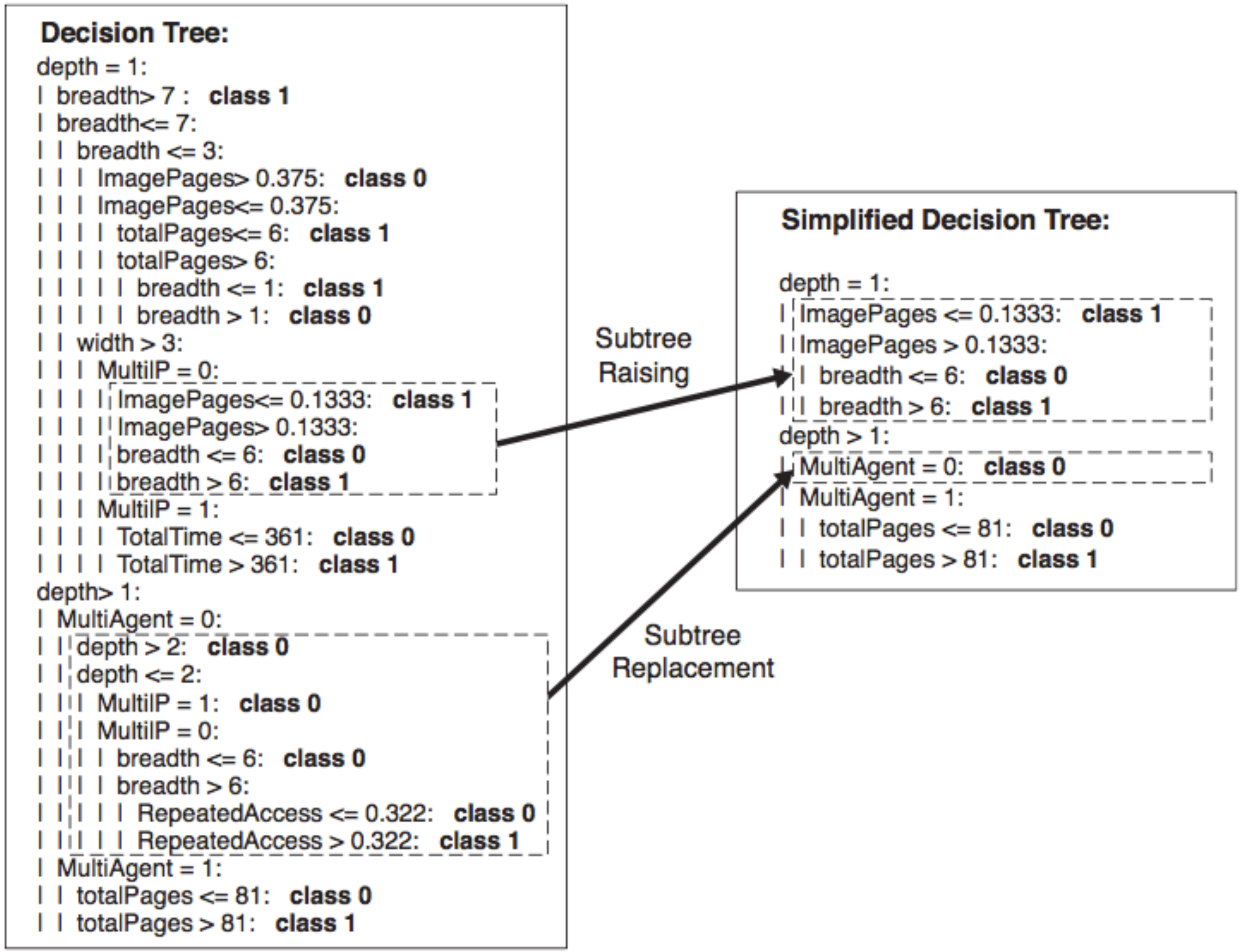


Figure 4.29. Post-pruning of the decision tree for Web robot detection.

