hierarchical set of rules

Decision Trees

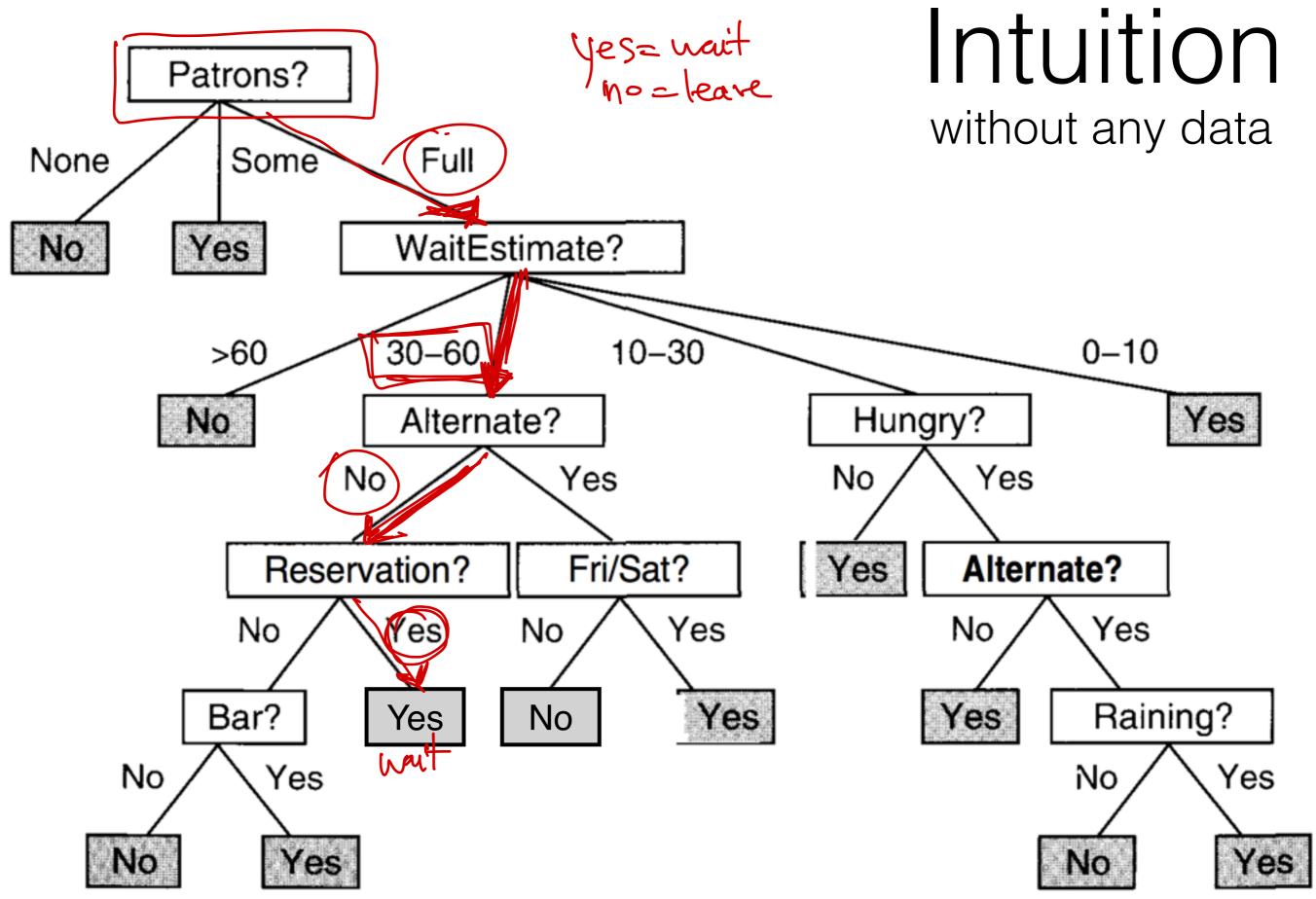
Sourav Sen Gupta CDS 2015 | PGDBA | 6 Oct 2015

Will you eat/wait?

Deciding factors may be

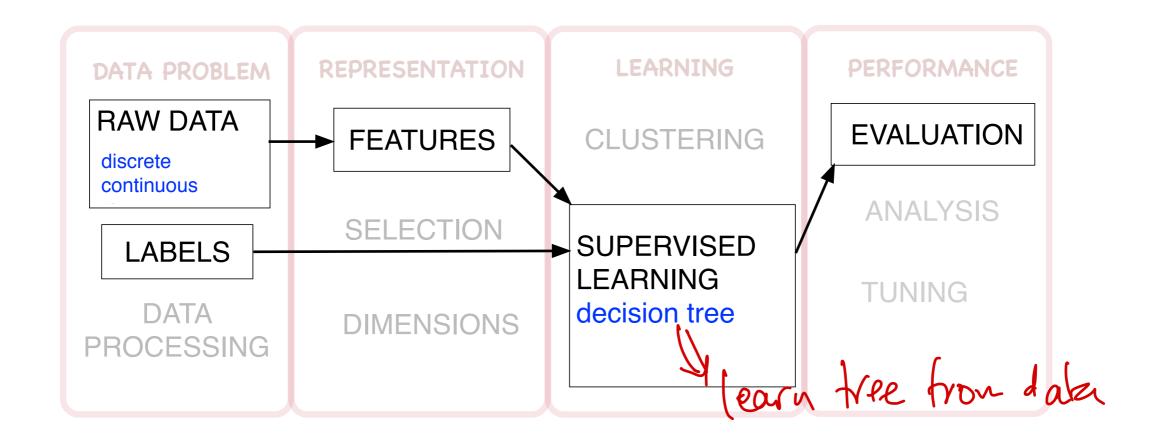
```
2 heuristic rules
```

- If there are patrons (people inside) Yes/No If you are hungry already Yes / No
- Alternative options in the vicinity Yes / No The estimated time for waiting In minutes
- If you already have a reservation Yes/No
- If it is a Friday/Saturday night Yes/No
 If there is a Bar area to wait Yes/No
 The range of price at the place High/Medium/Low
- If it is raining at the time Yes/No
 The genre of cuisine French, Italian, Thai, Burger



Ref. — "Artificial Intelligence : A Modern Approach" — Stuart J. Russell and Peter Norvig

ML Pipeline



Training Data

Example	L.	₽	4	4	A	ttributes	\$ €	4			Goal
	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est	WillWai
\widehat{X}_1	Yes	No	No	Yes	Some	\$\$\$	No	Yes	French	0–10	Yes
X_2 X_3	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
$(\widehat{T_5})$	Yes	No	Yes	No	Full	\$\$\$	No	Yes	French	>60	(No
(X_6)	No	Yes	No	Yes	Some	\$\$	Yes	Yes	Italian	0-10	Yes
$\langle \widehat{X}_7 \rangle$	No	Yes	No	No	None	\$	Yes	No	Burger	0-10	No
X_8	No	No	No	Yes	Some	\$\$	Yes	Yes	Thai	0-10	Yes
	No	Yes	Yes	No	Full	\$	Yes	No	Burger	>60	No
Λ_{10}	Yes	Yes	Yes	Yes	Full	\$\$\$	No	Yes	Italian	10–30	No
$\langle \chi_{11} \rangle$	No	No	No	No	None	\$	No	No	Thai	0-10	No
X_{12}	Yes	Yes	Yes	Yes	Full	\$	No	No	Burger	30–60	Yes

