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BBM406

Fundamentals of Machine Learning

Lecture 18:

Decision Trees

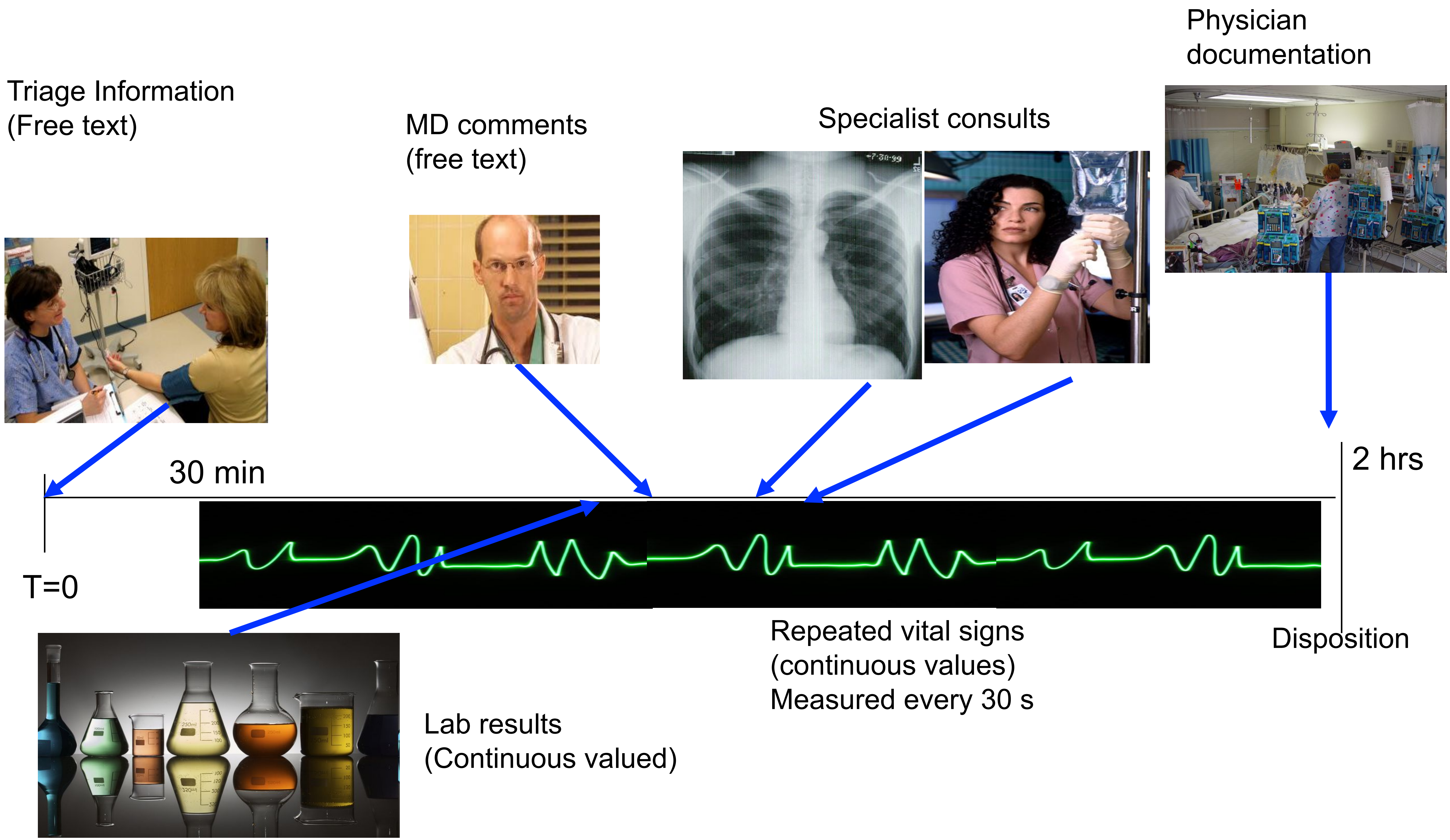
HACETTEPE UNIVERSITY COMPUTER VISION LAB

Aykut Erdem // Hacettepe University // Fall 2019

Today

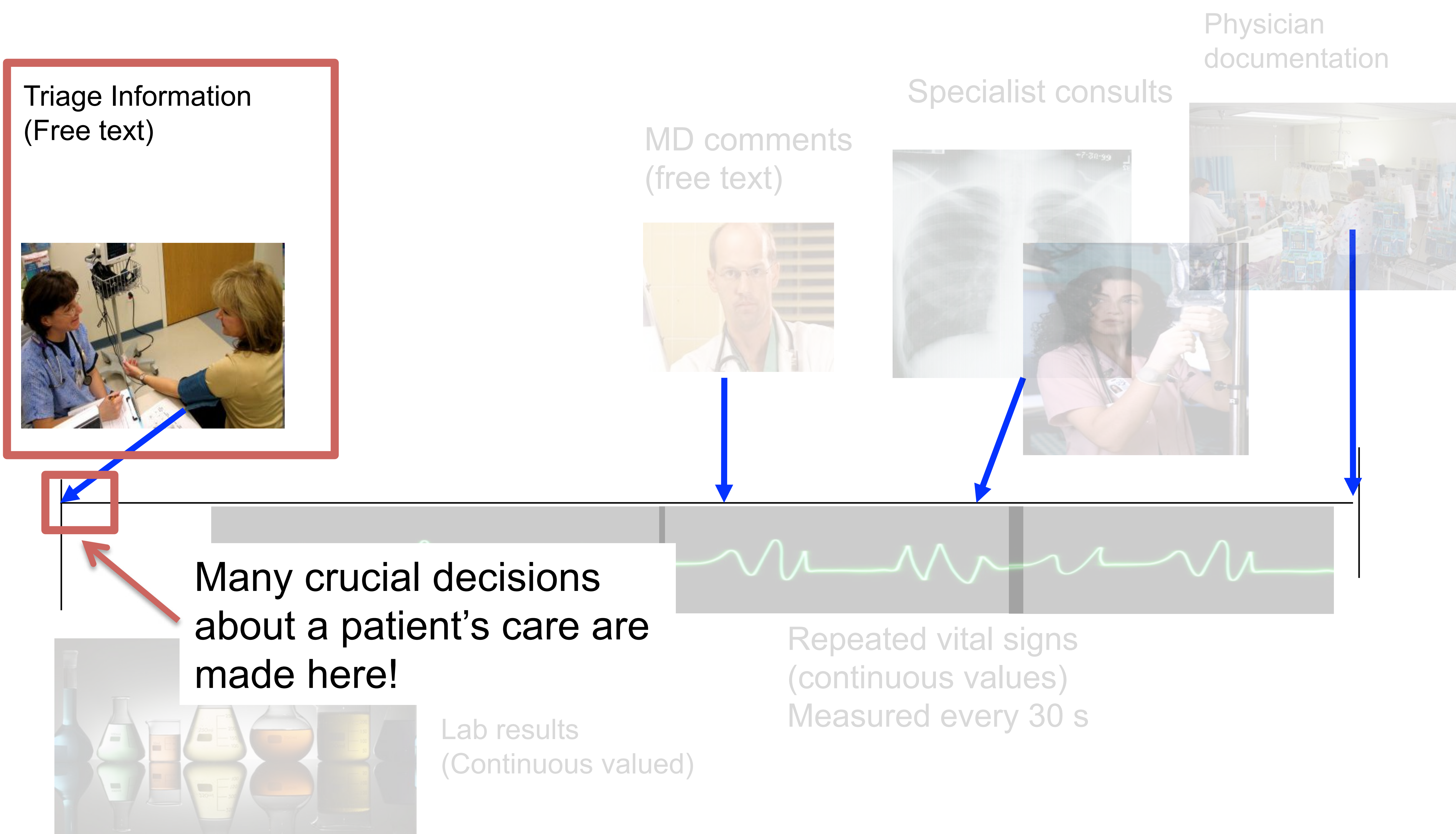
- Decision Trees
- Tree construction
- Overfitting
- Pruning
- Real-valued inputs

Machine Learning in the ER



slide by David Sontag

Can we predict infection?

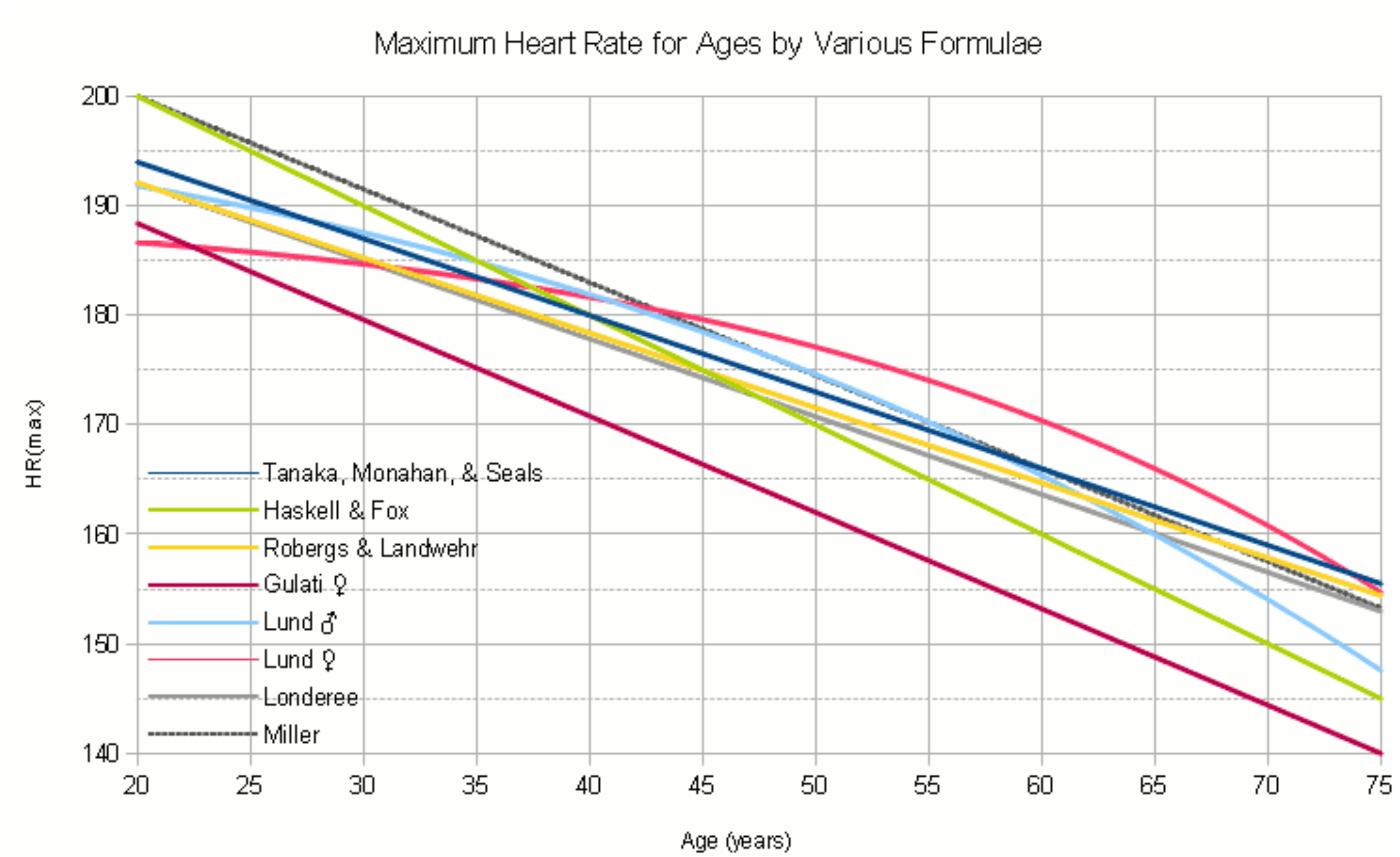


slide by David Sontag

Can we predict infection

- Previous automatic approaches based on simple criteria:
  - Temperature < 96.8 °F or > 100.4 °F
  - Heart rate > 90 beats/min
  - Respiratory rate > 20 breaths/min

- Too simplified... e.g., heart rate depends on age!



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Can we predict infection?

