Decision Trees

Machine Learning – CSEP546

Carlos Guestrin

University of Washington

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Linear separability

- A dataset is **linearly separable** iff there exists a **separating hyperplane**:
  - Exists **w**, such that:
    - $w_0 + \sum_i w_i x_i > 0$; if $\mathbf{x}=\{x_1,\ldots,x_k\}$ is a positive example
    - $w_0 + \sum_i w_i x_i < 0$; if $\mathbf{x}=\{x_1,\ldots,x_k\}$ is a negative example

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Not linearly separable data

- Some datasets are **not linearly separable!**

Addressing non-linearly separable data – Option 1, non-linear features

- Choose non-linear features, e.g.,
  - □ Typical linear features: $w_0 + \sum_i w_i x_i$
  - □ Example of non-linear features:
    - Degree 2 polynomials, $w_0 + \sum_i w_i x_i + \sum_{ij} w_{ij} x_i x_j$
- Classifier $h_{\mathbf{w}}(\mathbf{x})$ still linear in parameters $\mathbf{w}$
  - □ As easy to learn
  - □ Data is linearly separable in higher dimensional spaces

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Addressing non-linearly separable data – Option 2, non-linear classifier

- Choose a classifier $h_{\mathbf{w}}(\mathbf{x})$ that is non-linear in parameters **w**, e.g.,
  - Decision trees, boosting, nearest neighbor, neural networks…
- More general than linear classifiers
- But, can often be harder to learn (non-convex/concave optimization required)
- But, but, often very useful

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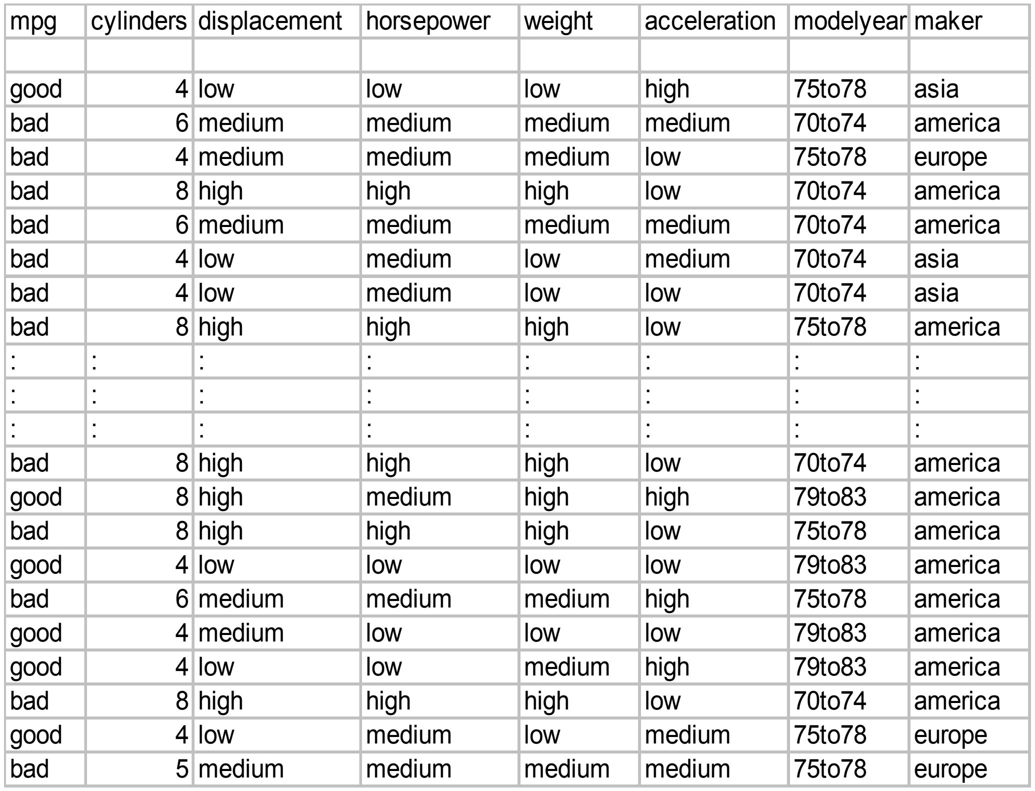
A small dataset: Miles Per Gallon

Suppose we want to predict MPG



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

40 training examples

From the UCI repository (thanks to Ross Quinlan)

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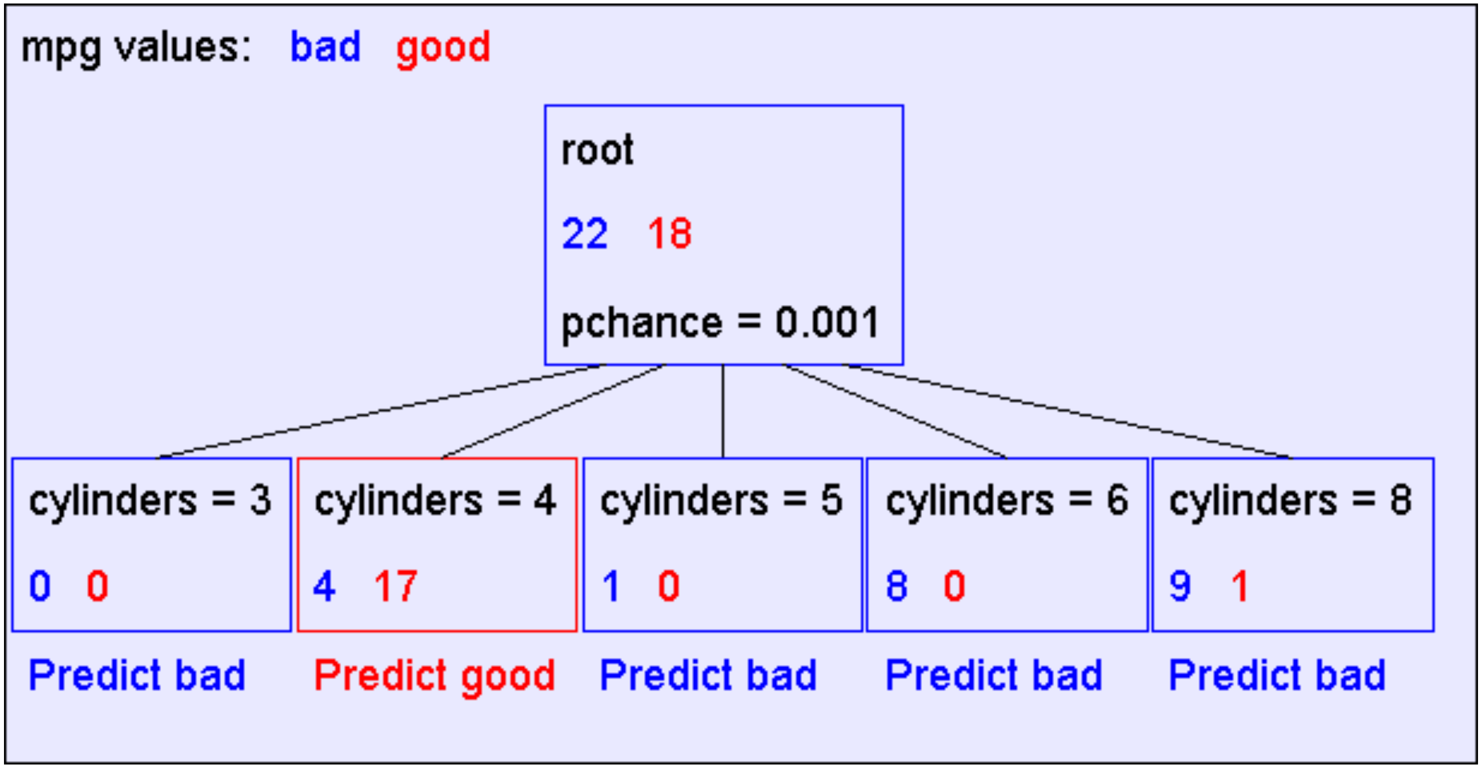
A Decision Stump



mpg values: bad good

root

22 18

pchance = 0.001

cylinders = 3

0 0

Predict bad

cylinders = 4

4 17

Predict good

cylinders = 5

1 0

Predict bad

cylinders = 6

8 0

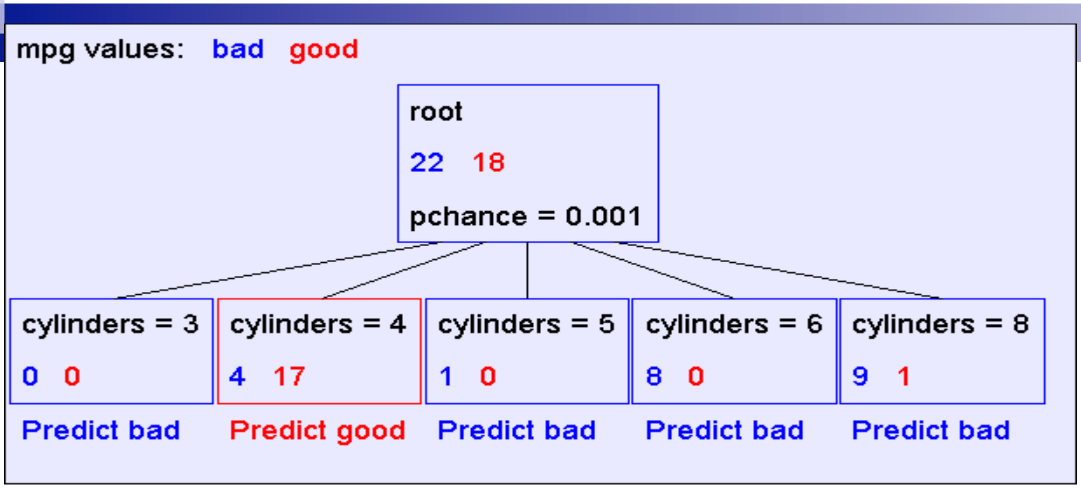
Predict bad

cylinders = 8

9 1

Predict bad

Recursion Step

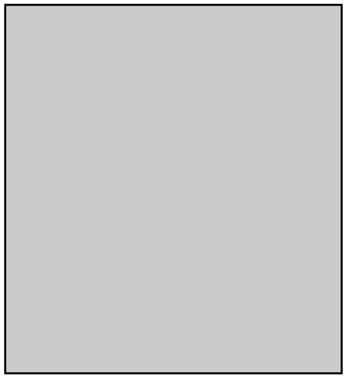


mpg values: bad good

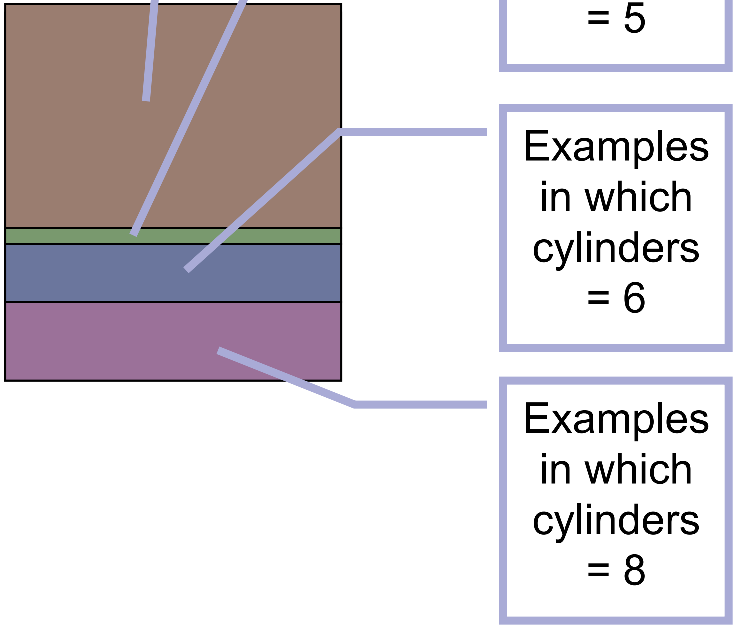
root
22 18
pchance = 0.001

cylinders = 3	cylinders = 4	cylinders = 5	cylinders = 6	cylinders = 8
0 0	4 17	1 0	8 0	9 1
Predict bad	Predict good	Predict bad	Predict bad	Predict bad

Take the Original Dataset..



