Predictive Modelling

Classification - Decisions Trees

Jonathan Mwaura

Khoury College of Computer Sciences

July 23, 2024

The Roux Institute
at Northeastern University

Introduction

Acknowledgements

These slides have been adapted from the following Professors:

1) Andrew Ng - Stanford
2) Eric Eaton - UPenn
3) David Sontag - MIT
4) Alina Oprea - Northeastern

Review: Naïve Bayes Classifier

- For each class label k
  1. Estimate prior $P[Y = k]$ from the data
  2. For each value v of attribute X_j
     - Estimate $\mathrm{P}[X_j = v | Y = k]$

- Classify a new point via:

$$h(\mathbf{x}) = \arg\max_{y_k} \log P(Y = k) + \sum_{j=1}^{d} \log P(X_j = x_j \mid Y = k)$$

- In practice, the independence assumption doesn't often hold true, but Naïve Bayes performs very well despite it

Review Naïve Bayes

- Density Estimators can estimate joint probability distribution from data
- Risk of overfitting and curse of dimensionality
- Naïve Bayes assumes that features are independent given labels
  - Reduces the complexity of density estimation
  - Even though the assumption is not always true, Naïve Bayes works well in practice
- Applications: text classification with bag-of-words representation
  - Naïve Bayes becomes a linear classifier

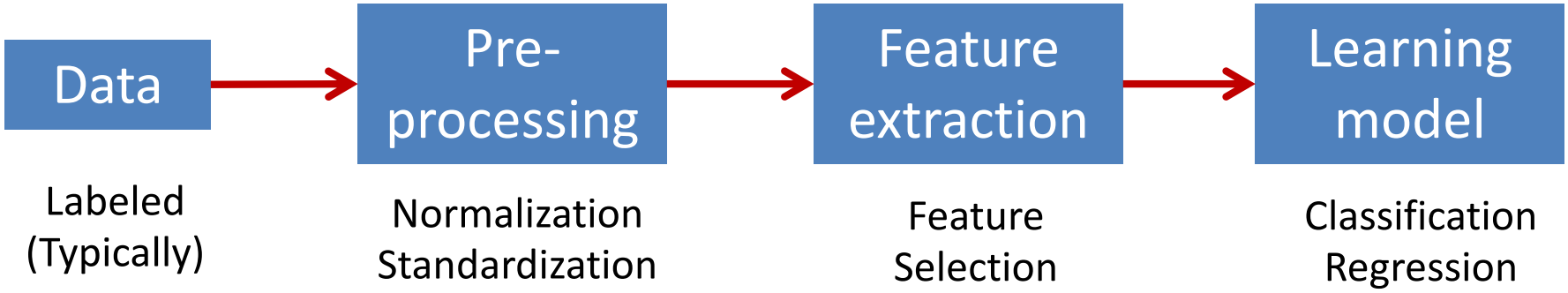
Generative model

Outline

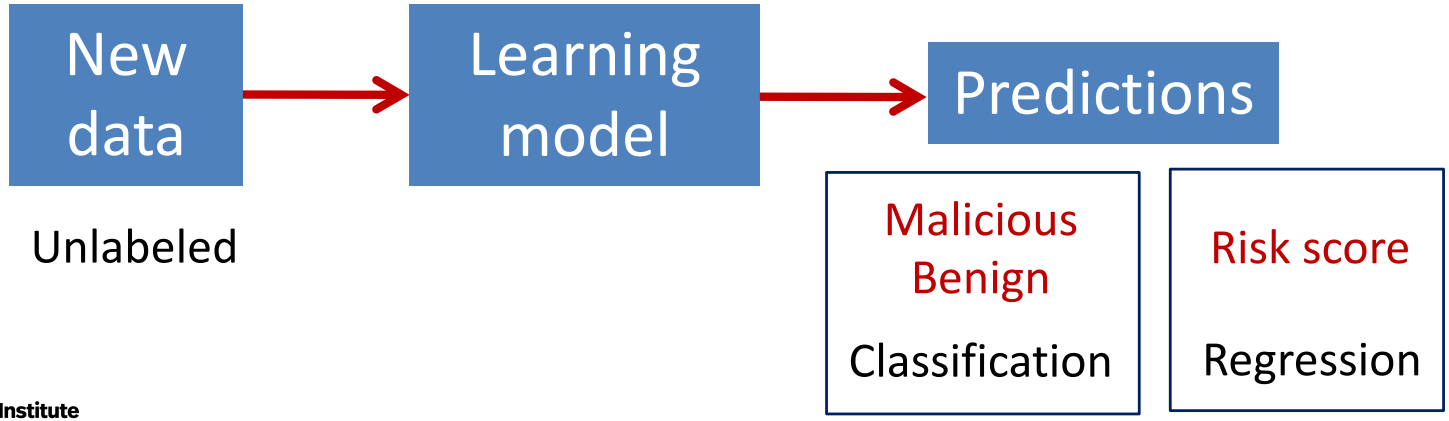
- Feature selection
  - Wrapper
  - Filter
  - Embedded methods
- Decision trees
  - Information Gain
  - ID3 algorithm
  - Pruning decision trees

Supervised Learning Process

Training



Testing



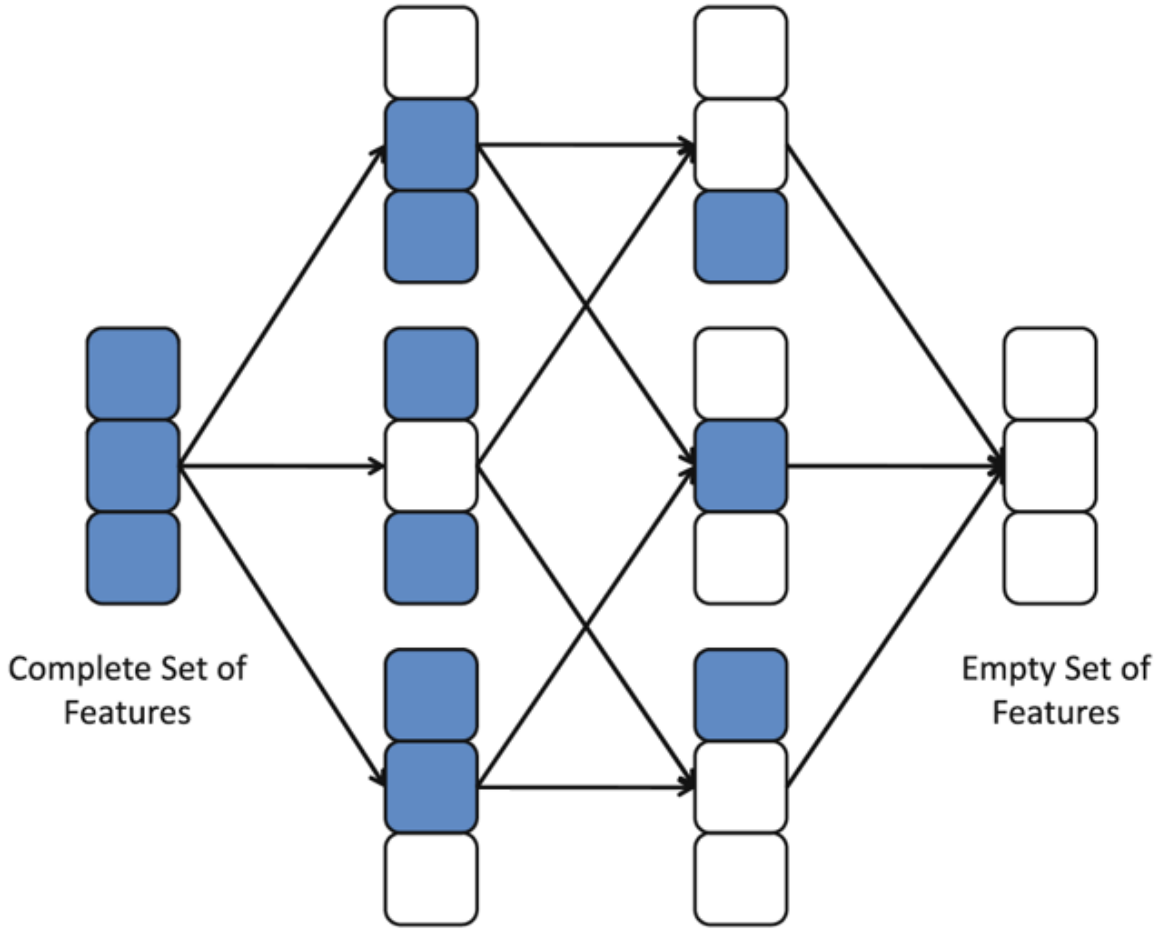
Feature selection

- *Feature Selection*
  - Process for choosing an optimal subset of features according to a certain criteria

- Why we need Feature Selection:
  1. To improve performance (in terms of speed, predictive power, simplicity of the model).
  2. To visualize the data for model selection.
  3. To reduce dimensionality and remove noise.

Feature Search Space

Search Space:



Exponentially large!

Methods for Feature Selection

- Wrappers
  - Select subset of features that gives best prediction accuracy (using cross-validation)
  - Model-specific
- Filters
  - Compute some statistical metrics (correlation coefficient, mutual information)
  - Select features with statistics higher than threshold
- Embedded methods
  - Feature selection done as part of training
  - Example: Regularization (Lasso, L1 regularization)

Feature Engineering

- Feature engineering is crucial to getting good results
- Strategy: overshoot and regularize
  - Define as many features as you can
  - Use regularization for models that support it
  - Use other feature selection methods (e.g., filters) otherwise
- Do cross-validation to evaluate selected features on multiple runs
- When feature selection is frozen, evaluate on test set

Wrappers: Search Strategy

- With an **exhaustive search**

$$10111000000100010000100000000100101010$$

With d features $\rightarrow$ 2^d possible feature subsets.

20 features … 1 million feature sets to check
25 features … 33.5 million sets
30 features … 1.1 billion sets

- Need for **a search strategy**
  - Sequential forward selection
  - Recursive backward elimination
  - Genetic algorithms
  - Simulated annealing
  - …

Wrappers: Sequential Forward Selection

Start with the empty set $S = \emptyset$

While *stopping criteria not met*

For each feature X_f not in S

- Define $S' = S \cup \{X_f\}$
- Train model using the features in S'
- Compute the accuracy on validation set

