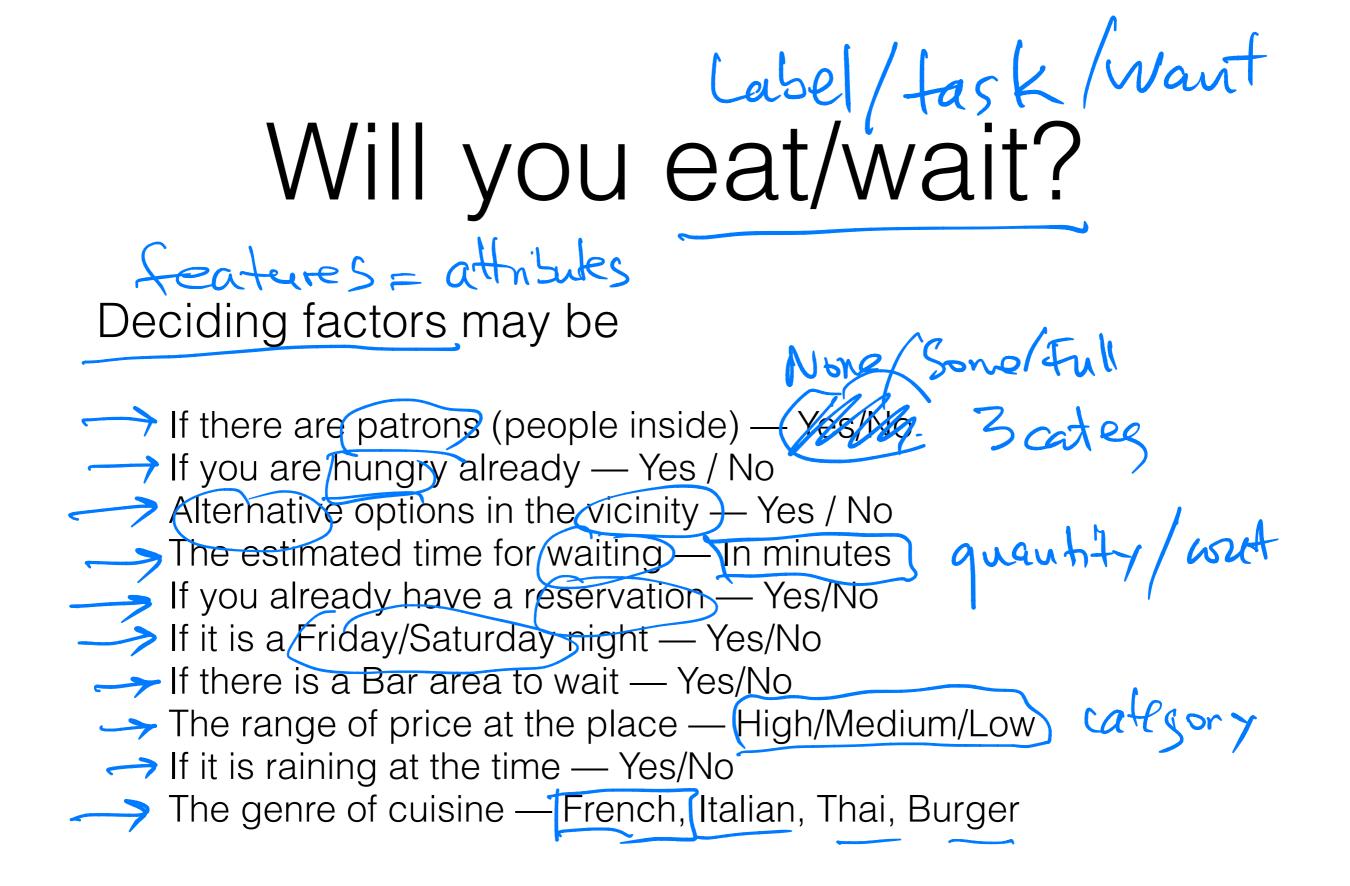
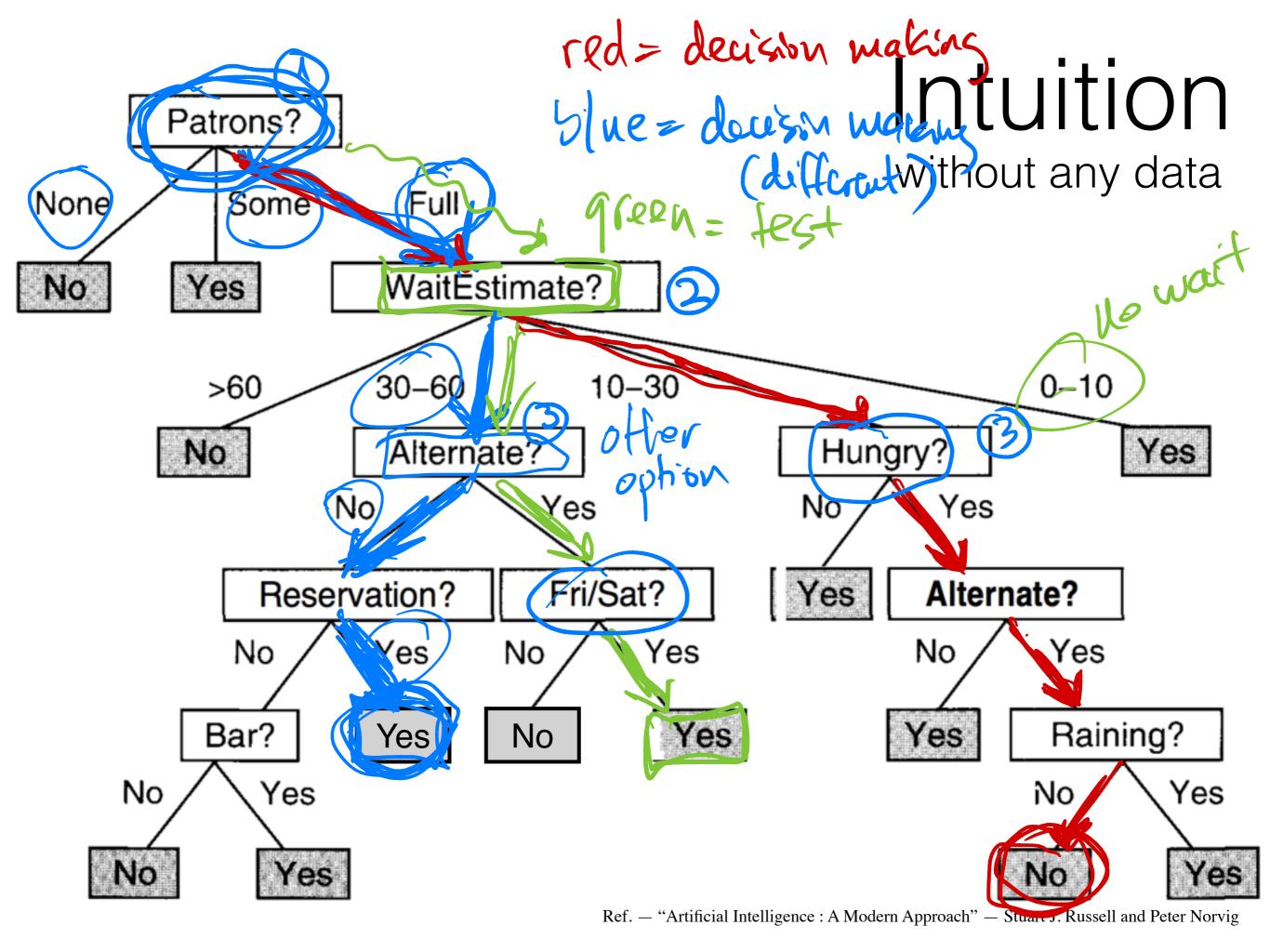
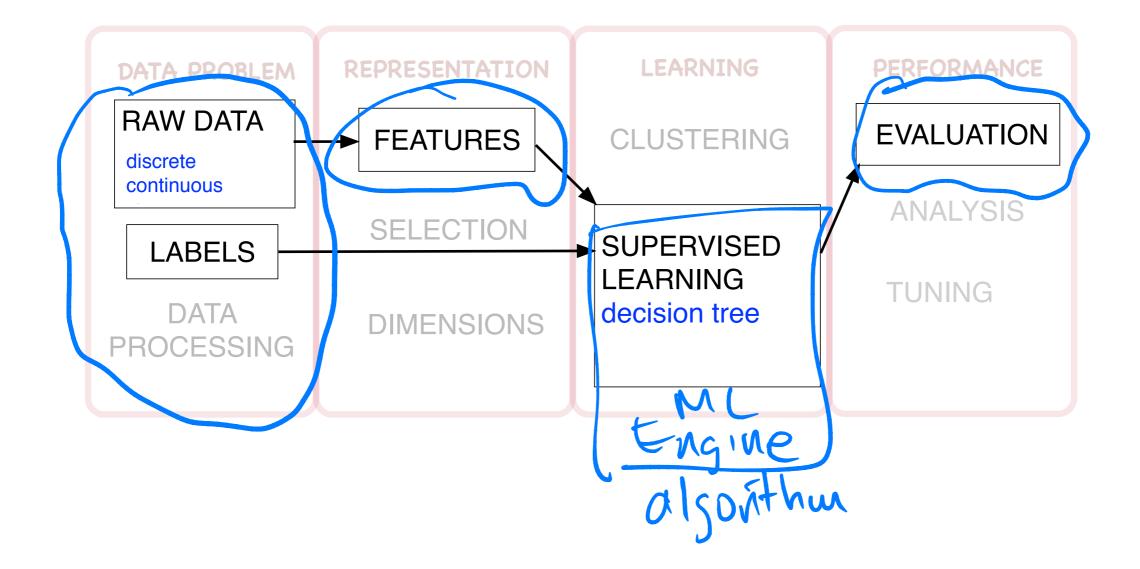