\$\$\$

No

No

Thai

Full

Yes Yes

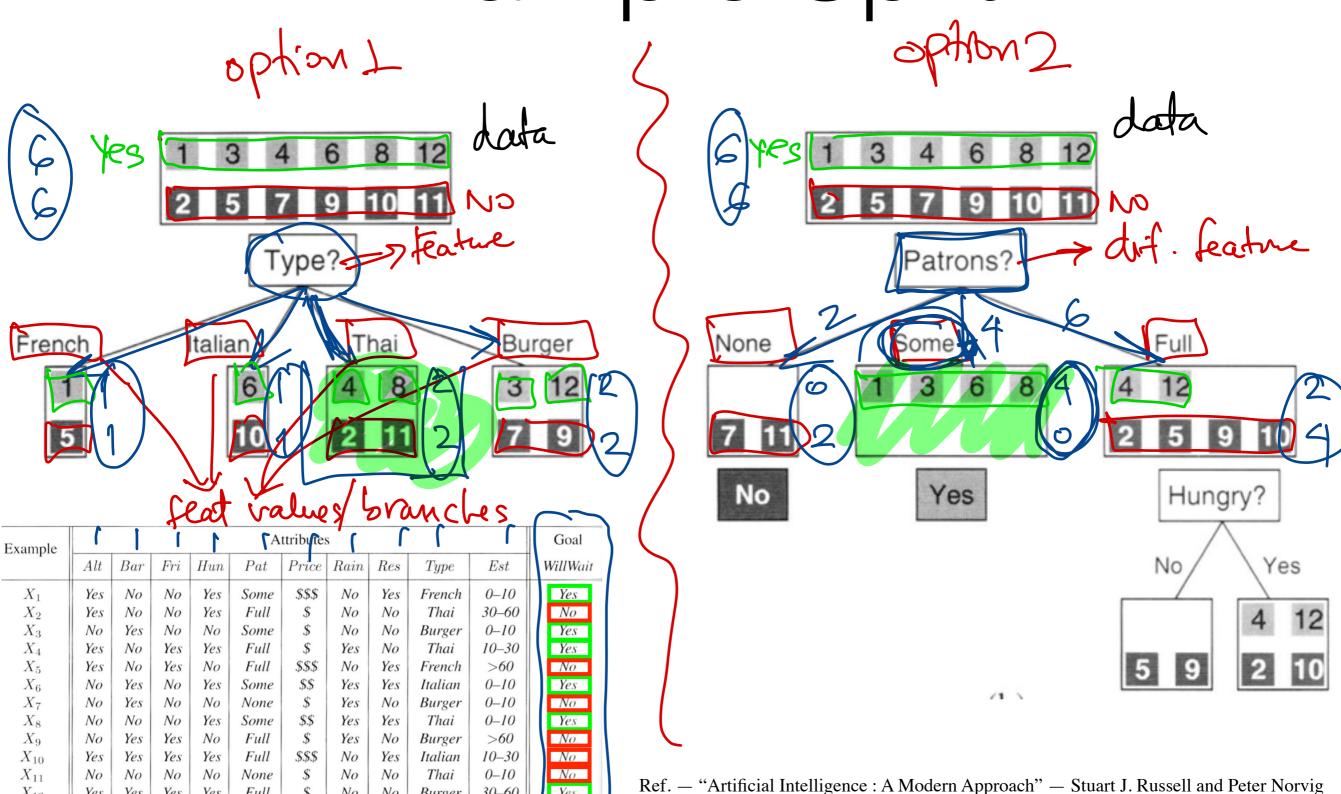
TEST

Yes

No

30-60





Yes

30-60

No

No

Burger

Yes

Yes

Yes

Yes

Full

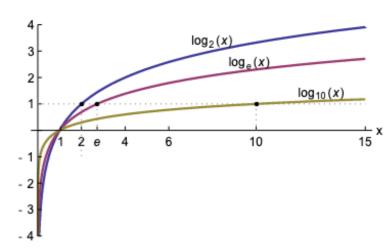
Entropy & Information Gain

Why a logarithm function?

$$log(p_1 \times p_2) = log(p_1) + log(p_2)$$

Shannon Entropy:

$$H(p_1, ..., p_N) = -\sum_{i=1}^{N} p_i . log(p_i) = \text{weakings}$$



Issue: increasing number of events shrinks the probability.

Solution: use logarithm of probability instead and take the average.

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

Idea: a good attribute splits the examples into subsets that are (ideally) "all positive" or "all negative"



For a training set containing
$$p$$
 positive examples and n negative examples, we have:
$$H(\frac{p}{p+n}, \frac{n}{p+n}) = -\frac{p}{p+n} \log_2 \frac{p}{p+n} - \frac{n}{p+n} \log_2 \frac{n}{p+n}$$

Information Gain

Reduction in Entropy

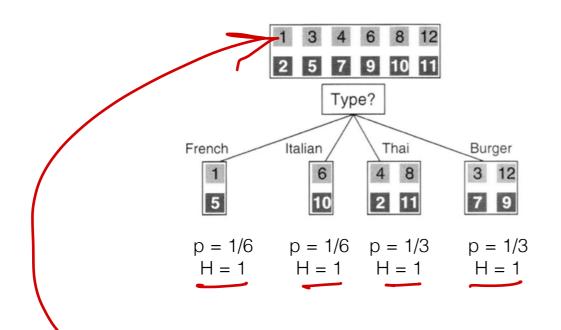
Information Gain = Parent Entropy — E(Child Entropy)

$$I = H(S) - \sum_{\text{untopy of labe(s)}} \frac{|S^i|}{|S|} H(S^i)$$
 entropy of labels whose split $i \in \{L,R\}$ entropy of labels after the split

One notion of entropy is that of Shannon Entropy

$$H(\mathcal{S}) = -\sum_{c \in \mathcal{C}} p(c) \log(p(c))$$

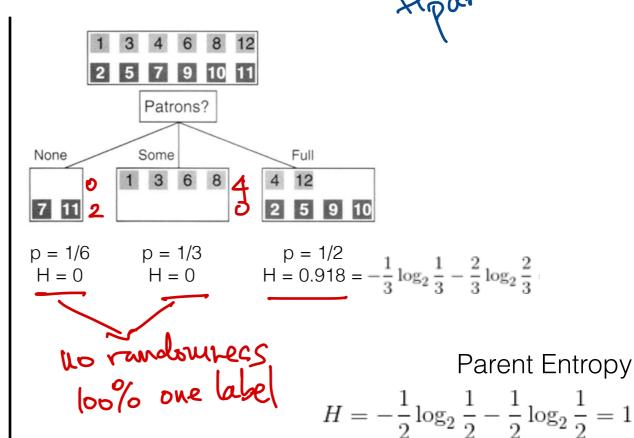
Compare Gain = reduction in entropy weight supposed to the state of th



Parent Entropy

$$H = -\frac{1}{2}\log_2\frac{1}{2} - \frac{1}{2}\log_2\frac{1}{2} = 1$$

E(Child Entropy)



E(Child Entropy)

How to pick nodes?