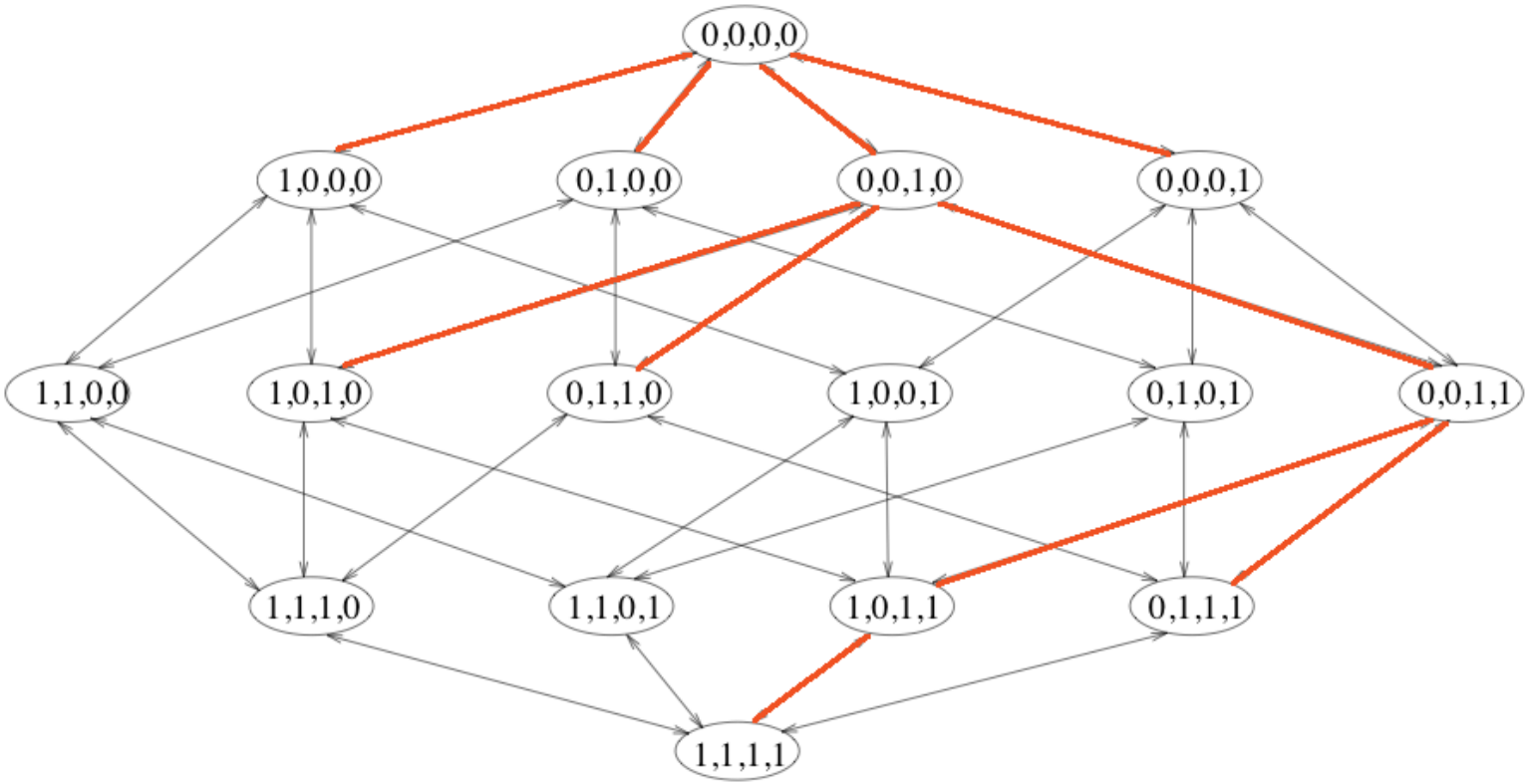
End

$S = S'$ where S' is the feature set with the greatest accuracy

End

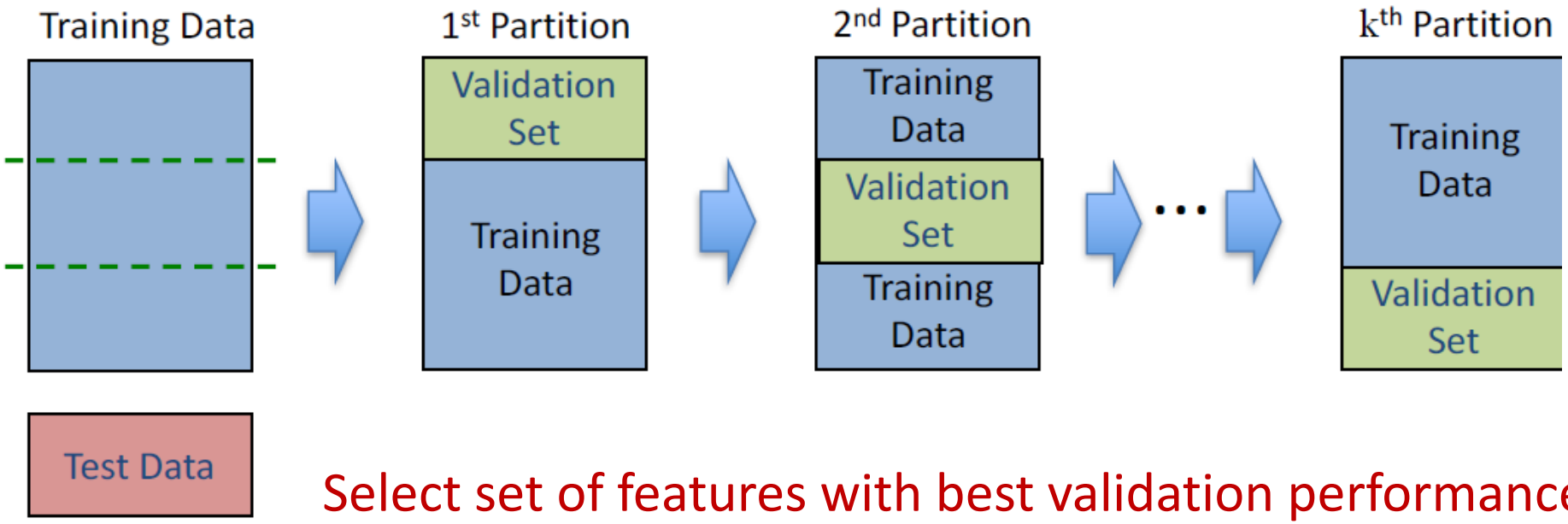
Backward feature selection starts with all features and eliminates backward

Search complexity for sequential forward selection



- Evaluates $\frac{d(d+1)}{2}$ features sets instead of 2^d

Cross Validation



Select set of features with best validation performance

- k-fold CV
  - Split data into k partitions of equal size
- Leave-one-out CV (LOOCV)
- k=n (validation set only one point)

Filters

Principle: *replace evaluation of model with quick to compute statistics* $J(X_f)$

k	$J(X_k)$
35	0.846
42	0.811
10	0.810
654	0.611
22	0.443
59	0.388
...	...
212	0.09
39	0.05

For each feature X_f

- Compute $J(X_f)$

End

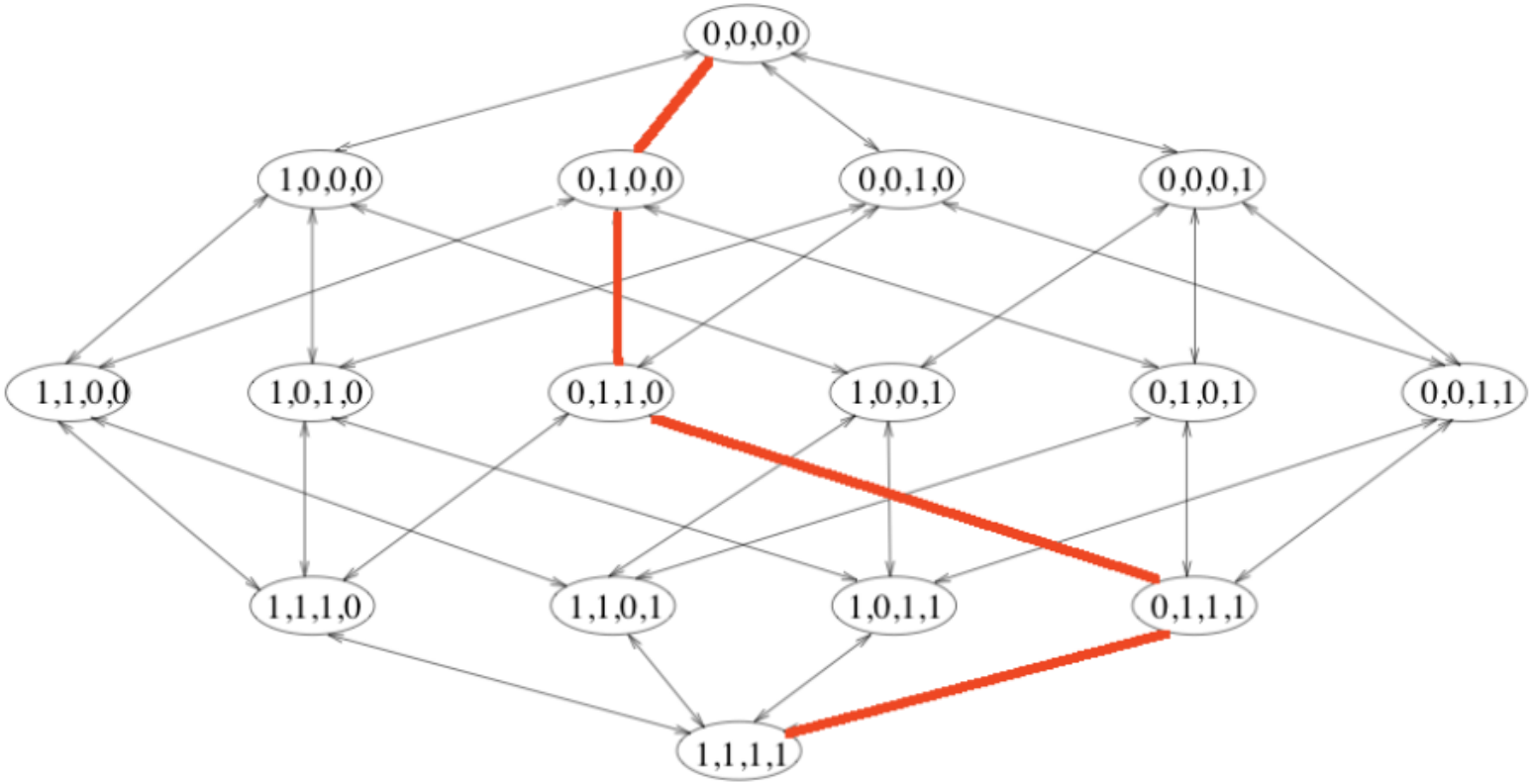
Rank features according to $J(X_f)$

Choose manual cut-off point

Examples of filtering criterion

- The mutual information with the target variable $J(X_f) = I(X_f; Y)$
- The correlation with the target variable
- χ^2 - statistic

Search Complexity for Filter Methods



Pros:

- A lot less expensive!

Cons:

- Not model-oriented

Embedded methods: Regularization

Lasso regression

$$J(\theta) = \underbrace{\sum_{i=1}^{N} (h_\theta(x_i) - y_i)^2}_{\text{Squared Residuals}} + \lambda \underbrace{\sum_{j=1}^{d} |\theta_j|}_{\text{Regularization}}$$

- L1 norm for regularization
- No closed form solution
- Algorithms based on sub-gradient descent

Embedded methods: Regularization

Principle: the classifier performs feature selection as part of the learning procedure

Example: the logistic LASSO (Tibshirani, 1996)

$$f(\boldsymbol{x}) = \frac{1}{1 + e^{-(\boldsymbol{w}^T \boldsymbol{x})}} = P(Y = 1|\boldsymbol{x})$$

With Error Function:

$$E = \underbrace{-\sum_{i=1}^{N} \{y_i \log f(\boldsymbol{x}_i) + (1 - y_i) \log(1 - f(\boldsymbol{x}_i))\}}_{\text{Cross-entropy error}} + \underbrace{\lambda \sum_{f=1}^{d} |w_f|}_{\text{Regularizing term}}$$

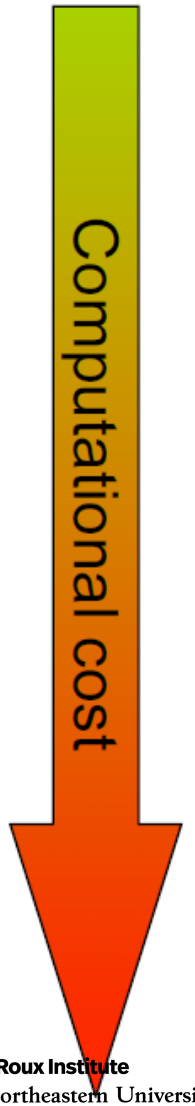
Pros:

- Performs feature selection as part of learning the procedure

Cons:

- Computationally demanding

Summary: Feature Selection



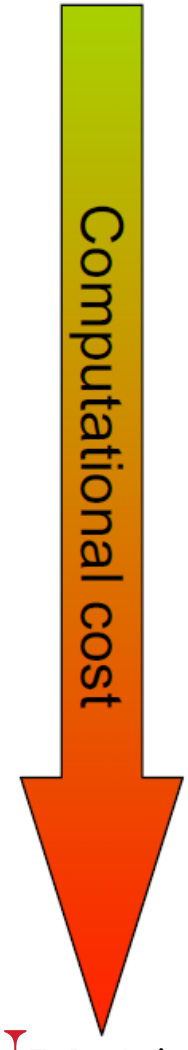
- Filtering
- L_1 regularization (embedded methods)
- Wrappers
  - Forward selection
  - Backward selection
  - Other search
  - Exhaustive

Summary: Feature Selection

- *Filtering*
- L_1 regularization (embedded methods)
- Wrappers
  - Forward selection
  - Backward selection
  - Other search
  - Exhaustive

- Good preprocessing step
- Fails to capture relationship between features

Summary: Feature Selection



- Filtering
- L_1 regularization (embedded methods)
- Wrappers
  - Forward selection
  - Backward selection
  - Other search
  - Exhaustive

- Can add regularization in optimization objective
- Can be solved with Gradient Descent
- Can be applied to many models (e.g., linear or logistic regression)
- Can not be applied to all methods (e.g., kNN)

Summary: Feature Selection

- Filtering
- L_1 regularization (embedded methods)
- *Wrappers*
  - Forward selection
  - Backward selection
  - Other search
  - Exhaustive

- Most directly optimize prediction performance
- Can be very expensive, even with greedy search methods
- Cross-validation is a good objective function to start with

Outline

- Feature selection
  - Wrapper
  - Filter
  - Embedded methods
- Decision trees
  - Information Gain
  - ID3 algorithm
  - Pruning decision trees
- Lab decision trees

Sample Dataset

- Columns denote features X_i
- Rows denote labeled instances $< x_i, y_i >$
- Class label denotes whether a tennis game was played

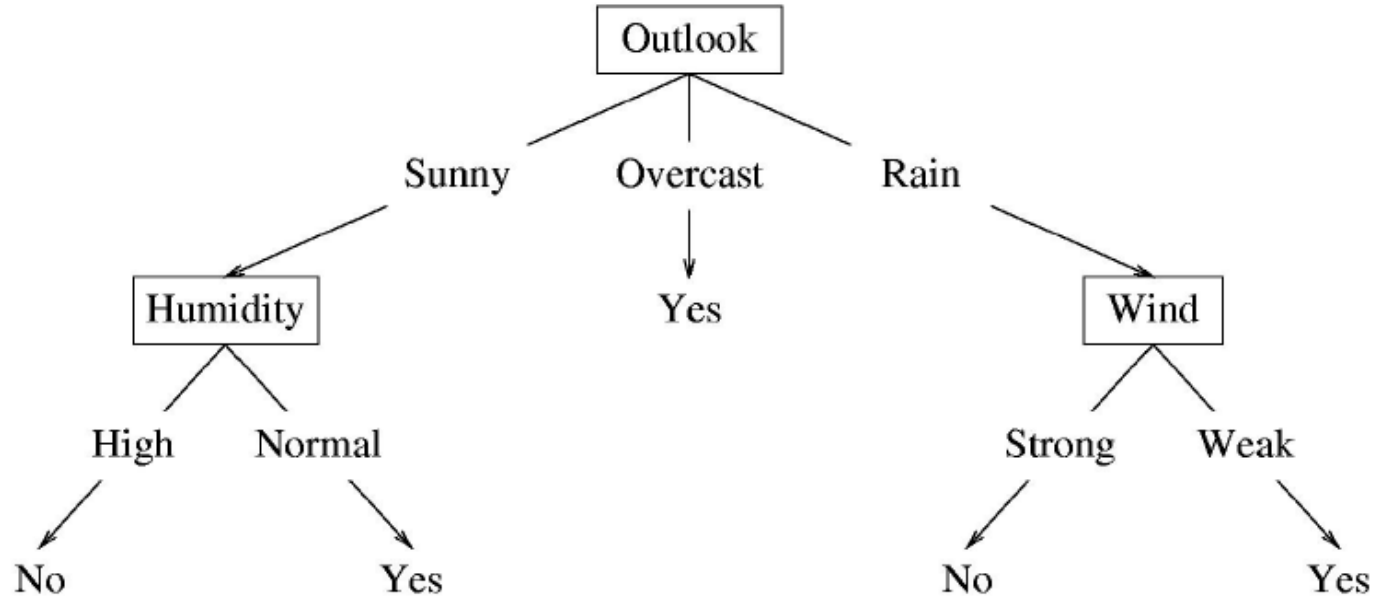
$< x_i, y_i >$

Predictors				Response
Outlook	**Temperature**	**Humidity**	**Wind**	**Class**
Sunny	Hot	High	Weak	No
Sunny	Hot	High	Strong	No
Overcast	Hot	High	Weak	Yes
Rain	Mild	High	Weak	Yes
Rain	Cool	Normal	Weak	Yes
Rain	Cool	Normal	Strong	No
Overcast	Cool	Normal	Strong	Yes
Sunny	Mild	High	Weak	No
Sunny	Cool	Normal	Weak	Yes
Rain	Mild	Normal	Weak	Yes
Sunny	Mild	Normal	Strong	Yes
Overcast	Mild	High	Strong	Yes
Overcast	Hot	Normal	Weak	Yes
Rain	Mild	High	Strong	No

Categorical data

Decision Tree

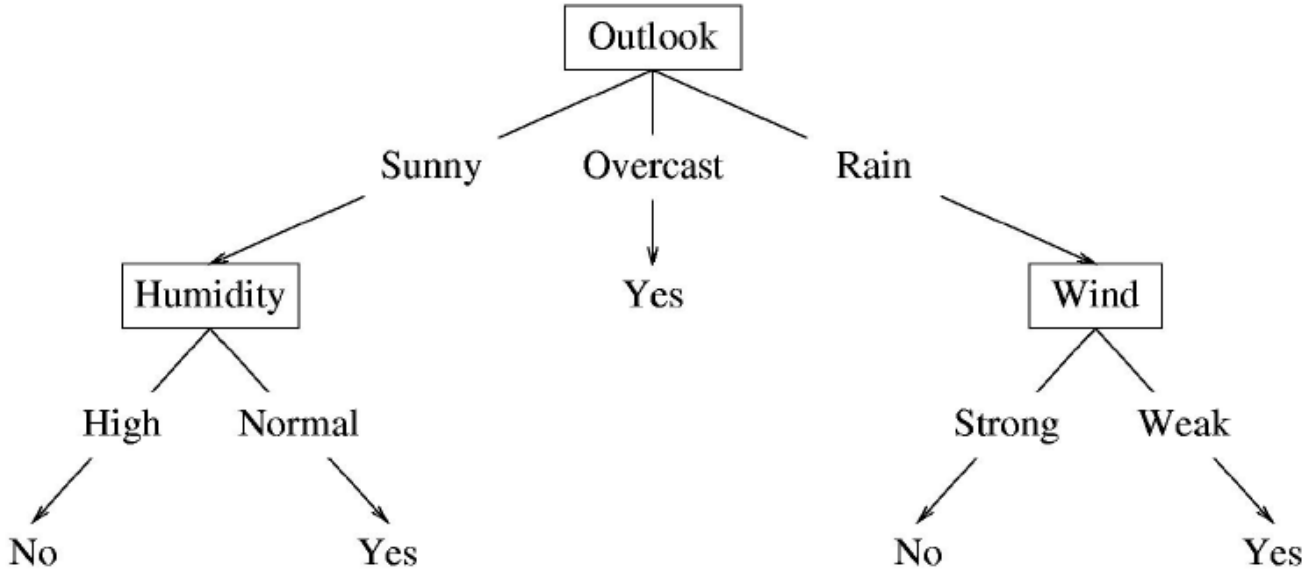
- A possible decision tree for the data:



- Each internal node: test one attribute X_i
- Each branch from a node: selects one value for X_i
- Each leaf node: predict Y (or $p(Y \mid x \in \text{leaf})$)

Decision Tree

- A possible decision tree for the data:



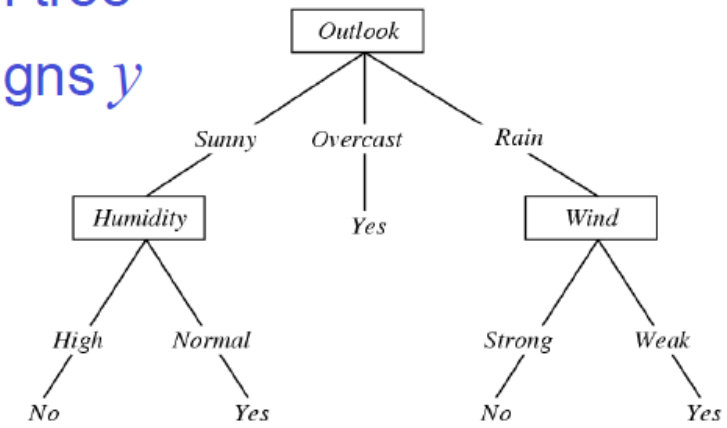
- What prediction would we make for

  <outlook=sunny, temperature=hot, humidity=high, wind=weak> ?

Decision Tree Learning

Problem Setting:

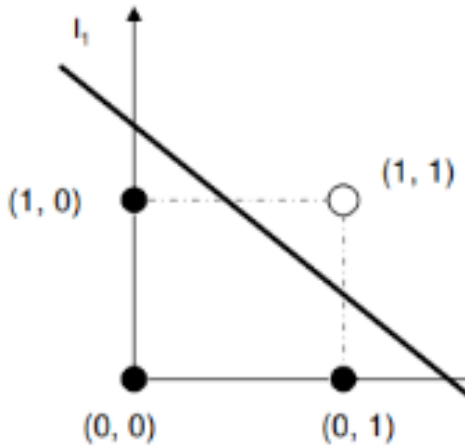
- Set of possible instances X
  - each instance x in X is a feature vector
  - e.g., <*Humidity=low, Wind=weak, Outlook=rain, Temp=hot*>
- Unknown target function $f : X \rightarrow Y$
  - Y is discrete valued
- Set of function hypotheses $H=\{ h \mid h : X \rightarrow Y \}$
  - each hypothesis h is a decision tree
  - trees sorts x to leaf, which assigns y



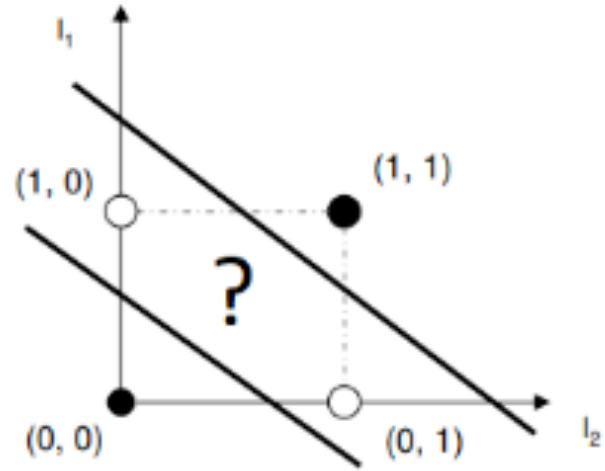
Slide by Tom Mitchell

Learning Boolean Functions

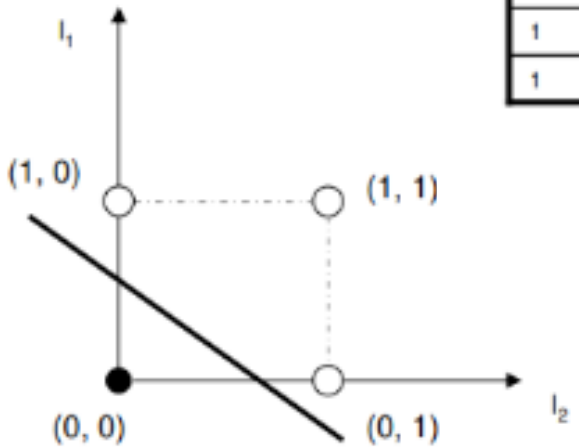
AND		
I_1	I_2	out
0	0	0
0	1	0
1	0	0
1	1	1