Sourav Sen Gupta CDS 2015 | PGDBA | 6 Oct 2015

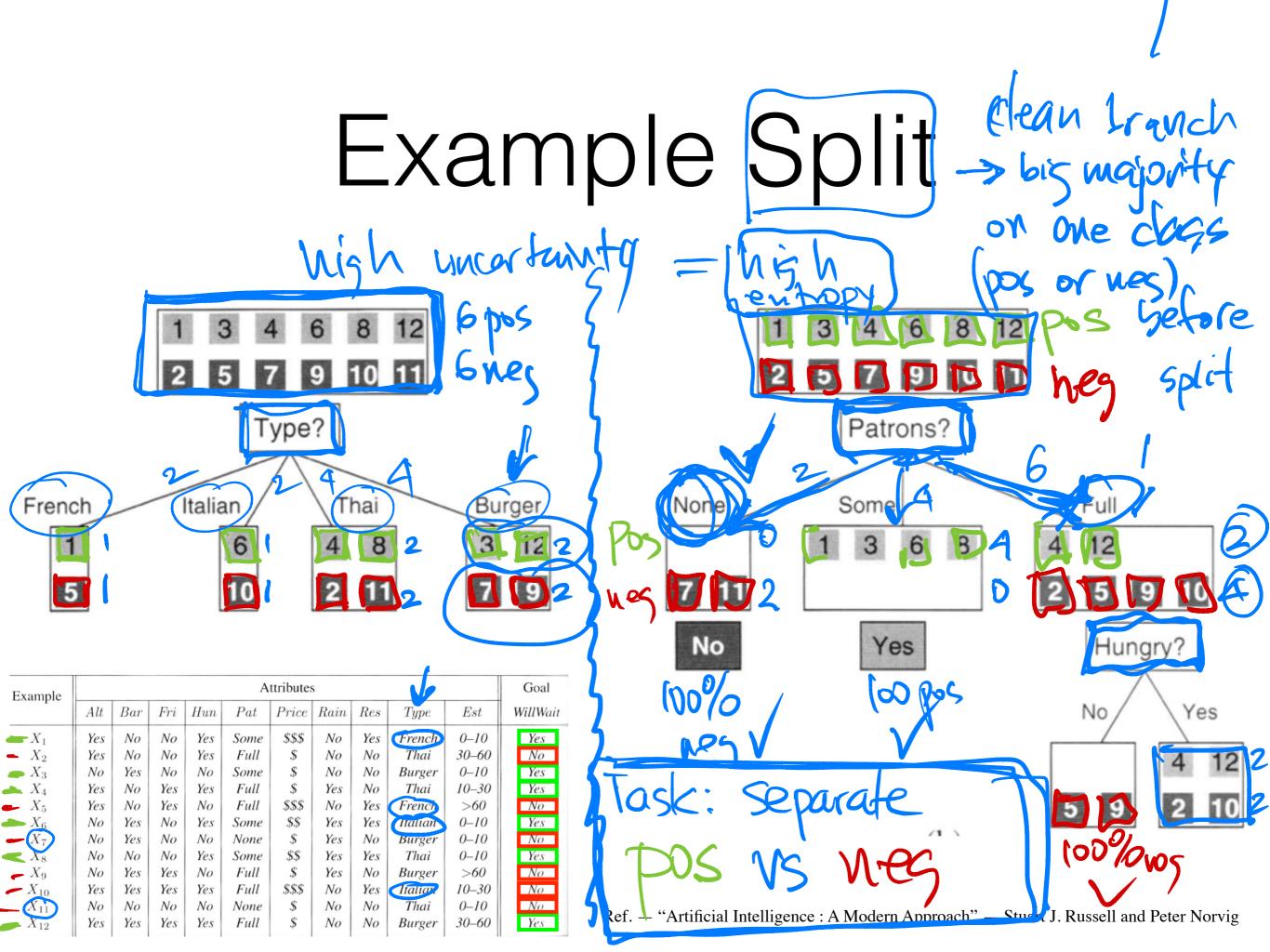


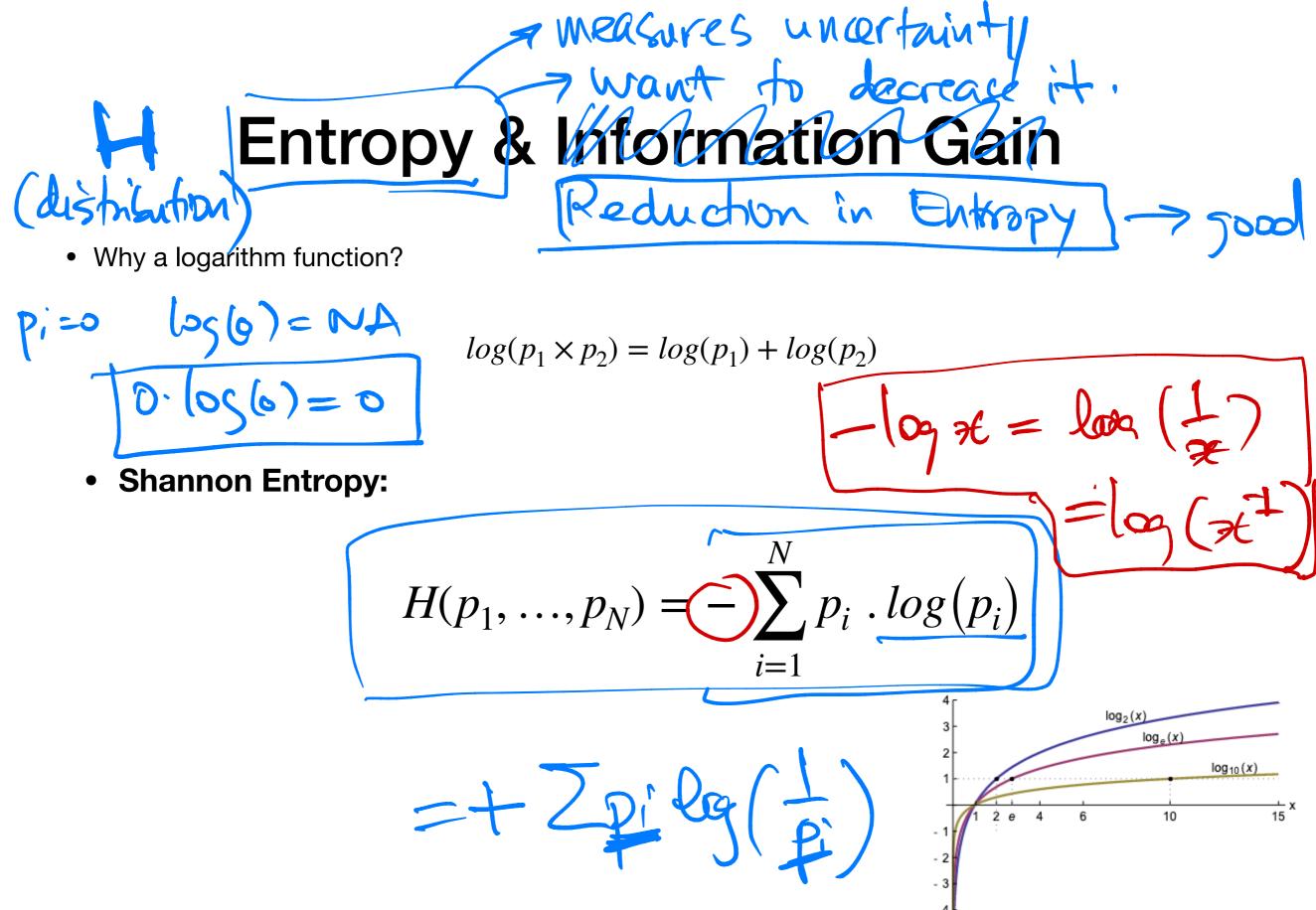


#### **ML** Pipeline



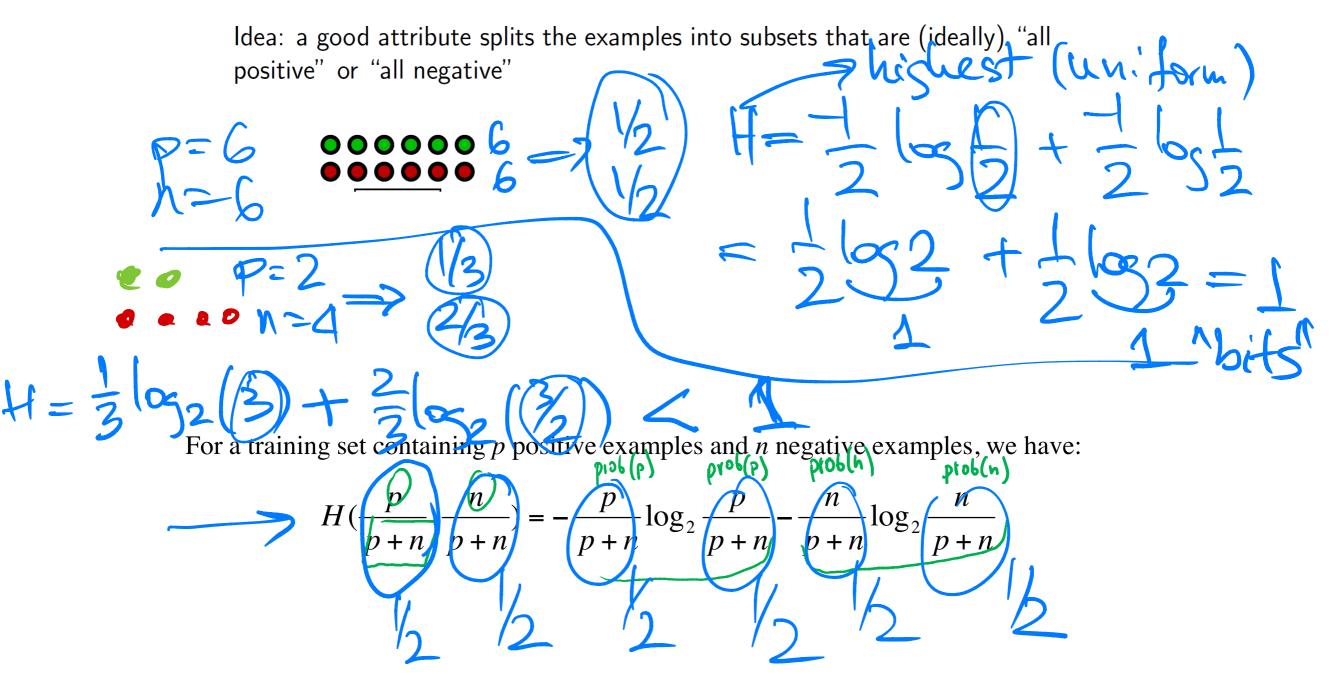
Example					A	ttributes	5			Vaft	Goal
Example	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est	WillWait
$X_1$	Yes	No	No	Yes	Some	\$\$\$	(No)	Yes	French	0-10	Yes
$X_2$	Yes	No	No	Yes	Full	\$	No	No	Thai	30–60	No
$X_3$	No	Yes	No	No	Some	\$	No	No	Burger	0–10	Yes
$X_4$	Yes	No	Yes	Yes	Full	\$	Yes	No	Thai	10-30	Yes
$X_5$	Yes	No	Yes	No	Full	\$\$\$	No	Yes	French	>60	No
$X_6$	No	Yes	No	Yes	Some	\$\$	Yes	Yes	Italian	0–10	Yes
$X_7$	No	Yes	No	No	None	\$	Yes	No	Burger	0–10	No Yes
$X_8$	No	No	No	Yes	Some	\$\$	Yes	Yes	Thai	0–10	Yes
$X_9$	No	Yes	Yes	No	Full	\$	Yes	No	Burger	>60	No
$X_{10}$	Yes	Yes	Yes	Yes	Full	\$\$\$	No	Yes	Italian	10–30	No
$X_{11}$	No	No	No	No	None	\$	No	No	Thai	0–10	No
$X_{12}$	Yes	Yes	Yes	Yes	Full	\$	No	No	Burger	30–60	Yes
TEST	Yes	Yes	Yes	No	Full	\$\$\$	No	No	Thai	30-60	pleal)