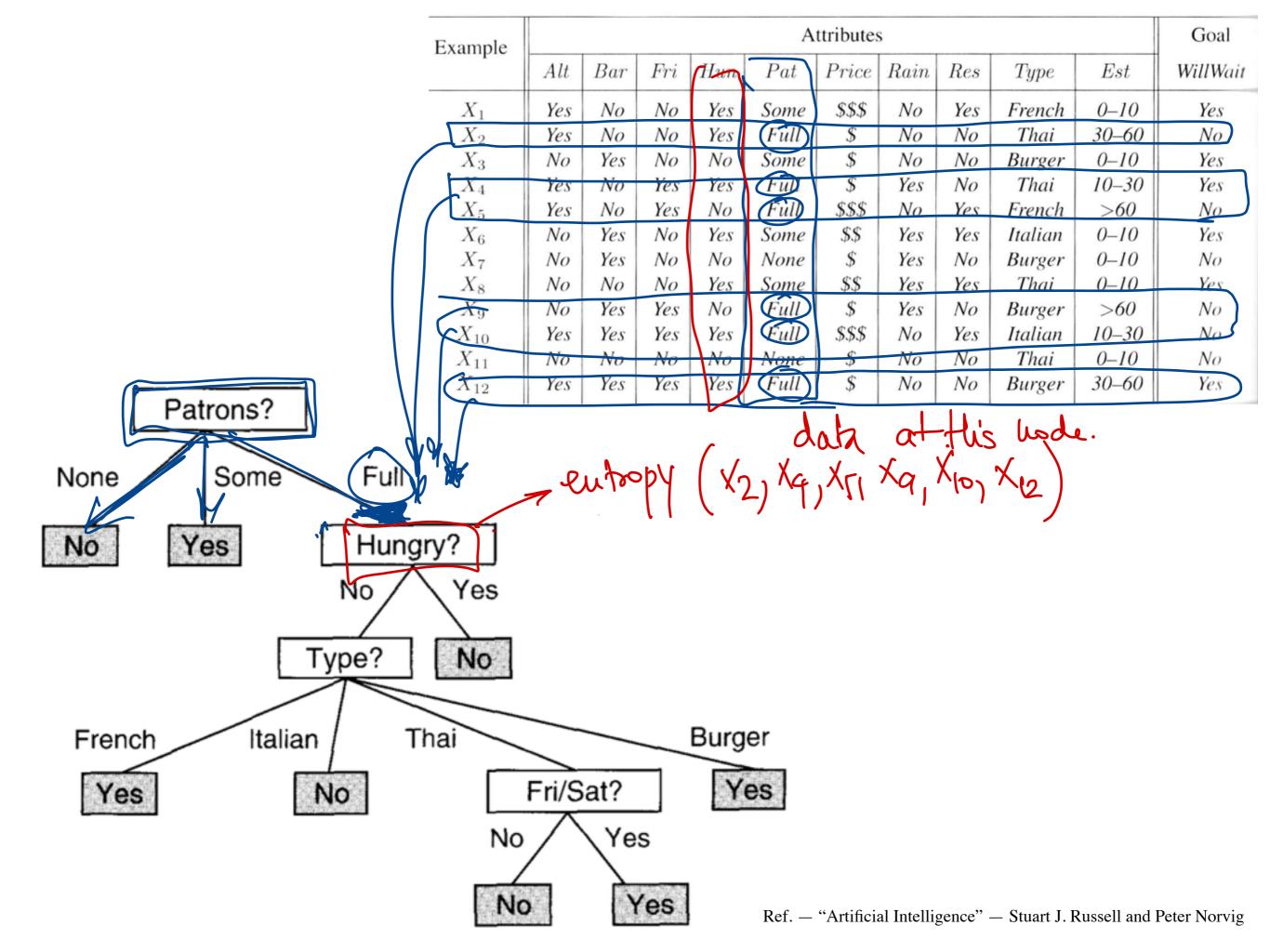
- \square A chosen attribute A, with K distinct values, divides the training set E into subsets E_1, \ldots, E_K .
- The Expected Entropy (EH) remaining after trying attribute A (with branches i=1,2,...,K) is

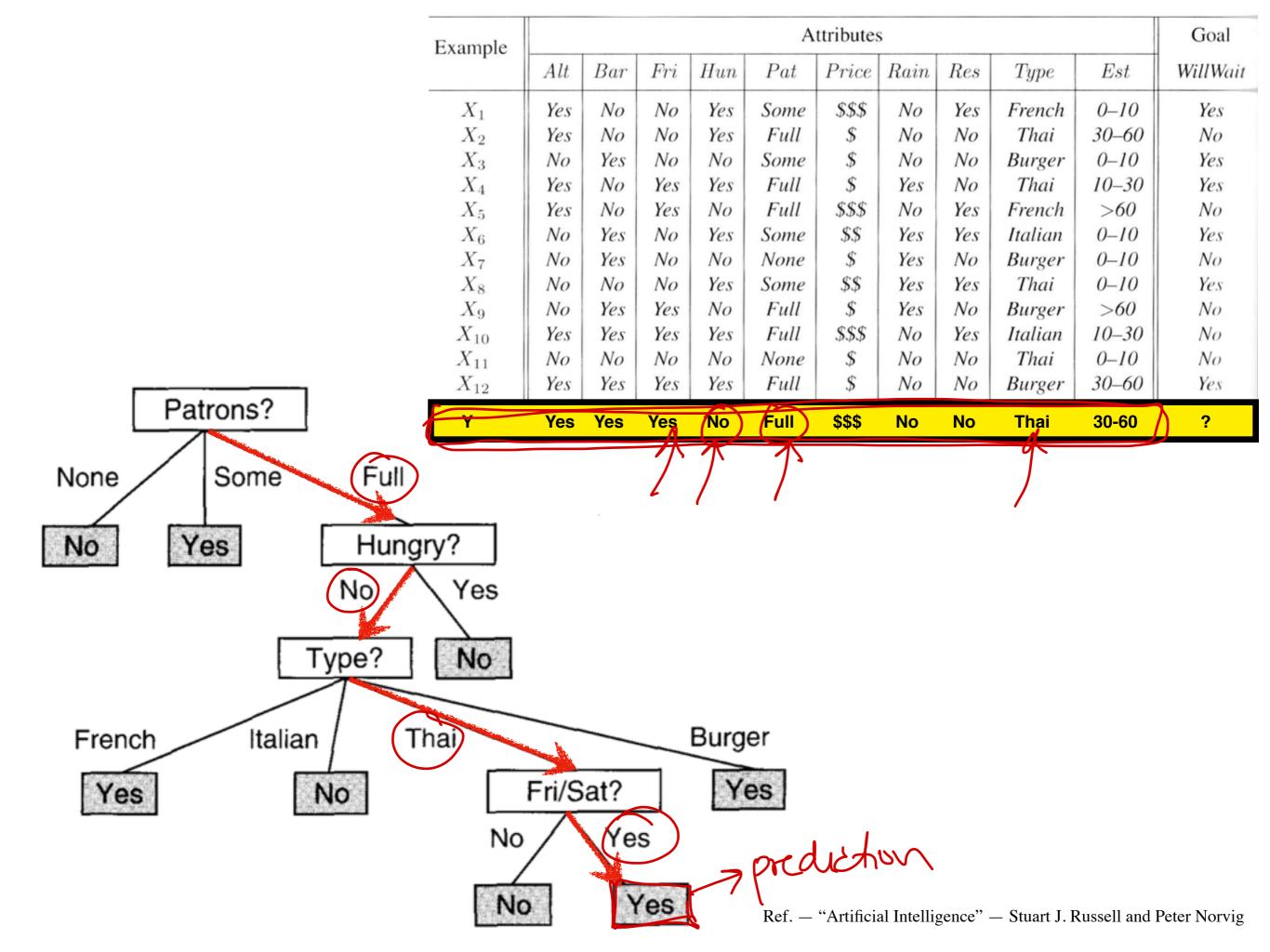
(with branches
$$i=1,2,...,K$$
) is
$$EH(A) = \sum_{i=1}^{K} \underbrace{\frac{p_i + n_i}{p_i + n_i}}_{P_i + n_i} H(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i})$$