XOR		
I_1	I_2	out
0	0	0
0	1	1
1	0	1
1	1	0



OR		
I_1	I_2	out
0	0	0
0	1	1
1	0	1
1	1	1



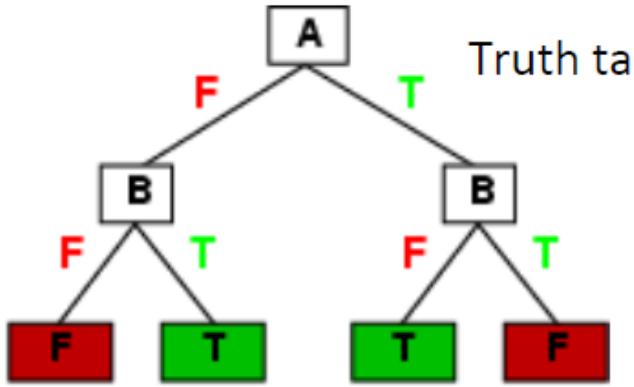
The Roux Institute at Northeastern University

XOR cannot be learned with linear classifiers

Expressiveness

- Decision trees can represent any boolean function of the input attributes

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



Truth table row → path to leaf

- In the worst case, the tree will require exponentially many nodes

Occam's Razor

- Principle stated by William of Ockham (1285-1347)
  - "*non sunt multiplicanda entia praeter necessitatem*"
  - entities are not to be multiplied beyond necessity
  - AKA Occam's Razor, Law of Economy, or Law of Parsimony

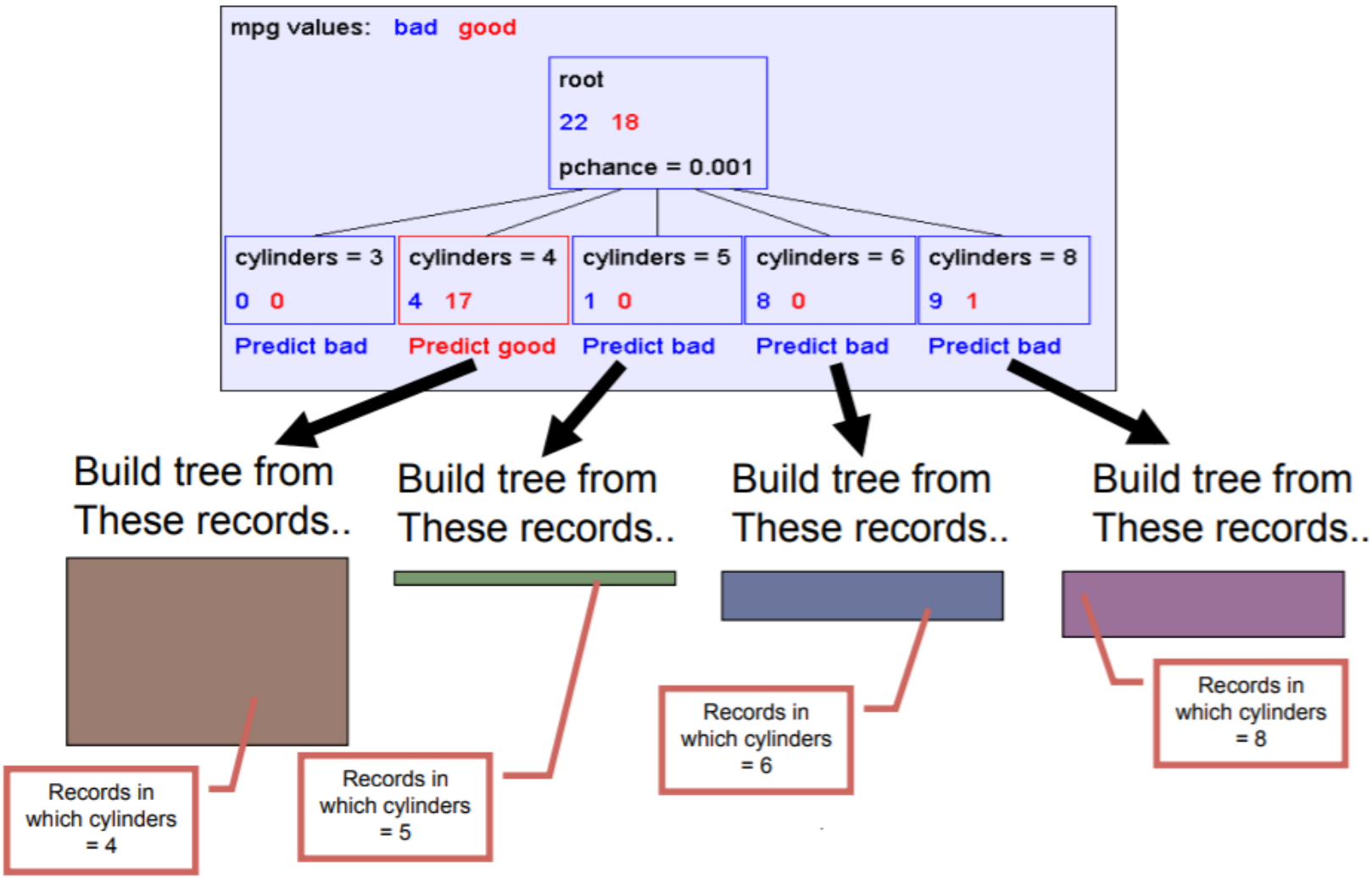
Idea: The simplest consistent explanation is the best

- Therefore, the smallest decision tree that correctly classifies all of the training examples is best
  - Finding the provably smallest decision tree is NP-hard
  - ...So instead of constructing the absolute smallest tree consistent with the training examples, construct one that is pretty small