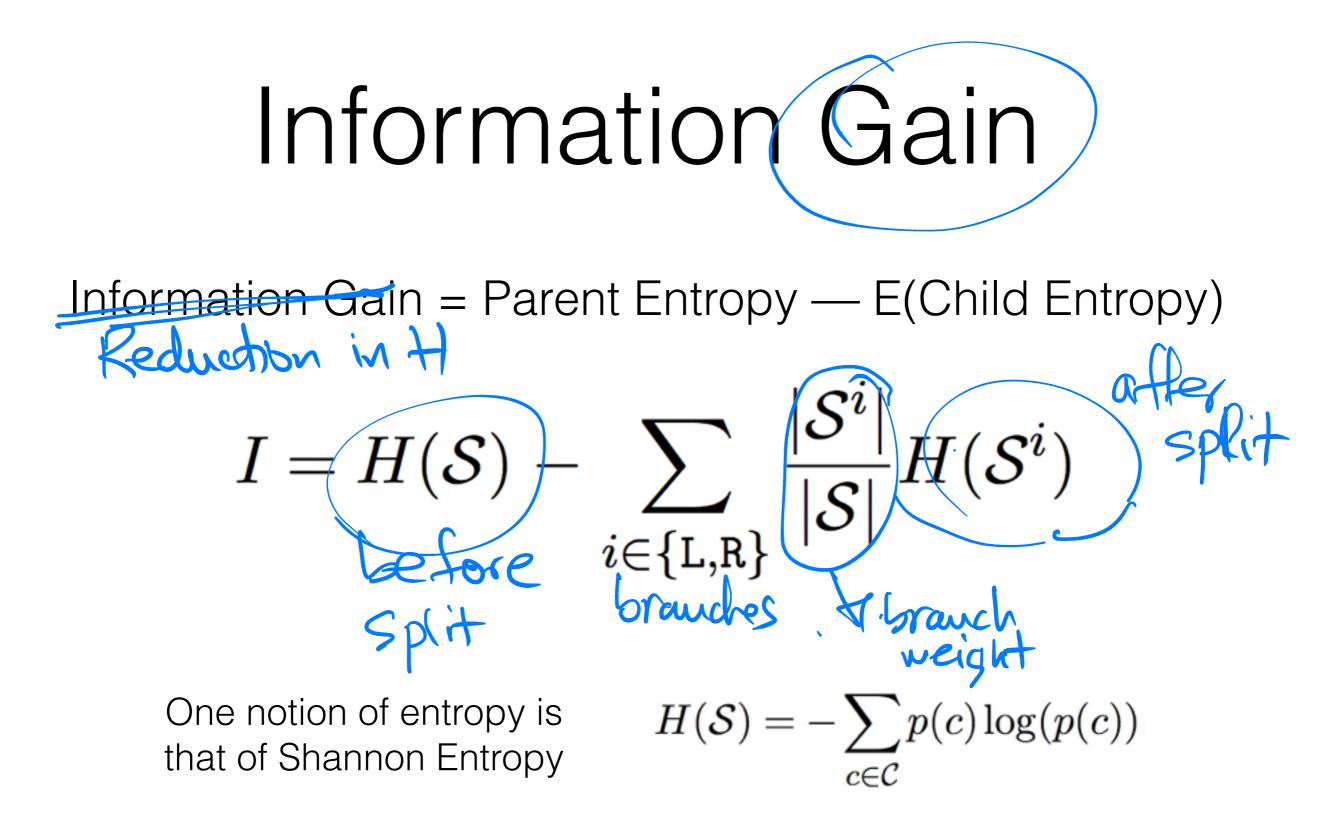


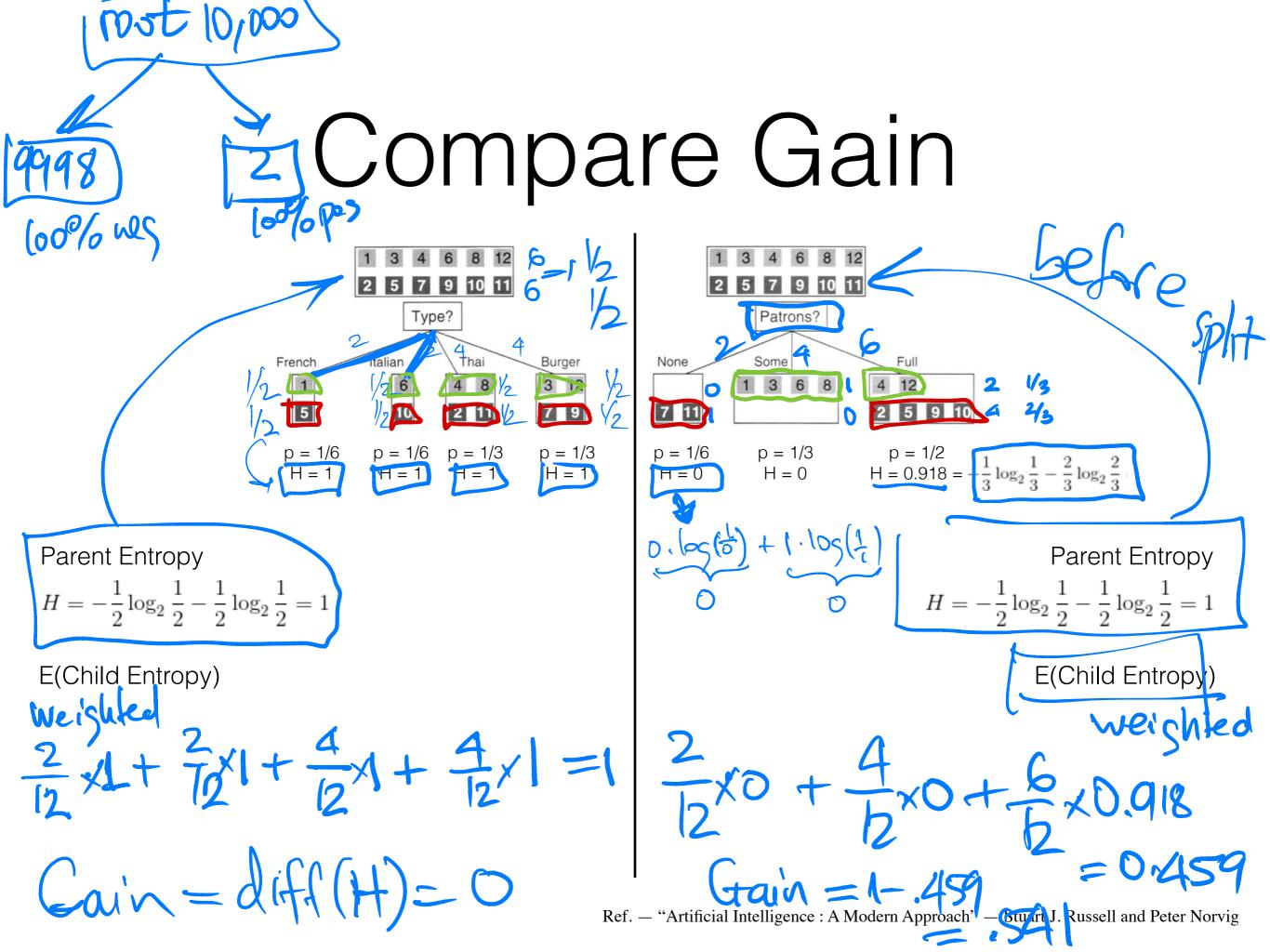


**Issue:** increasing number of events shrinks the probability. **Solution:** use **Iogarithm of probability** instead and take **the average**.

# How do we construct the tree ? i.e., how to pick attribute (nodes)?







## How to pick nodes?

- □ A chosen attribute *A*, with *K* distinct values, divides the training set *E* into subsets  $E_1, \ldots, E_K$ .
- The Expected Entropy (EH) remaining after trying attribute A (with branches i=1,2,...,K) is points in child i

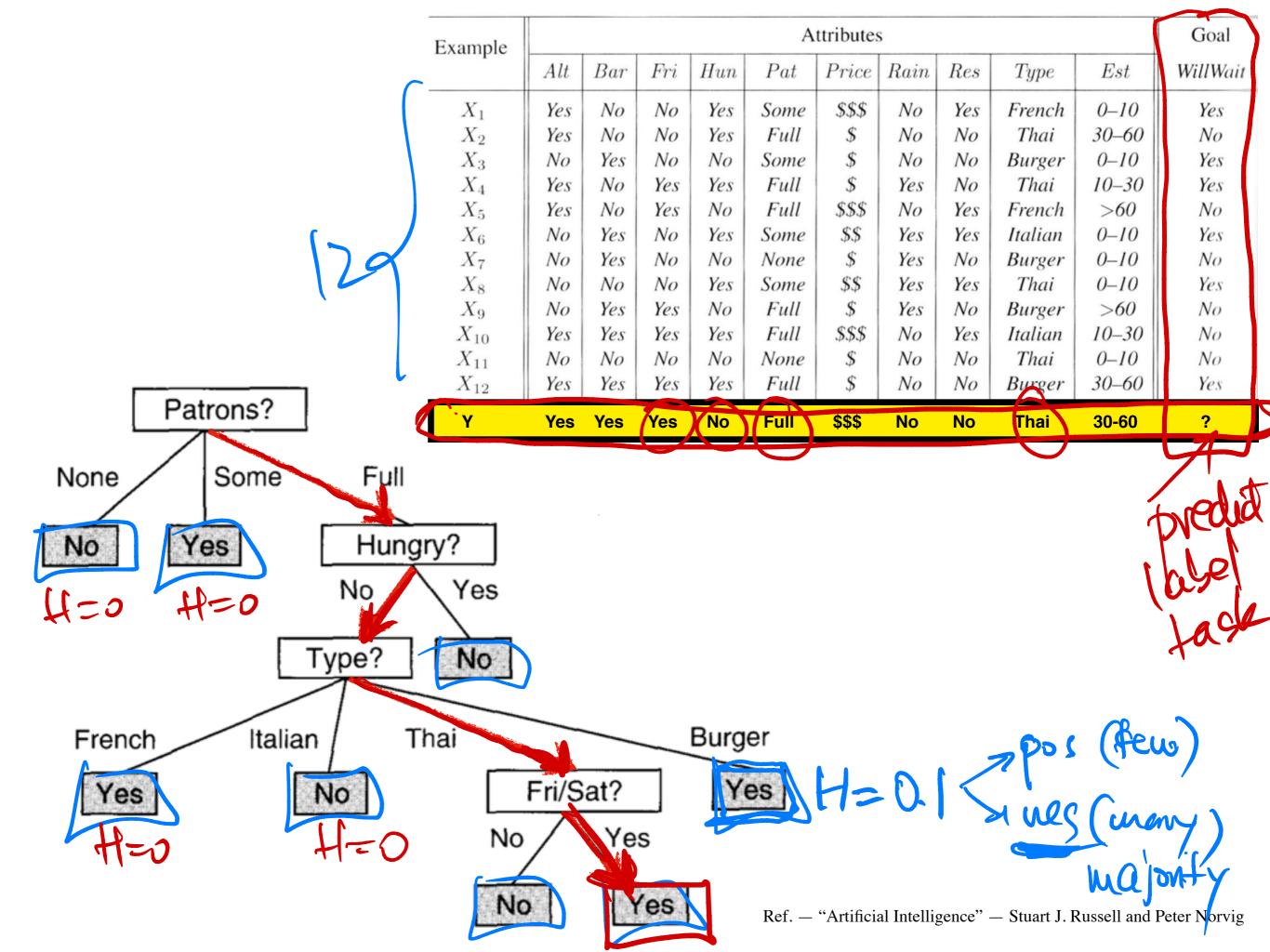
$$EH(A) = \sum_{i=1}^{K} \underbrace{\frac{p_i + n_i}{p_i + n_i}}_{p_i + n_i} H(\underbrace{\frac{p_i}{p_i + n_i}}_{p_i + n_i}, \frac{n_i}{p_i + n_i})$$