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



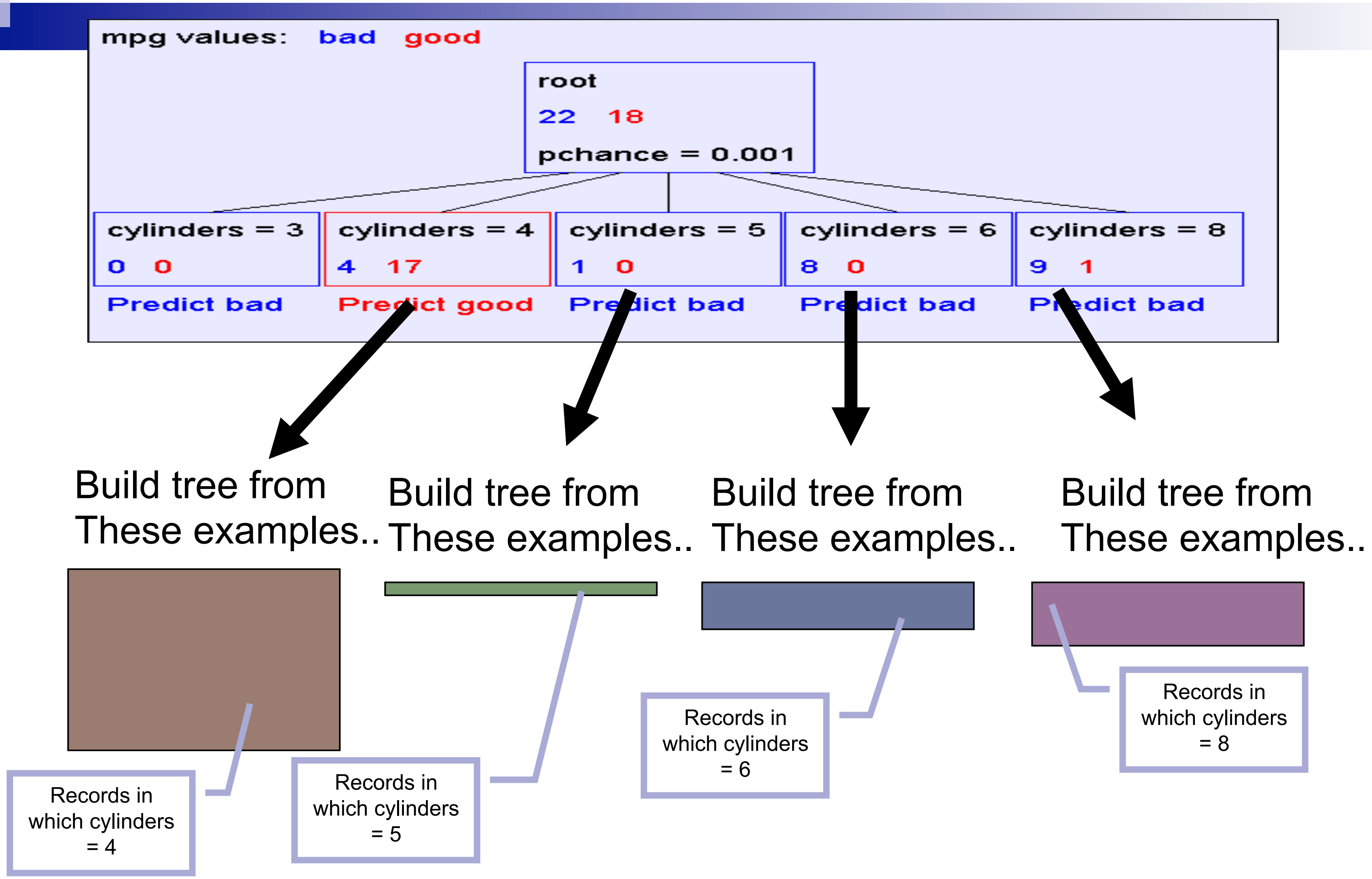
Examples in which cylinders = 4

Examples in which cylinders = 5

Examples in which cylinders = 6

Examples in which cylinders = 8

Recursion Step



mpg values: bad good

root
22 18
pchance = 0.001

cylinders = 3	cylinders = 4	cylinders = 5	cylinders = 6	cylinders = 8
0 0	4 17	1 0	8 0	9 1
Predict bad	Predict good	Predict bad	Predict bad	Predict bad

Build tree from These examples..

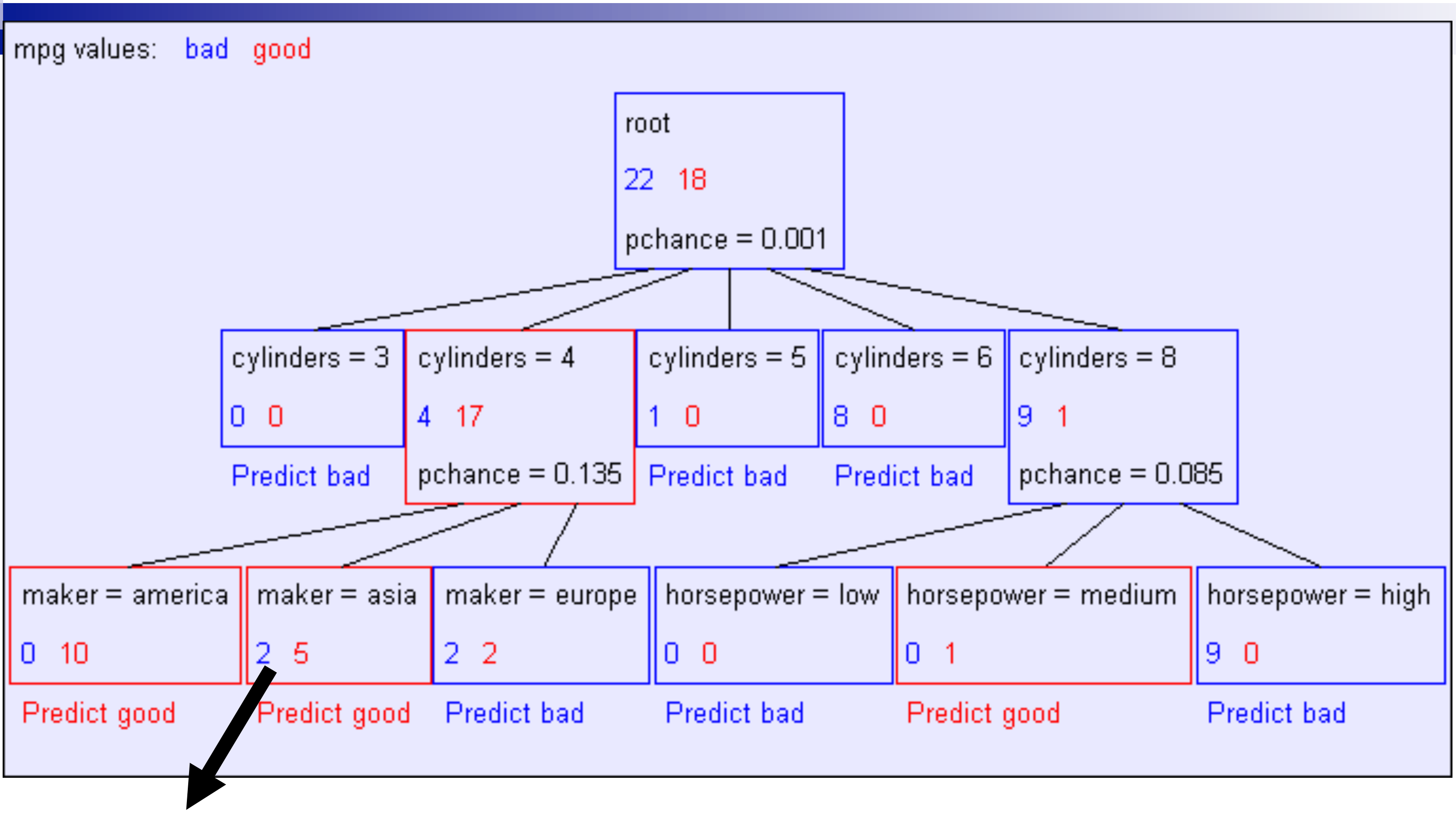
Build tree from These examples..

Build tree from These examples..

Build tree from These examples..