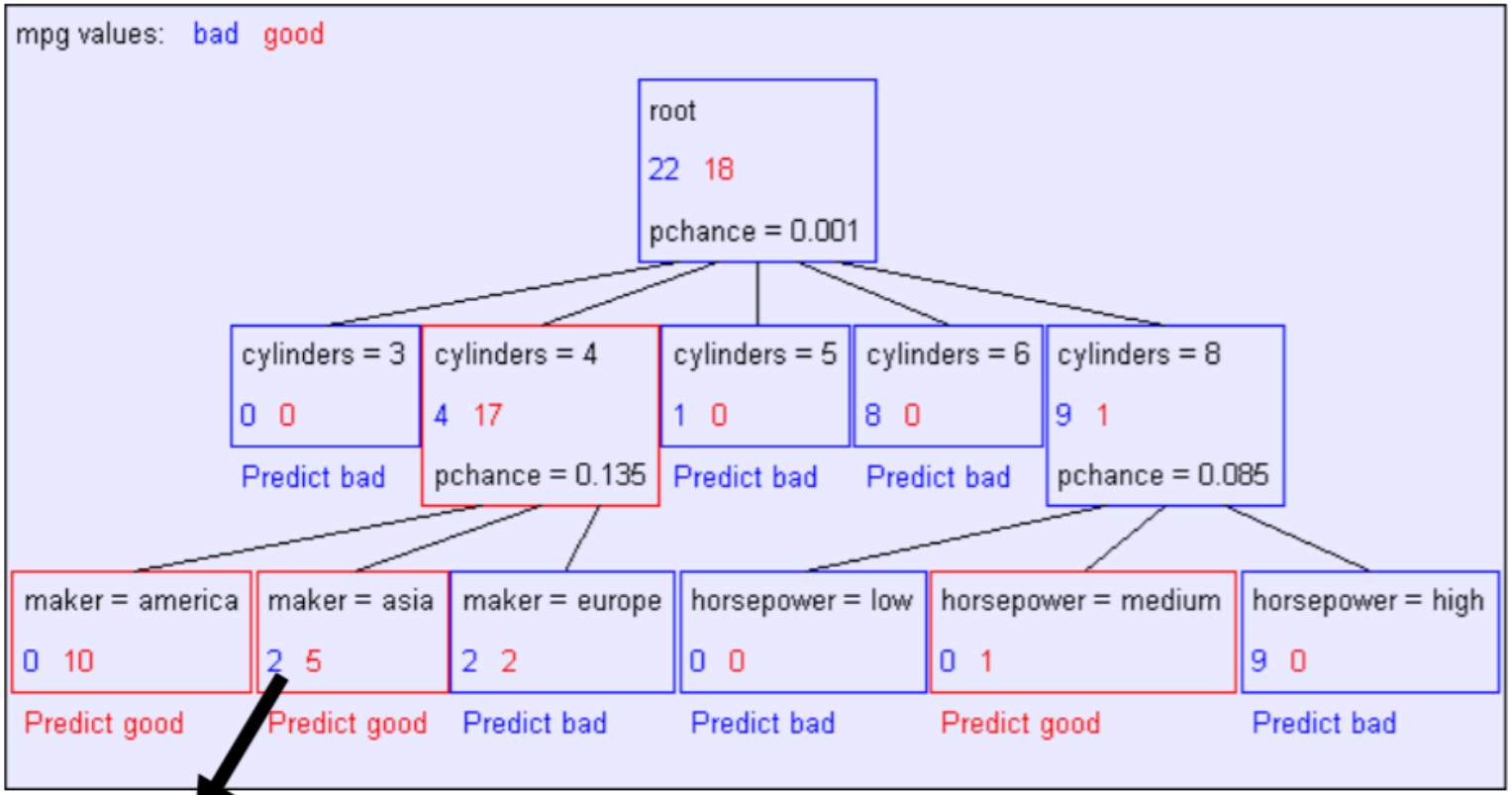
Learning Decision Trees

- 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

Key Idea: Use Recursion Greedily



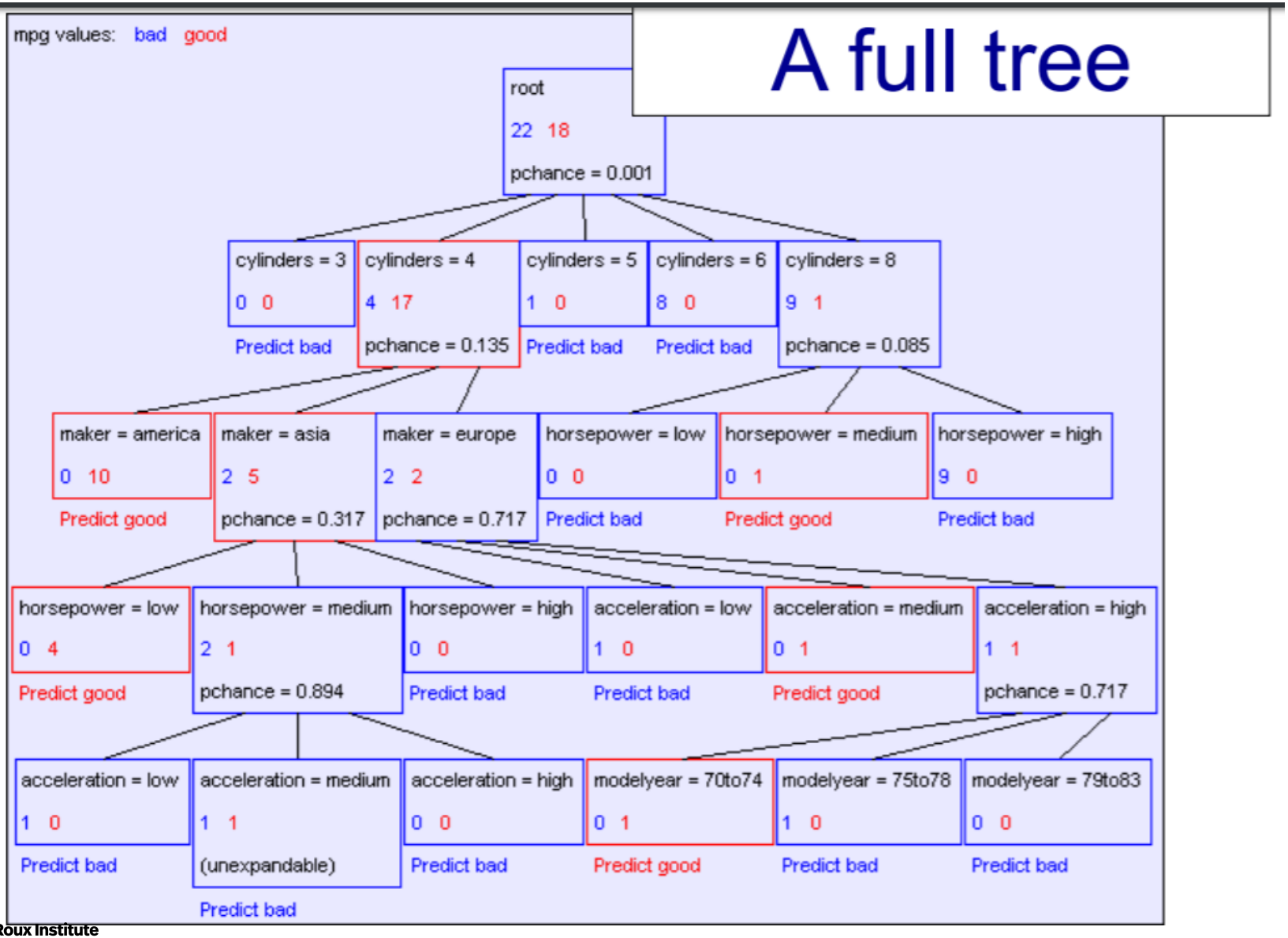
Second Level



Recursively build a tree from the seven records in which there are four cylinders and the maker was based in Asia

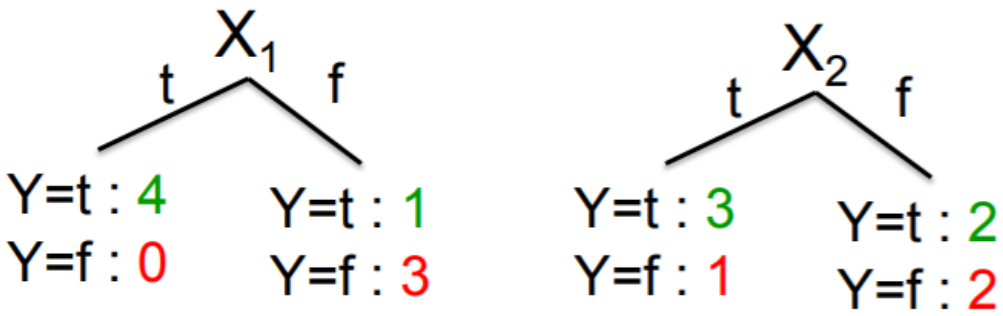
(Similar recursion in the other cases)

Full Tree


A full tree
mpg values: bad good
root
22 18
pchance = 0.001
cylinders = 3
0 0
Predict bad
cylinders = 4
4 17
pchance = 0.135
cylinders = 5
1 0
Predict bad
cylinders = 6
8 0
Predict bad
cylinders = 8
9 1
pchance = 0.085
maker = america
0 10
Predict good
maker = asia
2 5
pchance = 0.317
maker = europe
2 2
pchance = 0.717
horsepower = low
0 0
Predict bad
horsepower = medium
0 1
Predict good
horsepower = high
9 0
Predict bad
horsepower = low
0 4
Predict good
horsepower = medium
2 1
pchance = 0.894
horsepower = high
0 0
Predict bad
acceleration = low
1 0
Predict bad
acceleration = medium
0 1
Predict good
acceleration = high
1 1
pchance = 0.717
acceleration = low
1 0
Predict bad
acceleration = medium
1 1
(unexpandable)
Predict bad
acceleration = high
0 0
Predict bad
modelyear = 70to74
0 1
Predict good
modelyear = 75to78
1 0
Predict bad
modelyear = 79to83
0 0
Predict bad

Splitting

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!

Use entropy-based measure (Information Gain)

Transmitting Bits

You are watching a set of independent random samples of X

You see that X has four possible values

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

So you might see: BAACBADCDADDDA…

You transmit data over a binary serial link. You can encode each reading with two bits (e.g. A = 00, B = 01, C = 10, D = 11)

01000010010011101100111111100…

Use Fewer Bits

Someone tells you that the probabilities are not equal

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

It's possible…

…to invent a coding for your transmission that only uses 1.75 bits on average per symbol. How?

Use Fewer Bits

Someone tells you that the probabilities are not equal

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

It's possible...

...to invent a coding for your transmission that only uses 1.75 bits on average per symbol. How?

A	0
B	10
C	110
D	111

(This is just one of several ways)

General case

Suppose X can have one of *m* values... $V_1, V_2, \ldots V_m$

$P(X=V_1) = p_1$	$P(X=V_2) = p_2$	….	$P(X=V_m) = p_m$

What's the smallest possible number of bits, on average, per symbol, needed to transmit a stream of symbols drawn from X's distribution? It's

$$H(X) = -p_1 \log_2 p_1 - p_2 \log_2 p_2 - \ldots - p_m \log_2 p_m$$

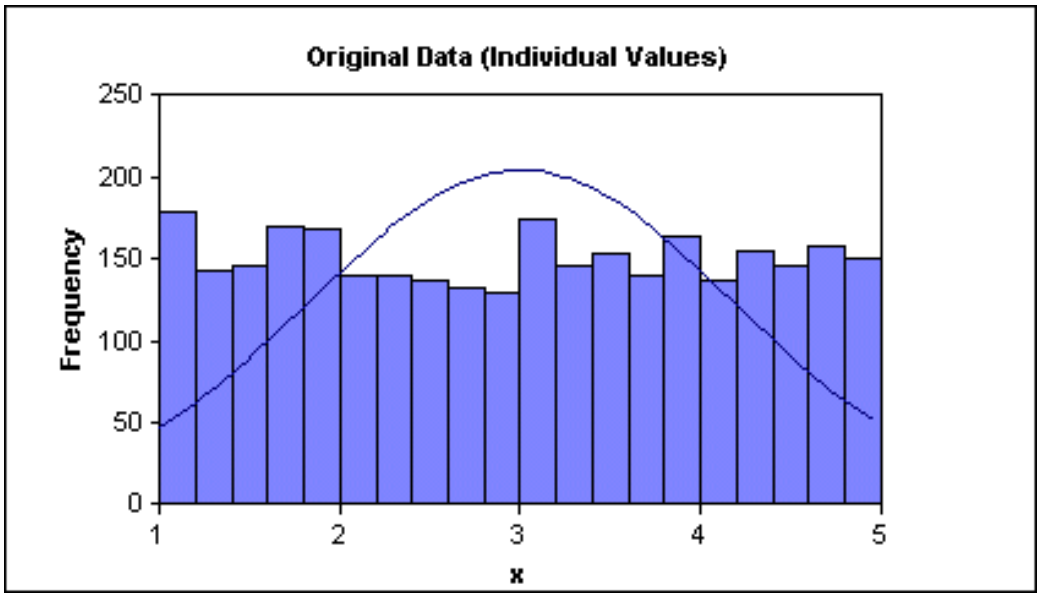
$$= -\sum_{j=1}^{m} p_j \log_2 p_j$$

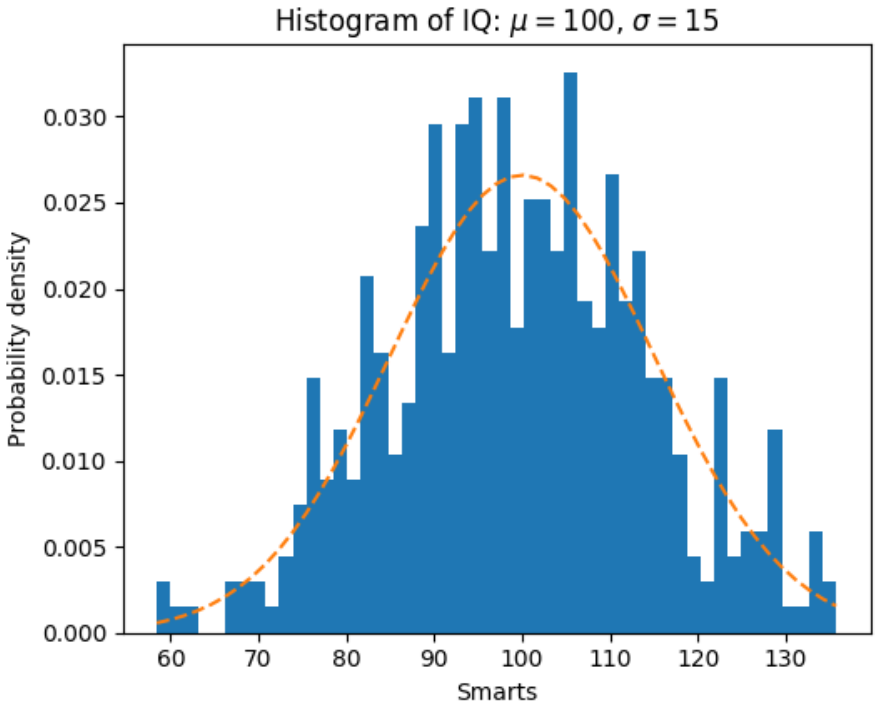
H(X) = The entropy of X

- "High Entropy" means X is from a uniform (boring) distribution
- "Low Entropy" means X is from varied (peaks and valleys) distribution

High/Low Entropy

Which distribution has high entropy?