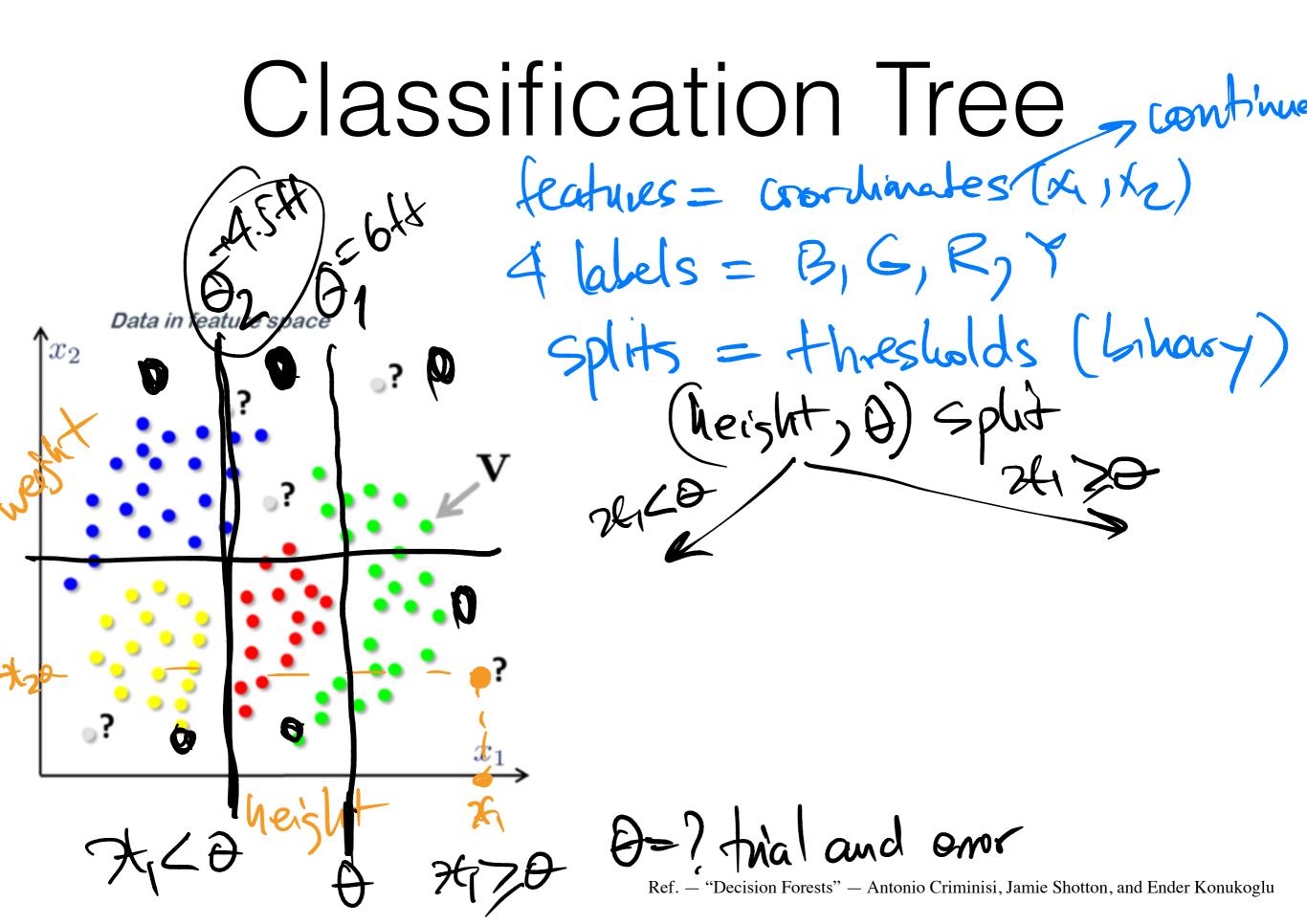
□ Information gain (I) or reduction in entropy for this attribute is:

$$I(A) = H(\frac{p}{p+n}, \frac{n}{p+n}) \cdot EH(A)$$
  
= Entropy in the parent node - remaining Expected Entropy in the child nodes

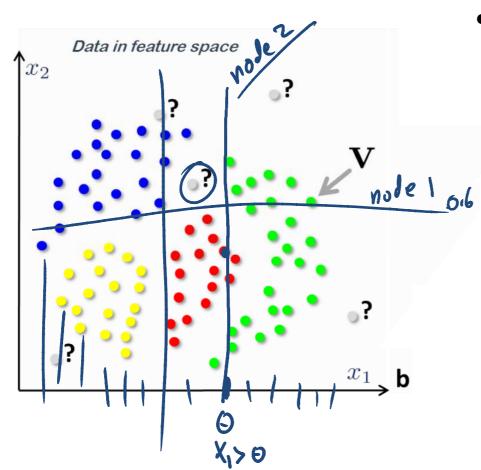
[Hwee Tou Ng & Stuart Russell]

F	Example					A	ttributes					Goal
	minple	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est	WillWait
	$X_1$	Yes	No	No	Yes	Some	\$\$\$	No	Yes	French	0–10	Yes
	$X_2$	Yes	No	No	Yes		\$	No	No	Thai	30-60	No
	$X_3$	No	Yes	No	No	Some	\$	No	No	Burger	0–10	Yes
	$X_4$	Yes	No	Yes	Yes	Full	\$	Yes	No	Thai	10-30	Yes
	$X_5$	Yes	No	Yes	No	Füll	\$\$\$	No	Yes	French	>60	No
	$X_6$	No	Yes	No	Yes	Some	\$\$	Yes	Yes	Italian	0–10	Yes
	$X_7$	No	Yes	No	No	None	\$	Yes	No	Burger	0–10	No
	$X_8$	No	No	No	Yes	Some	\$\$	Yes	Yes	Thai	0–10	Yes
	$X_9$	No	Yes	Yes	No	Full	\$	Yes	No	Burger	>60	No
	$X_{10}$	Yes	Yes	Yes	Yes	Full	\$\$\$	No	Yes	Italian	10–30	No
	$X_{11}$	No	No	No	No	None	\$	No	No	Thai	0–10	No
Patrons?	$X_{12}$	Yes	Yes	Yes	Yes	Full	\$	No	No	Burger	30–60	Yes
None Some Full No Yes Hungry No Type?	Yes	9 (1	0		7	f (	he IG	U Le For	sp st du	lifts (hig chan	) pla host in e fdo	ck uhopy) da
French Italian Tha	ai				Burg	er	(	4	) <sup>[2</sup>			
Yes		Fri/S	at?		Y	es		. 2	5,	9,10	1	
	No	$\wedge$	Ye	S			ov		of a	r ch	"Fi	ull
	No	)	Ì	'es		Ref. —	"Artificia	al Intellig	gence" -	— Stuart J. F	Russell and I	Peter Norvig