Records in which cylinders = 4
Records in which cylinders = 5
Records in which cylinders = 6
Records in which cylinders = 8

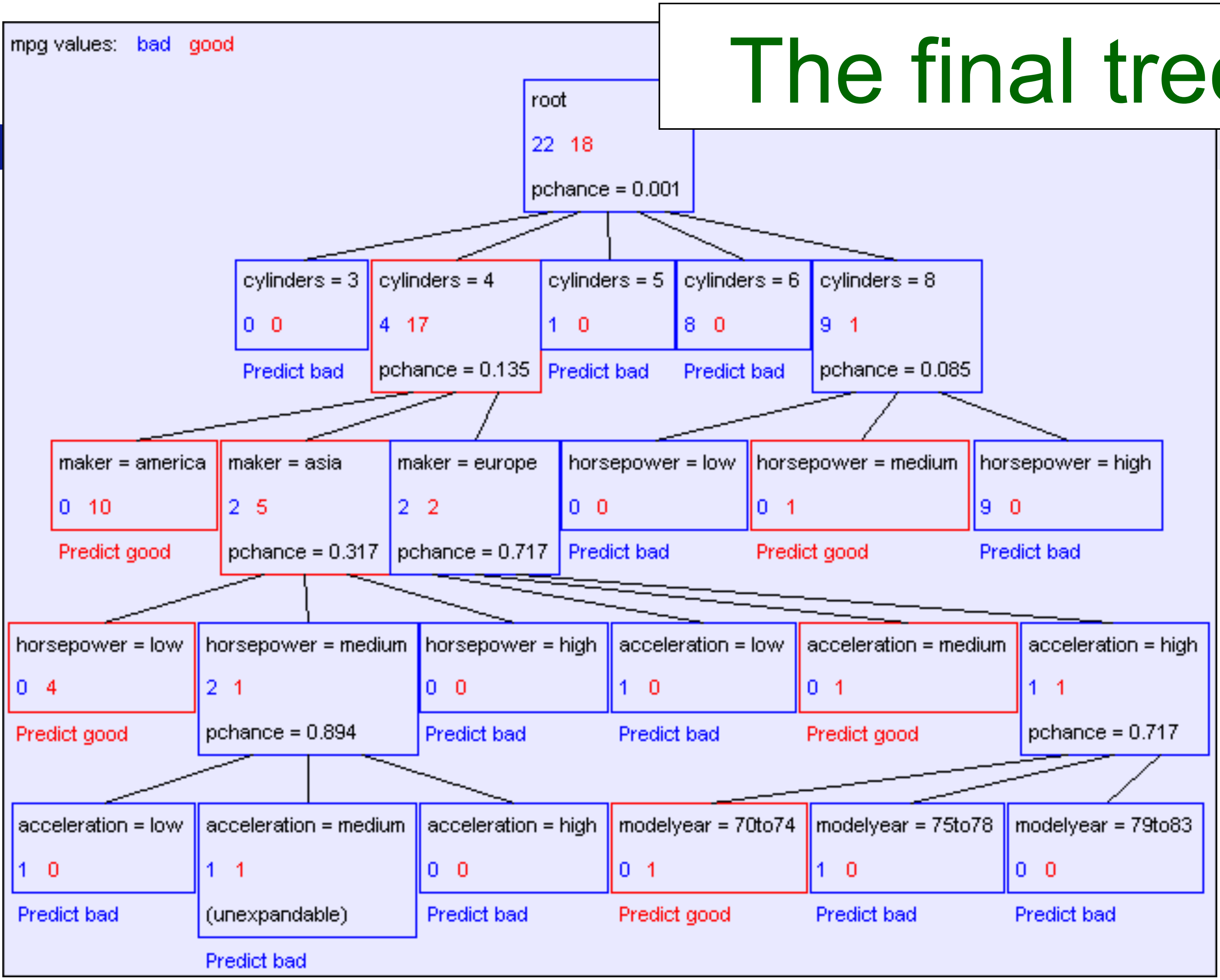
Second level of tree



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

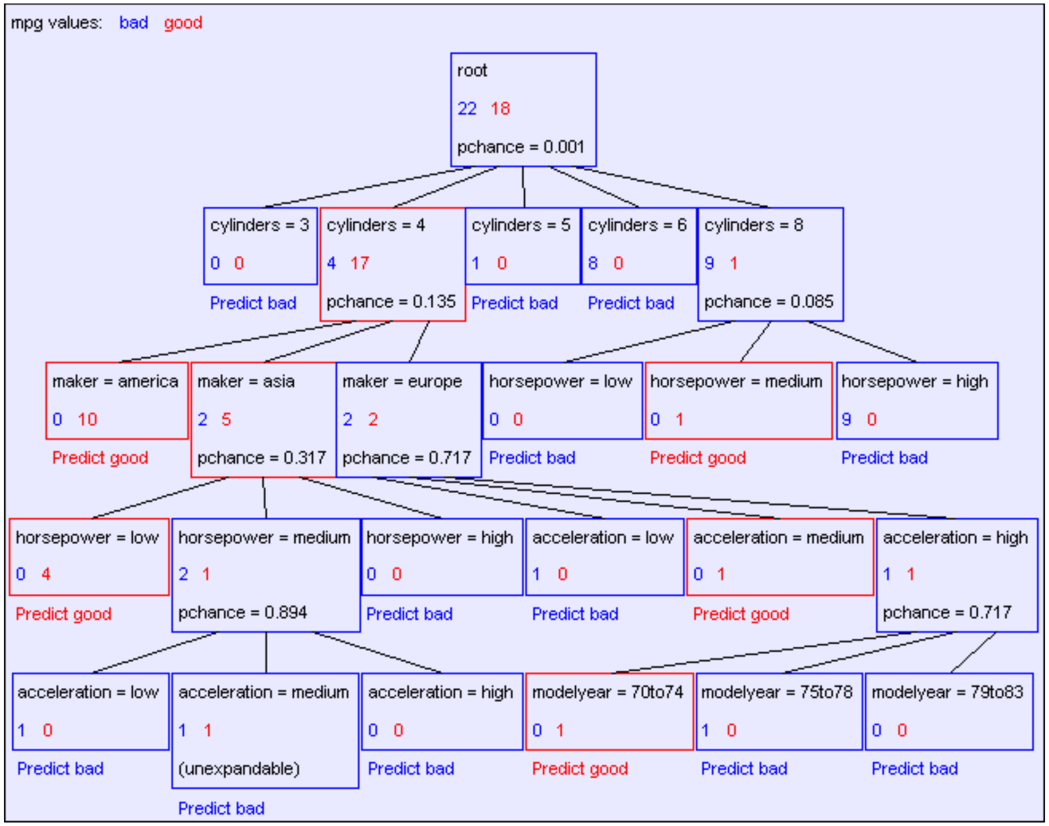
(Similar recursion in the other cases)

The final tree



Classification of a new example

- Classifying a test example – traverse tree and report leaf label



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

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))

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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

Choosing a good attribute

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

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Measuring uncertainty

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

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

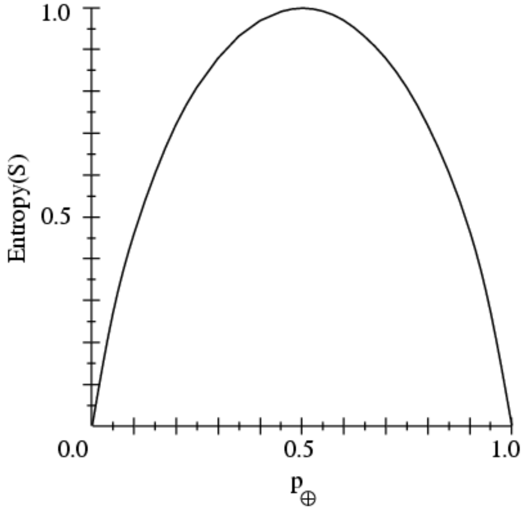
Entropy

Entropy *H(X)* 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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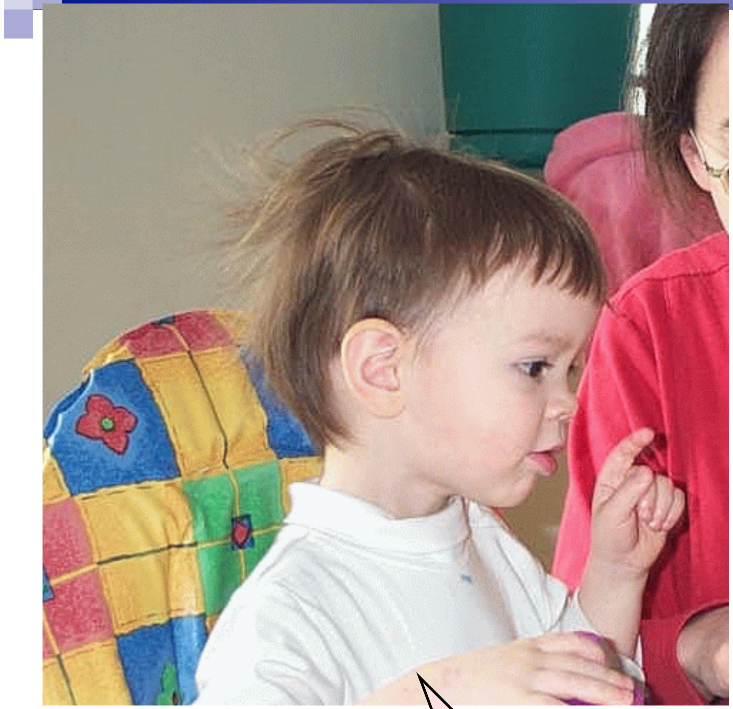
Andrew Moore's Entropy in a nutshell

Low Entropy

High Entropy

Andrew Moore’s Entropy in a nutshell



Low Entropy

..the values (locations of soup) sampled entirely from within the soup bowl

High Entropy

..the values (locations of soup) unpredictable... almost uniformly sampled throughout our dining room

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Information gain

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

- Advantage of attribute – decrease in uncertainty
  - Entropy of Y before you split
  - Entropy after split
    - Weight by probability of following each branch, i.e., normalized number of records

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

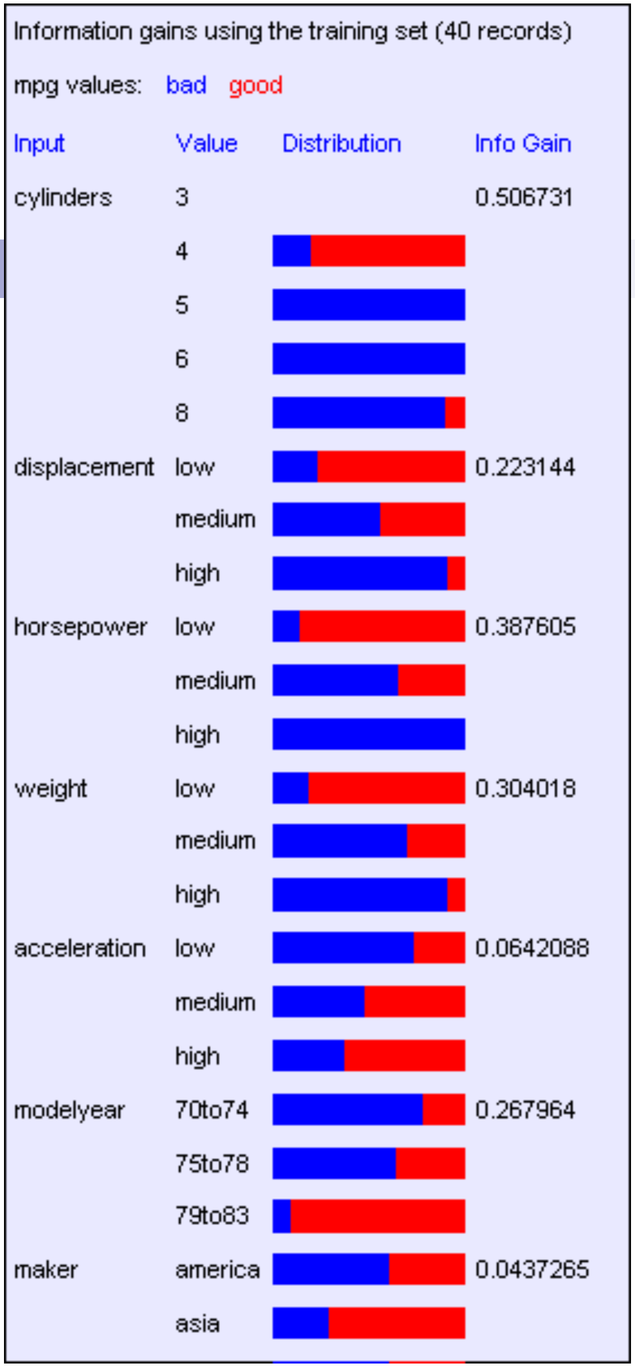
- Information gain is difference $IG(X) = H(Y) - H(Y \mid X)$