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

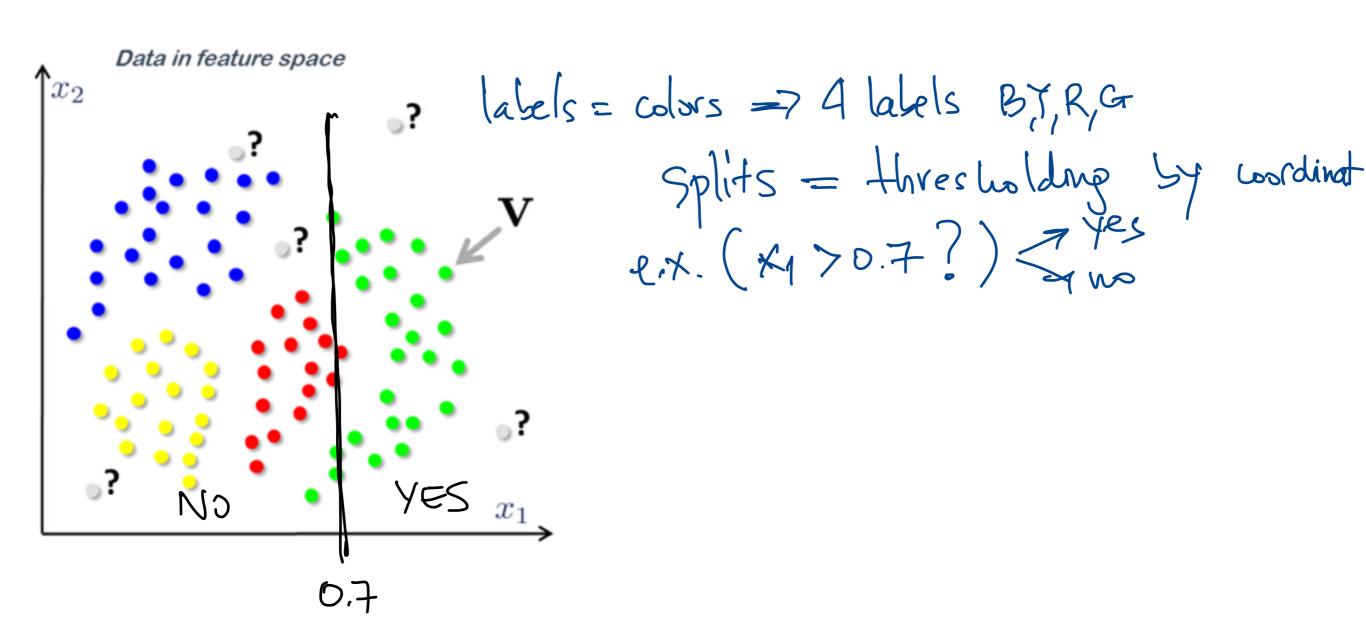
$$I(A) = H(\frac{p}{p+n}, \frac{n}{p+n}) - EH(A)$$