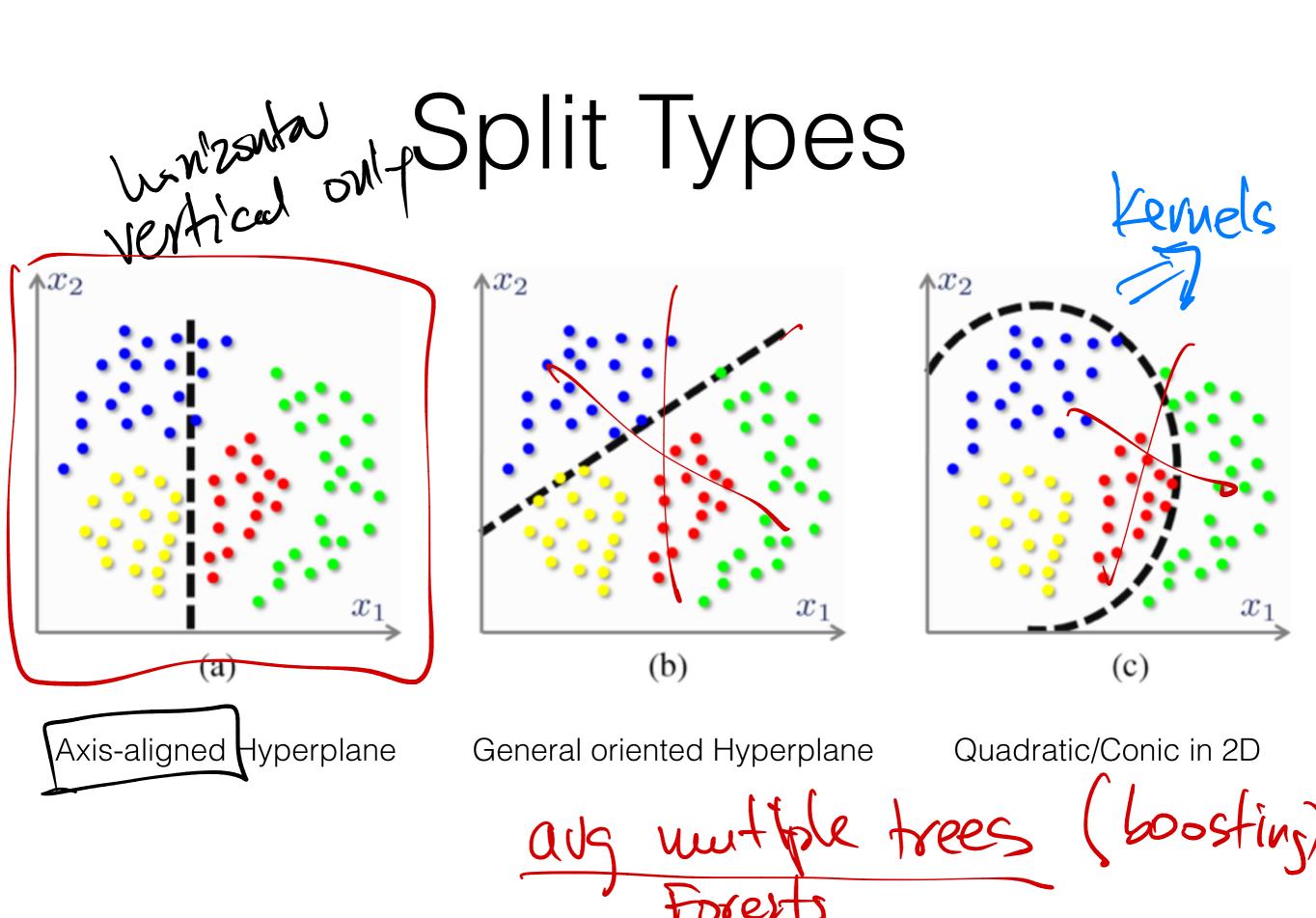


#### Classification tree



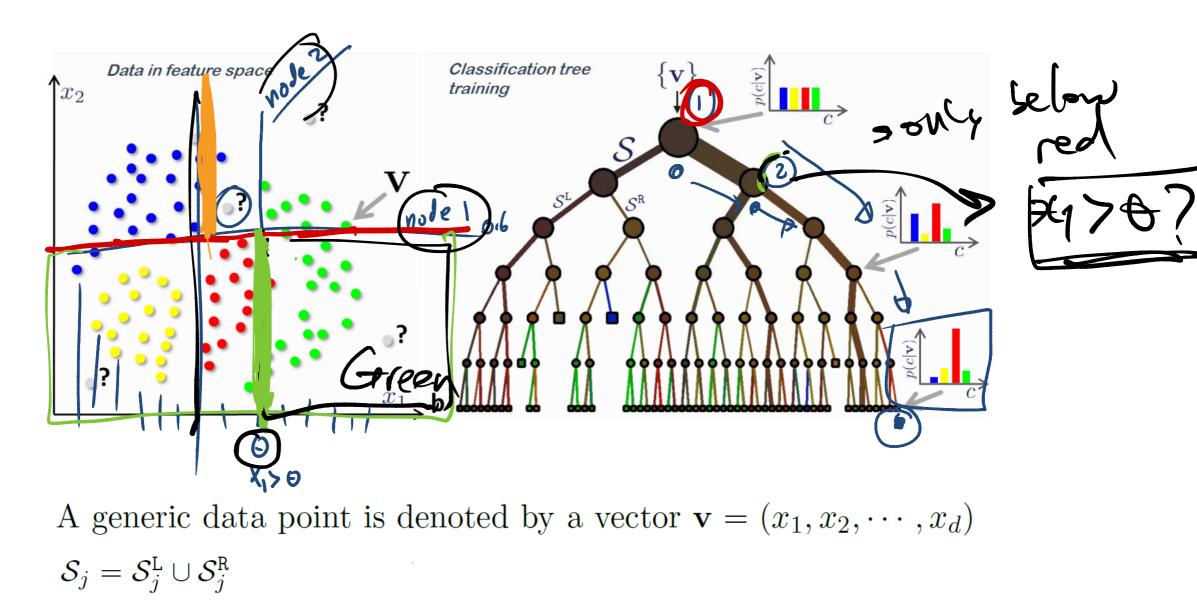
- How to deal with *continuous features*?
  - Create the splits **randomly**
  - Compute information gain for each split
  - Choose the one with **maximum gain**

A generic data point is denoted by a vector  $\mathbf{v} = (x_1, x_2, \cdots, x_d)$ 



- "Decision Forests" — Antonio Criminisi, Jamie Shotton, and Ender Konukoglu

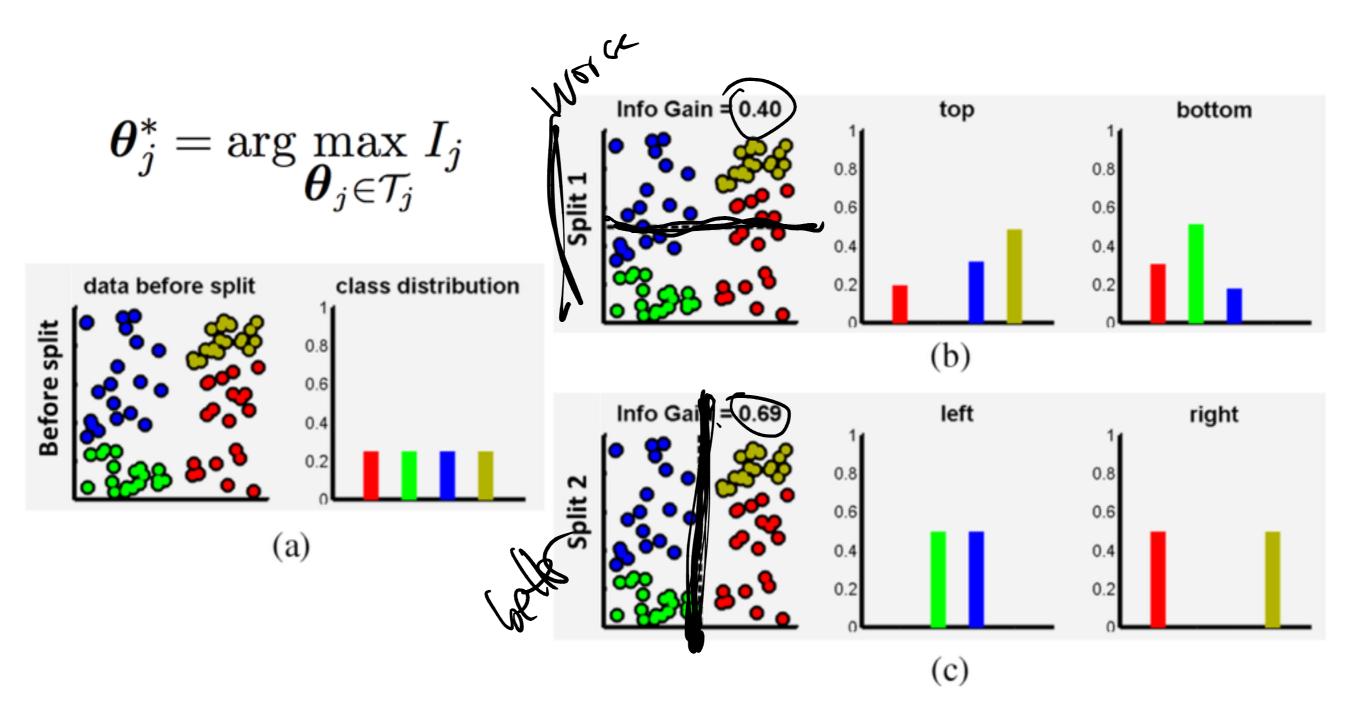
#### Classification tree



Note that the histogram shows the posterior distribution for each class:

p(Class | Data)

# Choosing Split



#### **Expressiveness of decision trees**

The tree on previous slide is a Boolean decision tree:

- ✓ the decision is a binary variable (true, false), and
- ✓ the attributes are discrete.
- ✓ It returns ally iff the input attributes satisfy one of the paths leading to an ally leaf:

 $ally \Leftrightarrow (neck = tie \land smile = yes) \lor (neck = \neg tie \land body = triangle),$ 

i.e. in general

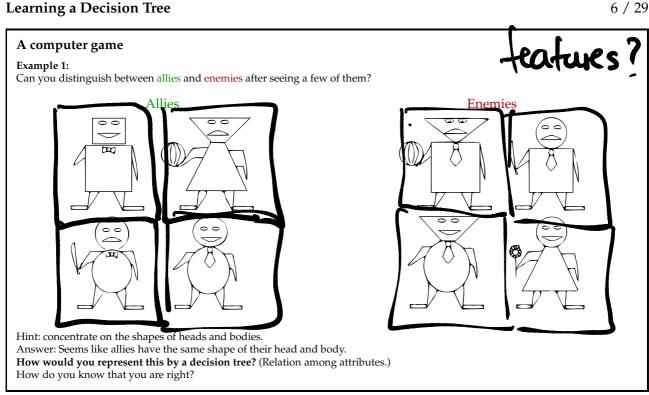
- ★ Goal  $\Leftrightarrow$  (*Path*<sub>1</sub>  $\lor$  *Path*<sub>2</sub>  $\lor$  ...), where
- **★** *Path* is a conjuction of attribute-value tests, i.e.
- ★ the tree is equivalent to a DNF of a function.

Any function in propositional logic can be expressed as a dec. tree.

- ✓ Trees are a suitable representation for some functions and unsuitable for others.
- ✓ What is the cardinality of the set of Boolean functions of *n* attributes?
  - **x** It is equal to the number of truth tables that can be created with *n* attributes.
  - **x** The truth table has  $2^n$  rows, i.e. there is  $2^{2^n}$  different functions.
  - **x** The set of trees is even larger; several trees represent the same function.
- ✔ We need a clever algorithm to find good hypotheses (trees) in such a large space.