Learning decision trees

- Start from empty decision tree
- Split on **next best attribute (feature)**
  - Use, for example, information gain to select attribute
  - Split on $\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$
- Recurse

Suppose we want to predict MPG

Look at all the information gains…

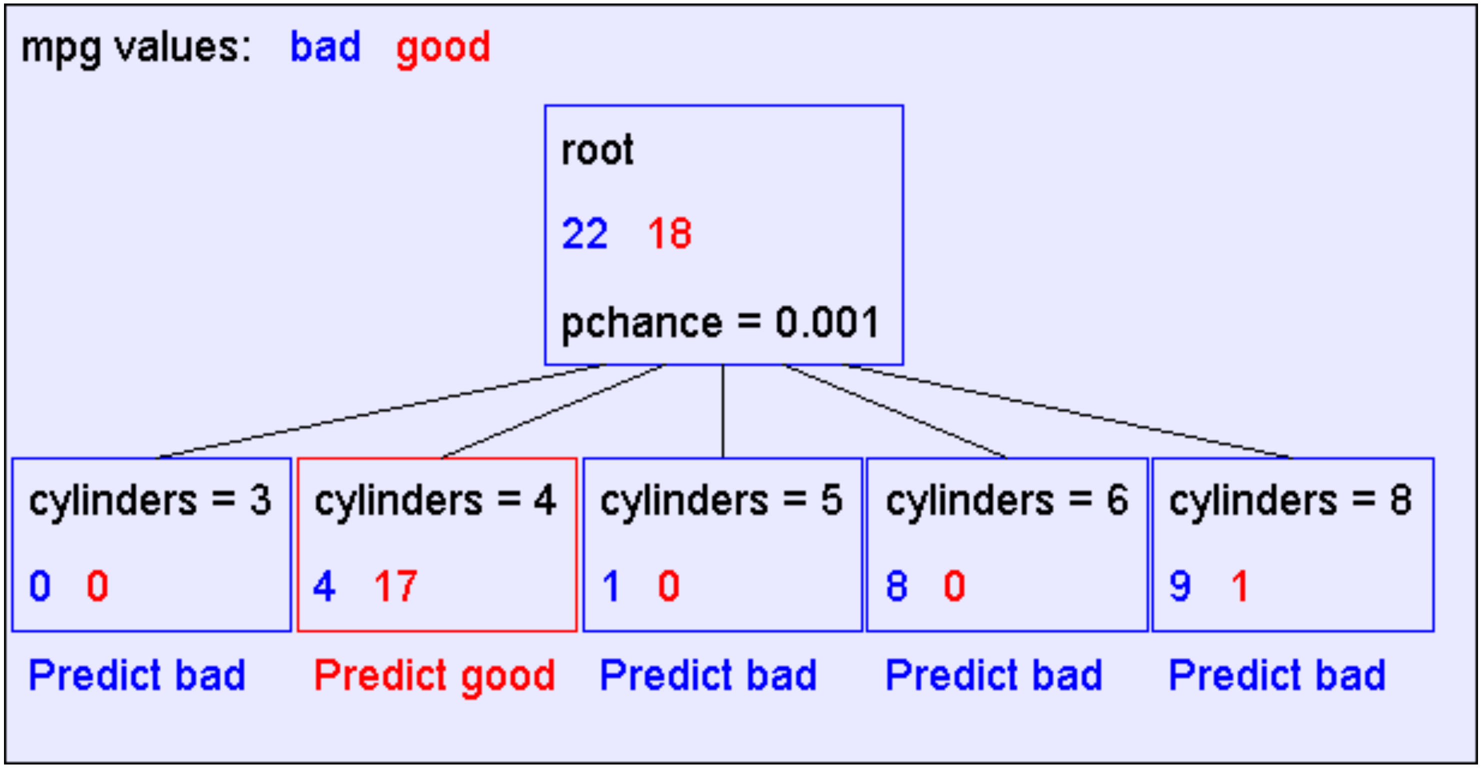


Information gains using the training set (40 records)

mpg values: bad good

Input	Value	Distribution	Info Gain
cylinders	3		0.506731
	4		
	5		
	6		
	8		
displacement	low		0.223144
	medium		
	high		
horsepower	low		0.387605
	medium		
	high		
weight	low		0.304018
	medium		
	high		
acceleration	low		0.0642088
	medium		
	high		
modelyear	70to74		0.267964
	75to78		
	79to83		
maker	america		0.0437265
	asia		