High

Low

Conditional Entropy

Suppose I'm trying to predict output Y and I have input X

X = College Major

Y = Likes "Gladiator"

X	Y
Math	Yes
History	No
CS	Yes
Math	No
Math	No
CS	Yes
History	No
Math	Yes

Let's assume this reflects the true probabilities

E.G. From this data we estimate

- *P(LikeG = Yes) = 0.5*
- *P(Major = Math & LikeG = No) = 0.25*
- *P(Major = Math) = 0.5*
- *P(LikeG = Yes | Major = History) = 0*

Note:

- *H(X) = 1.5*
- *H(Y) = 1*

Conditional Entropy

X = College Major

Y = Likes "Gladiator"

X	Y
Math	Yes
History	No
CS	Yes
Math	No
Math	No
CS	Yes
History	No
Math	Yes

Definition of Specific Conditional Entropy:

$H(Y|X=v)$ = **The entropy of Y among only those records in which X has value v**

Example:

- $H(Y|X=Math) = 1$
- $H(Y|X=History) = 0$
- $H(Y|X=CS) = 0$

Conditional Entropy

X = College Major

Y = Likes "Gladiator"

X	Y
Math	Yes
History	No
CS	Yes
Math	No
Math	No
CS	Yes
History	No
Math	Yes

Definition of Conditional Entropy:

$H(Y|X)$ = The average specific conditional entropy of Y

= if you choose a record at random what will be the conditional entropy of Y, conditioned on that row's value of X

= Expected number of bits to transmit Y if both sides will know the value of X

$= \Sigma_j Prob(X=v_j)\ H(Y \mid X = v_j)$

Conditional Entropy

X = College Major

Y = Likes "Gladiator"

X	Y
Math	Yes
History	No
CS	Yes
Math	No
Math	No
CS	Yes
History	No
Math	Yes

Definition of Conditional Entropy:

$H(Y|X)$ = The average conditional entropy of Y

$= \Sigma_j Prob(X=v_j)\, H(Y \mid X = v_j)$

Example:

v_j	$Prob(X=v_j)$	$H(Y \mid X = v_j)$
Math	0.5	1
History	0.25	0
CS	0.25	0

$H(Y|X) = 0.5 * 1 + 0.25 * 0 + 0.25 * 0 = 0.5$

Information Gain

X = College Major

Y = Likes "Gladiator"

X	Y
Math	Yes
History	No
CS	Yes
Math	No
Math	No
CS	Yes
History	No
Math	Yes

Definition of Information Gain:

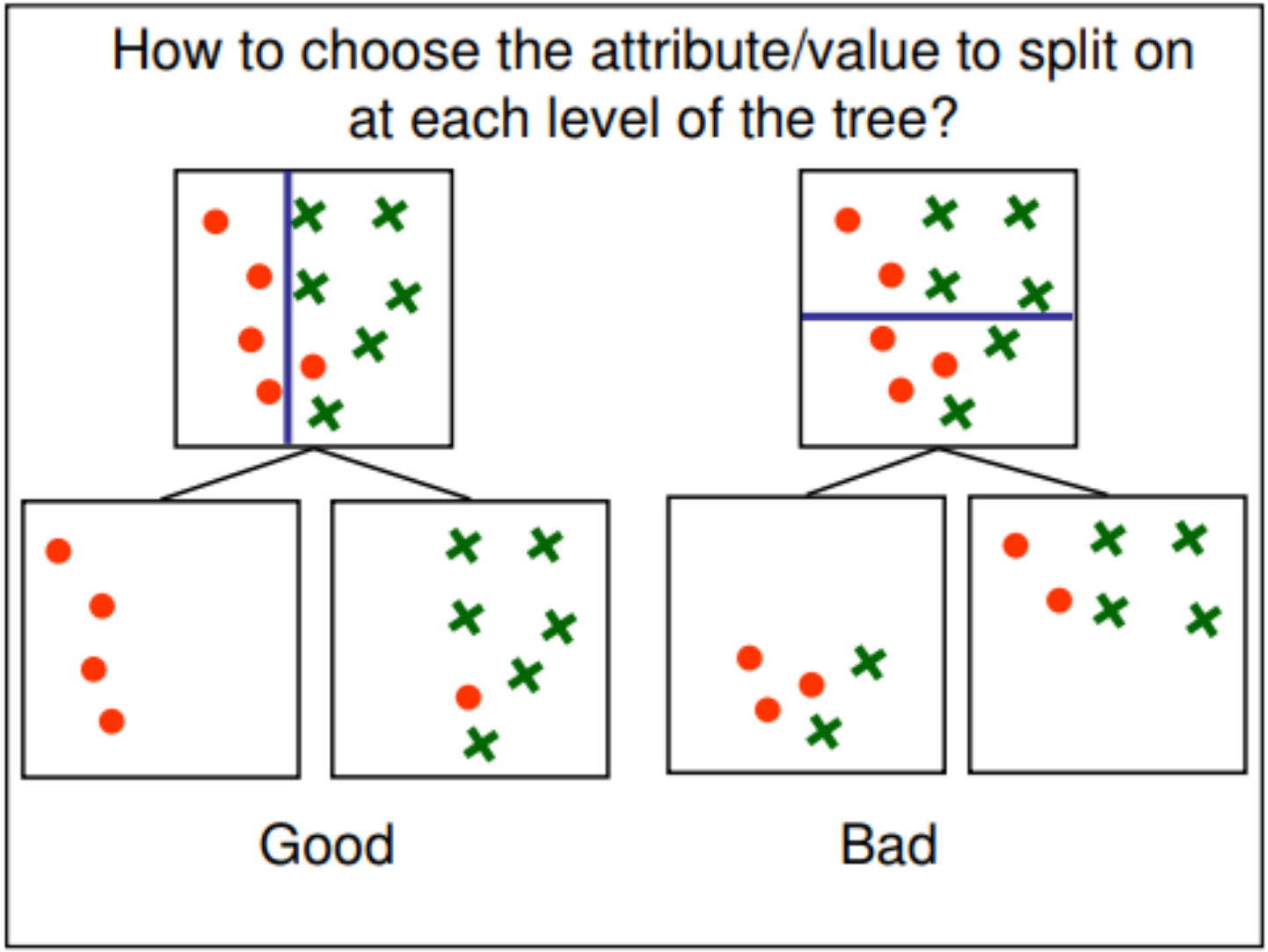
$IG(Y|X)$ = **I must transmit** Y. **How many bits on average would it save me if both ends of the line knew** X**?**

$$IG(Y|X) = H(Y) - H(Y|X)$$

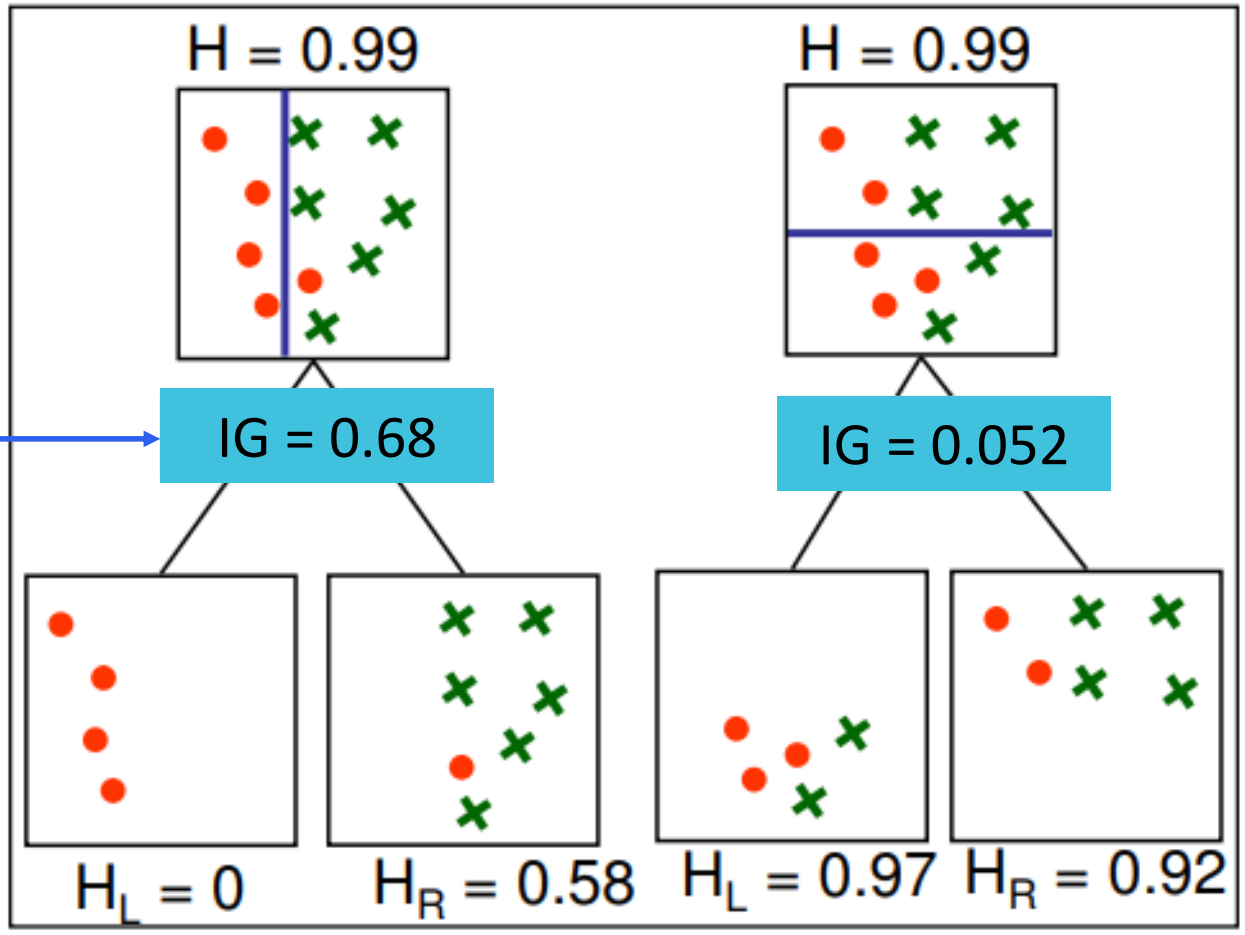
Example:

- **H(Y) = 1**
- **H(Y|X) = 0.5**
- **Thus IG(Y|X) = 1 – 0.5 = 0.5**

Example


How to choose the attribute/value to split on at each level of the tree?
Good
Bad

Example Information Gain



Max Information Gain

Pure node

Learning Decision Trees

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

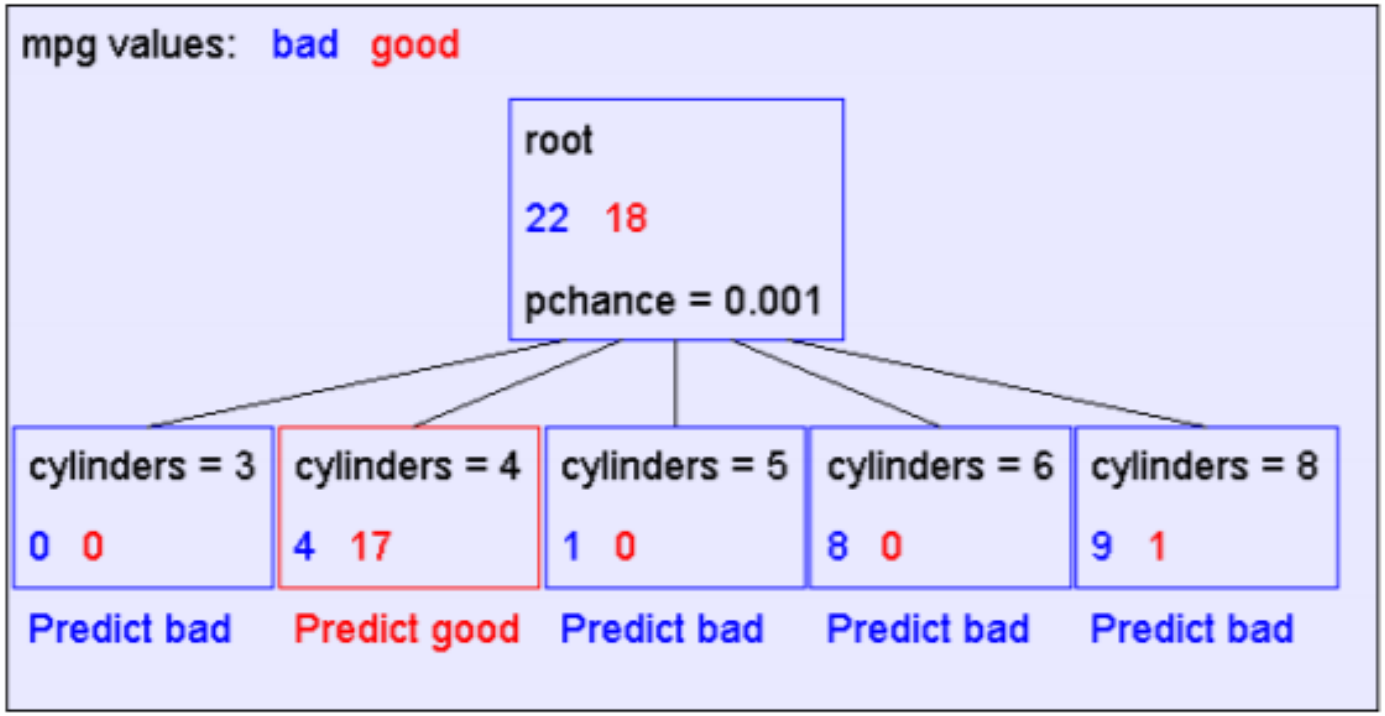
$$\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$$