= Entropy in the parent node - remaining Expected Entropy in the child nodes



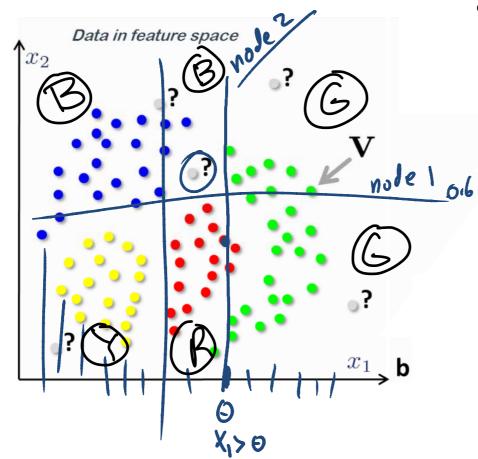


Classification Tree



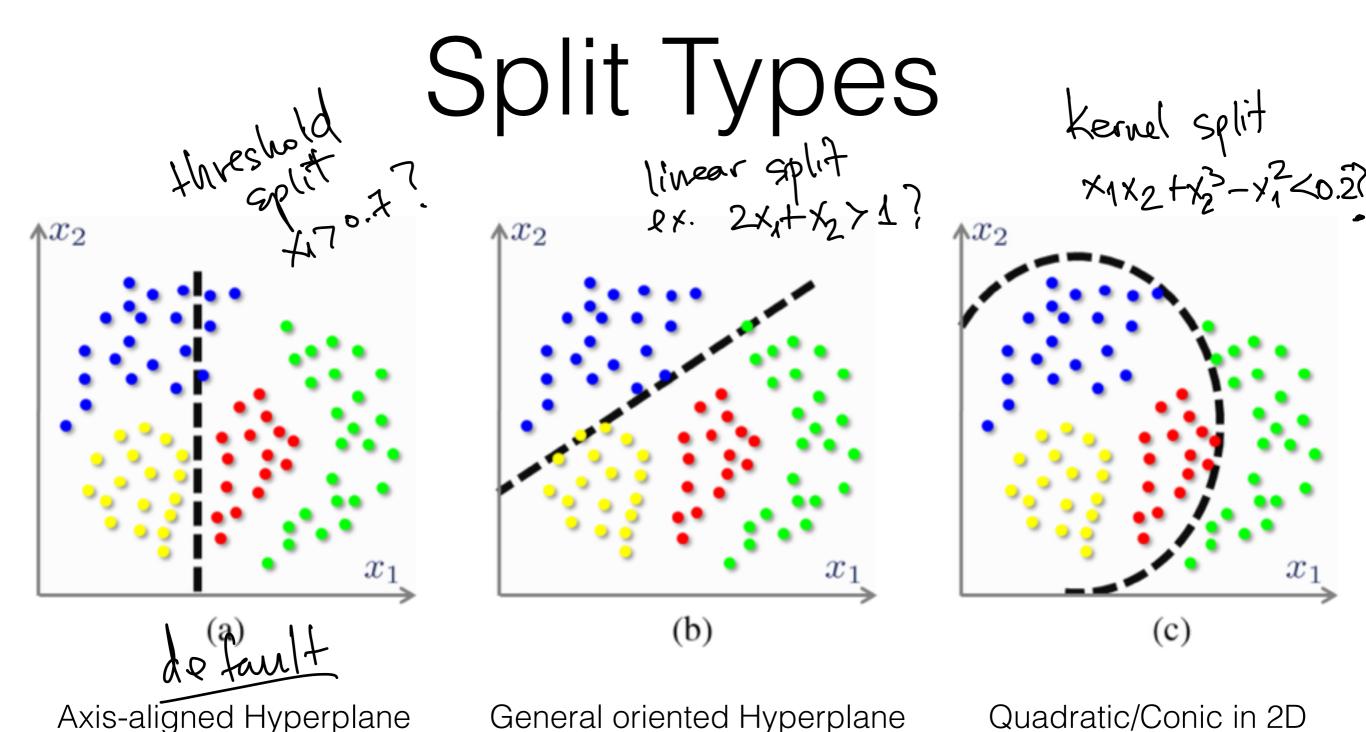
Classification tree



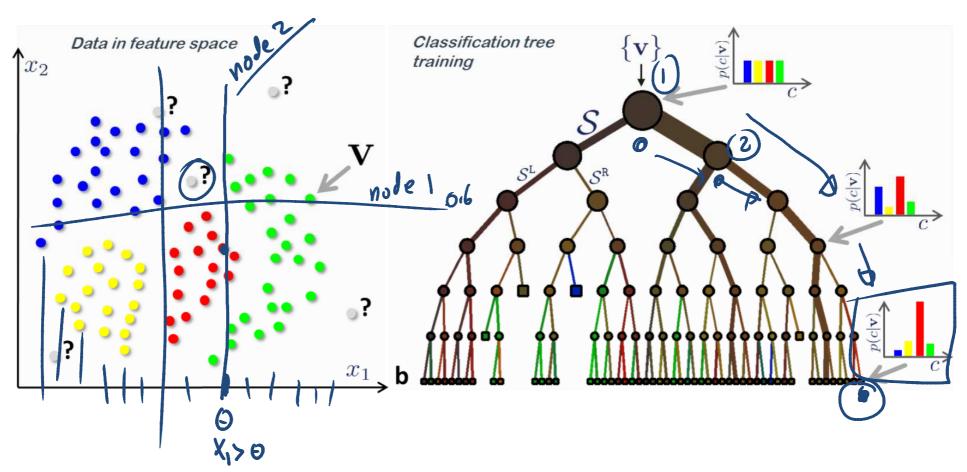


- How to deal with continuous features?
 - Create the splits randomly
 - Compute information gain for each split
 - Choose the one with maximum gain

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



Classification tree



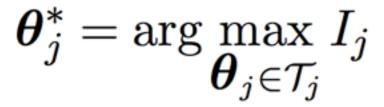
A generic data point is denoted by a vector $\mathbf{v} = (x_1, x_2, \dots, x_d)$ $\mathcal{S}_j = \mathcal{S}_j^{\mathsf{L}} \cup \mathcal{S}_j^{\mathsf{R}}$

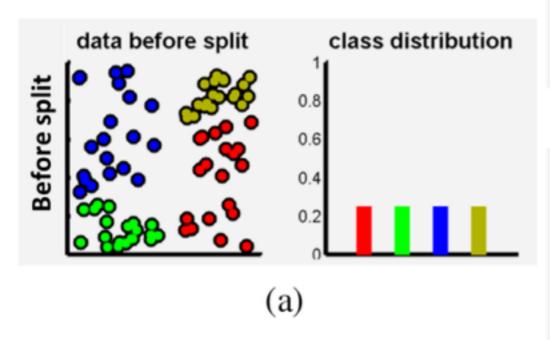
[Criminisi et al, 2011]

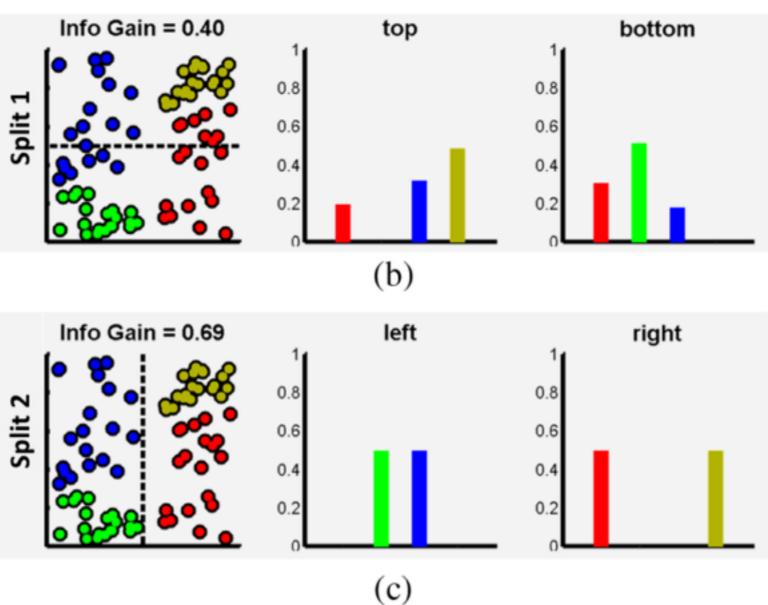
• Note that the **histogram** shows the **posterior distribution** for each class:

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

- **x** $Goal \Leftrightarrow (Path_1 \vee Path_2 \vee ...)$, where
- **x** *Path* is a conjuction of attribute-value tests, i.e.
- **x** the tree is equivalent to a DNF of a function.

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

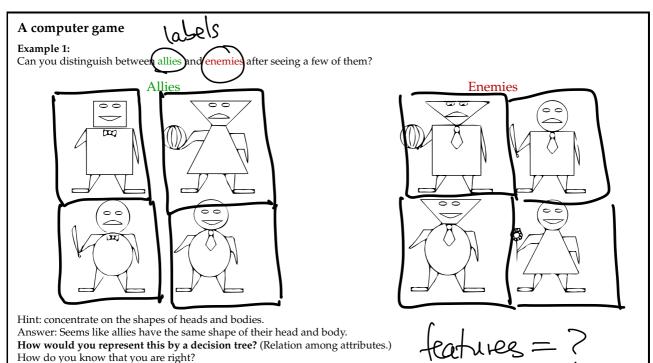
- ✔ Trees are a suitable representation for some functions and unsuitable for others.
- What is the cardinality of the set of Boolean functions of *n* attributes?
 - \mathbf{x} It is equal to the number of truth tables that can be created with n attributes.
 - **x** The truth table has 2^n rows, i.e. 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.

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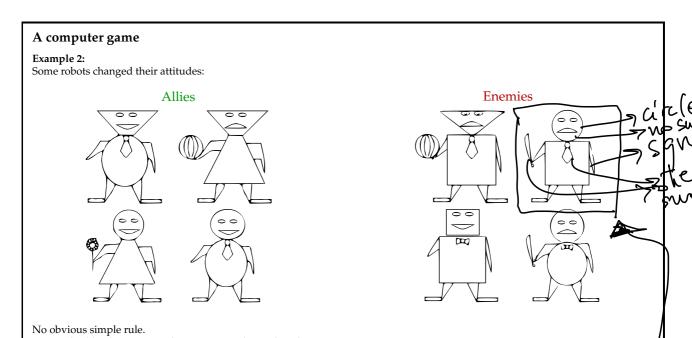
Learning a Decision Tree

How do you know that you are right?

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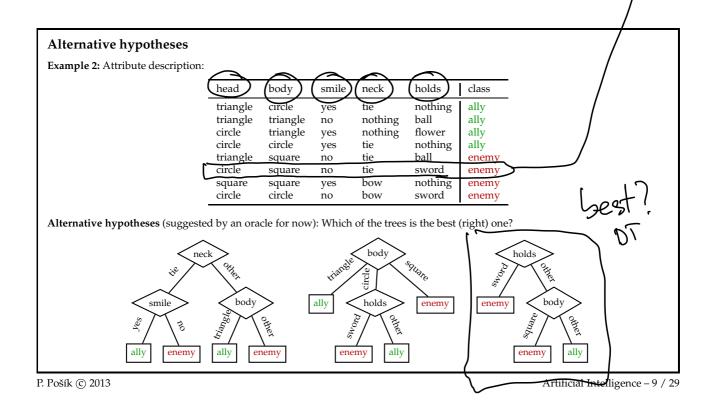
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How to build a decision tree discriminating the 2 robot classes?

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Artificial Intelligence – 8



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?

✓ The right-hand side one is the simplest one:

		left	middle	right
:	depth	2	2	2
	leaves	4	4	3
	conditions	3	2	2

Will it work for new data?

- ✔ We have no idea!
- ✓ We need a set of new testing data (different data from the same source).

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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.