- These are the attributes we have for each patient:
  - Temperature
  - Heart rate (HR)
  - Respiratory rate (RR)
  - Age
  - Acuity and pain level
  - Diastolic and systolic blood pressure (DBP, SBP)
  - Oxygen Saturation (SaO2)
- We have these attributes + label (infection) for 200,000 patients!
- Let's **learn** to classify infection

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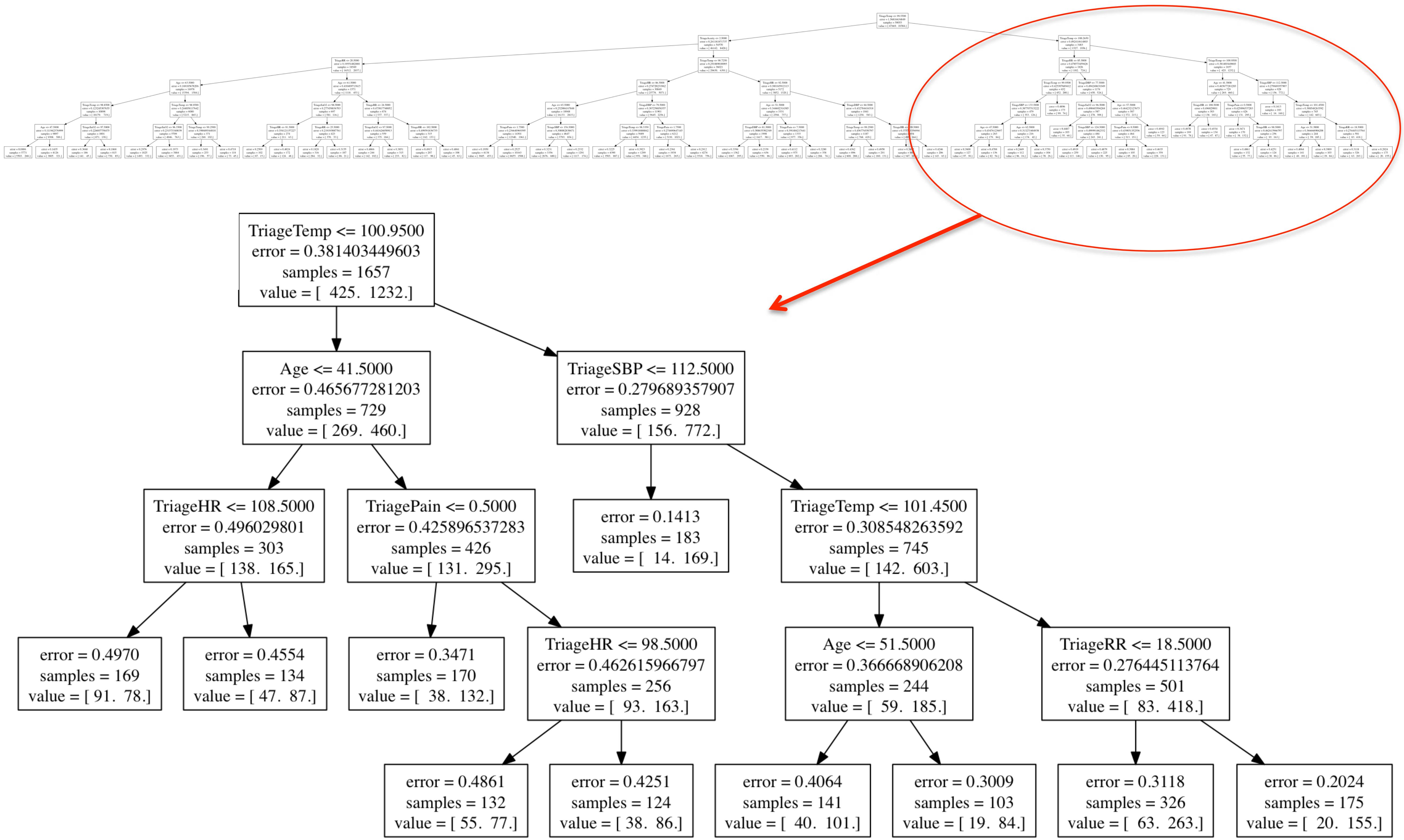
Predicting infection using decision trees



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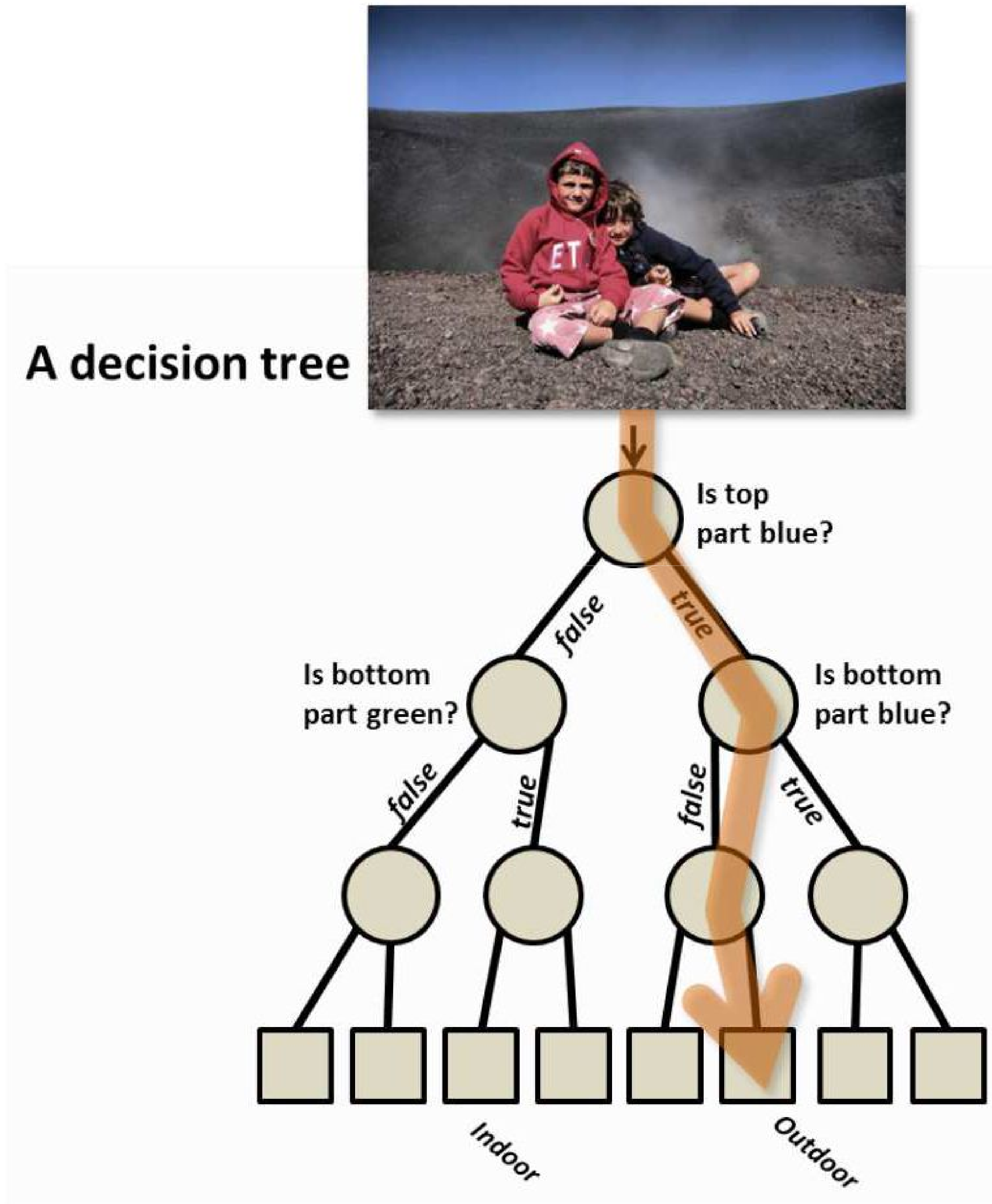
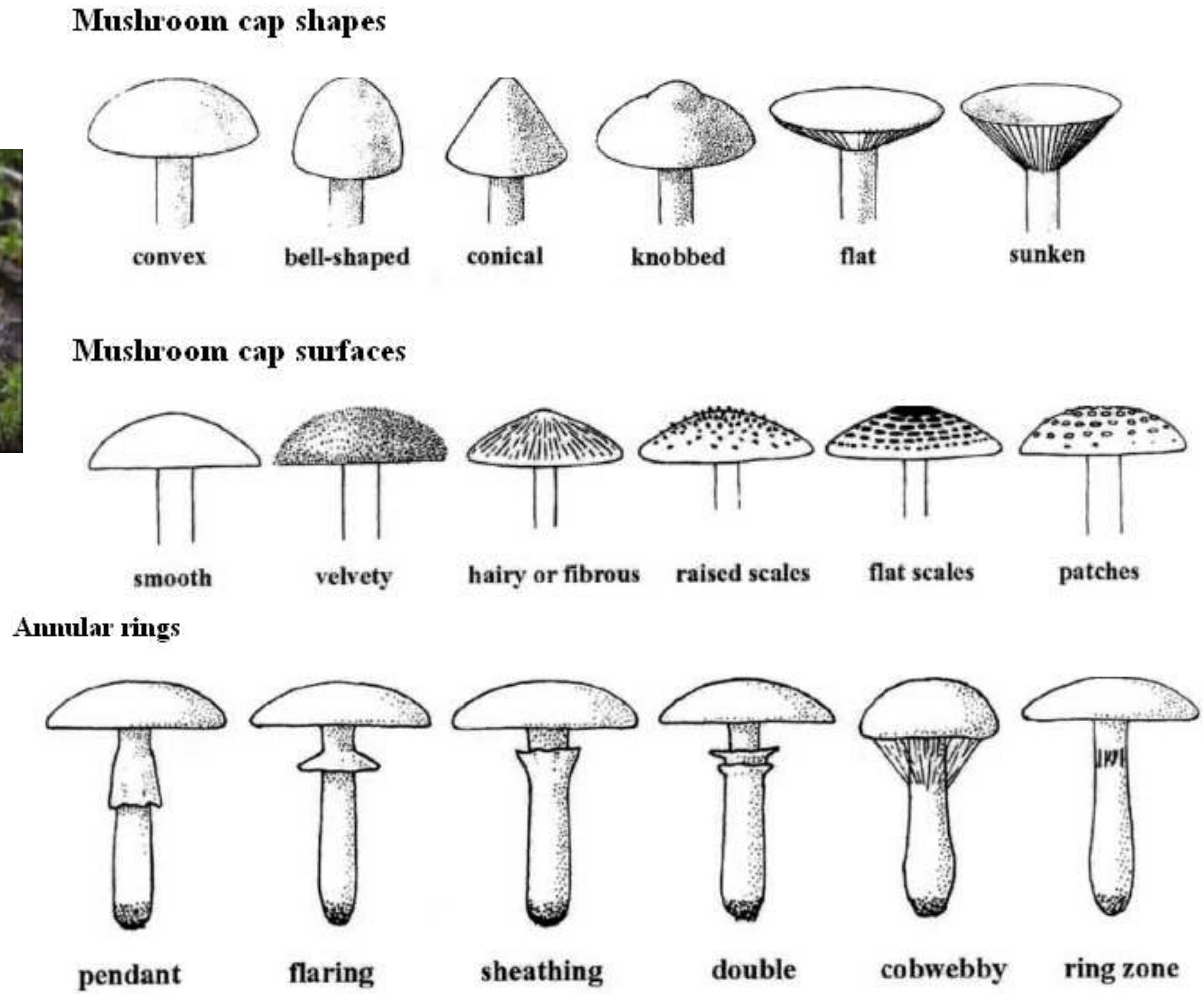
Example: Image Classification



[Criminisi et al, 2011]

slide by Nando de Freitas

Example: Mushrooms



http://www.usask.ca/biology/fungi/

slide by Jerry Zhu

Mushroom features

1. **cap-shape:** bell=b, conical=c, convex=x, flat=f, knobbed=k, sunken=s
2. **cap-surface:** fibrous=f, grooves=g, scaly=y, smooth=s
3. **cap-color:** brown=n, buff=b, cinnamon=c, gray=g, green=r, pink=p,purple=u, red=e, white=w, yellow=y
4. **bruises?:** bruises=t,no=f
5. **odor:** almond=a, anise=l, creosote=c, fishy=y, foul=f, musty=m, none=n, pungent=p, spicy=s
6. **gill-attachment:** attached=a, descending=d, free=f, notched=n
7. ...

slide by Jerry Zhu

Two mushrooms

x_1=x,s,n,t,p,f,c,n,k,e,e,s,s,w,w,p,w,o,p,k,s,u

y_1=p

x_2=x,s,y,t,a,f,c,b,k,e,c,s,s,w,w,p,w,o,p,n,n,g

y_2=e

1. cap-shape: bell=b,conical=c,convex=x,flat=f, knobbed=k,sunken=s
2. cap-surface: fibrous=f,grooves=g,scaly=y,smooth=s
3. cap-color: brown=n,buff=b,cinnamon=c,gray=g,green=r, pink=p,purple=u,red=e,white=w,yellow=y
4. …

slide by Jerry Zhu

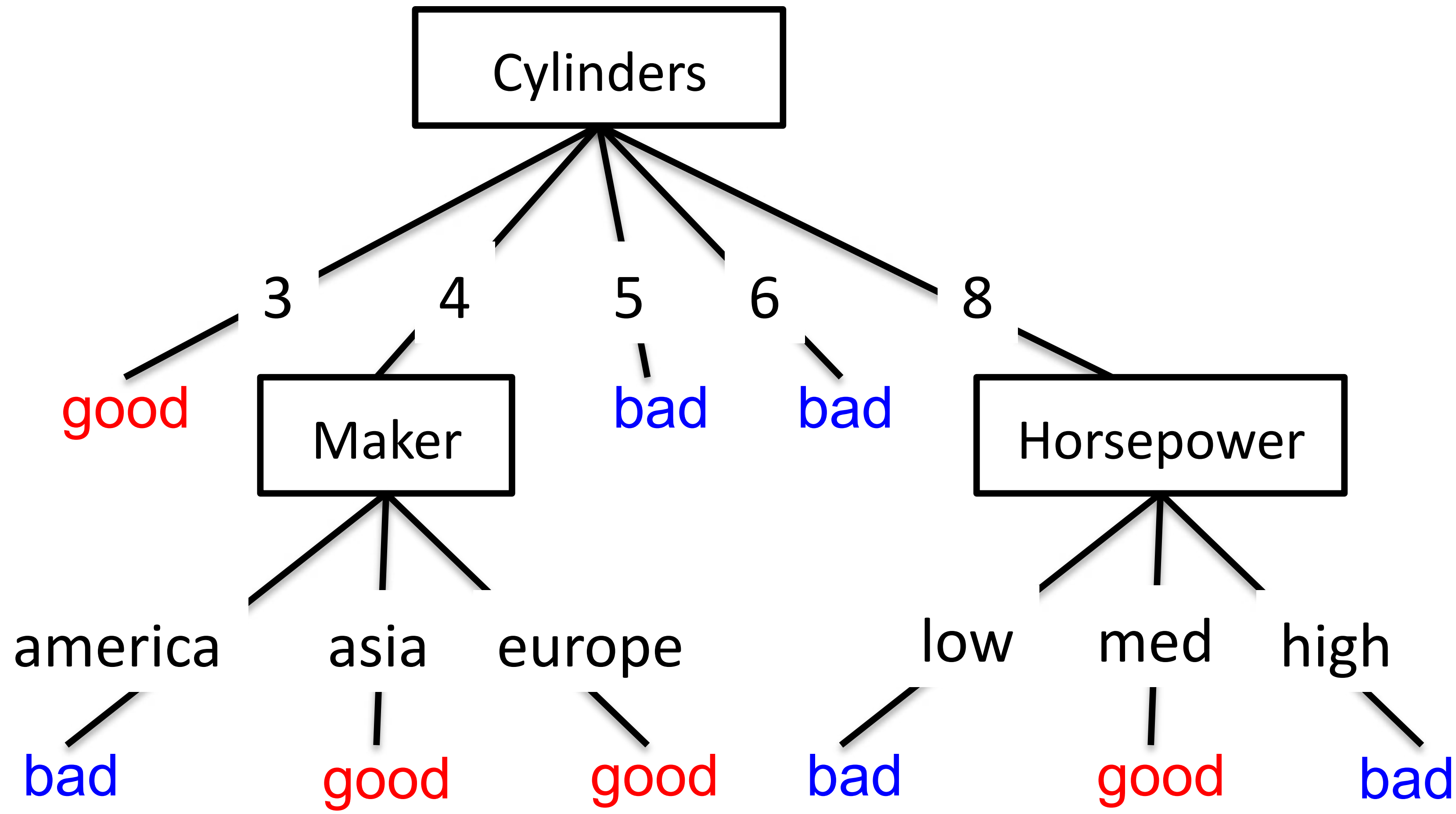
Example: Automobile Miles-per-gallon prediction

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
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
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

slide by Jerry Zhu

Hypotheses: decision trees $f : X \to Y$

- Each internal node tests an attribute x_i
- Each branch assigns an attribute value $x_i = v$
- Each leaf assigns a class y
- To classify input x: traverse the tree from root to leaf, output the labeled y



Human interpretable!