A Decision Stump



mpg values: bad good

root

22 18

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cylinders = 3

0 0

Predict bad

cylinders = 4

4 17

Predict good

cylinders = 5

1 0

Predict bad

cylinders = 6

8 0

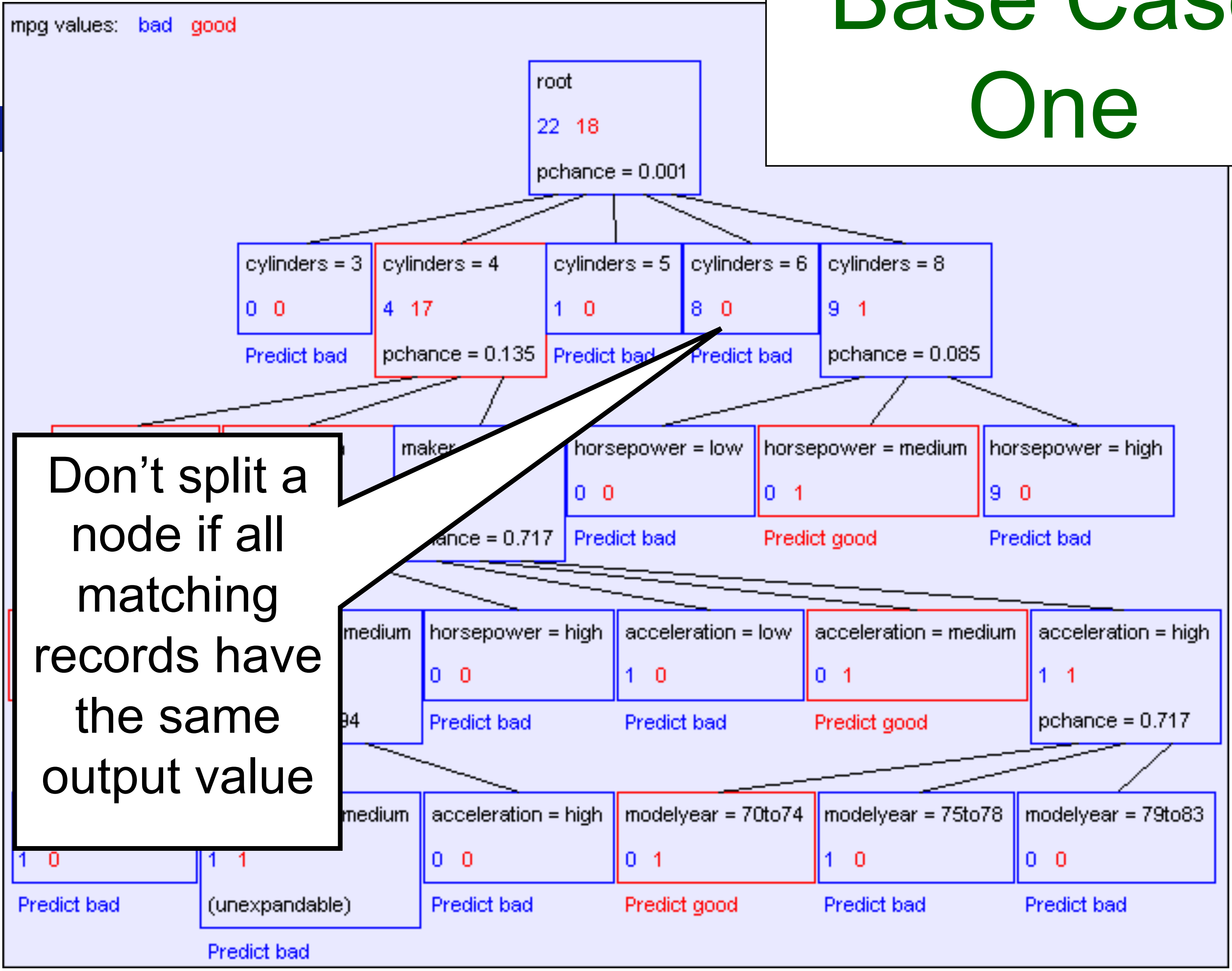
Predict bad

cylinders = 8

9 1

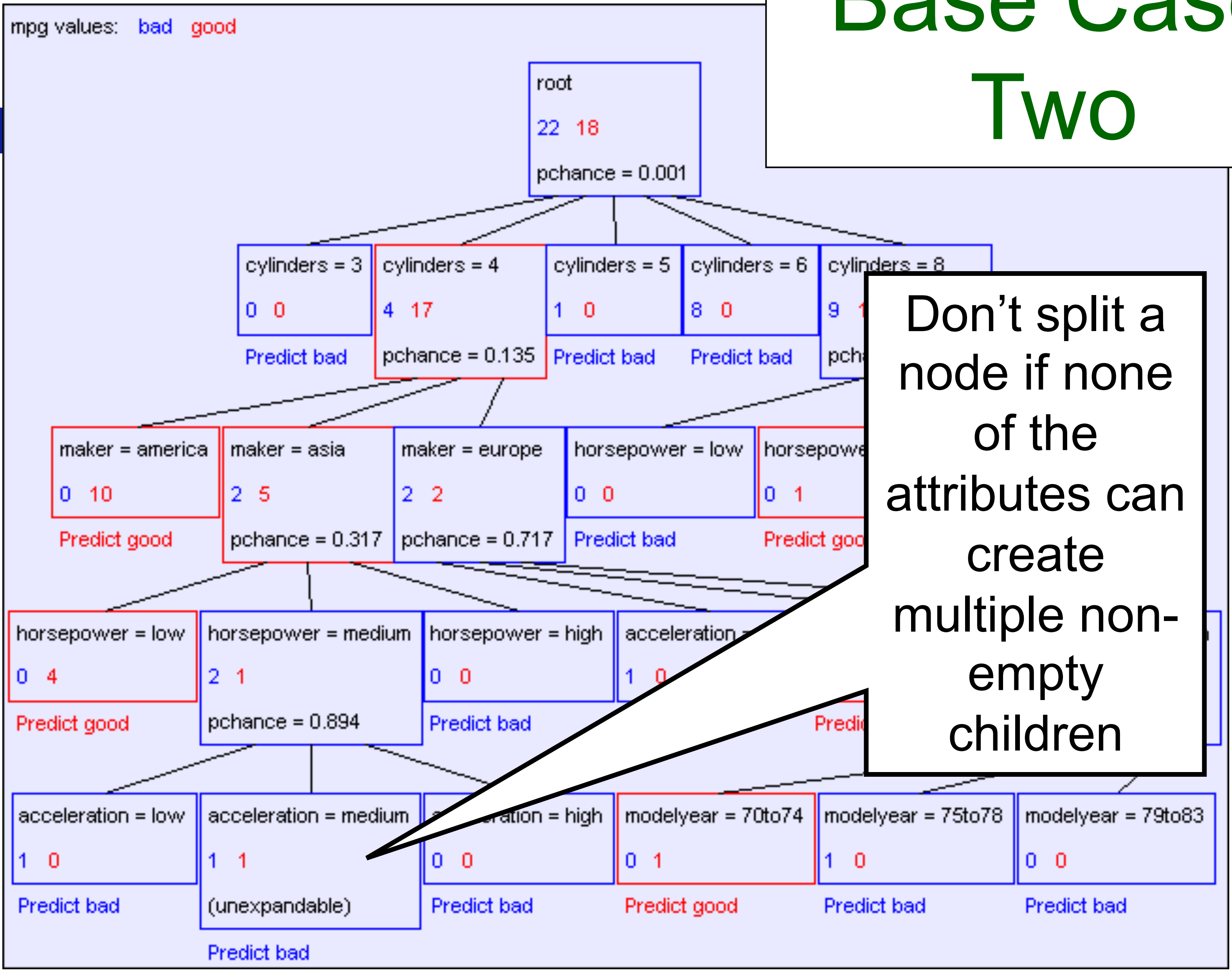
Predict bad

Base Case One



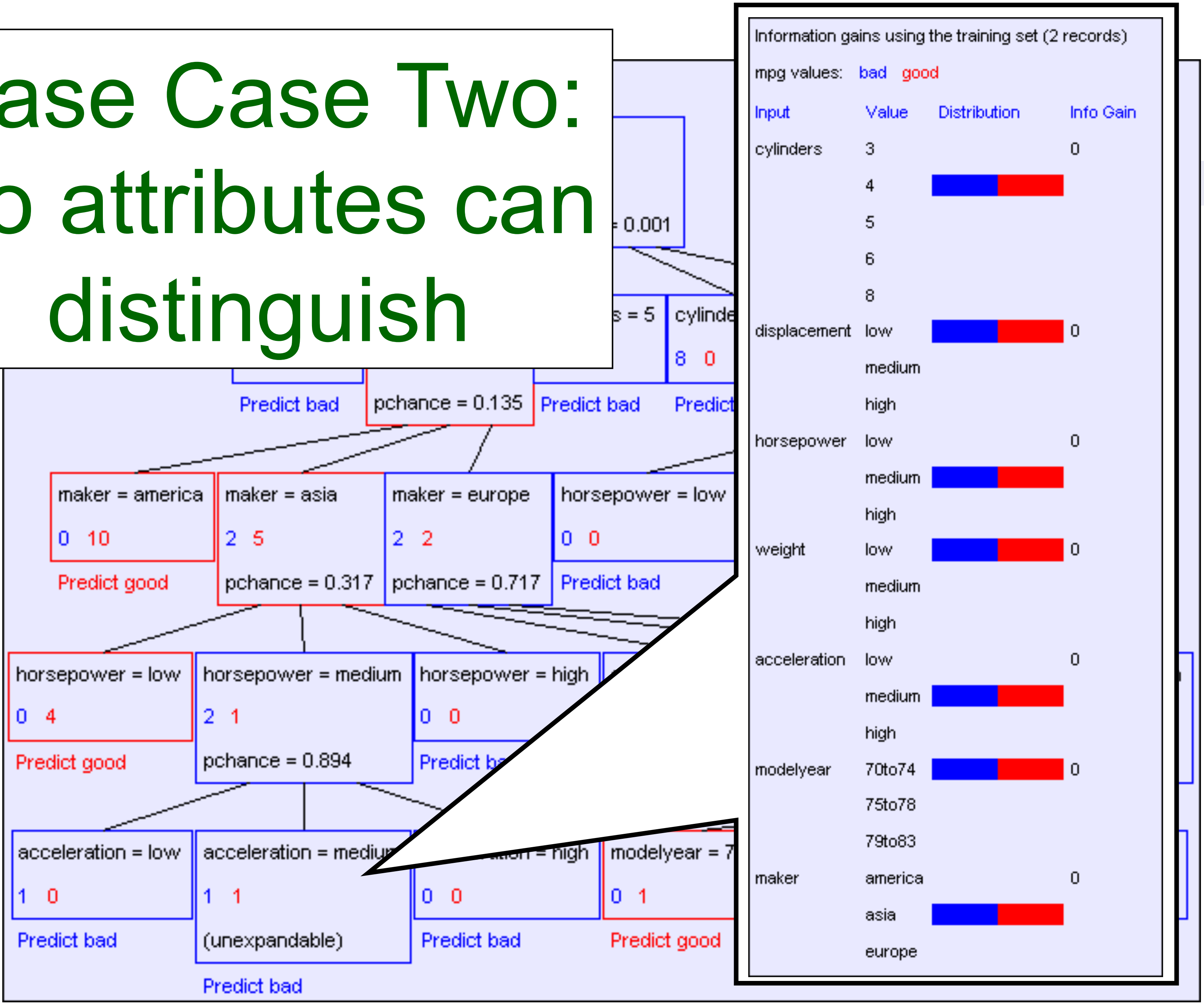
Don’t split a node if all matching records have the same output value

Base Case Two



Don’t split a node if none of the attributes can create multiple non-empty children

Base Case Two: No attributes can distinguish



Information gains using the training set (2 records)

mpg values: bad good

Input	Value	Distribution	Info Gain
cylinders	3		0
	4	🟦🟥	
	5		
	6		
	8		
displacement	low	🟦🟥	0
	medium		
	high		
horsepower	low		0
	medium	🟦🟥	
	high		
weight	low	🟦🟥	0
	medium		
	high		
acceleration	low		0
	medium	🟦🟥	
	high		
modelyear	70to74	🟦🟥	0
	75to78		
	79to83		
maker	america		0
	asia	🟦🟥	
	europe		

Base Cases

- 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

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 zero information gain then don't recurse

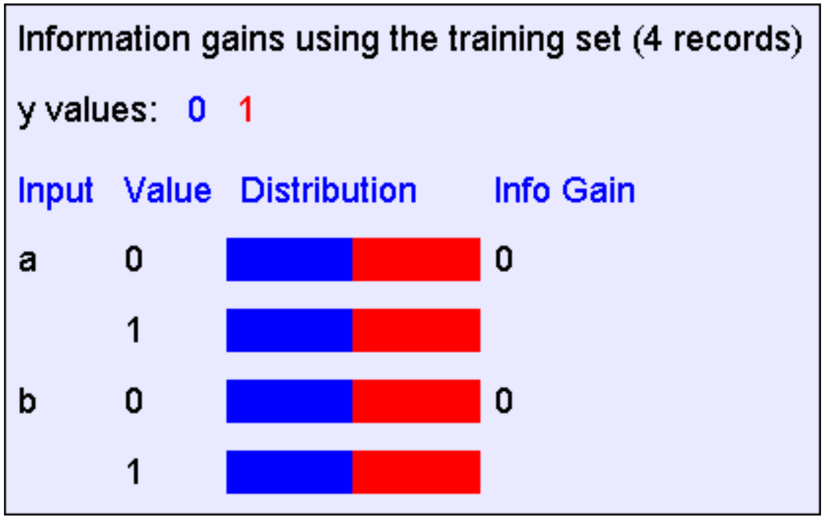
•*Is this a good idea?*

The problem with Base Case 3

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

Y = A XOR B

The information gains:

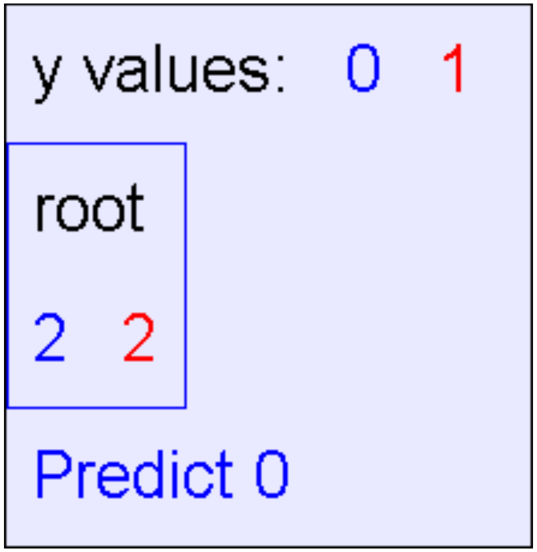


Information gains using the training set (4 records)

y values: 0 1

Input	Value	Distribution	Info Gain
a	0	🟦🟥	0
	1	🟦🟥	
b	0	🟦🟥	0
	1	🟦🟥	

The resulting bad decision tree:



y values: 0 1

root

2 2

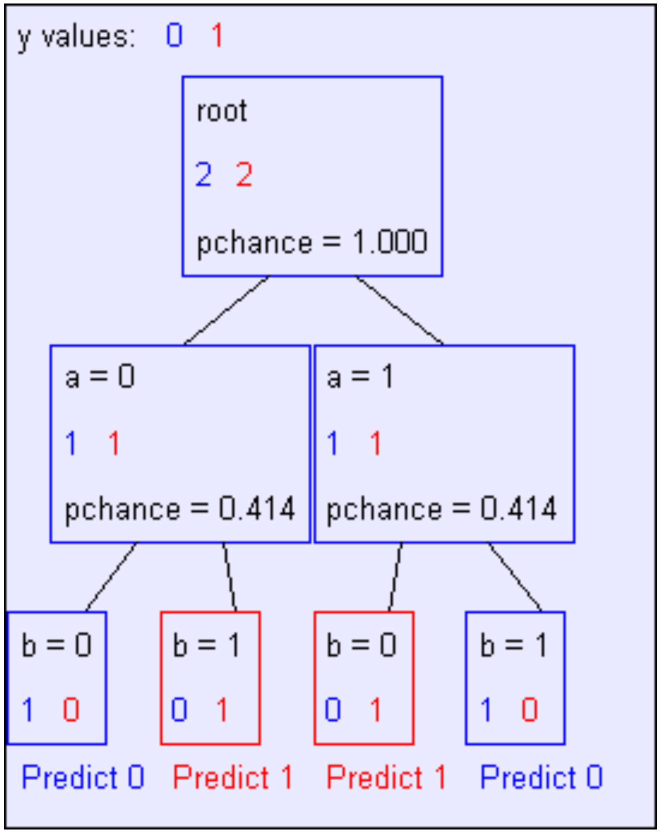
Predict 0

If we omit Base Case 3:

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

y = a XOR b

The resulting decision tree:



Basic Decision Tree Building Summarized

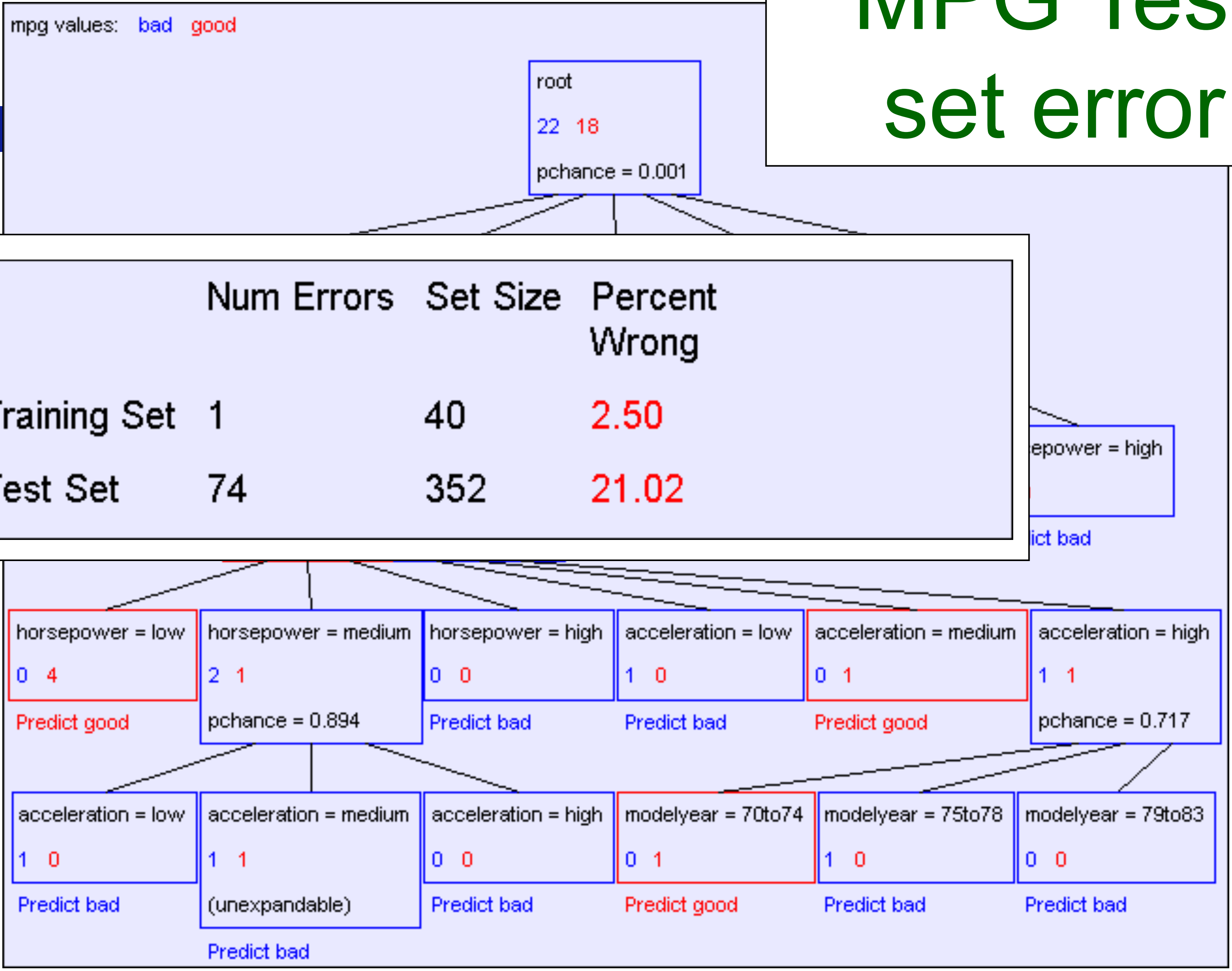
BuildTree(*DataSet,Output*)

- 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 and return a non-leaf node with n_X children.
  - The *i*'th child should be built by calling

    BuildTree(DS_i,*Output*)

    Where DS_i built consists of all those records in DataSet for which X = *i*th distinct value of X.

MPG Test set error



	Num Errors	Set Size	Percent Wrong
Training Set	1	40	2.50
Test Set	74	352	21.02

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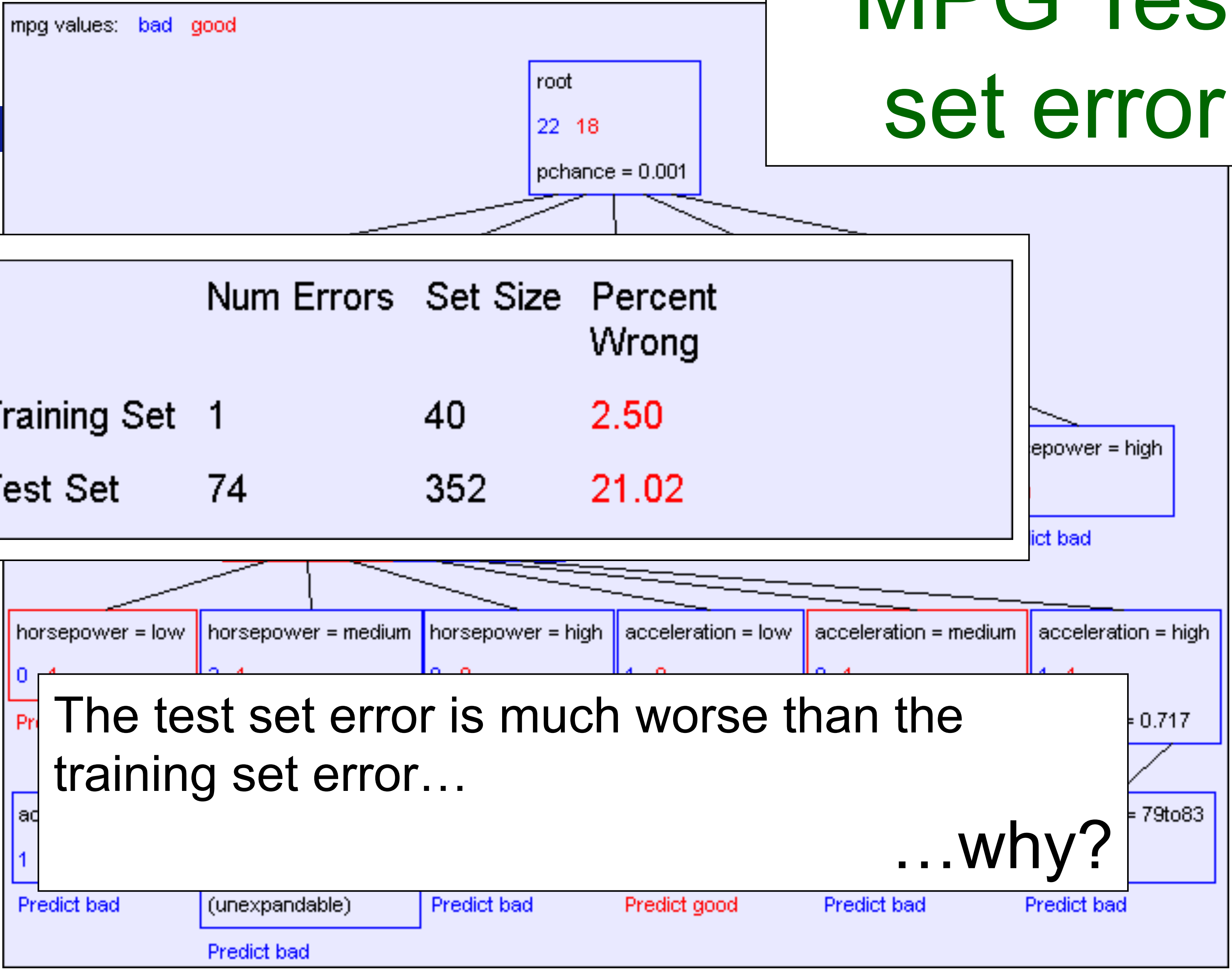
MPG Test set error

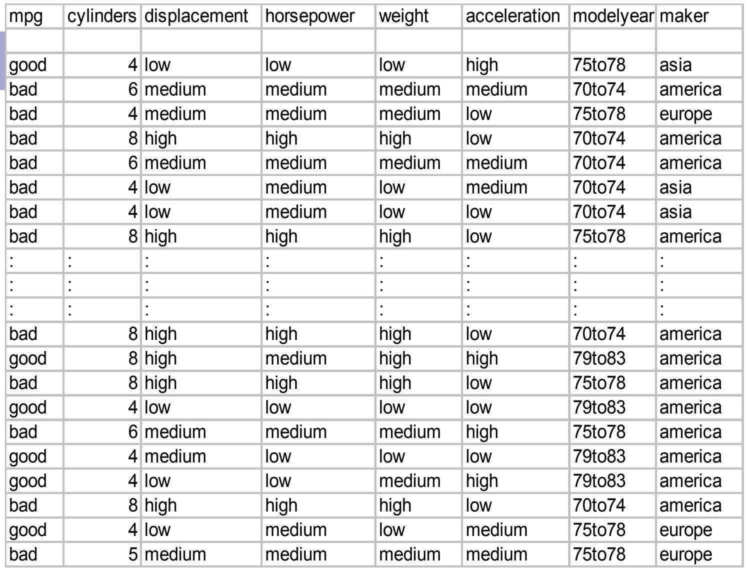


	Num Errors	Set Size	Percent Wrong
Training Set	1	40	2.50
Test Set	74	352	21.02

The test set error is much worse than the training set error…

…why?