$\textbf{Top-Down Induction of Decision Trees} \ (\texttt{TDIDT}) :$

- ✔ 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.

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

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Choosing the test attribute

Information gain:

- ✔ Formalization of the terms "useless", "perfect", "more useful".
- \checkmark 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):

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

 \checkmark 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).

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Artificial Intelligence – 13 / 29

Choosing the test attribute (special case: binary classification)

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

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

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

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

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Choosing the test attribute (example)

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

head:

$$\begin{array}{l} p(S_{\text{head=tri}}) = \frac{3}{8}; H(C, S_{\text{head=tri}}) = H_B\left(\frac{2}{2+1}\right) = 0.92 \\ p(S_{\text{head=cir}}) = \frac{4}{8}; H(C, S_{\text{head=cir}}) = H_B\left(\frac{2}{2+2}\right) = 1 \\ p(S_{\text{head=sq}}) = \frac{1}{8}; H(C, S_{\text{head=sq}}) = H_B\left(\frac{0}{0+1}\right) = 0 \\ H(C, S, head) = \frac{3}{8} \cdot 0.92 + \frac{4}{8} \cdot 1 + \frac{1}{8} \cdot 0 = 0.84 \\ Gain(head, S) = 1 - 0.84 = 0.16 \end{array}$$

body:

$$\begin{array}{l} p(S_{\rm body=tri}) = \frac{2}{8}; H(C,S_{\rm body=tri}) = H_B\left(\frac{2}{2+0}\right) = 0 \\ p(S_{\rm body=cir}) = \frac{3}{8}; H(C,S_{\rm body=cir}) = H_B\left(\frac{2}{2+1}\right) = 0.92 \\ p(S_{\rm body=sq}) = \frac{3}{8}; H(C,S_{\rm body=sq}) = H_B\left(\frac{0}{0+3}\right) = 0 \\ H(C,S,body) = \frac{2}{8} \cdot 0 + \frac{3}{8} \cdot 0.92 + \frac{3}{8} \cdot 0 = 0.35 \\ Gain(body,S) = 1 - 0.35 = 0.65 \end{array}$$

smile:

$$\begin{array}{l} p(S_{\rm smile=yes}) = \frac{4}{8}; H(C,S_{\rm yes}) = H_B \left(\frac{3}{3+1}\right) = 0.81 \\ p(S_{\rm smile=no}) = \frac{4}{8}; H(C,S_{\rm no}) = H_B \left(\frac{1}{1+3}\right) = 0.81 \\ H(C,S,smile) = \frac{4}{8} \cdot 0.81 + \frac{4}{8} \cdot 0.81 + \frac{3}{8} \cdot 0 = 0.81 \\ Gain(smile,S) = 1 - 0.81 = 0.19 \end{array}$$

neck:

$$\begin{array}{l} P(S_{\text{neck=tie}}) = \frac{4}{8}; \, H(C, S_{\text{neck=tie}}) = H_B \left(\frac{2}{2+2}\right) = 1 \\ p(S_{\text{neck=bow}}) = \frac{2}{8}; \, H(C, S_{\text{neck=bow}}) = H_B \left(\frac{0}{0+2}\right) = 0 \\ p(S_{\text{neck=no}}) = \frac{2}{8}; \, H(C, S_{\text{neck=no}}) = H_B \left(\frac{2}{2+0}\right) = 0 \\ H(C, S, neck) = \frac{4}{8} \cdot 1 + \frac{2}{8} \cdot 0 + \frac{2}{8} \cdot 0 = 0.5 \\ Gain(neck, S) = 1 - 0.5 = 0.5 \end{array}$$

holds:

$$\begin{array}{l} p(S_{\rm holds=ball}) = \frac{2}{8}; H(C,S_{\rm holds=ball}) = H_B \left(\frac{1}{1+1}\right) = 1 \\ p(S_{\rm holds=swo}) = \frac{2}{8}; H(C,S_{\rm holds=swo}) = H_B \left(\frac{0}{0+2}\right) = 0 \\ p(S_{\rm holds=flo}) = \frac{1}{8}; H(C,S_{\rm holds=flo}) = H_B \left(\frac{1}{1+0}\right) = 0 \\ p(S_{\rm holds=no}) = \frac{3}{8}; H(C,S_{\rm holds=no}) = H_B \left(\frac{2}{2+1}\right) = 0.92 \\ H(C,S,holds) = \frac{2}{8} \cdot 1 + \frac{2}{8} \cdot 0 + \frac{1}{8} \cdot 0 + \frac{2}{8} \cdot 0.92 = 0.6 \\ Gain(holds,S) = 1 - 0.6 = 0.4 \end{array}$$

The **body** attribute

- ${\color{red} \checkmark} \;\;$ brings us the largest information gain, thus
- ✓ it shall be chosen for the first test in the tree!

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Artificial Intelligence – 15 / 29

Entropy gain toy example

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

X ¹	X ²	Υ
Т	Т	Η
Т	F	Т
Т	Т	Т
Т	F	Т
F	Т	Т
F	F	F
F	Т	F
F	F	F

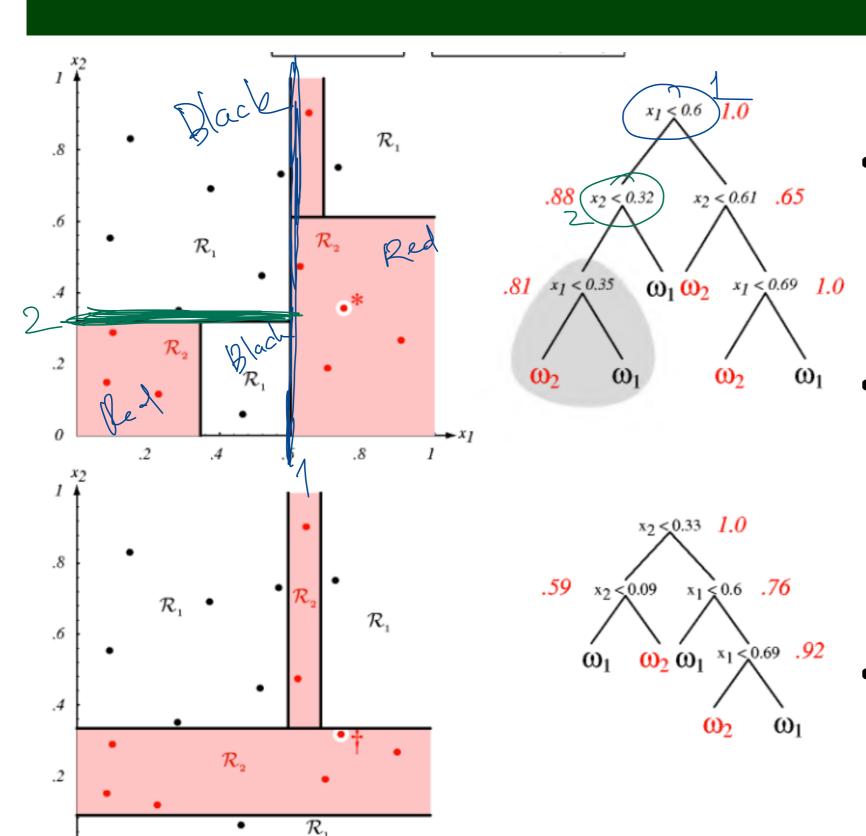
Figure 6: 2 possible features to split by