- Recurse

ID3 algorithm uses Information Gain

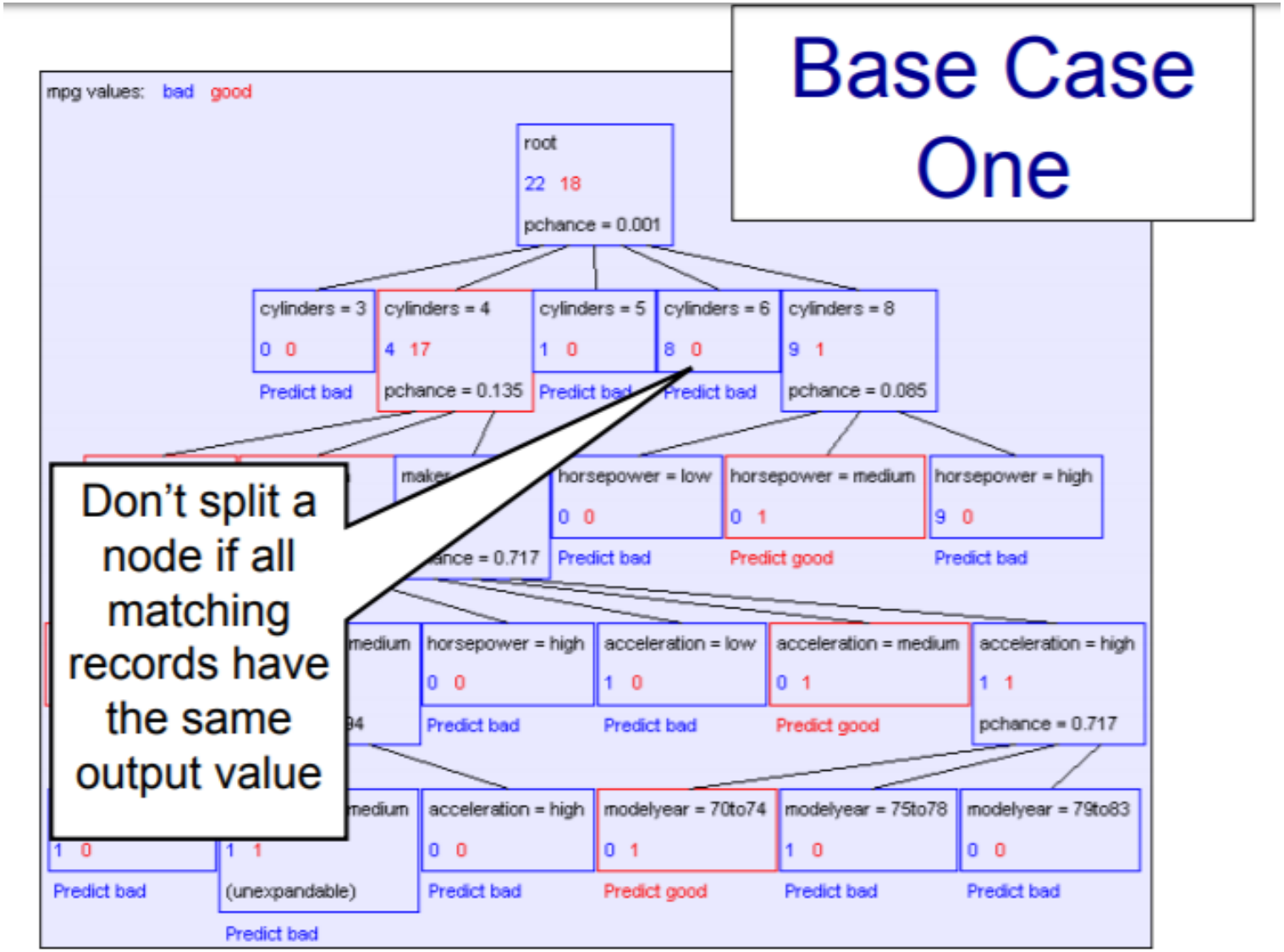
Information Gain reduces uncertainty on Y

When to stop?

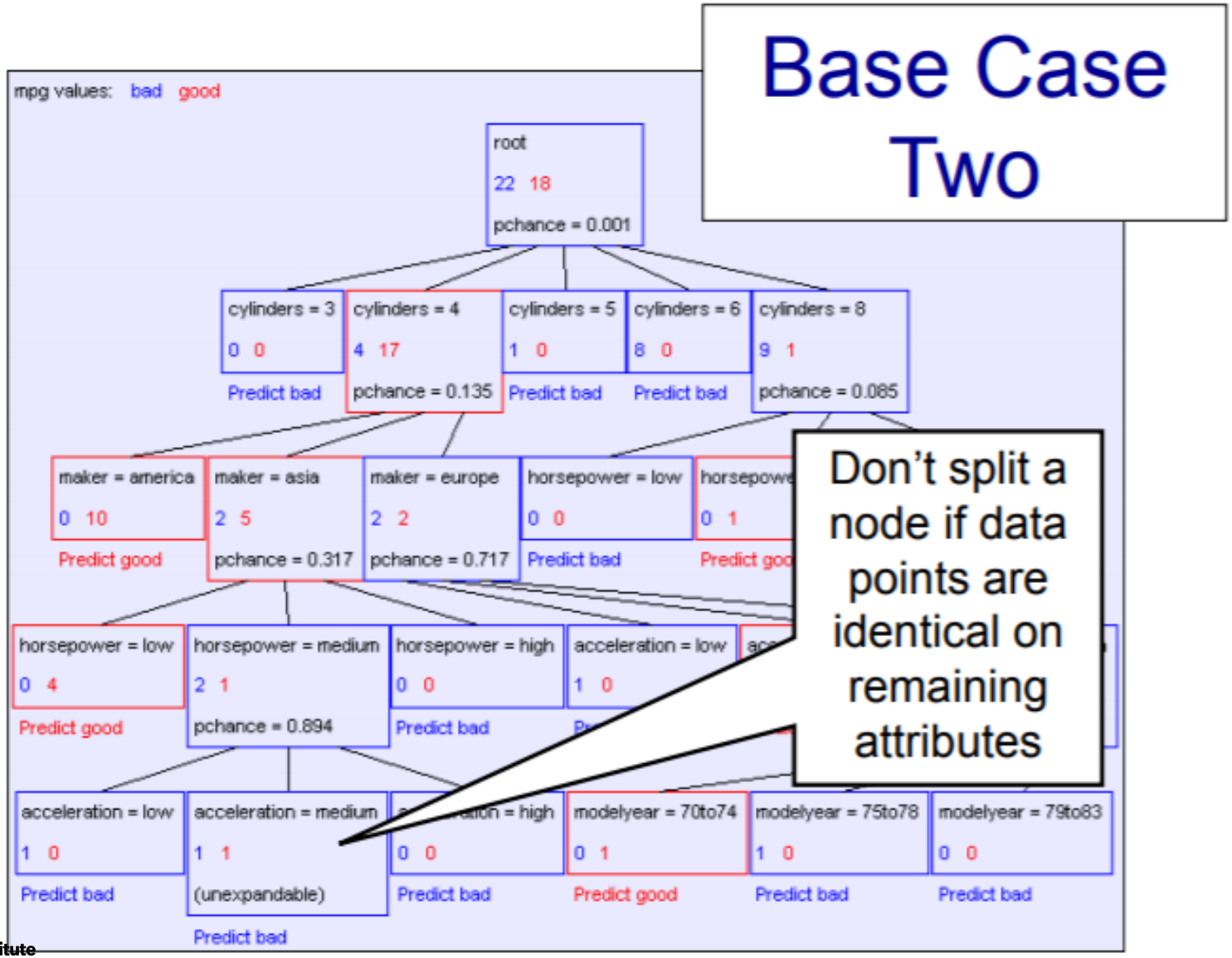


First split looks good! But, when do we stop?

Case 1


Base Case One
mpg values: bad good
root
22 18
pchance = 0.001
cylinders = 3
0 0
Predict bad
cylinders = 4
4 17
pchance = 0.135
cylinders = 5
1 0
Predict bad
cylinders = 6
8 0
Predict bad
cylinders = 8
9 1
pchance = 0.085
horsepower = low
0 0
Predict bad
horsepower = medium
0 1
Predict good
horsepower = high
9 0
Predict bad
horsepower = high
0 0
Predict bad
acceleration = low
1 0
Predict bad
acceleration = medium
0 1
Predict good
acceleration = high
1 1
pchance = 0.717
acceleration = high
0 0
Predict bad
modelyear = 70to74
0 1
Predict good
modelyear = 75to78
1 0
Predict bad
modelyear = 79to83
0 0
Predict bad
1 0
Predict bad
1 1
(unexpandable)
Predict bad
Don't split a node if all matching records have the same output value

Case 2


Base Case Two
mpg values: bad good
root
22 18
pchance = 0.001
cylinders = 3
0 0
Predict bad
cylinders = 4
4 17
pchance = 0.135
cylinders = 5
1 0
Predict bad
cylinders = 6
8 0
Predict bad
cylinders = 8
9 1
pchance = 0.085
maker = america
0 10
Predict good
maker = asia
2 5
pchance = 0.317
maker = europe
2 2
pchance = 0.717
horsepower = low
0 0
Predict bad
horsepower = low
0 4
Predict good
horsepower = medium
2 1
pchance = 0.894
horsepower = high
0 0
Predict bad
acceleration = low
1 0
acceleration = low
1 0
Predict bad
acceleration = medium
1 1
(unexpandable)
Predict bad
modelyear = 70to74
0 1
Predict good
modelyear = 75to78
1 0
Predict bad
modelyear = 79to83
0 0
Predict bad
Don't split a node if data points are identical on remaining attributes