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Hypothesis space

- How many possible hypotheses?
- What functions can be represented?

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
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
bad	8	high	high	high	low	70to74	america
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bad	8	high	high	high	low	75to78	america
good	4	low	low	low	low	79to83	america
bad	6	medium	medium	medium	high	75to78	america
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good	4	low	low	medium	high	79to83	america
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good	4	low	medium	low	medium	75to78	europe
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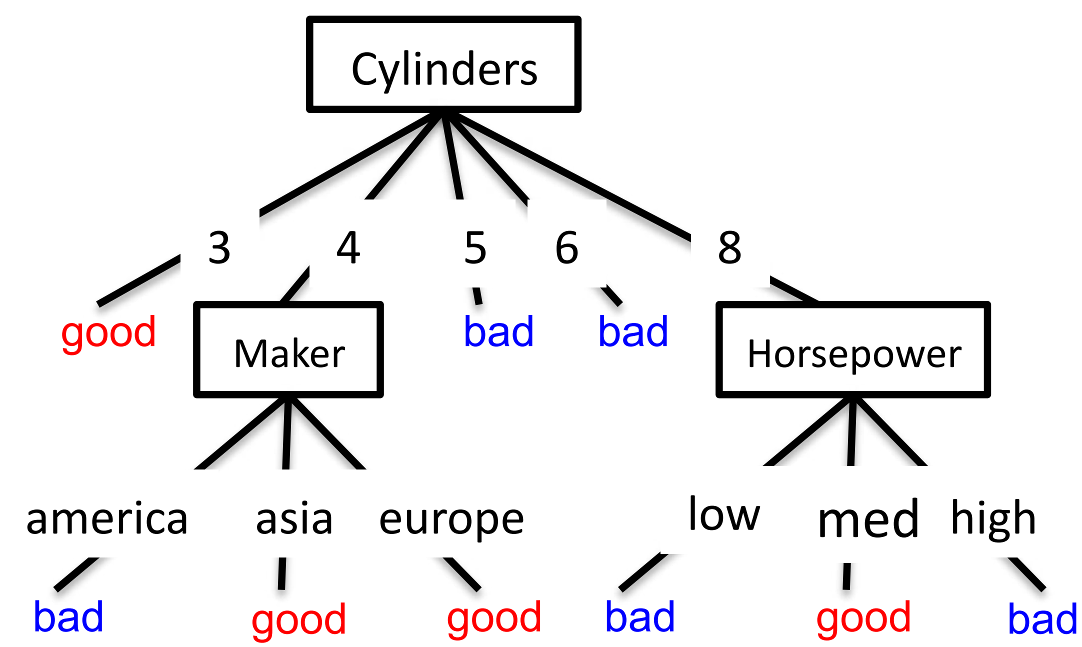

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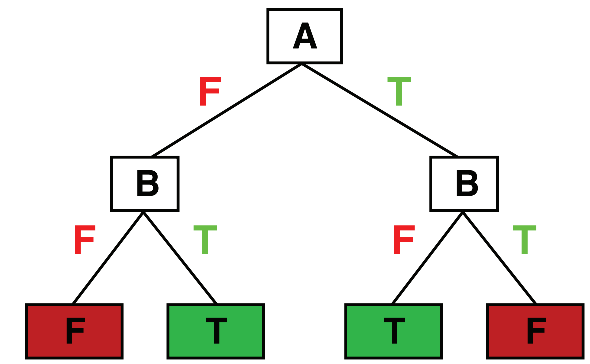
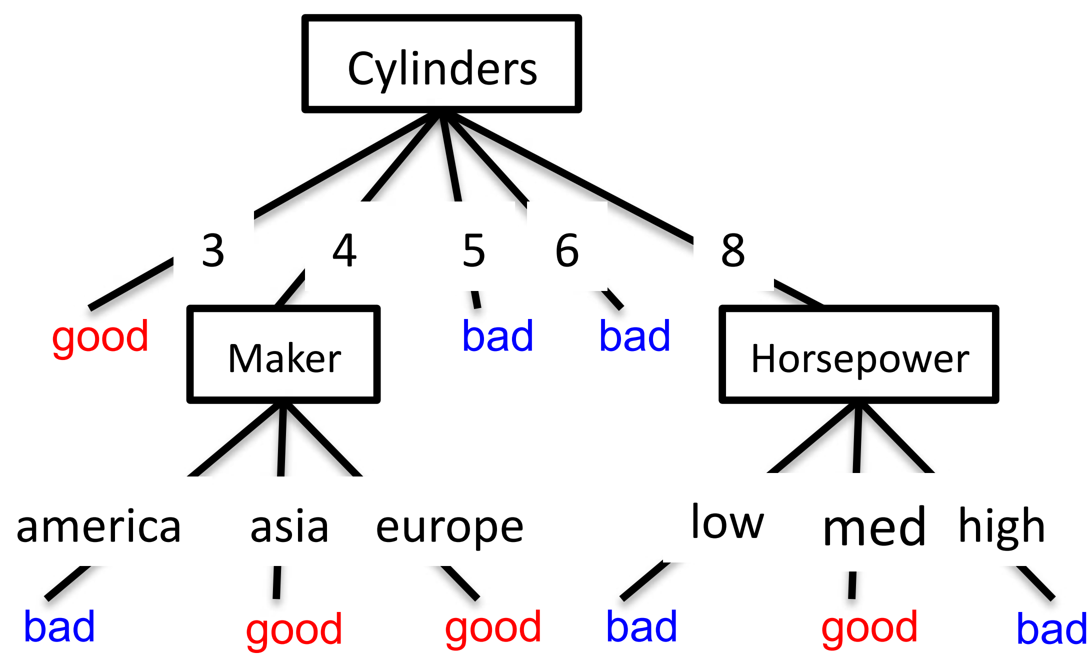
What functions can be represented?

- Decision trees can represent any function of the input attributes!
- For Boolean functions, path to leaf gives truth table row
- But, could require exponentially many nodes…

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



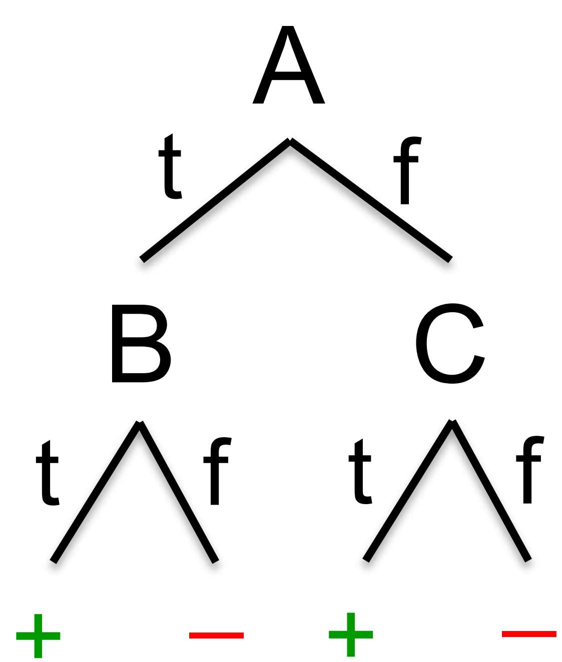
(Figure from Stuart Russell)

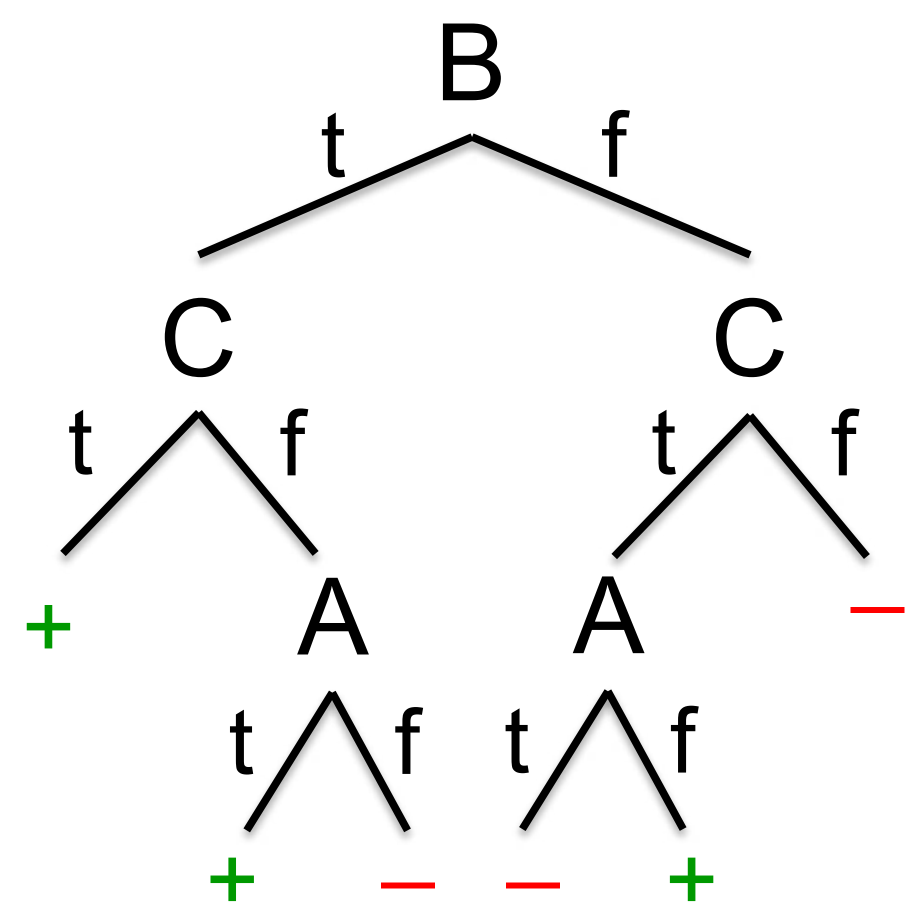


$$cyl=3 \vee (cyl=4 \wedge (maker=asia \vee maker=europe)) \vee \ldots$$

Are all decision trees equal?

- Many trees can represent the same concept
- But, not all trees will have the same size
  - e.g.,$\phi = (A \wedge B) \vee (\neg A \wedge C)$ — ((A and B) or (not A and C))





- Which tree do we prefer?

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Learning decision trees is hard!!!

- Learning the simplest (smallest) decision tree is an NP-complete problem [Hyafil & Rivest ’76]

- Resort to a greedy heuristic:
  - Start from empty decision tree
  - Split on next best attribute (feature)
  - Recurse

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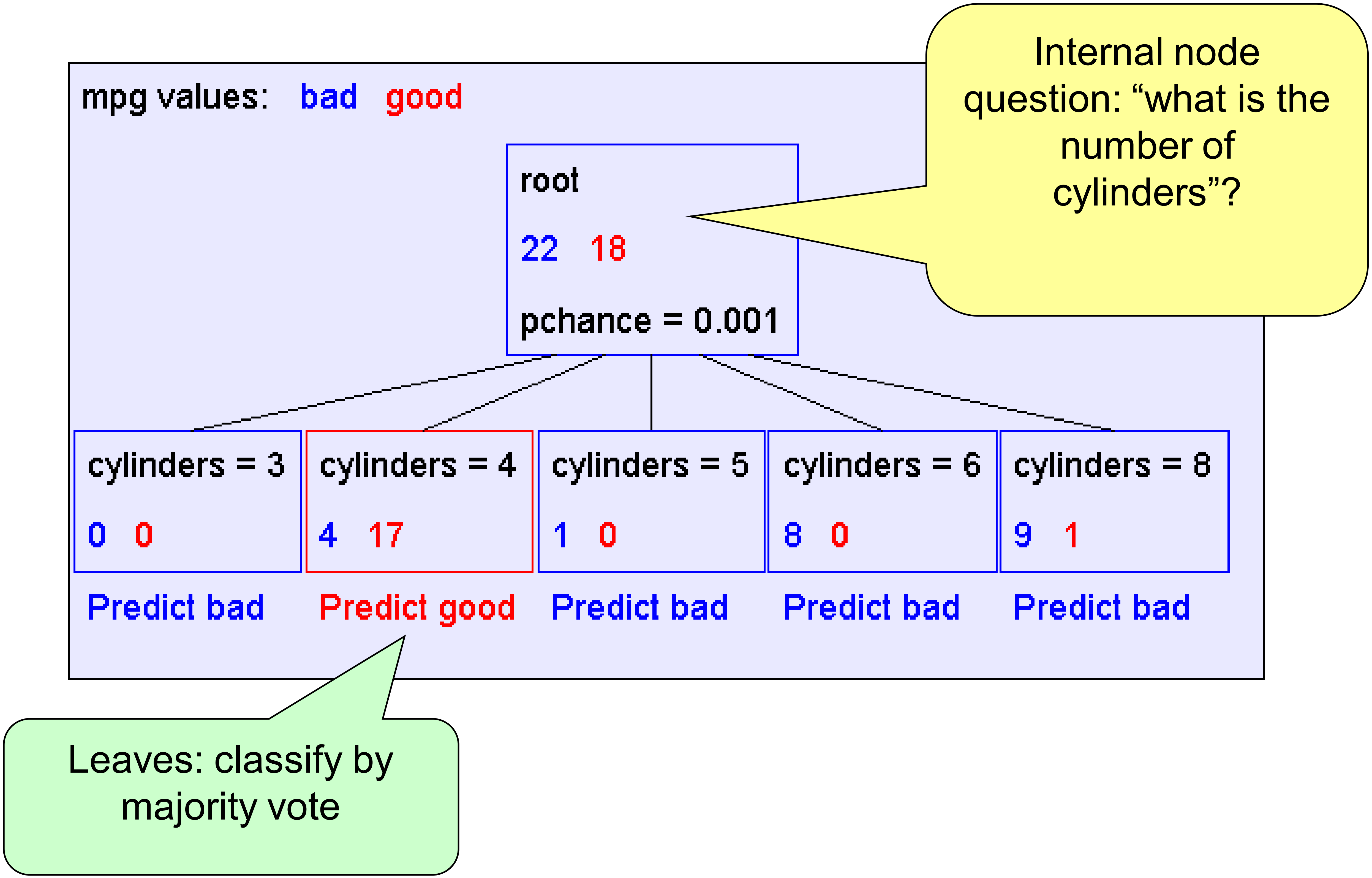
A Decision Stump