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

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

$$IG(X^{2}) = H(Y) - H(Y|X^{2}) = .954 - .905 = .049$$

Data Partition Rules



.8

X12 word wort

 $x_1,x_2 = data$ features

Each path in the tree corresponds to a region

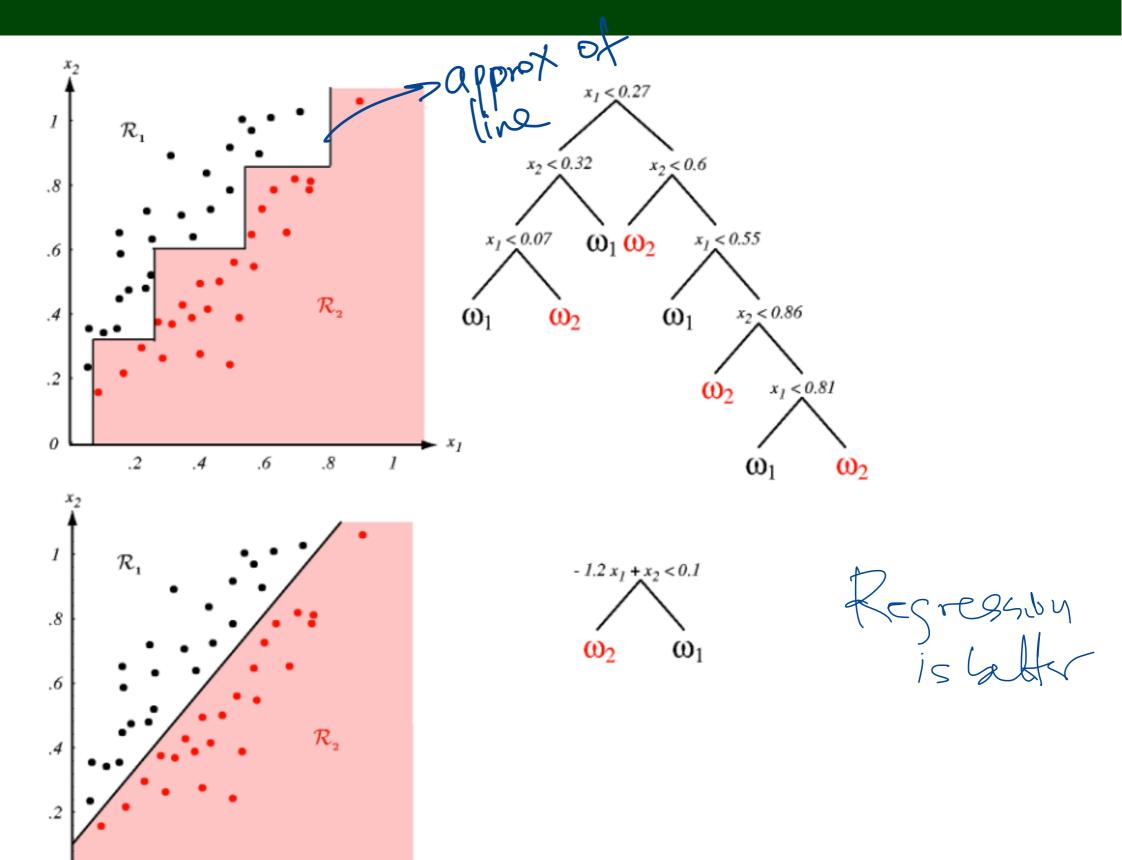
Deeper paths correspond to smaller regions