Decision trees & Learning Bias



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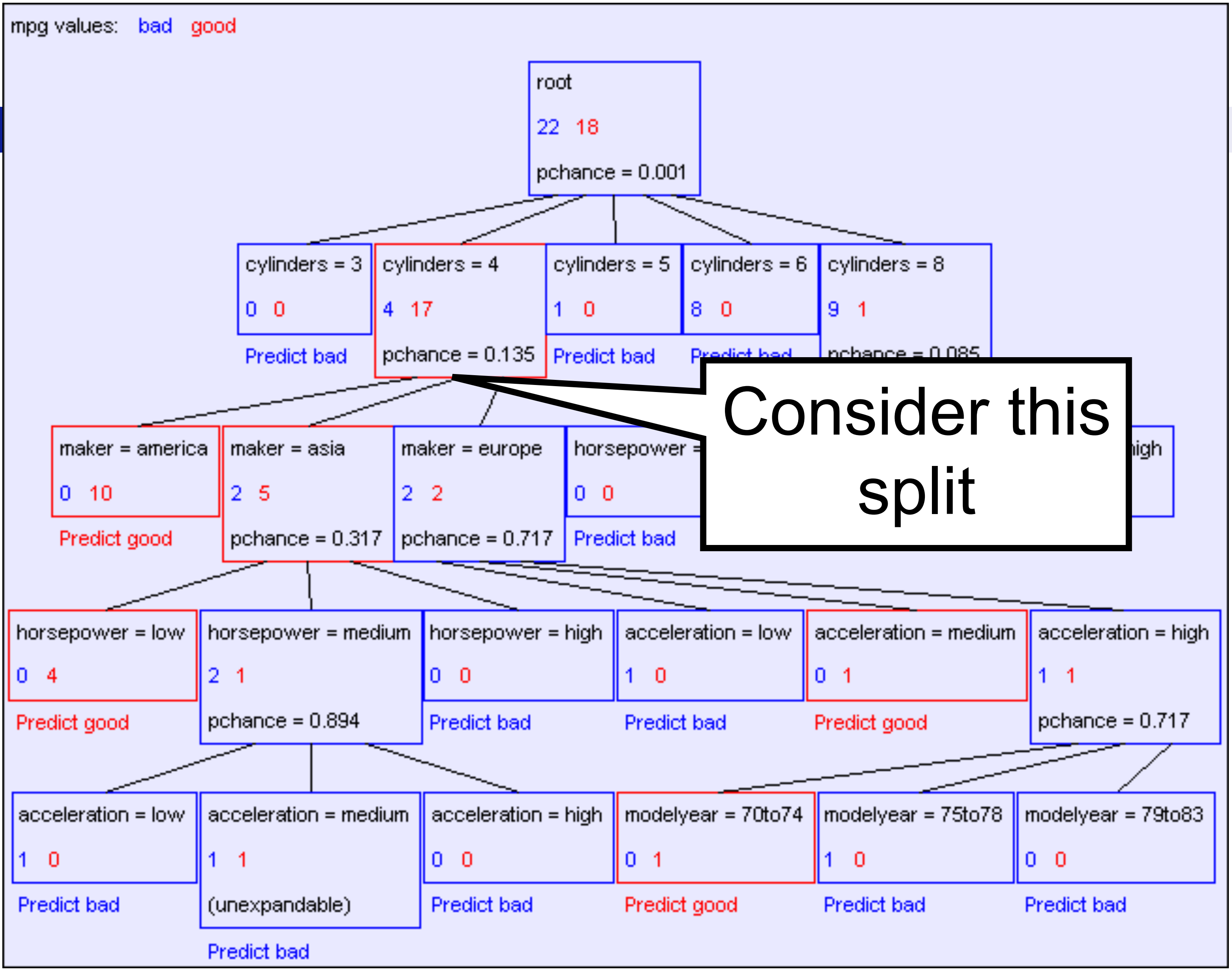
good	4	medium	low	low	low	79to83	america
good	4	low	low	medium	high	79to83	america
bad	8	high	high	high	low	70to74	america
good	4	low	medium	low	medium	75to78	europe
bad	5	medium	medium	medium	medium	75to78	europe

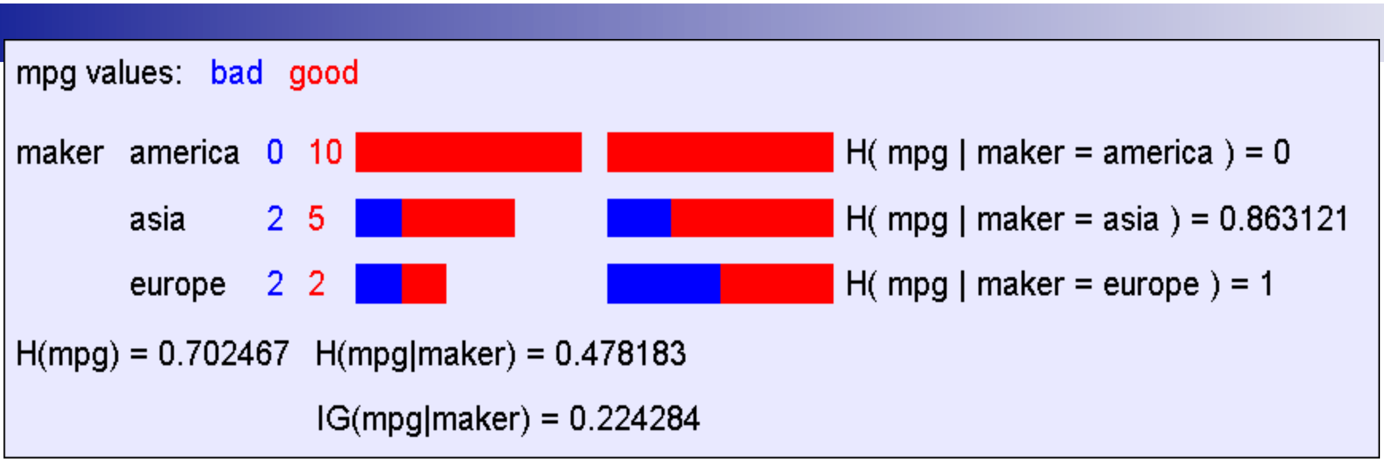
Decision trees will overfit

- Standard decision trees are have no learning bias
  - Training set error is always zero!
    - (If there is no label noise)
  - Lots of variance
  - Will definitely overfit!!!
  - Must bias towards simpler trees
- Many strategies for picking simpler trees:
  - Fixed depth
  - Fixed number of leaves
  - Or something smarter…



Consider this split

A chi-square test



mpg values: bad good

maker america 0 10 H(mpg | maker = america) = 0

asia 2 5 H(mpg | maker = asia) = 0.863121

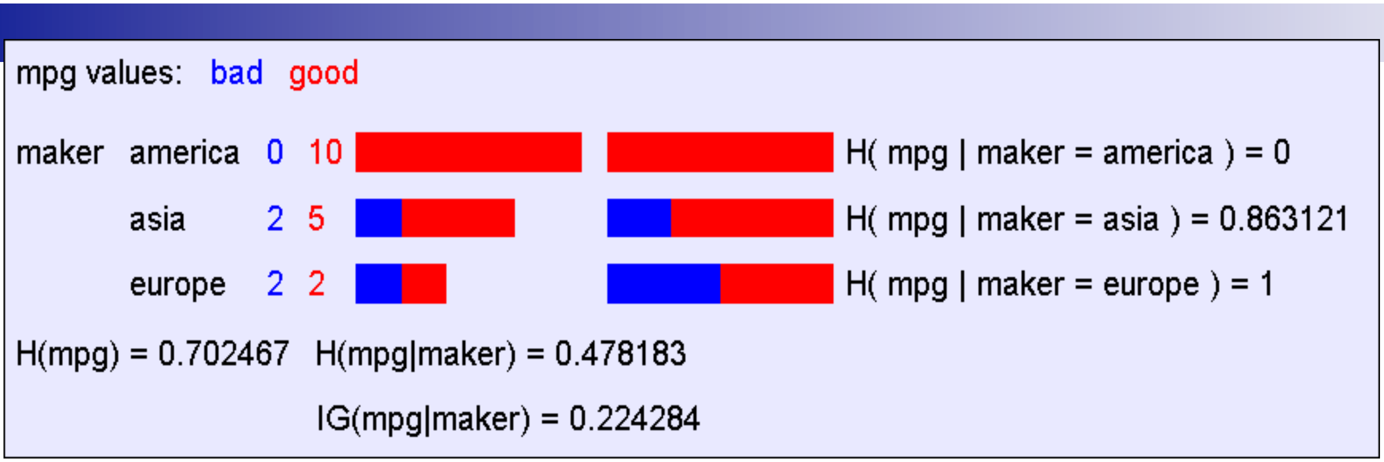
europe 2 2 H(mpg | maker = europe) = 1

H(mpg) = 0.702467 H(mpg|maker) = 0.478183

IG(mpg|maker) = 0.224284

- Suppose that MPG was completely uncorrelated with maker.
- What is the chance we'd have seen data of at least this apparent level of association anyway?

A chi-square test



```
mpg values:  bad  good

maker  america  0  10    H( mpg | maker = america ) = 0
       asia     2  5     H( mpg | maker = asia ) = 0.863121
       europe   2  2     H( mpg | maker = europe ) = 1

H(mpg) = 0.702467   H(mpg|maker) = 0.478183

                    IG(mpg|maker) = 0.224284
```

- Suppose that mpg was completely uncorrelated with maker.
- What is the chance we'd have seen data of at least this apparent level of association anyway?