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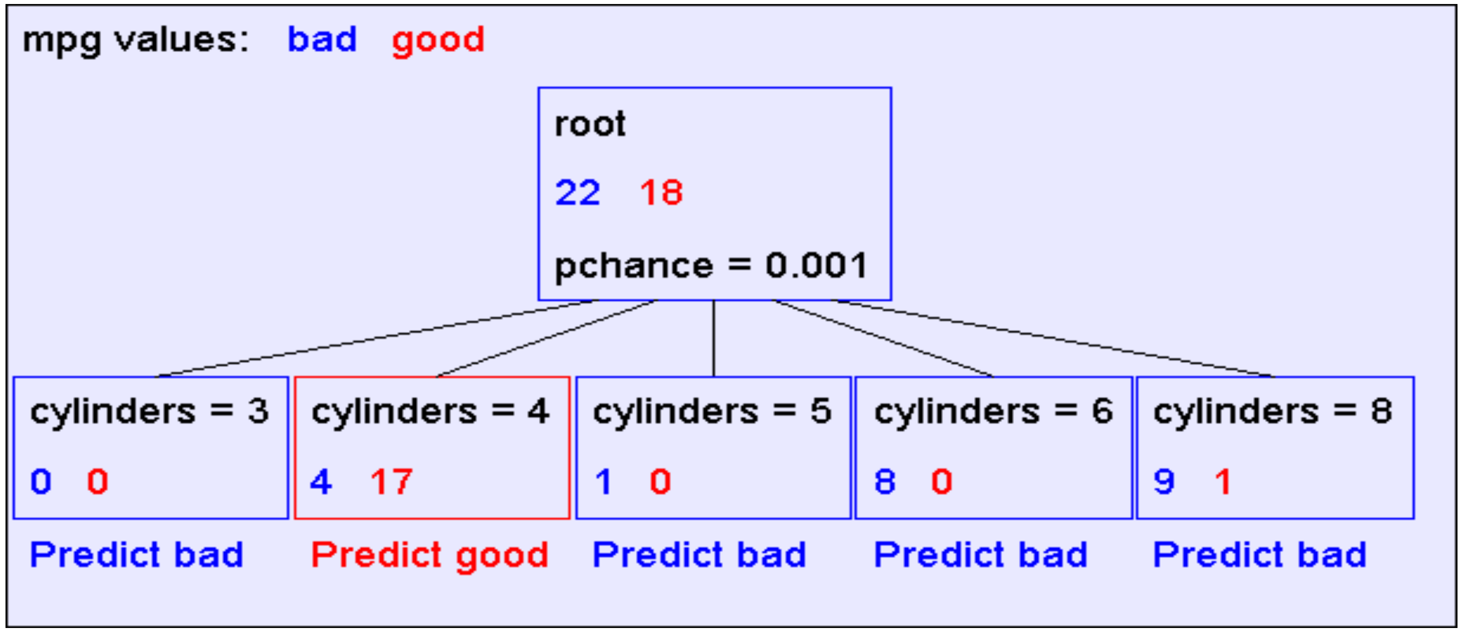
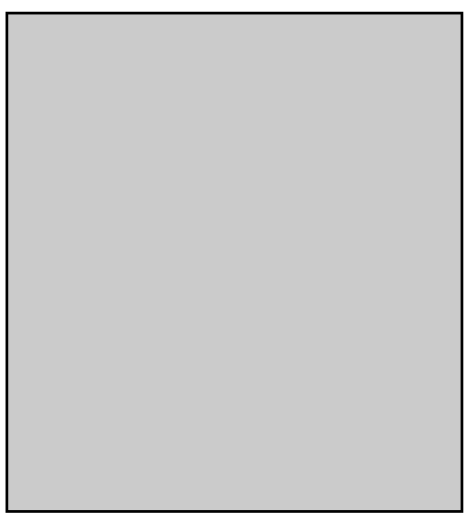
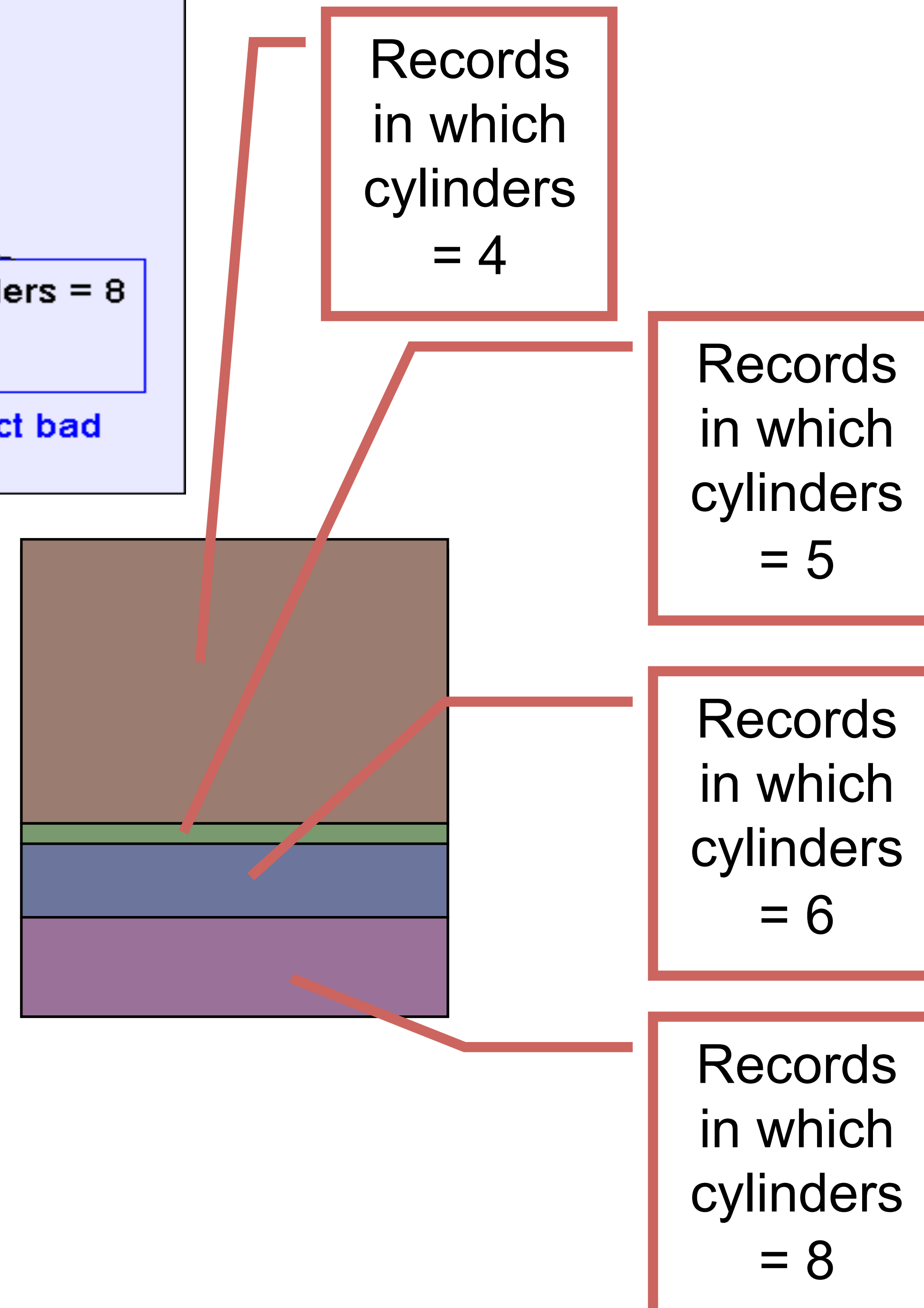
Key idea: Greedily learn trees using **recursion**



Take the Original Dataset..



And partition it according to the value of the attribute we split on



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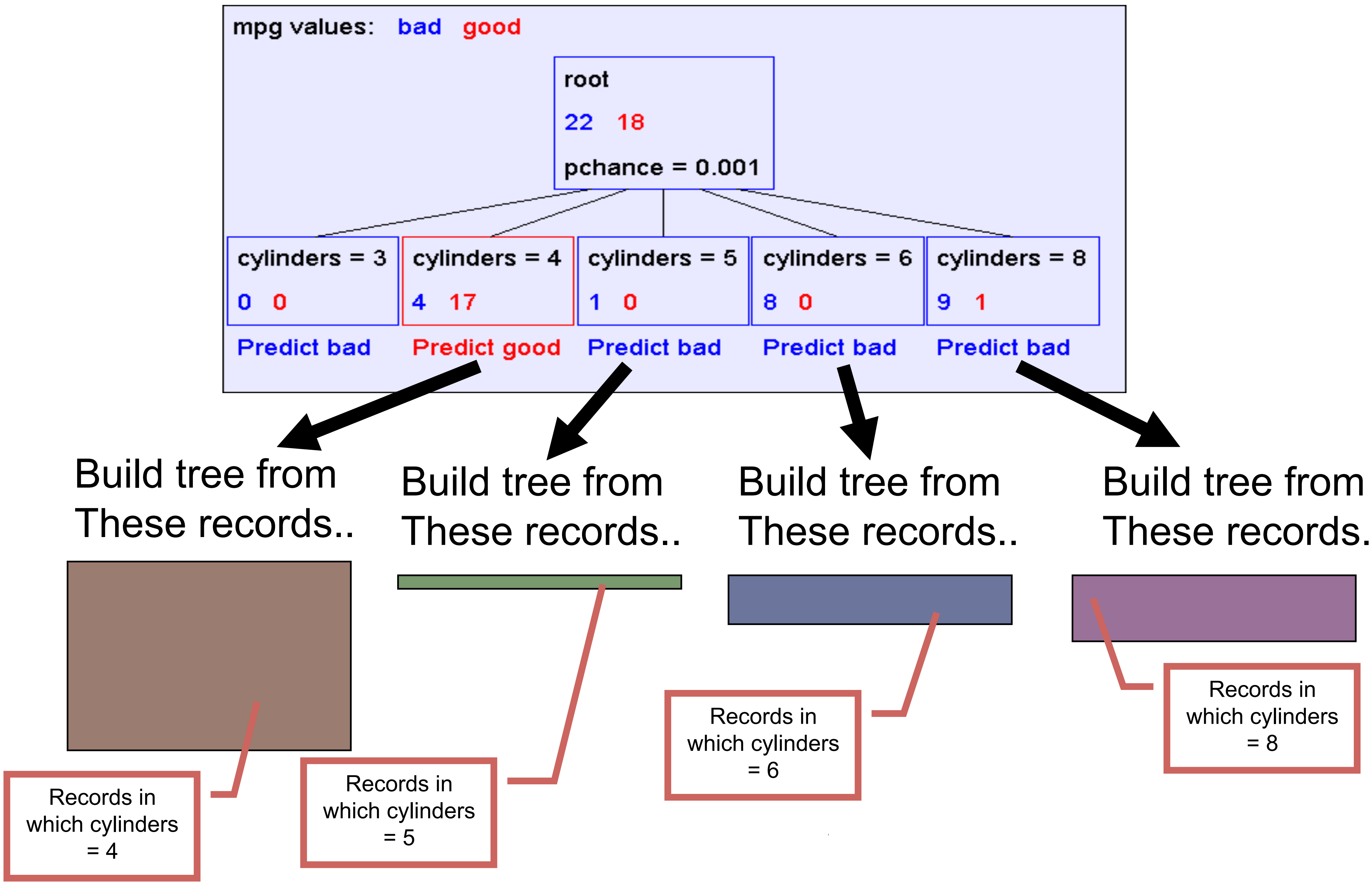
Recursive Step