V.PROS CONS USES

PROS AND CONS OF DECISION TREES

Pros:

- Extremely intuitive and simple to use
- Very easy to explain and visualize
- Can use any categorical or continuous variable without preprocessing!
- Can handle both numerical and categorical data and multiple classes easily

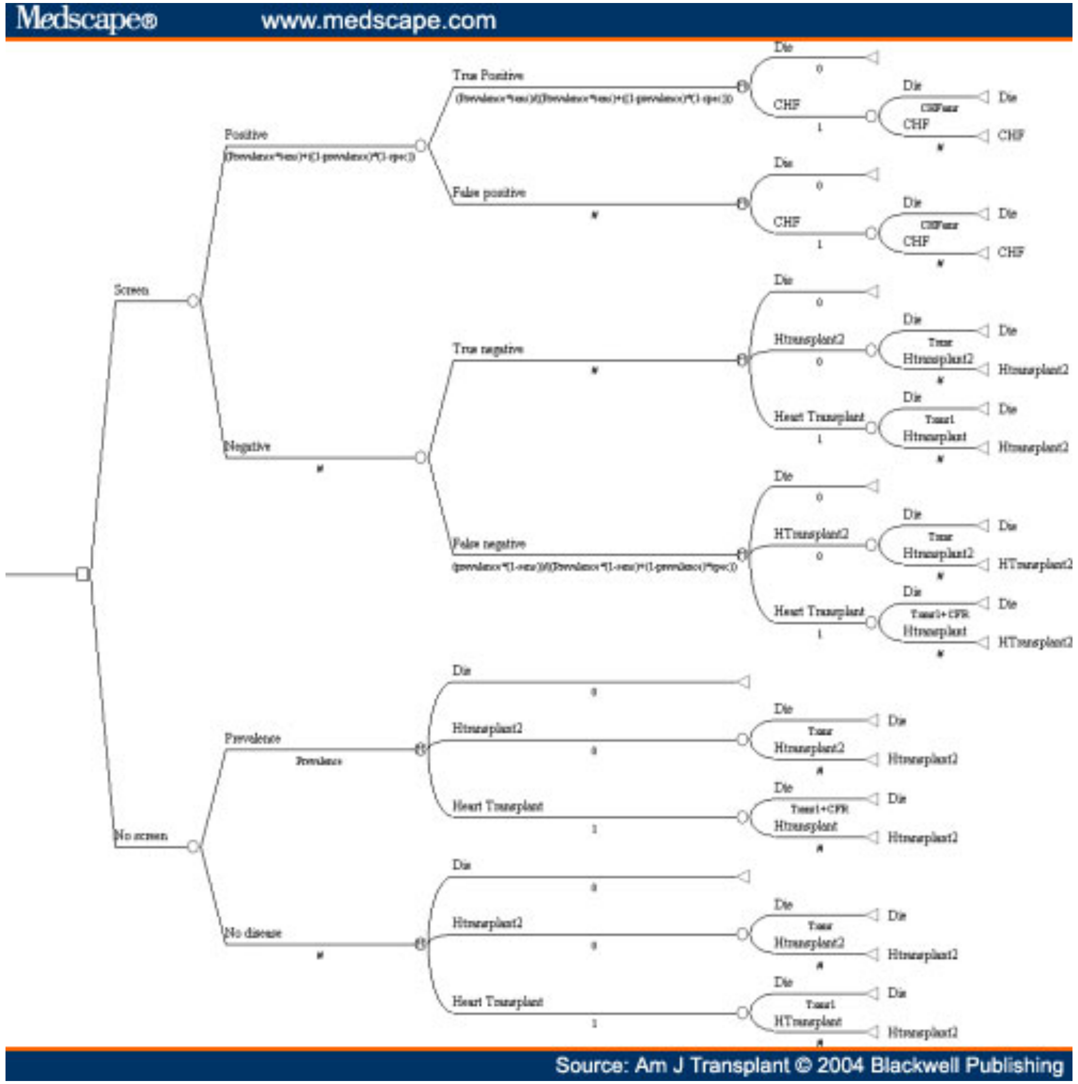
Cons:

- Prone to overfitting
- Creation of trees are unstable
- Heuristics used to create trees i.e. suboptimal
- Decision trees can create biased trees if the data is unbalanced