P. Pošík © 2013

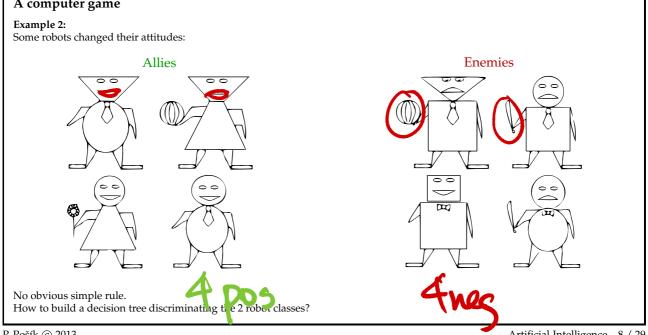
Artificial Intelligence - 5 / 29



P. Pošík © 2013

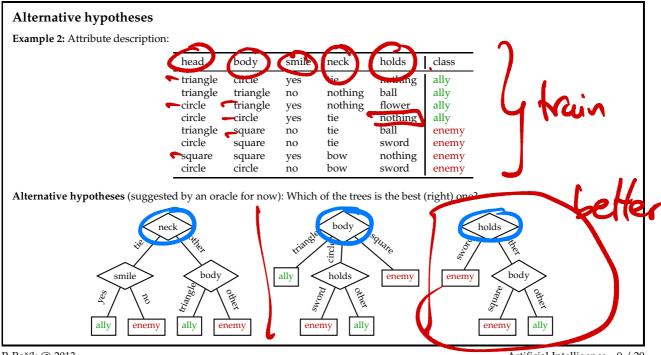
Artificial Intelligence - 7 / 29

#### A computer game



P. Pošík © 2013

Artificial Intelligence - 8 / 29



P. Pošík © 2013

Artificial Intelligence – 9 / 29

How to choose the best tree?				
We want a tree that is				
✓ consistent with the data,				
✓ is as small as possible, and				
✓ which also works for new data.				
Consistent with data?				
✓ All 3 trees are consistent.				
Small?				
		left	middle	right
✓ The right-hand side one is the simplest one:	depth	2	2	2
0	leaves	4	4	3
	conditions	3	2	2

P. Pošík © 2013

Artificial Intelligence - 10 / 29

#### Learning a Decision Tree

It is an intractable problem to find **the smallest consistent tree** among  $> 2^{2^n}$  trees. We can find approximate solution: **a small (but not the smallest) consistent tree**.

#### **Top-Down Induction of Decision Trees** (TDIDT):

- ✓ A greedy divide-and-conquer strategy.
- ✔ Progress:
  - 1. Test the most important attribute.
  - 2. Divide the data set using the attribute values.
  - 3. For each subset, build an independent tree (recursion).
- ✔ "Most important attribute": attribute that makes the most difference to the classification.
- ✓ All paths in the tree will be short, the tree will be shallow.

P. Pošík © 2013

Artificial Intelligence - 11 / 29

Attribute	e imp	ortance								
head		body		smile		neck		holds		class
triangle triangle circle circle triangle circle square circle		circle triangle triangle circle square square square circle		yes no yes yes no no yes no		tie nothing nothing tie tie tie bow bow		nothing ball flower nothing ball sword nothing sword		ally ally ally enemy enemy enemy enemy
triangle: circle: square:	2:1 2:2 0:1	triangle: circle: square:	2:0 2:1 0:3	yes: no:	3:1 1:3	tie: bow: nothing:	2:2 0:2 2:0	ball: sword: flower: nothing:	1:1 0:2 1:0 2:1	

A perfect attribute divides the examples into sets each of which contain only a single class. (Do you remember the simply created perfect attribute from Example 1?)

A useless attribute divides the examples into sets each of which contains the same distribution of classes as the set before splitting.

None of the above attributes is perfect or useless. Some are more useful than others.

P. Pošík © 2013

Artificial Intelligence - 12 / 29

#### Choosing the test attribute

Information gain:

- ✔ Formalization of the terms "useless", "perfect", "more useful".
- ✓ Based on entropy, a measure of the uncertainty of a random variable *V* with possible values  $v_i$ :

 $H(V) = -\sum_{i} p(v_i) \log_2 p(v_i)$ 

✓ Entropy of the target class *C* measured on a data set *S* (a finite-sample estimate of the true entropy):

$$H(C,S) = -\sum_{i} p(c_i) \log_2 p(c_i),$$

where  $p(c_i) = \frac{N_S(c_i)}{|S|}$ , and  $N_S(c_i)$  is the number of examples in *S* that belong to class  $c_i$ .

✓ The entropy of the target class *C* remaining in the data set *S* after splitting into subsets  $S_k$  using values of attribute *A* (weighted average of the entropies in individual subsets):

$$H(C, S, A) = \sum_{k} p(S_k) H(C, S_k), \quad \text{where } p(S_k) = \frac{|S_k|}{|S|}$$

✓ The information gain of attribute A for a data set S is

$$Gain(A,S) = H(C,S) - H(C,S,A).$$

Choose the attribute with the highest information gain, i.e. the attribute with the lowest H(C, S, A).

P. Pošík © 2013

Artificial Intelligence - 13 / 29

#### Choosing the test attribute (special case: binary classification)

 $\checkmark$  For a Boolean random variable *V* which is true with probability *q*, we can define:

$$H_B(q) = -q \log_2 q - (1-q) \log_2 (1-q)$$

• Entropy of the target class *C* measured on a data set *S* with  $N_p$  positive and  $N_n$  negative examples:

$$H(C,S) = H_B\left(\frac{N_p}{N_p + N_n}\right) = H_B\left(\frac{N_p}{|S|}\right)$$

P. Pošík © 2013

Artificial Intelligence - 14 / 29

Choosing the test at	tribute (	exam	ple)							
	head		body		smile		neck		holds	
	triangle: circle: square:	2:1 2:2 0:1	triangle: circle: square:	2:0 2:1 0:3	yes: no:	3:1 1:3	tie: bow: nothing:	2:2 0:2 2:0	ball: sword: flower: nothing:	1:1 0:2 1:0 2:1
<b>head:</b> Profilead=tri) = $\frac{3}{8}$ ; $H(C, S_{head=tr})$ $p(S_{head=cr}) = \frac{4}{8}$ ; $H(C, S_{head=tr})$ $p(S_{head=sq}) = \frac{1}{8}$ ; $H(C, S_{head=sc})$ $H(C, S, head) = \frac{3}{8} \cdot 0.92 + \frac{4}{8} \cdot C_{ain}(head, S) = 1 - 0.84 = 0.5$ <b>body</b> $p(S_{body=tri}) = \frac{2}{8}$ ; $H(C, S_{body=tr})$ $p(S_{body=cr}) = \frac{3}{8}$ ; $H(C, S_{body=tr})$ $p(S_{body=sq}) = \frac{3}{8}$ ; $H(C, S_{body=sr})$ $H(C, S, body) = \frac{2}{8} \cdot 0 + \frac{3}{8} \cdot 0.5$ Gain(body, S) = 1 - 0.35 = 0 <b>smile:</b> $p(S_{smile=yes}) = \frac{4}{8}$ ; $H(C, S_{yes}) = p(S_{smile=yes}) = \frac{4}{8}$ ; $H(C, S_{no}) = H(C, S, smile) = \frac{4}{8} \cdot 0.81 + \frac{4}{8}$ Gain(smile, S) = 1 - 0.81 = 0	$ \begin{aligned} H_{r} &= H_{B} \left( \frac{2}{2} + \frac{1}{2} + 1$	$ \begin{array}{l} \begin{array}{l} \hline 2 \\ \hline 2 \hline$				p(\$ p(\$ H( Ga hol p(\$ p(\$ p(\$ p(\$ p(\$ f(\$ Ga The	$\sum_{neck=tie}^{l} = \frac{4}{8}$ $\sum_{neck=tie}^{l} = \frac{4}{8}$ $\sum_{neck=no}^{l} = \frac{2}{8}$ $\sum_{neck=no}^{l} = \frac{2}{8}$ $\sum_{neck=no}^{l} = \frac{1}{8}$ $\sum_{nolds=ball}^{l} = \frac{1}{8}$ $\sum_{nolds=no}^{l} = \frac{1}{8}$ $\sum_{nolds=no}^{l$	$\frac{2}{8}; H(C, \frac{2}{8}; H(C, \frac{4}{8} \cdot 1 + \frac{1}{2} - 0))$ $\frac{2}{8}; H(C, \frac{2}{8}; H(C, \frac{2}{8}; H(C, \frac{1}{8}; H(C, \frac{1}; H(C, \frac$	$S_{\text{neck}=\text{bow}}) = \frac{1}{2} S_{\text{neck}=\text{bow}}) = \frac{1}{2} S_{\text{neck}=\text{bow}} = \frac{1}{2} S_{\text{neck}=\text$	$= H_B = H_B = H_B (\frac{1}{2}) = H_B = H_B (\frac{1}{2}) = H_B = H_B (\frac{1}{2}) = H_$

P. Pošík © 2013

Artificial Intelligence - 15 / 29

### Entropy gain toy example

At each split we are going to choose the feature that gives the highest information gain.

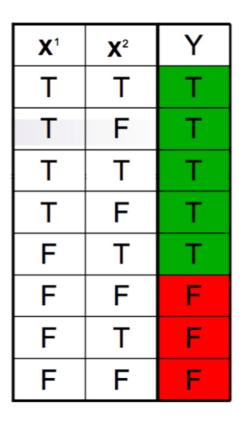
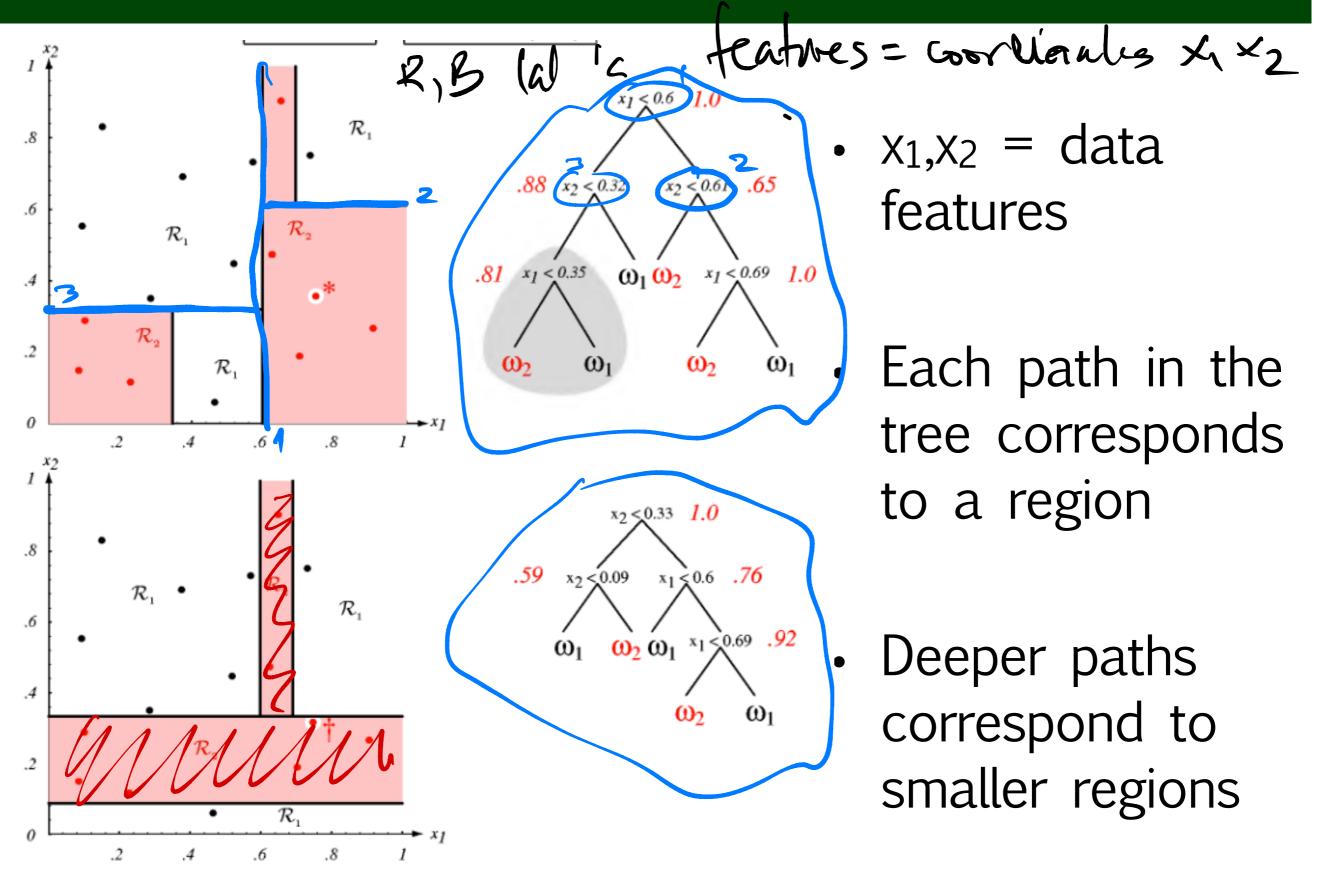