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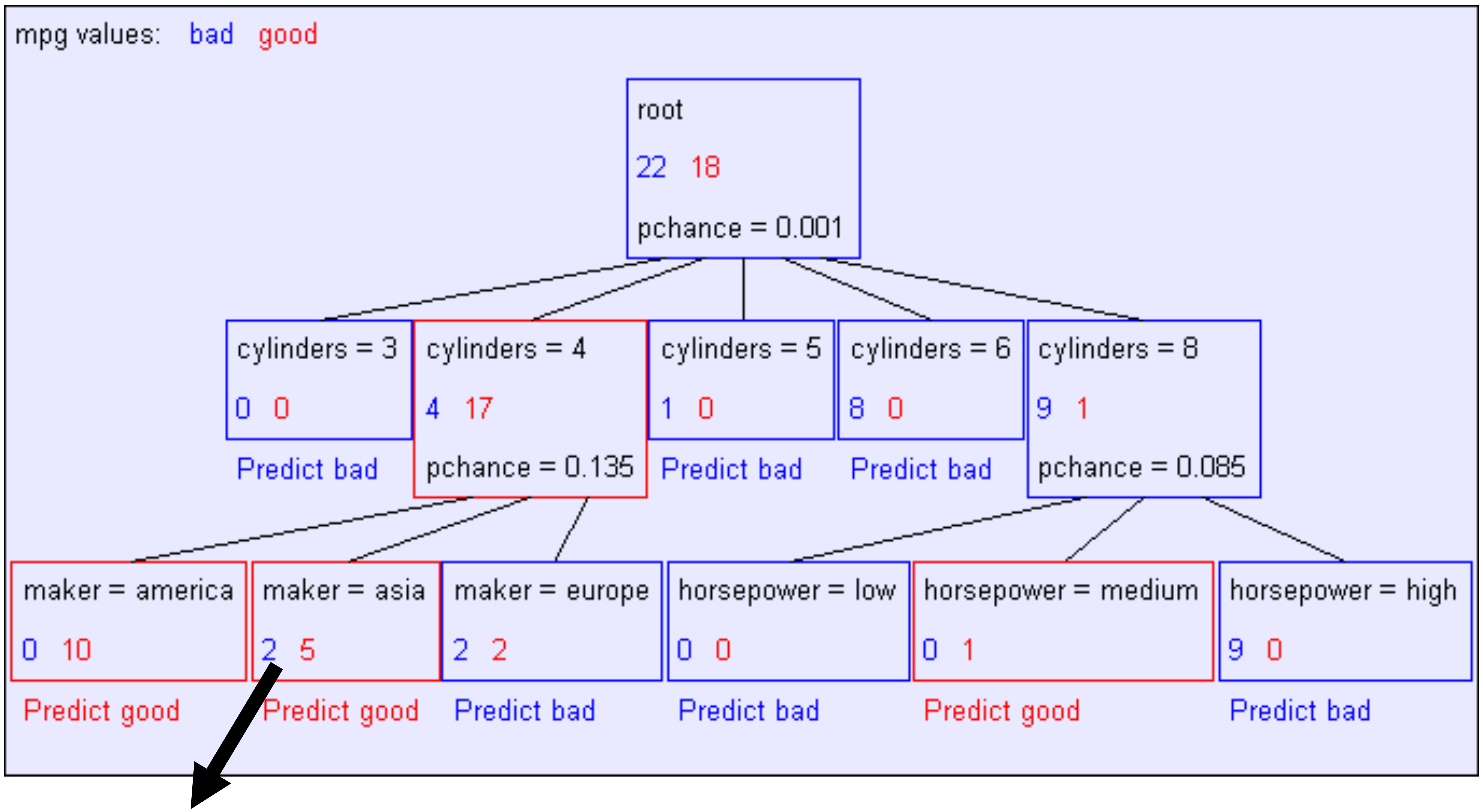
Second level of tree



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)

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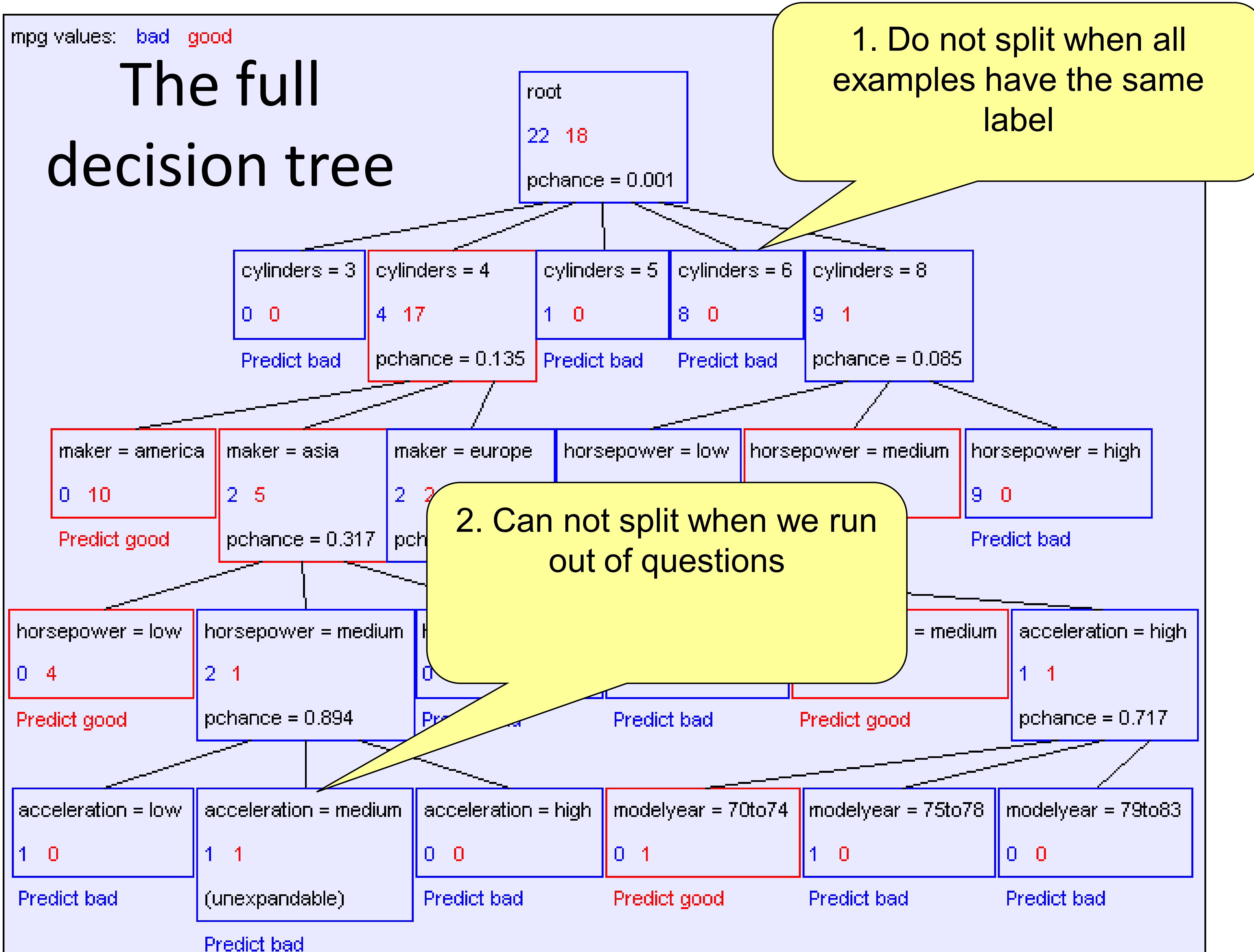
The full decision tree



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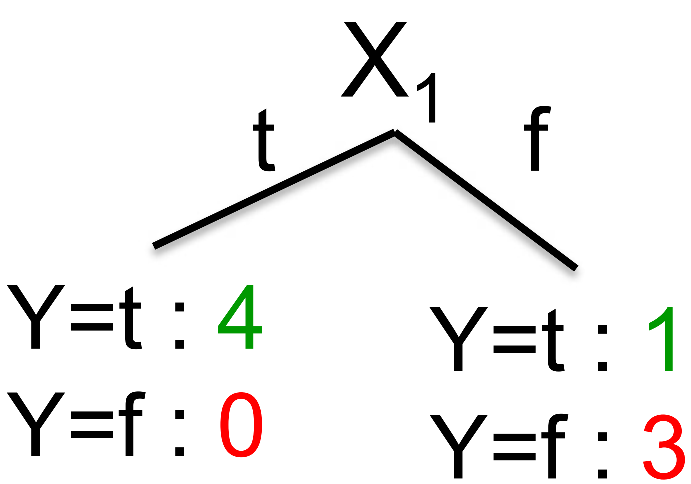
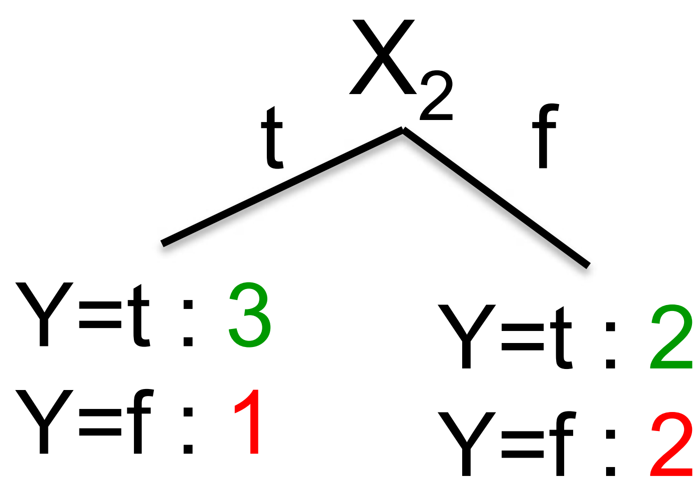
Splitting: Choosing a good attribute

- Would we prefer to split on X_1 or X_2?





X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F
F	T	F
F	F	F

Idea: use counts at leaves to define probability distributions, so we can measure uncertainty!

Measuring uncertainty

- Good split if we are more certain about classification after split
  - Deterministic good (all true or all false)
  - Uniform distribution bad
  - What about distributions in between?

P(Y=A) = 1/2	P(Y=B) = 1/4	P(Y=C) = 1/8	P(Y=D) = 1/8

P(Y=A) = 1/4	P(Y=B) = 1/4	P(Y=C) = 1/4	P(Y=D) = 1/4

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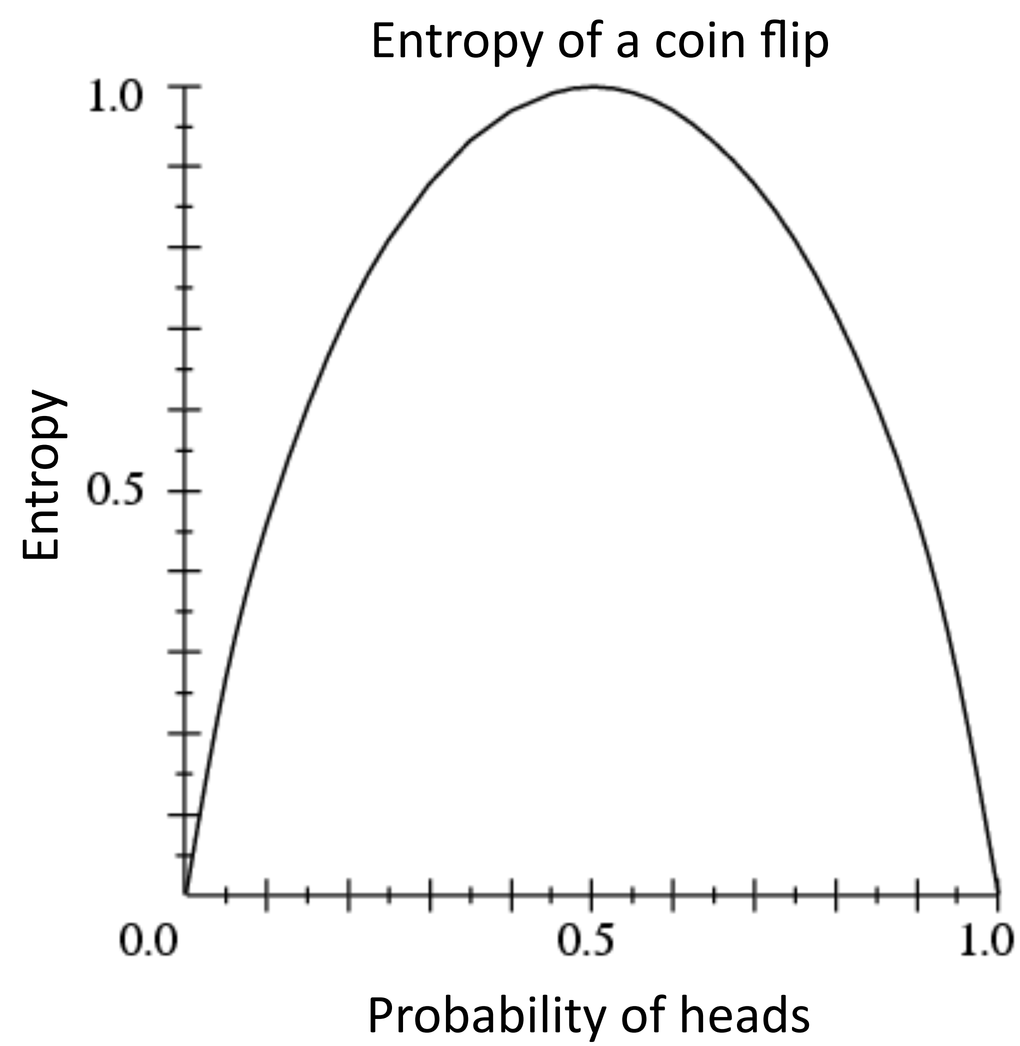
Entropy

- Entropy $H(Y)$ of a random variable Y

$$H(Y) = -\sum_{i=1}^{k} P(Y = y_i) \log_2 P(Y = y_i)$$

- **More uncertainty, more entropy!**
- Information Theory interpretation: $H(Y)$ is the expected number of bits needed to encode a randomly drawn value of Y (under most efficient code)



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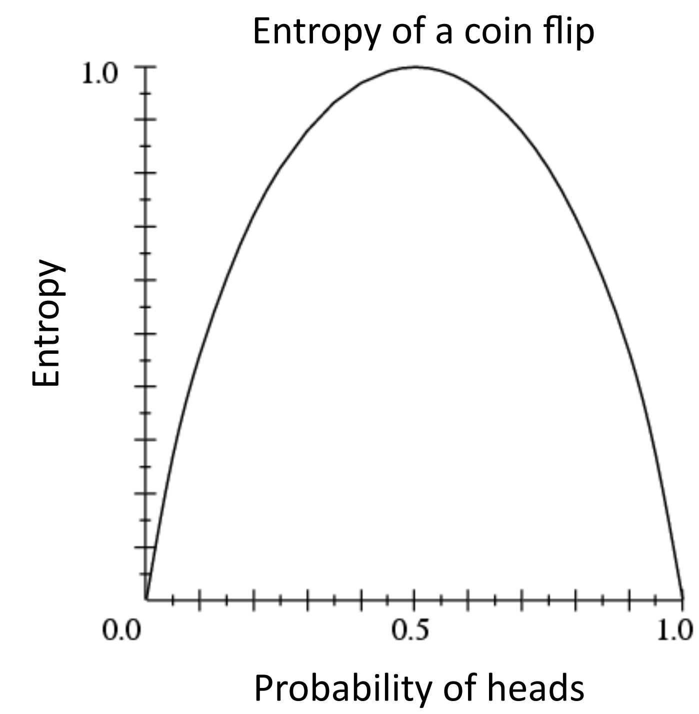
High, Low Entropy