Decision Trees

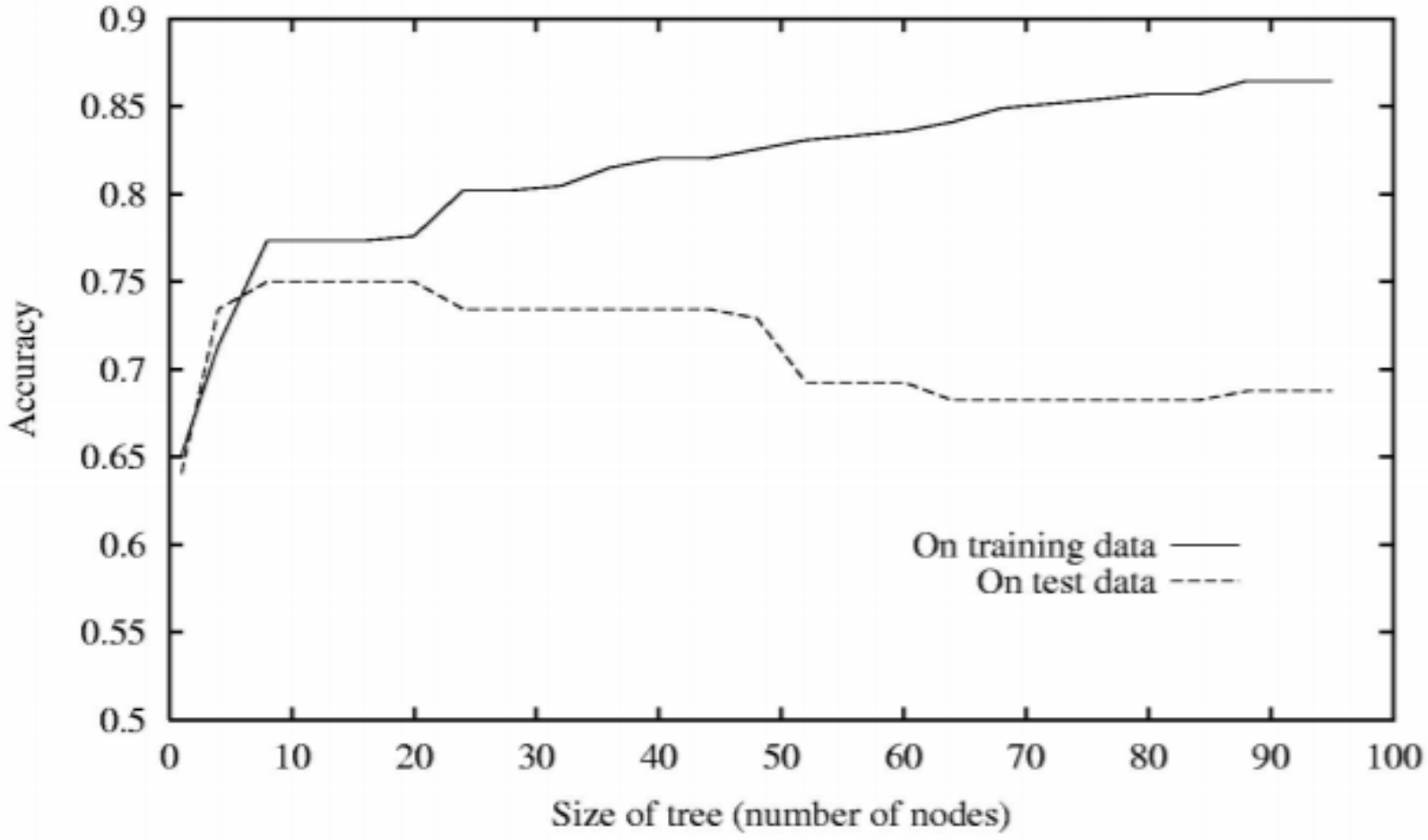
BuildTree(*DataSet,Output*)

- If all output values are the same in *DataSet*, return a leaf node that says "predict this unique output"
- If all input values are the same, return a leaf node that says "predict the majority output"
- Else find attribute *X* with highest Info Gain
- Suppose *X* has n_X distinct values (i.e. X has arity n_X).
  - Create a non-leaf node with n_X children.
  - The *i*'th child should be built by calling

    BuildTree(DS_i,*Output*)

    Where DS_i contains the records in DataSet where X = *i*th value of X.

Overfitting



Solutions against Overfitting

- 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
  - Minimum number of samples per leaf
- Pruning

Pruning Decision Trees

Split data into *training* and *validation* sets

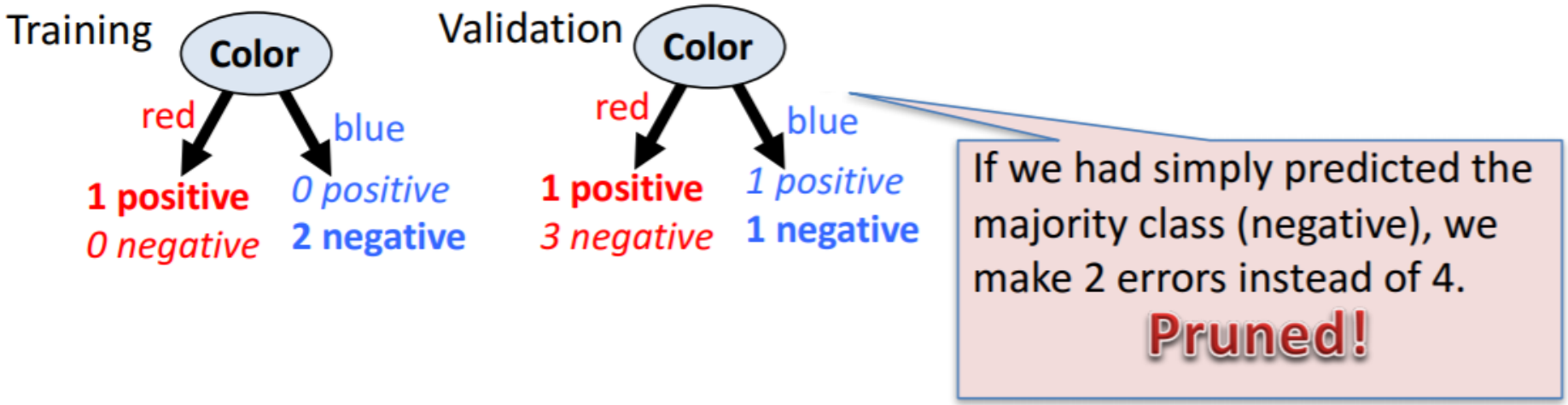
Grow tree based on *training set*

Do until further pruning is harmful:

1. Evaluate impact on validation set of pruning each possible node (plus those below it)
2. Greedily remove the node that most improves *validation set* accuracy

Pruning Decision Trees

- Pruning of the decision tree is done by replacing a whole subtree by a leaf node.
- The replacement takes place if a decision rule establishes that the expected error rate in the subtree is greater than in the single leaf.
- For example,



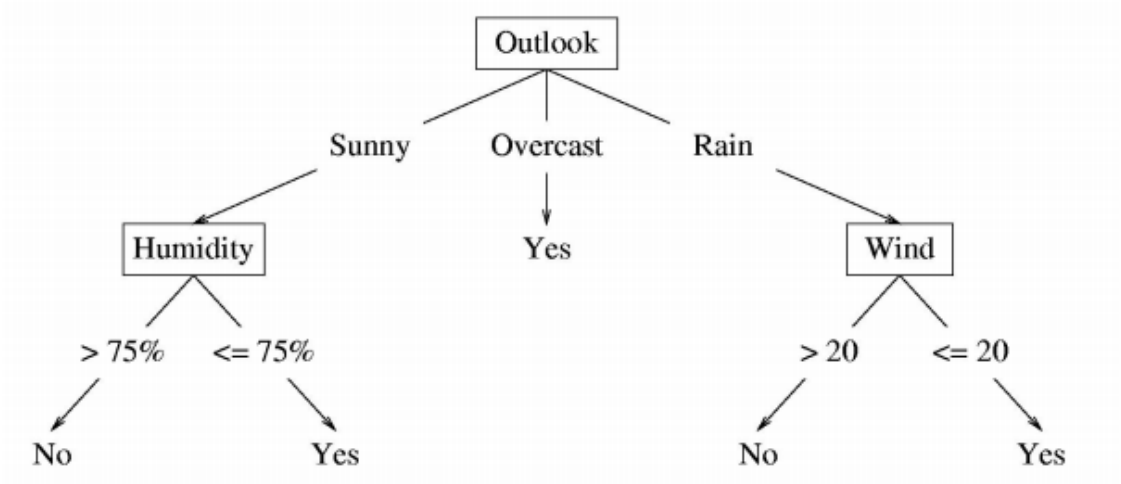
Real-Valued Inputs

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

Real-valued Features



- Change to binary splits by choosing a threshold
- One method:
  - Sort instances by value, identify adjacencies with different classes

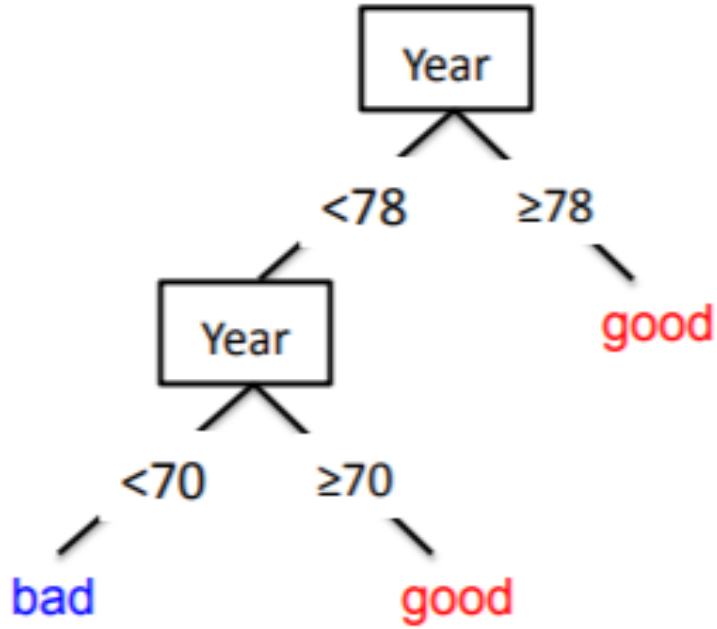
Temperature:	40	48	60	72	80	90
PlayTennis:	No	No	Yes	Yes	Yes	No

candidate splits

  - Choose among splits by InfoGain()

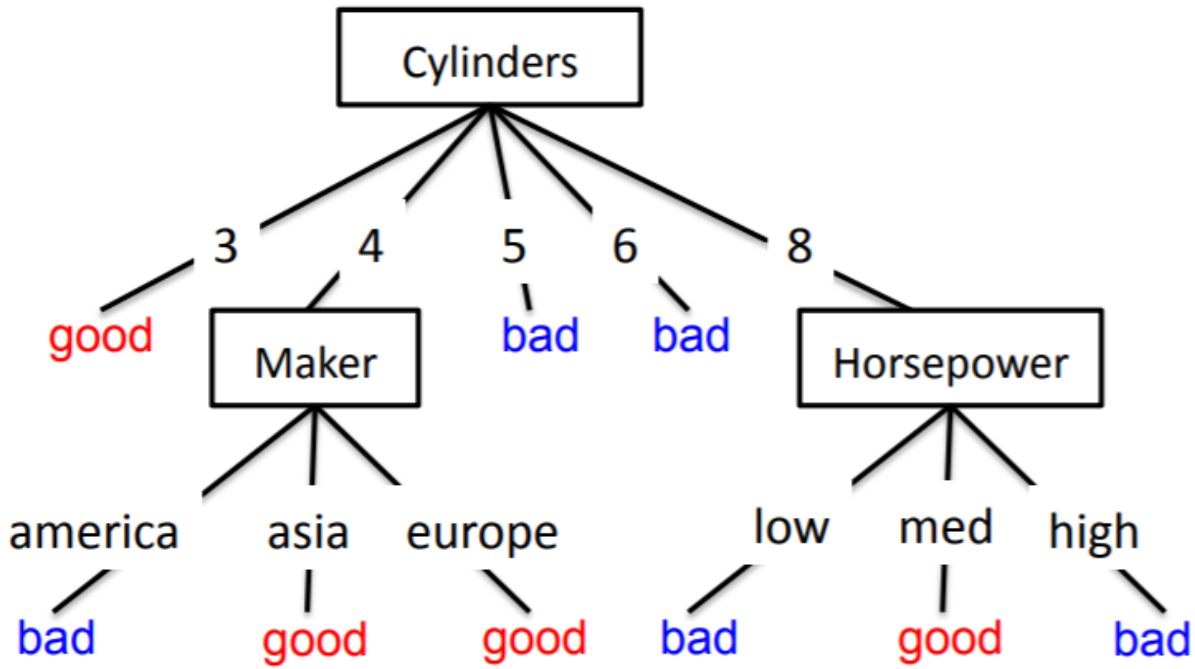
Threshold Splits

- **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**



Interpretability

- Each internal node tests an attribute x_i
- One branch for each possible 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!

Decision Boundary

- Decision trees divide the feature space into axis-parallel (hyper-)rectangles
- Each rectangular region is labeled with one label
  - or a probability distribution over labels