Figure 6: 2 possible features to split by

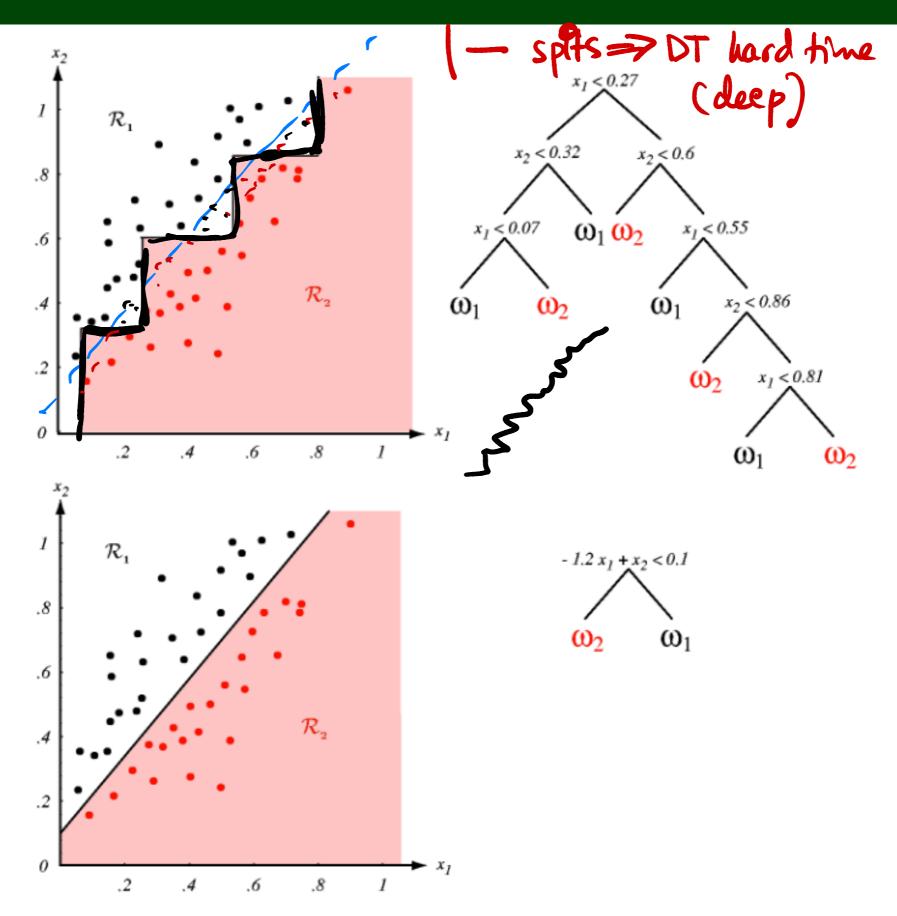
$$H(Y|X^{1}) = \frac{1}{2}H(Y|X^{1} = T) + \frac{1}{2}H(Y|X^{1} = F) = 0 + \frac{1}{2}(\frac{1}{4}\log_{2}\frac{1}{4} + \frac{3}{4}\log_{2}\frac{3}{4}) \approx .405$$
$$IG(X^{1}) = H(Y) - H(Y|X^{1}) = .954 - .405 = .549$$

$$H(Y|X^{2}) = \frac{1}{2}H(Y|X^{2} = T) + \frac{1}{2}H(Y|X^{2} = F) = \frac{1}{2}(\frac{1}{4}\log_{2}\frac{1}{4} + \frac{3}{4}\log_{2}\frac{3}{4}) + \frac{1}{2}(\frac{1}{2}\log_{2}\frac{1}{2} + \frac{1}{2}\log_{2}\frac{1}{2}) \approx .905$$
$$IG(X^{2}) = H(Y) - H(Y|X^{2}) = .954 - .905 = .049$$

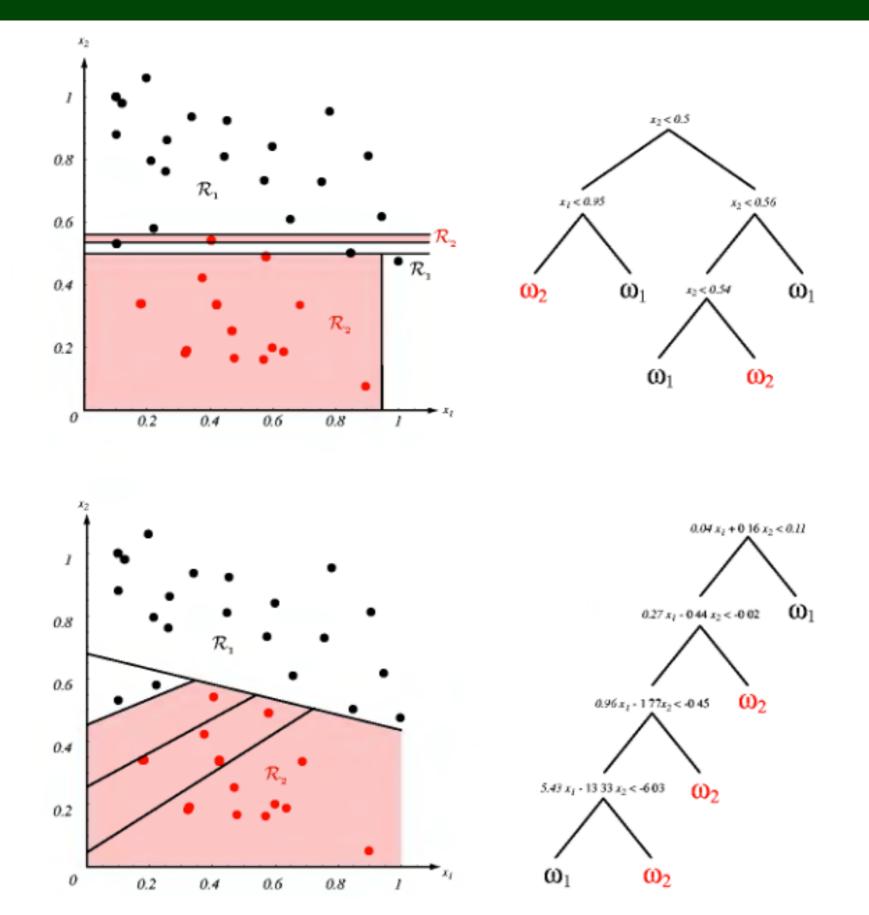
#### **Data Partition Rules**



#### **Data Partition Rules**



### **Data Partition Rules**



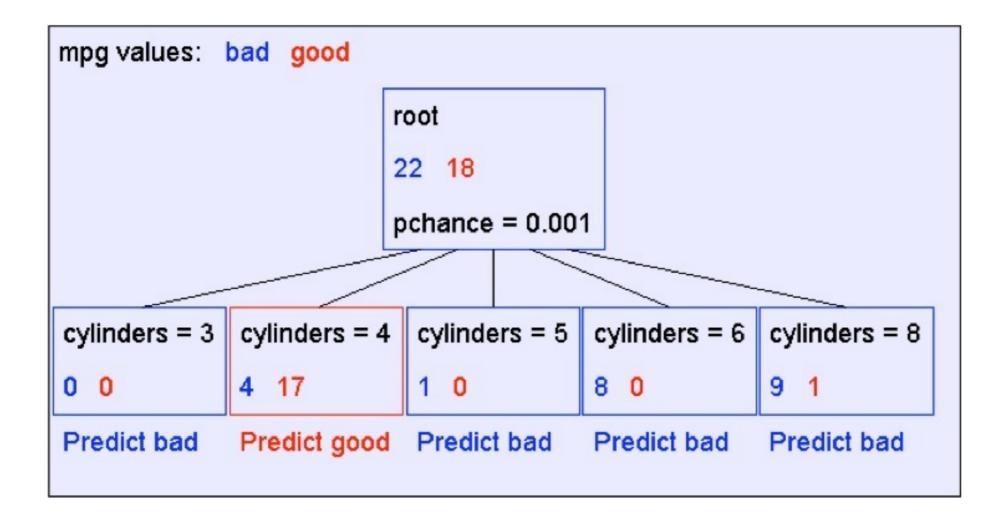
### Walkthrough Decision Tree Example

mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	low	low	low	high	75to78	asia
bad	6	medium	medium	medium	medium	70to74	america
bad	4	medium	medium	medium	low	75to78	europe
bad	8	high	high	high	low	70to74	america
bad	6	medium	medium	medium	medium	70to74	america
bad	4	low	medium	low	medium	70to74	asia
bad	4	low	medium	low	low	70to74	asia
bad	8	high	high	high	low	75to78	america
:	:	:	:	:	:	1	:
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
bad	8	high	high	high	low	70to74	america
good	8	high	medium	high	high	79to83	america
bad	8	high	high	high	low	75to78	america
good	4	low	low	low	low	79to83	america
bad	6	medium	medium	medium	high	75to78	america
good	4	medium	low	low	low	79to83	america
good	4	low	low	medium	high	79to83	america
bad	8	high	high	high	low	70to74	america
good	4	low	medium	low	medium	75to78	europe
bad	5	medium	medium	medium	medium	75to78	europe