- "High Entropy"
  - Y is from a uniform like distribution
  - Flat histogram
  - Values sampled from it are less predictable

- "Low Entropy"
  - Y is from a varied (peaks and valleys) distribution
  - Histogram has many lows and highs
  - Values sampled from it are more predictable

slide by Vibhav Gogate

Entropy Example



$$H(Y) = -\sum_{i=1}^{k} P(Y = y_i) \log_2 P(Y = y_i)$$

P(Y=t) = 5/6

P(Y=f) = 1/6

X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F

$H(Y) = -\ 5/6 \log_2 5/6 - 1/6 \log_2 1/6$

$= 0.65$

Conditional Entropy

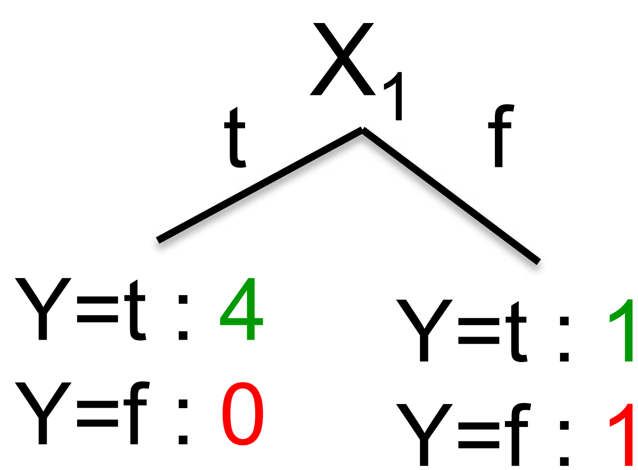
Conditional Entropy $H(Y|X)$ of a random variable Y conditioned on a random variable X

$$H(Y \mid X) = -\sum_{j=1}^{v} P(X = x_j) \sum_{i=1}^{k} P(Y = y_i \mid X = x_j) \log_2 P(Y = y_i \mid X = x_j)$$

Example:

$P(X_1=t) = 4/6$

$P(X_1=f) = 2/6$



X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F

$H(Y|X_1) = -\ 4/6\ (1 \log_2 1 + 0 \log_2 0)$

$\quad -\ 2/6\ (1/2 \log_2 1/2 + 1/2 \log_2 1/2)$

$= 2/6$

slide by David Sontag

Information gain

- Decrease in entropy (uncertainty) after splitting

$$IG(X) = H(Y) - H(Y \mid X)$$

In our running example:

$IG(X_1) = H(Y) – H(Y|X_1)$
$= 0.65 – 0.33$

$IG(X_1) > 0 \rightarrow$ we prefer the split!

X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F

slide by David Sontag

Learning decision trees

- Start from empty decision tree
- Split on **next best attribute (feature)**
  - Use, for example, information gain to select attribute:

$$\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$$

- Recurse

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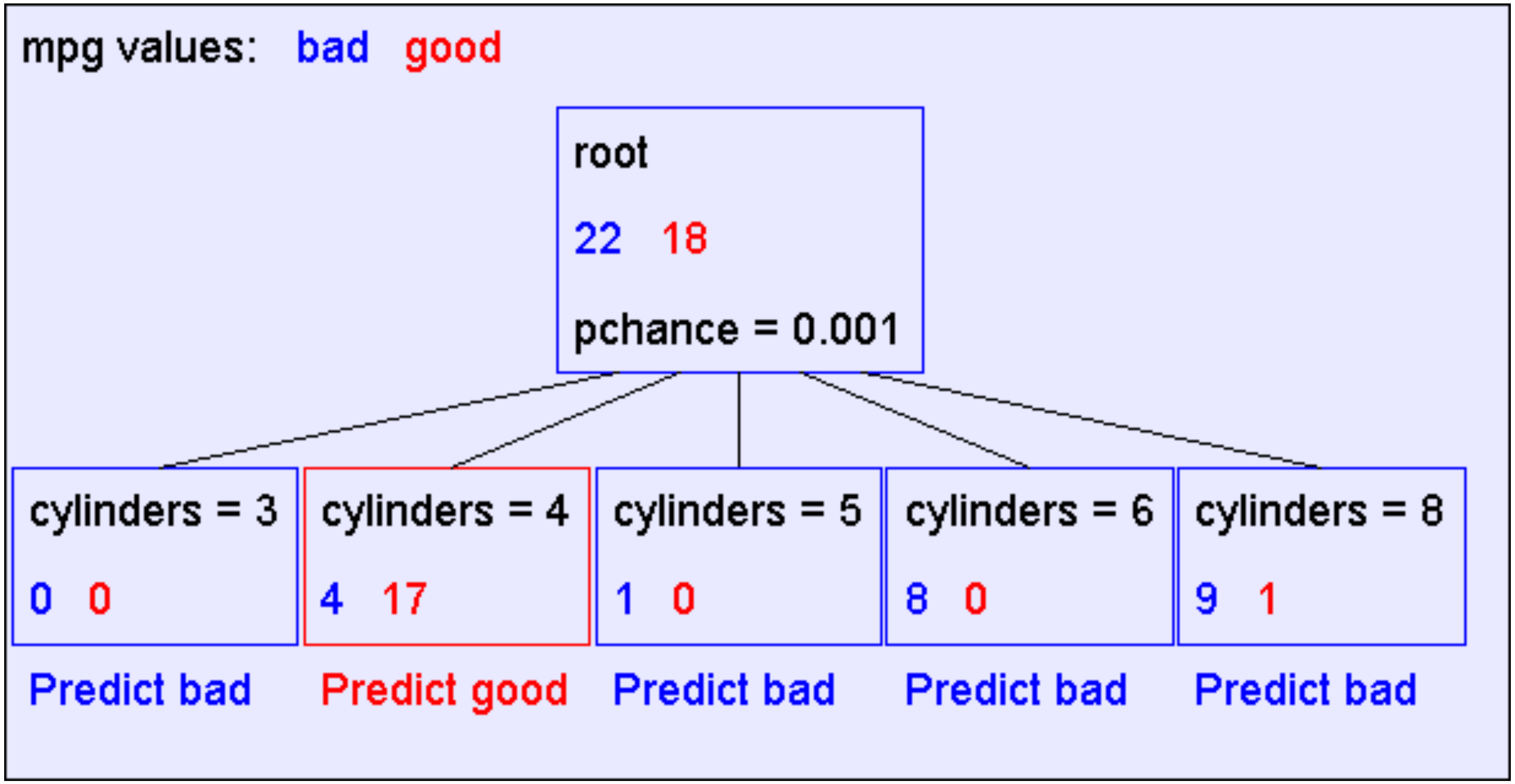
When to stop?



- First split looks good! But, when do we stop?

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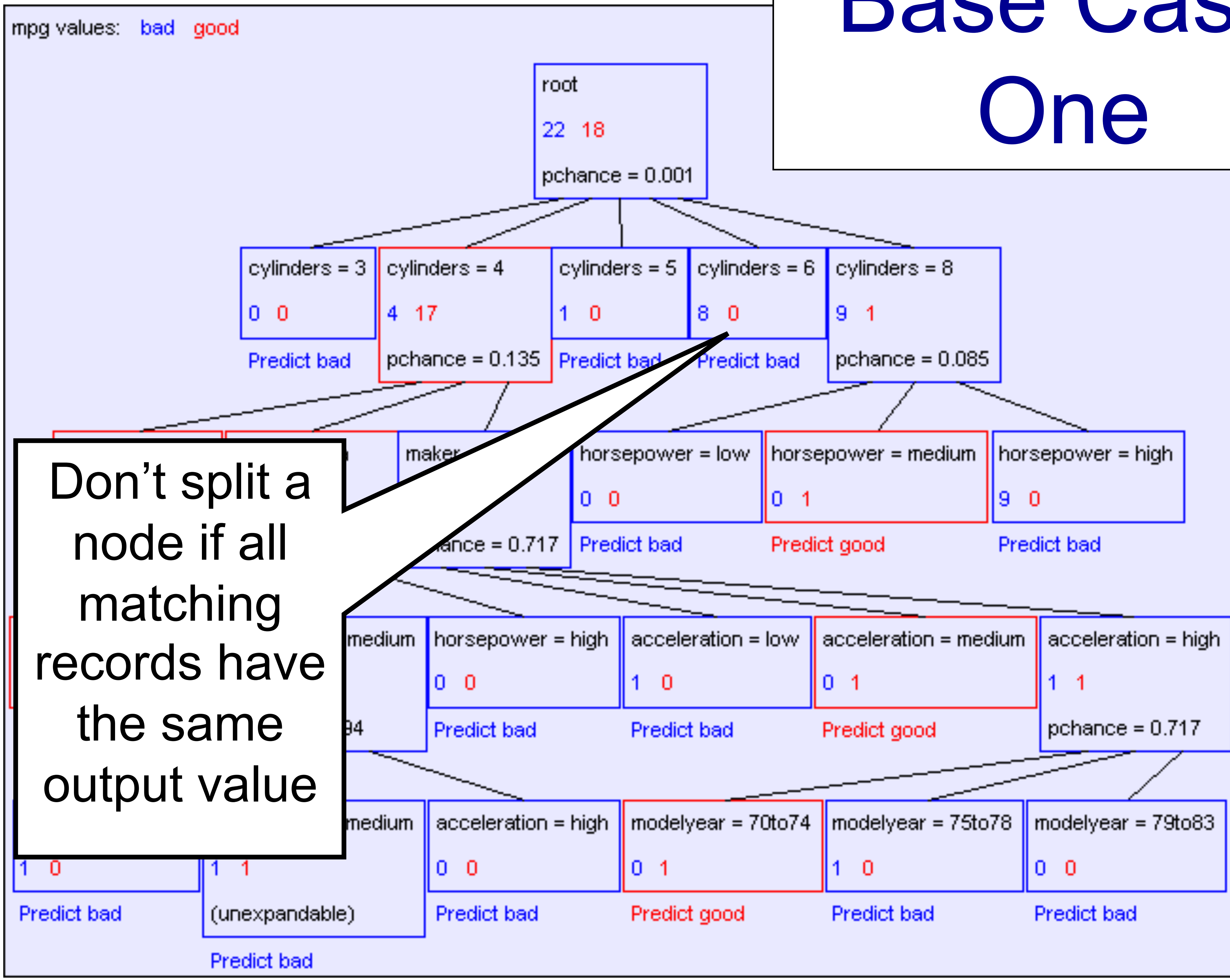
Base Case One



Don't split a node if all matching records have the same output value

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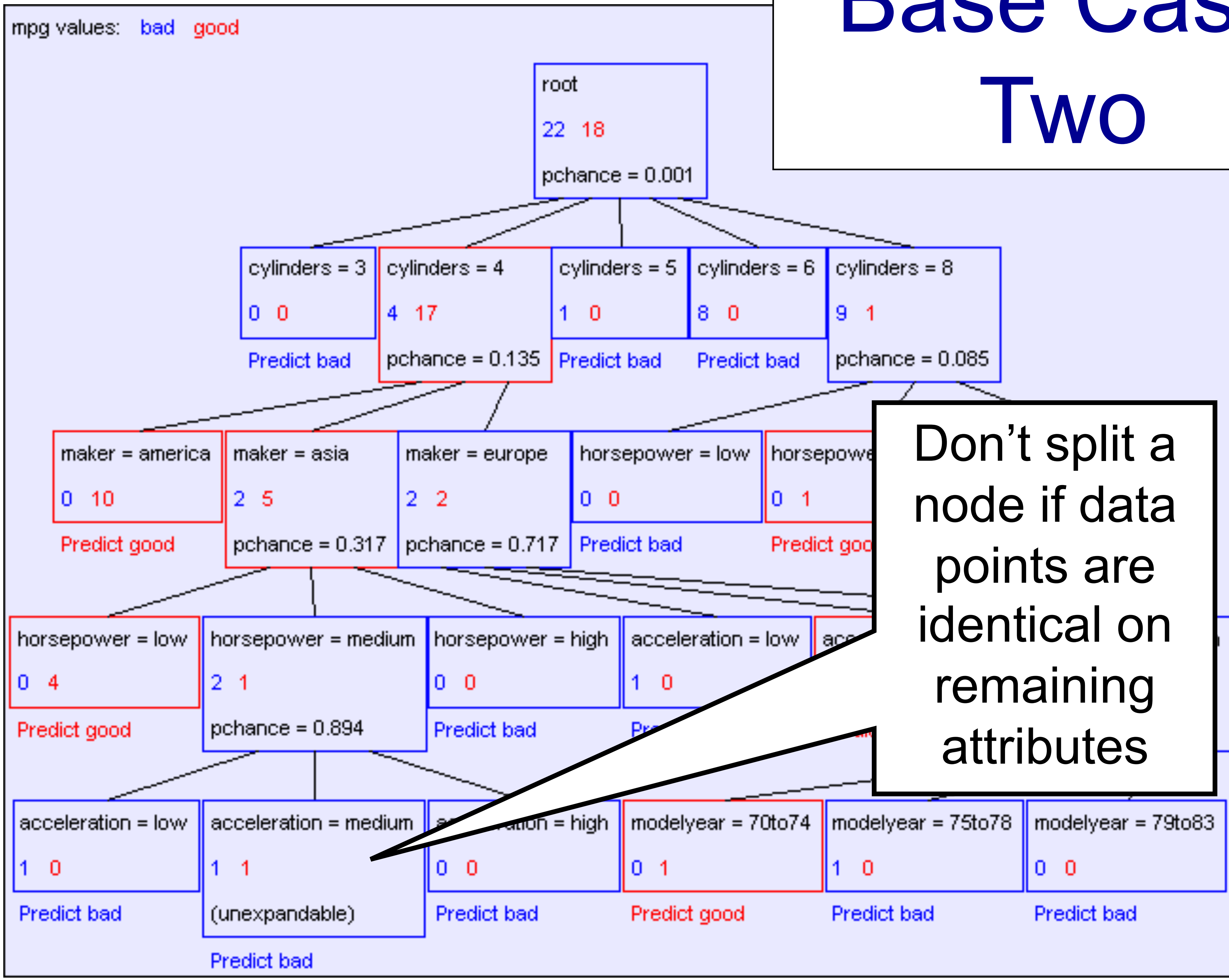
Base Case Two