Data Partition Rules

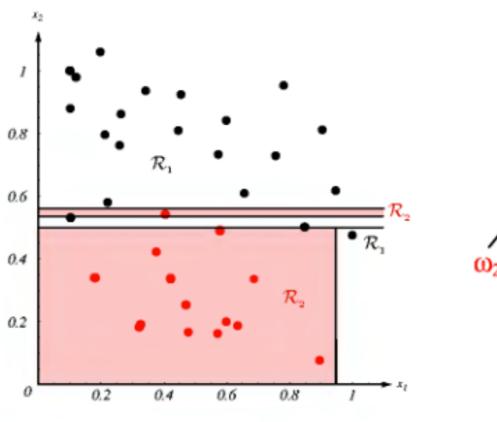
.2

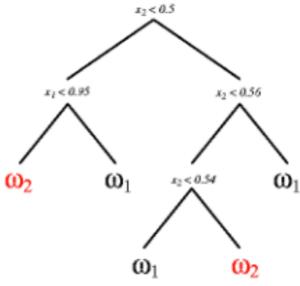
.6

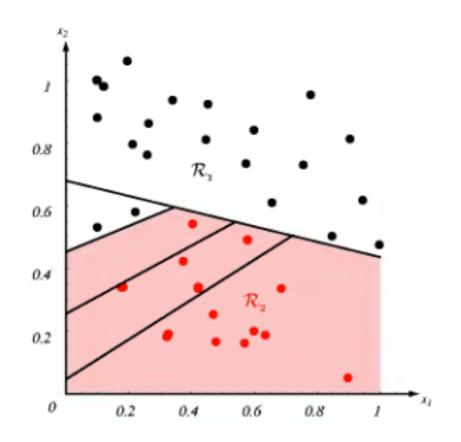
.8

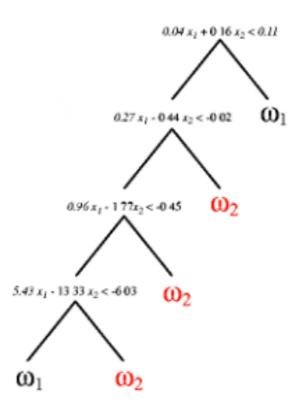


Data Partition Rules









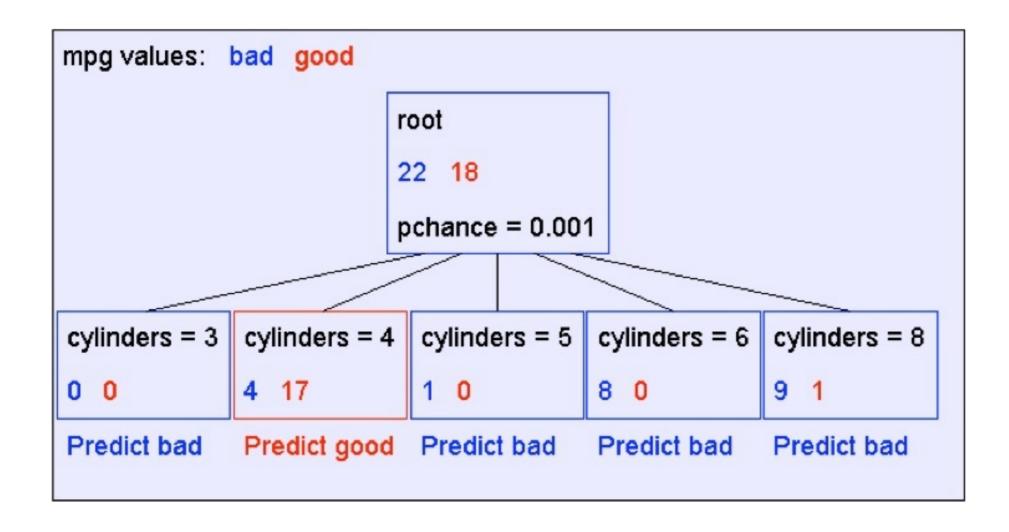
Walkthrough Decision Tree Example

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

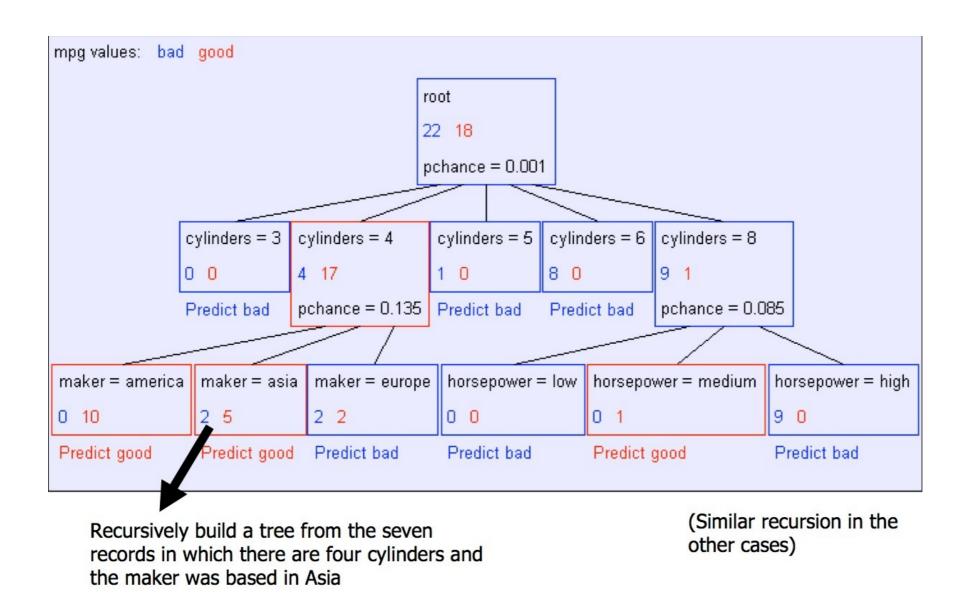
- Data (matrix) example: automobiles
- Target: mpg ∈ {good, bad} 2 class /binary problem

Decision Tree Split



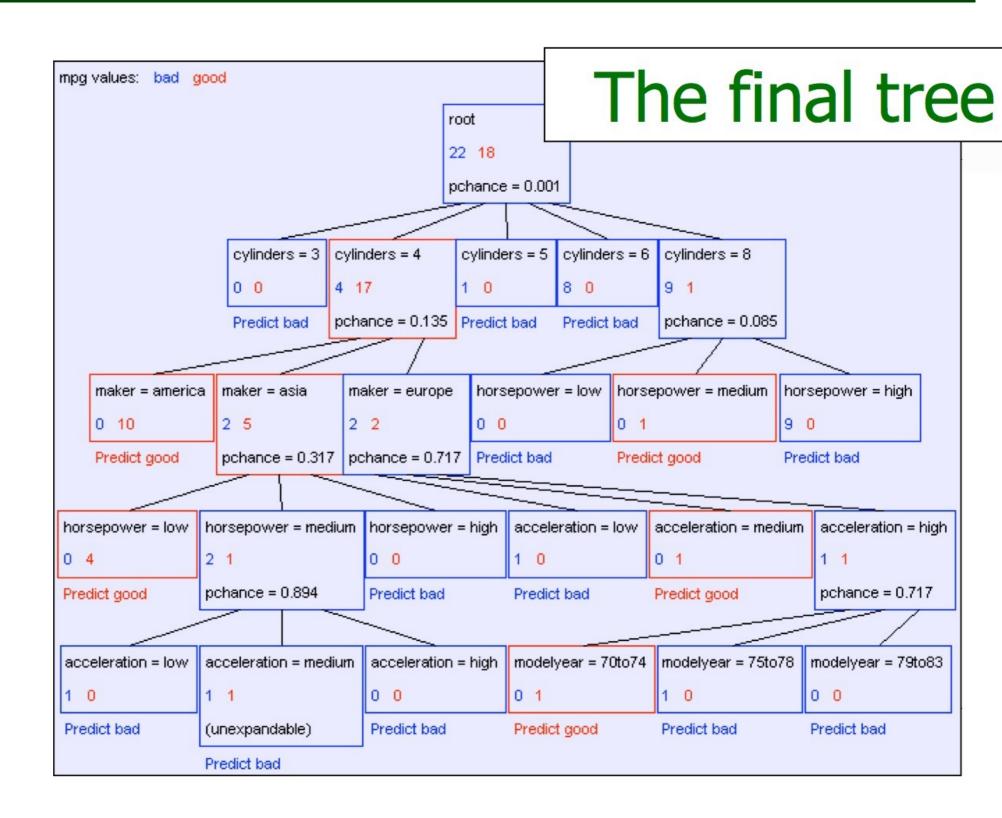
 Split by feature "cylinders", using feature values for branches

Decision Tree Splits



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

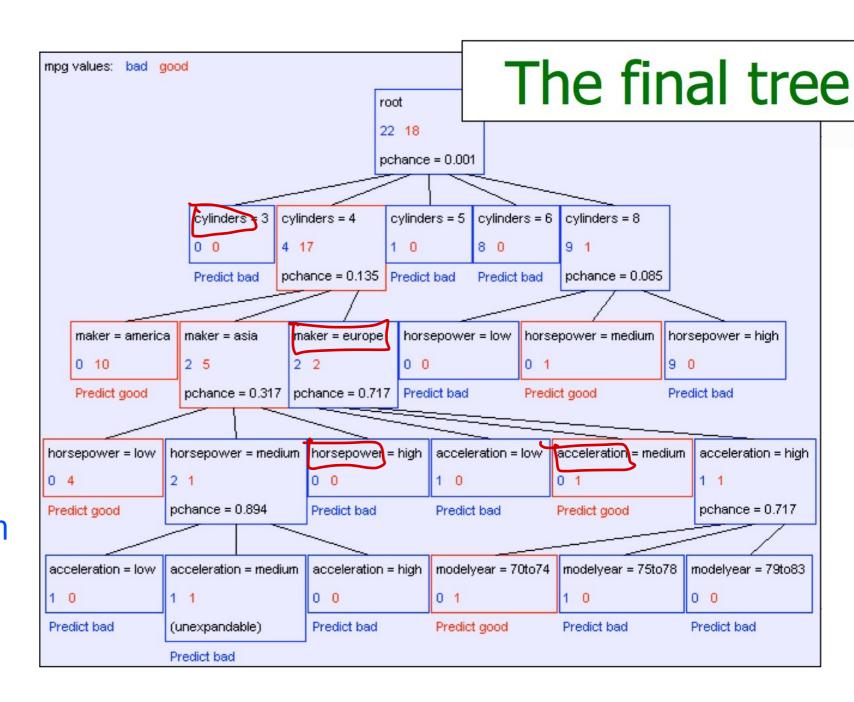
Decision Tree Splits



Prediction with a tree

testpoint:

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



Regression Tree

· 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

labels: 1, 2, 2, 3, 10, 12, 14, 15

$$g = \frac{1+2+2+3+10+12+14+15}{8} = 7.37$$

$$Error = \sum_{i} (label_i - g)^2 = 247.87$$

labels: 1, 2, 2, 3

$$g = \frac{1+2+2+3}{4} = 2$$

$$Error = \sum_{i} (label_i - g)^2 = 2$$

labels: 10, 12, 14, 15

$$g = \frac{10 + 12 + 14 + 15}{4} = 12.75$$

$$Error = \sum_{i} (label_i - g)^2 = 14.75$$

- $Error = \sum_{i} (label_i g)^2 = 2$ Choose a split criteria to minimize the weightedor total error at children nodes
 - in the example total error after the split is 14.75 + 2 = 16.75

Prediction with a tree

• for each test datapoint $x=(x^1,x^2,...,x^d)$ 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