#### 40 Records

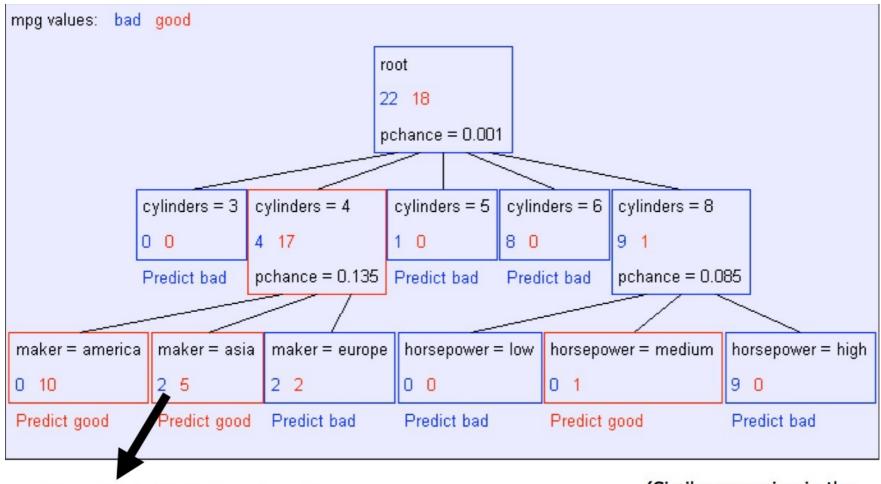
- Data (matrix) example : automobiles
- Target : mpg  $\in$  {good, bad} 2 class /binary problem

### **Decision Tree Split**



 Split by feature "cylinders", using feature values for branches

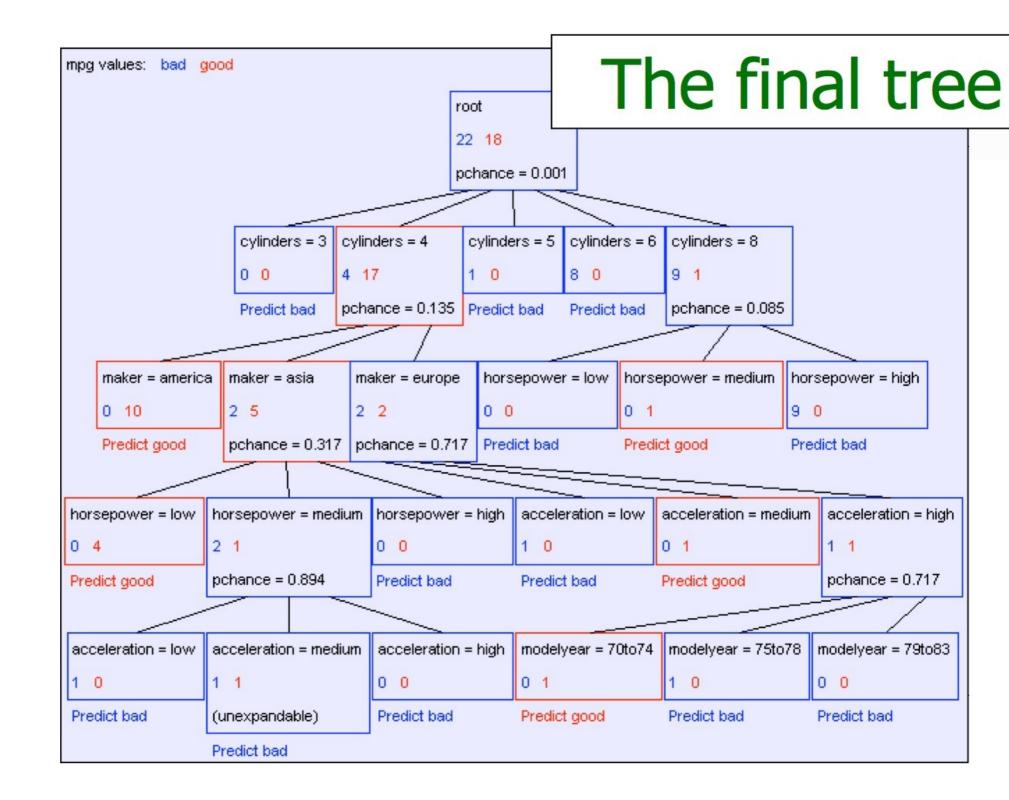
### **Decision Tree Splits**



Recursively build a tree from the seven records in which there are four cylinders and the maker was based in Asia (Similar recursion in the other cases)

 each terminal leaf is labeled by majority (at that leaf). This leaf-label is used for prediction.

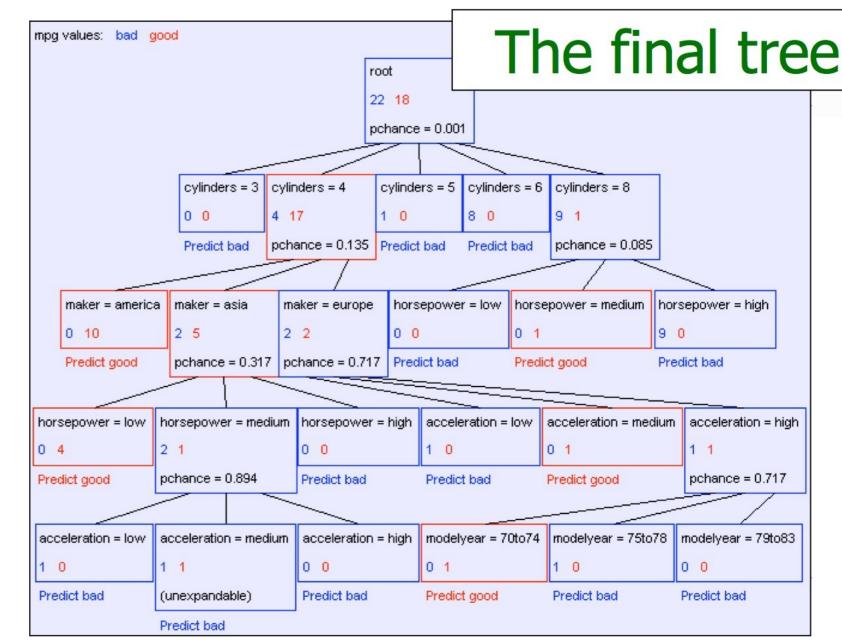
#### **Decision Tree Splits**



### Prediction with a tree

#### • testpoint:

- cylinder=4
- maker=asia
- horsepower=low
- weight=low
- displacement=medium
- modelyear=75to78



- same tree structure, split criteria
- assume numerical labels
- for each terminal node compute the node label (predicted value) and the mean square error

Estimate a predicted value per tree node

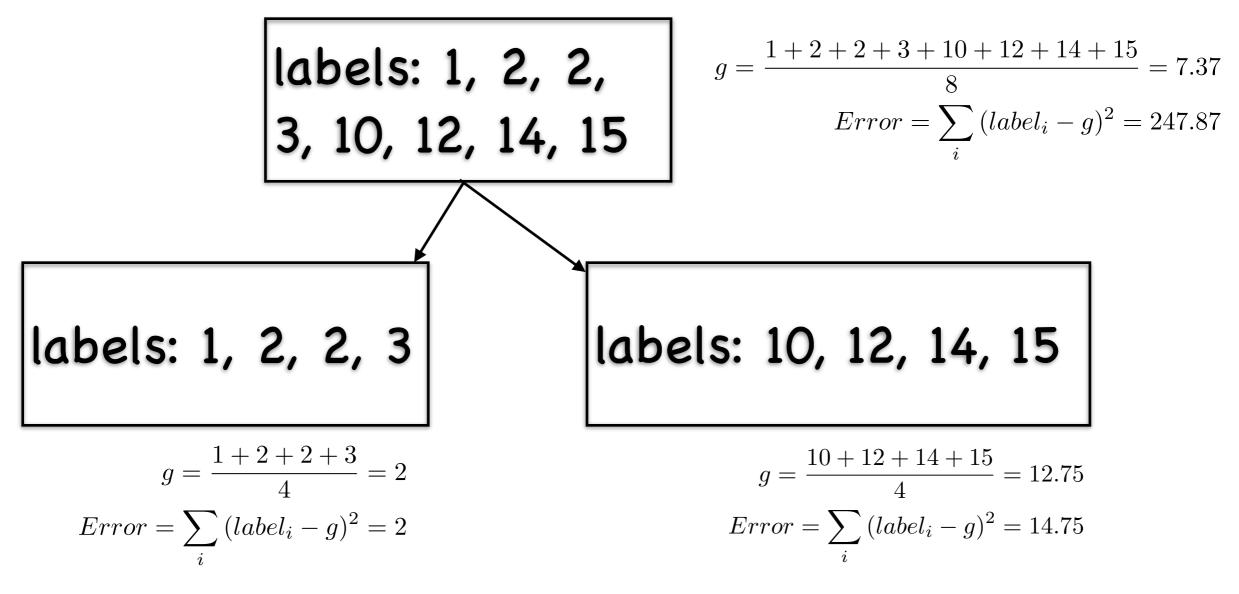
$$g_m = \frac{\sum_{t \in \chi_m} y_t}{|\chi_m|}$$

Calculate mean square error

$$E_m = \frac{\sum_{t \in \chi_m} (y_t - g_m)^2}{|\chi_m|}$$

 choose a split criteria to minimize the weighted error at children nodes

#### **Regression Tree**



- choose a split criteria to minimize the weighted or total error at children nodes
  - in the example total error after the split is 14.75 + 2=16.75

- for each test datapoint x=(x<sup>1</sup>,x<sup>2</sup>,...,x<sup>d</sup>) follow the corresponding path to reach a terminal node n
- predict the value/label associated with node n

## Overfitting

- decision trees can overfit quite badly
  - in fact they are designed to do so due to high complexity of the produced model
  - if a decision tree training error doesn't approach zero, it means that data is inconsistent
- some ideas to prevent overfitting:
  - create more than one tree, each using a different subset of features; average/vote predictions
  - do not split nodes in the tree that have very few datapoints (for example less than 10)
  - only split if the improvement is massive

# Pruning

- done also to prevent overfitting
- construct a full decision tree
- then walk back from the leaves and decide to "merge" overfitting nodes
  - when split complexity overwhelms the gain obtained by the spit