USES OF DECISION TREES

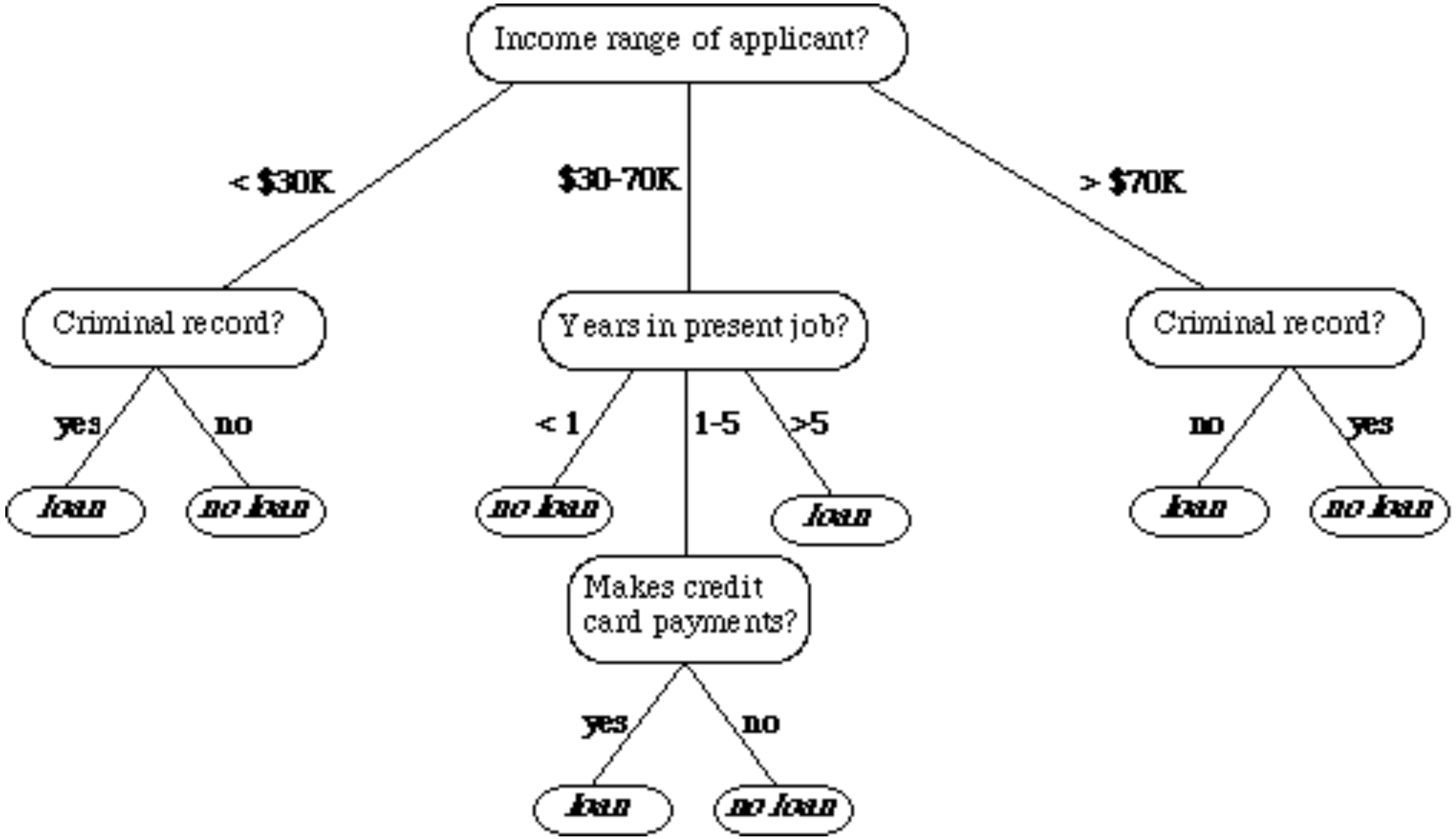
Netflix challenge

USES OF DECISION TREES



Medical diagnostics

USES OF DECISION TREES



Financial applications (i.e. intuition and explainability)

USES OF DECISION TREES

dmlc
XGBoost eXtreme Gradient Boosting

Underlying mechanism for EXTREME models

VI. DECISION TREE LAB

VII.RANDOM FORESTS

RANDOM FORESTS

A random forest is an ***ensemble*** *of decision trees where each base classifier is grown using a random effect.*

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For a small number of features, we can also create linear combinations of features and select splits from the enhanced feature set (Forest-RC)

*A random forest is an **ensemble** of decision trees where each base classifier is grown using a random effect.*

One way to do this is to choose the top feature amongst k randomly chosen features.

For a small number of features, we can also create linear combinations of features and select splits from the enhanced feature set (Forest-RC)
Or we can select splitting features completely at random (Forest-RI)

THAT'S IT!

- Exit Tickets: DAT1 - Lesson 12 - Trees
- Pretty good video series https://www.youtube.com/watch?v=p17C9q2M00Q
- Milestone 3 is due Feb 17 https://github.com/brianchandbound/ga-ds/blob/master/extra/project.md
- Peer Reviews
- Next week, we build upon trees into Ensemble methods