Don't split a node if data points are identical on remaining attributes

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Base Cases: An idea

- **Base Case One:** If all records in current data subset have the same output then don’t recurse
- **Base Case Two:** If all records have exactly the same set of input attributes then don’t recurse

Proposed Base Case 3:
If all attributes have small information gain then don’t recurse

- *This is not a good idea*

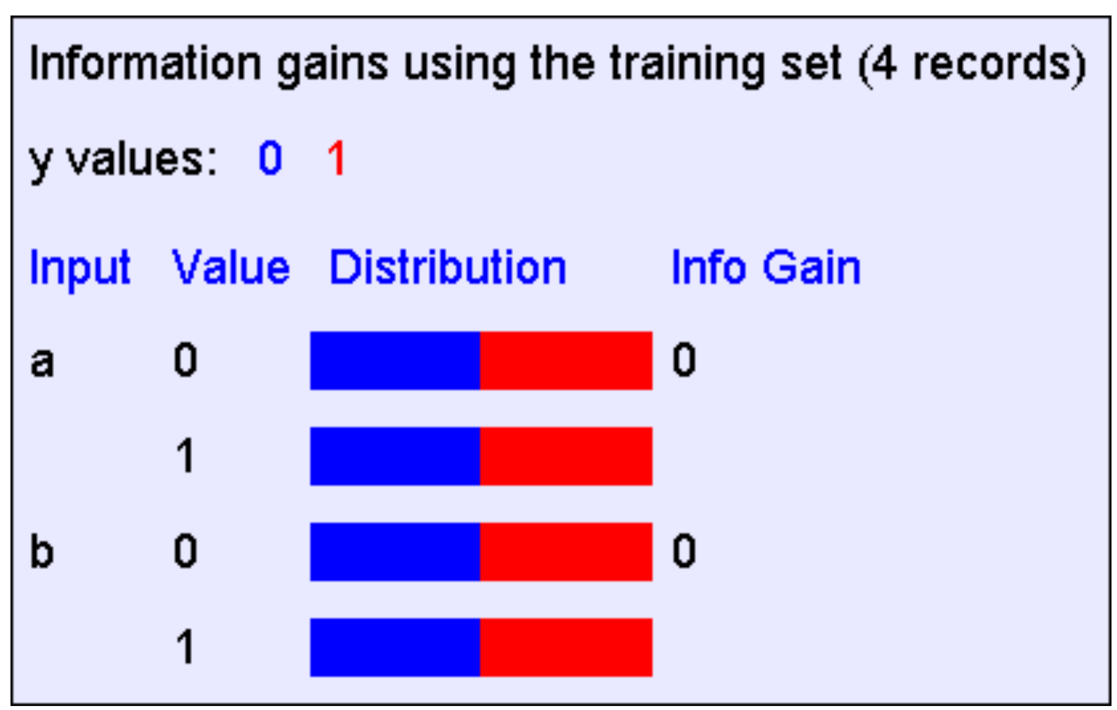
slide by David Sontag

The problem with proposed case 3

y = a XOR b

a	b	y
0	0	0
0	1	1
1	0	1
1	1	0

The information gains:



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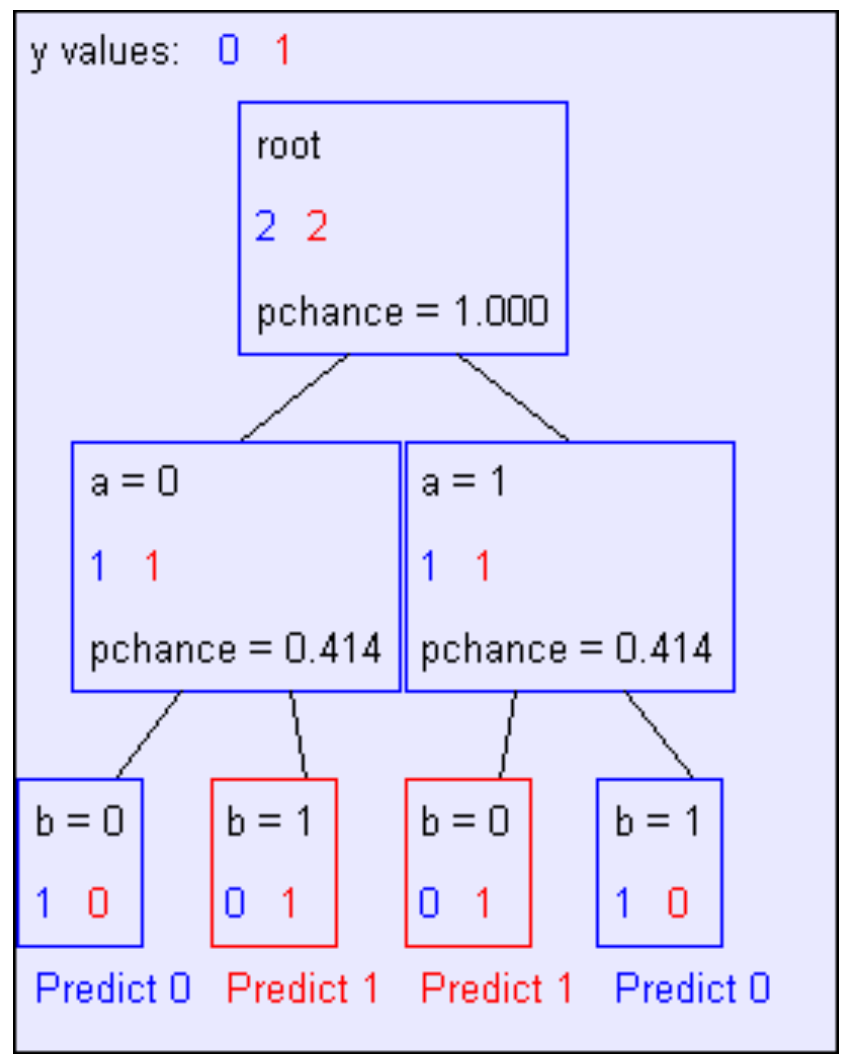
If we omit proposed case 3:

y = a XOR b

a	b	y
0	0	0
0	1	1
1	0	1
1	1	0

The resulting decision tree:



Instead, perform **pruning** after building a tree

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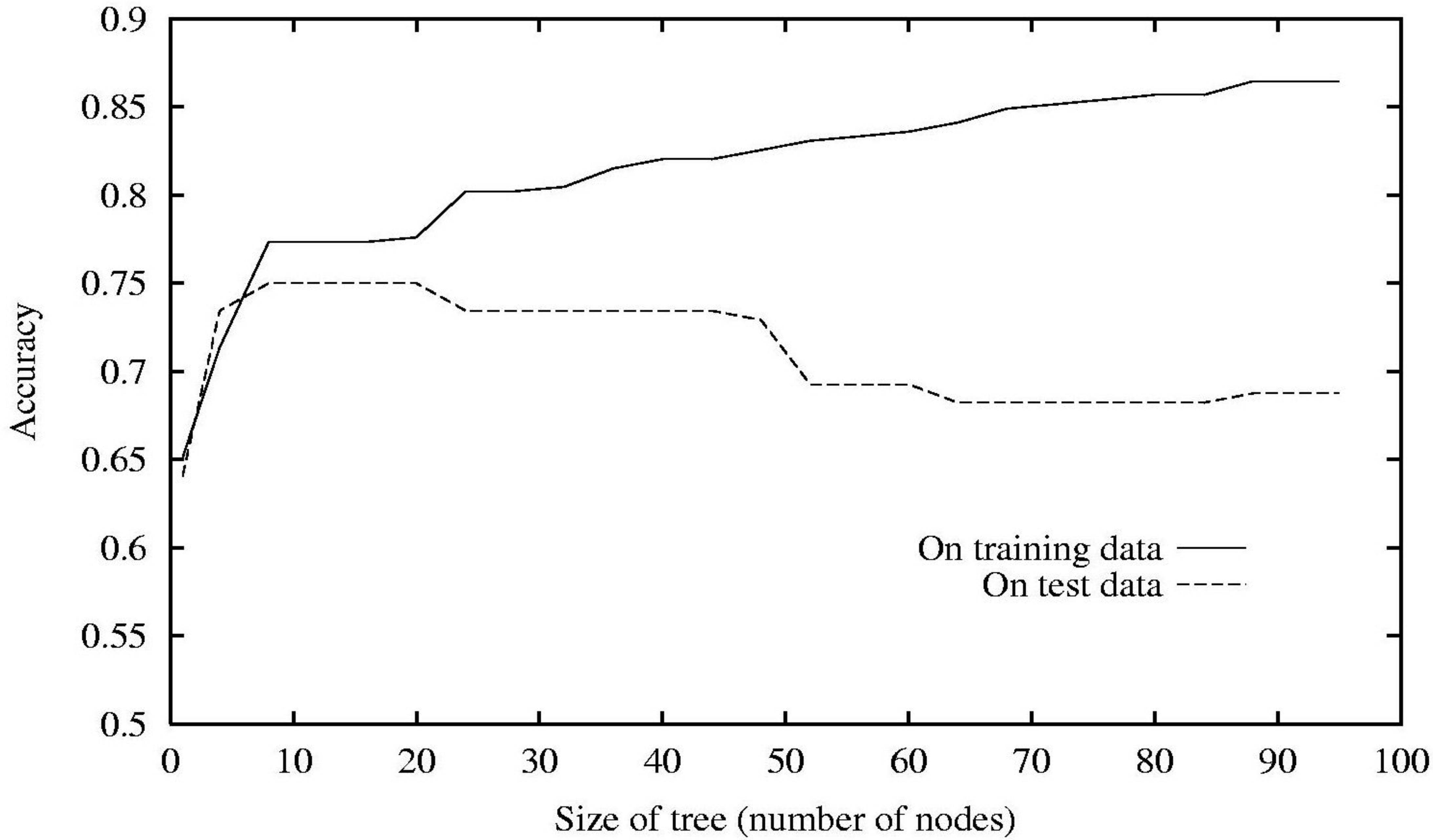
Decision trees will overfit



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Decision trees will overfit

- Standard decision trees have no learning bias
  - Training set error is always zero!
    - (If there is no label noise)
  - Lots of variance
  - Must introduce some bias towards simpler trees

- Many strategies for picking simpler trees
  - Fixed depth
  - Fixed number of leaves

- Random forests

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Real-valued inputs

- What should we do if some of the inputs are real-valued?

Infinite number of possible split values!!!

mpg	cylinders	displacemen	horsepower	weight	acceleration	modelyear	maker
good	4	97	75	2265	18.2	77	asia
bad	6	199	90	2648	15	70	america
bad	4	121	110	2600	12.8	77	europe
bad	8	350	175	4100	13	73	america
bad	6	198	95	3102	16.5	74	america
bad	4	108	94	2379	16.5	73	asia
bad	4	113	95	2228	14	71	asia
bad	8	302	139	3570	12.8	78	america
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
good	4	120	79	2625	18.6	82	america
bad	8	455	225	4425	10	70	america
good	4	107	86	2464	15.5	76	europe
bad	5	131	103	2830	15.9	78	europe

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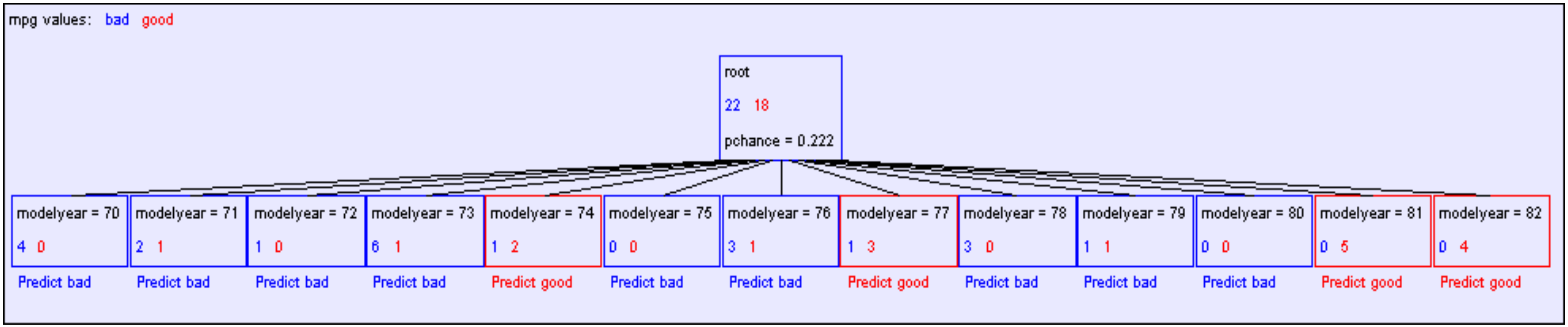
“One branch for each numeric value” idea:



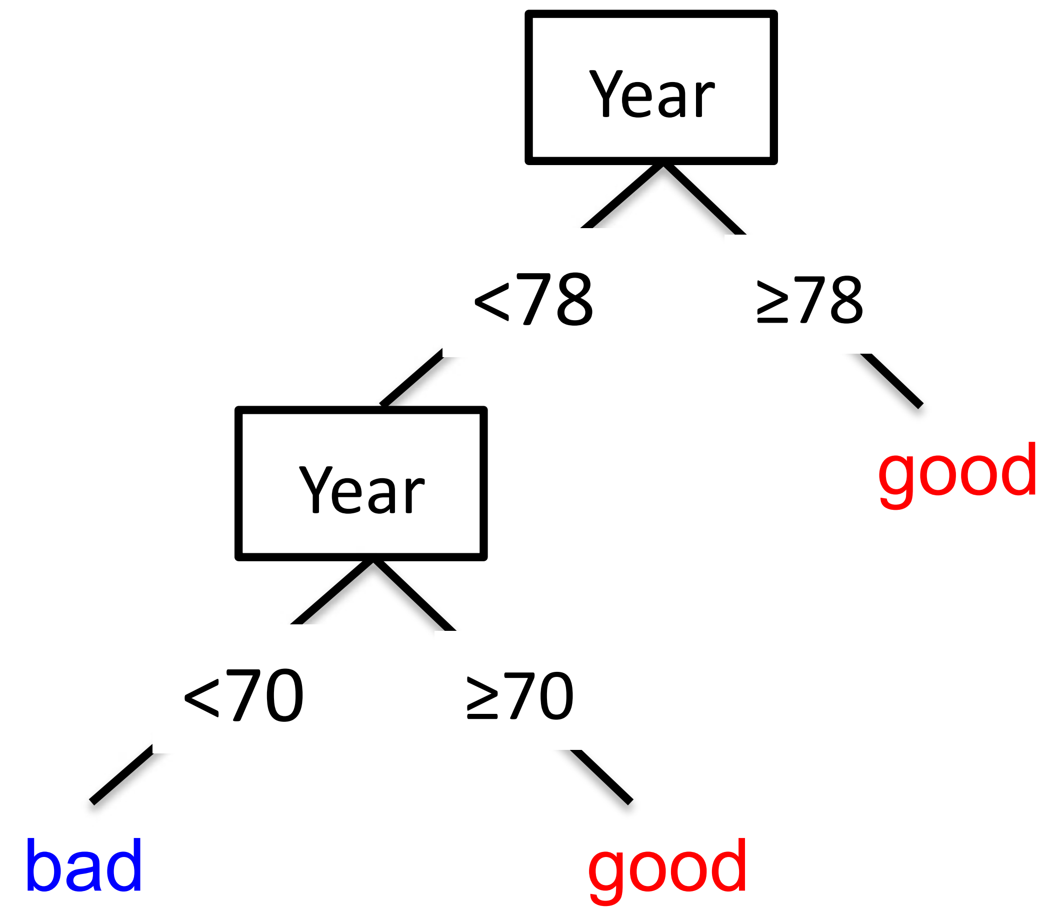
Hopeless: hypothesis with such a high branching factor will shatter **any** dataset and overfit

slide by David Sontag

Threshold splits

- Binary tree: split on attribute X at value t
  - One branch: X < t
  - Other branch: X ≥ t

- Requires small change
  - Allow repeated splits on same variable **along a path**



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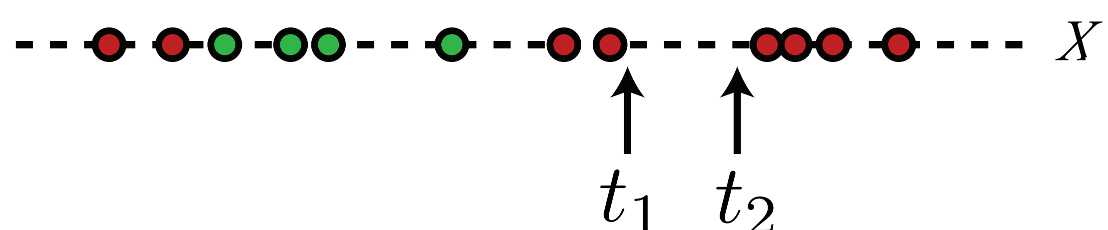
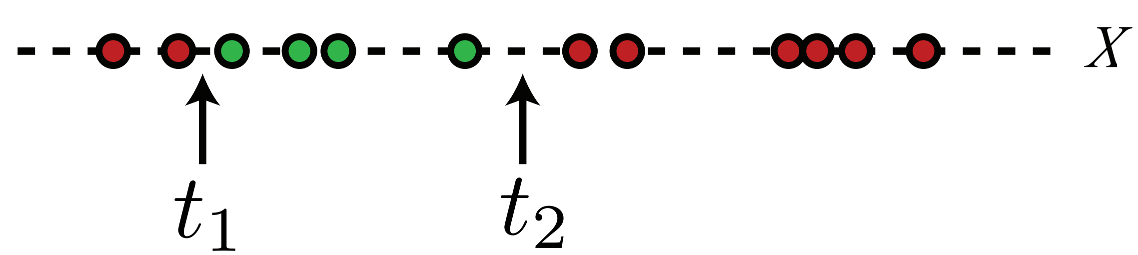
The set of possible thresholds

- Binary tree, split on attribute X
  - One branch: $X < t$
  - Other branch: $X \geq t$
- Search through possible values of t
  - Seems hard!!!
- But only a finite number of t's are important:



- Sort data according to X into $\{x_1,\ldots,x_m\}$
- Consider split points of the form $x_i + (x_{i+1} - x_i)/2$
- Moreover, only splits between examples from different classes matter!



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Picking the best threshold

- Suppose X is real valued with threshold t
- Want $IG(Y \mid X{:}t)$, the information gain for Y when testing if X is greater than or less than t
- Define:
  - $H(Y \mid X{:}t) = p(X<t)H(Y \mid X<t)+p(X>=\mathrm{t})H(Y \mid X>=t)$
  - $IG(Y \mid X{:}t) = H(Y) - H(Y \mid X{:}t)$
  - $IG^*(Y \mid X) = \max_t IG(Y \mid X{:}t)$
- Use: $IG^*(Y \mid X)$ for continuous variables

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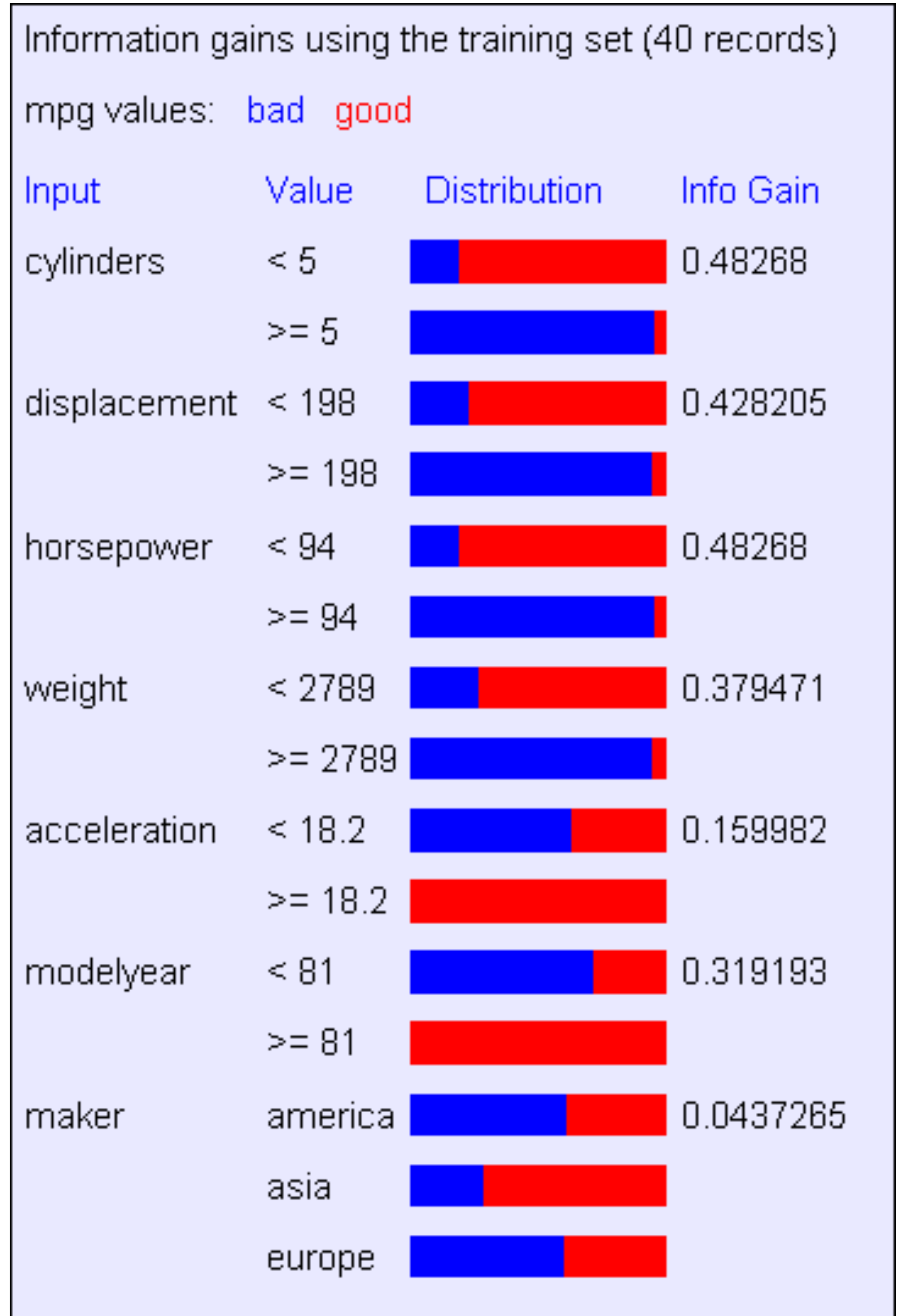
Example with MPG



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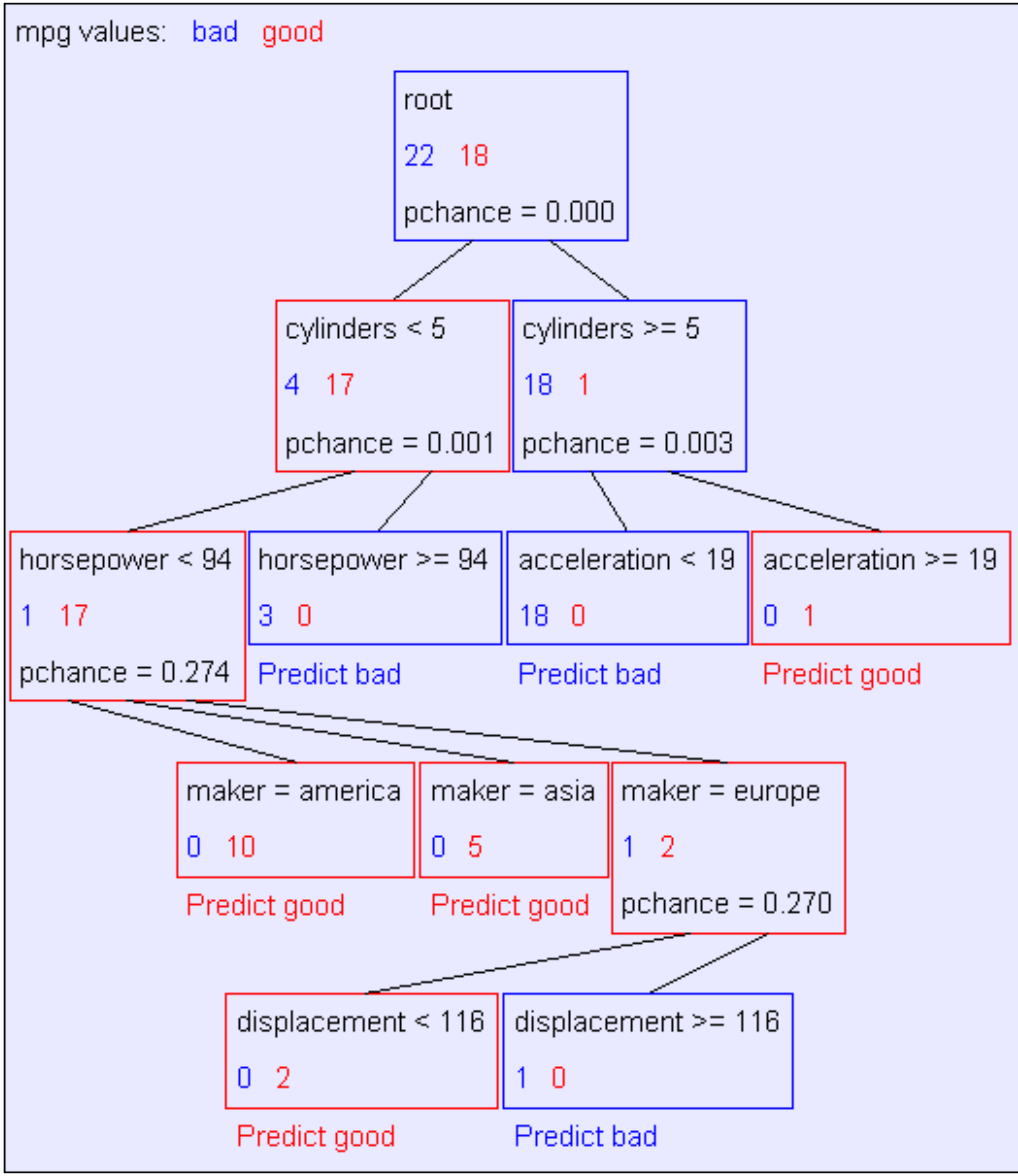
Example tree for our continuous dataset



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Demo time…

What you need to know about decision trees

- Decision trees are one of the most popular ML tools
  - Easy to understand, implement, and use
  - Computationally cheap (to solve heuristically)
- Information gain to select attributes (ID3, C4.5,...)
- Presented for classification, can be used for regression and density estimation too
- Decision trees will overfit!!!
  - Must use tricks to find "simple trees", e.g.,
    - Fixed depth/Early stopping
    - Pruning
  - Or, use ensembles of different trees (random forests)

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Decision Trees vs SVM

Characteristic	SVM	Trees
Natural handling of data of “mixed” type	▼	▲
Handling of missing values	▼	▲
Robustness to outliers in input space	▼	▲
Insensitive to monotone transformations of inputs	▼	▲
Computational scalability (large N)	▼	▲
Ability to deal with irrelevant inputs	▼	▲
Ability to extract linear combinations of features	▲	▼
Interpretability	▼	◆
Predictive power	▲	▼

slide by Vibhav Gogate

Hastie et al.,”The Elements of Statistical Learning: Data Mining, Inference, and Prediction”, Springer (2009)