By using a particular kind of chi-square test, the answer is 7.2%

(Such simple hypothesis tests are very easy to compute, unfortunately, not enough time to cover in the lecture, but see readings…)

Using Chi-squared to avoid overfitting

- Build the full decision tree as before
- But when you can grow it no more, start to prune:
  - □ Beginning at the bottom of the tree, delete splits in which p_{chance} > *MaxPchance*
  - □ Continue working you way up until there are no more prunable nodes

MaxPchance is a magic parameter you must specify to the decision tree, indicating your willingness to risk fitting noise

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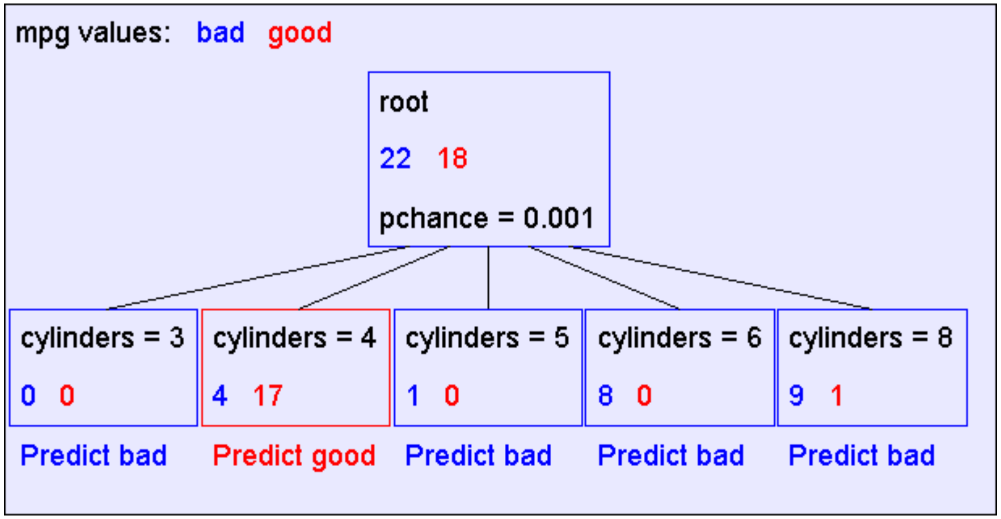
Pruning example

- With MaxPchance = 0.1, you will see the following MPG decision tree:



mpg values: bad good

root
22 18
pchance = 0.001

cylinders = 3
0 0
Predict bad

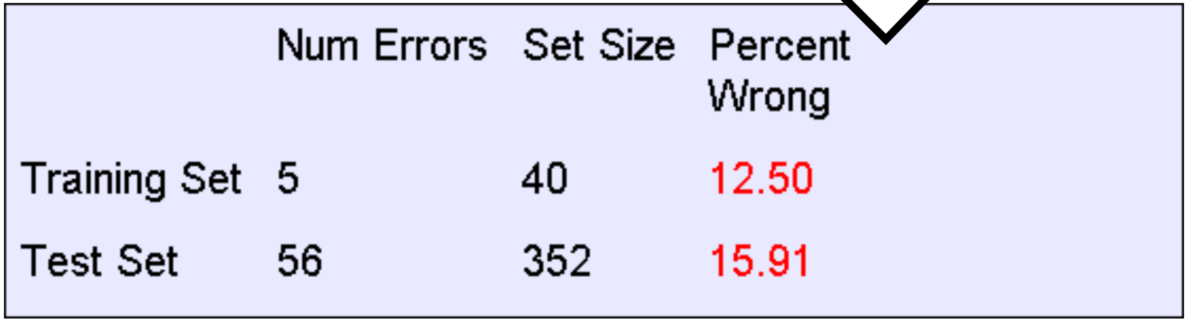
cylinders = 4
4 17
Predict good

cylinders = 5
1 0
Predict bad

cylinders = 6
8 0
Predict bad

cylinders = 8
9 1
Predict bad

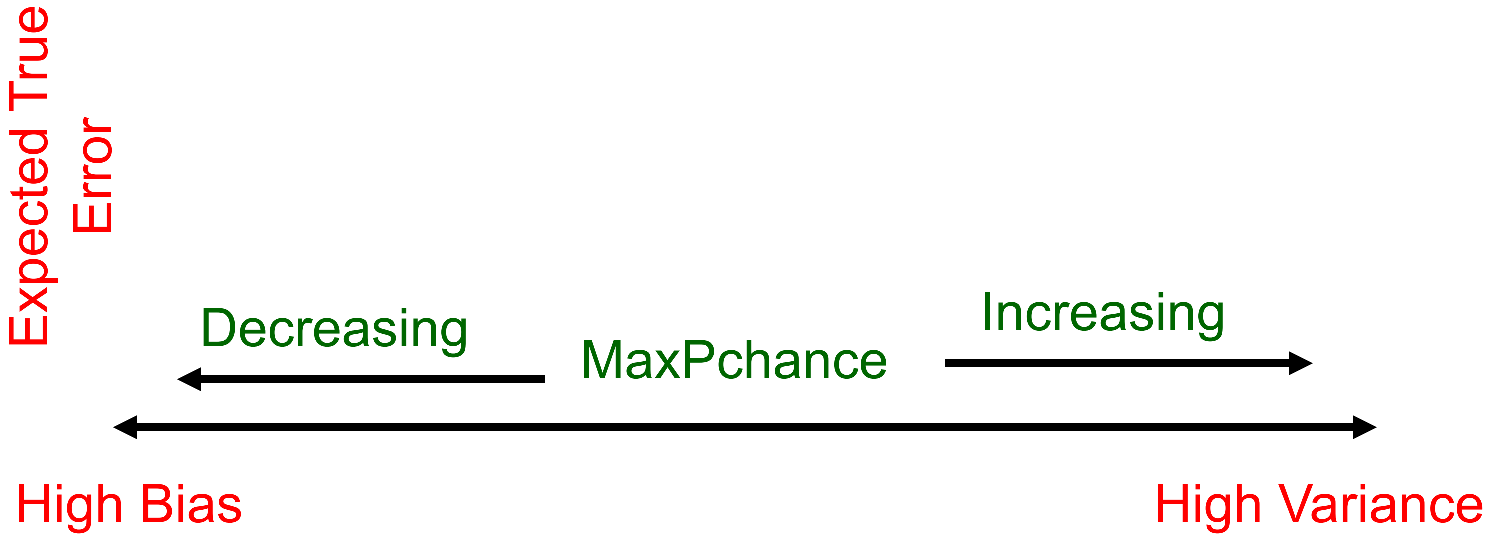
Note the improved test set accuracy compared with the unpruned tree



	Num Errors	Set Size	Percent Wrong
Training Set	5	40	12.50
Test Set	56	352	15.91

MaxPchance

- Technical note MaxPchance is a regularization parameter that helps us bias towards simpler models



Expected True Error

Decreasing

MaxPchance

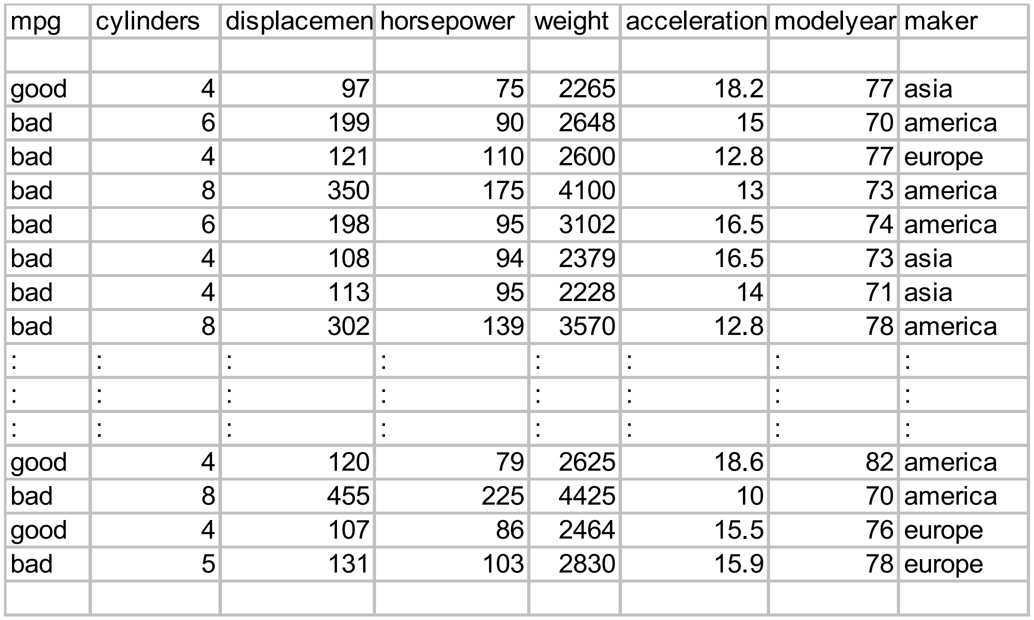
Increasing

High Bias

High Variance

Real-Valued inputs

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



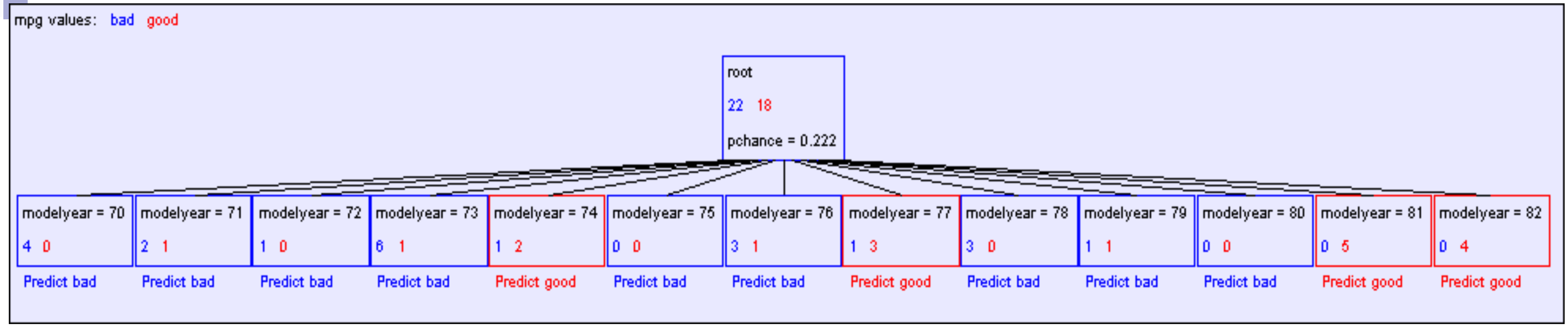
mpg	cylinders	displacemen	horsepower	weight	acceleration	modelyear	maker
good	4	97	75	2265	18.2	77	asia
bad	6	199	90	2648	15	70	america
bad	4	121	110	2600	12.8	77	europe
bad	8	350	175	4100	13	73	america
bad	6	198	95	3102	16.5	74	america
bad	4	108	94	2379	16.5	73	asia
bad	4	113	95	2228	14	71	asia
bad	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

Infinite number of possible split values!!!

Finite dataset, only finite number of relevant splits!

Idea One: Branch on each possible real value

“One branch for each numeric value” idea:



Hopeless: with such high branching factor will shatter the dataset and overfit

Threshold splits

- Binary tree, split on attribute X
  - One branch: $X < t$
  - Other branch: $X \geq t$

Choosing threshold split

- 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 finite number of *t*'s are important
  - Sort data according to X into $\{x_1,\ldots,x_m\}$
  - Consider split points of the form $x_i + (x_{i+1} - x_i)/2$

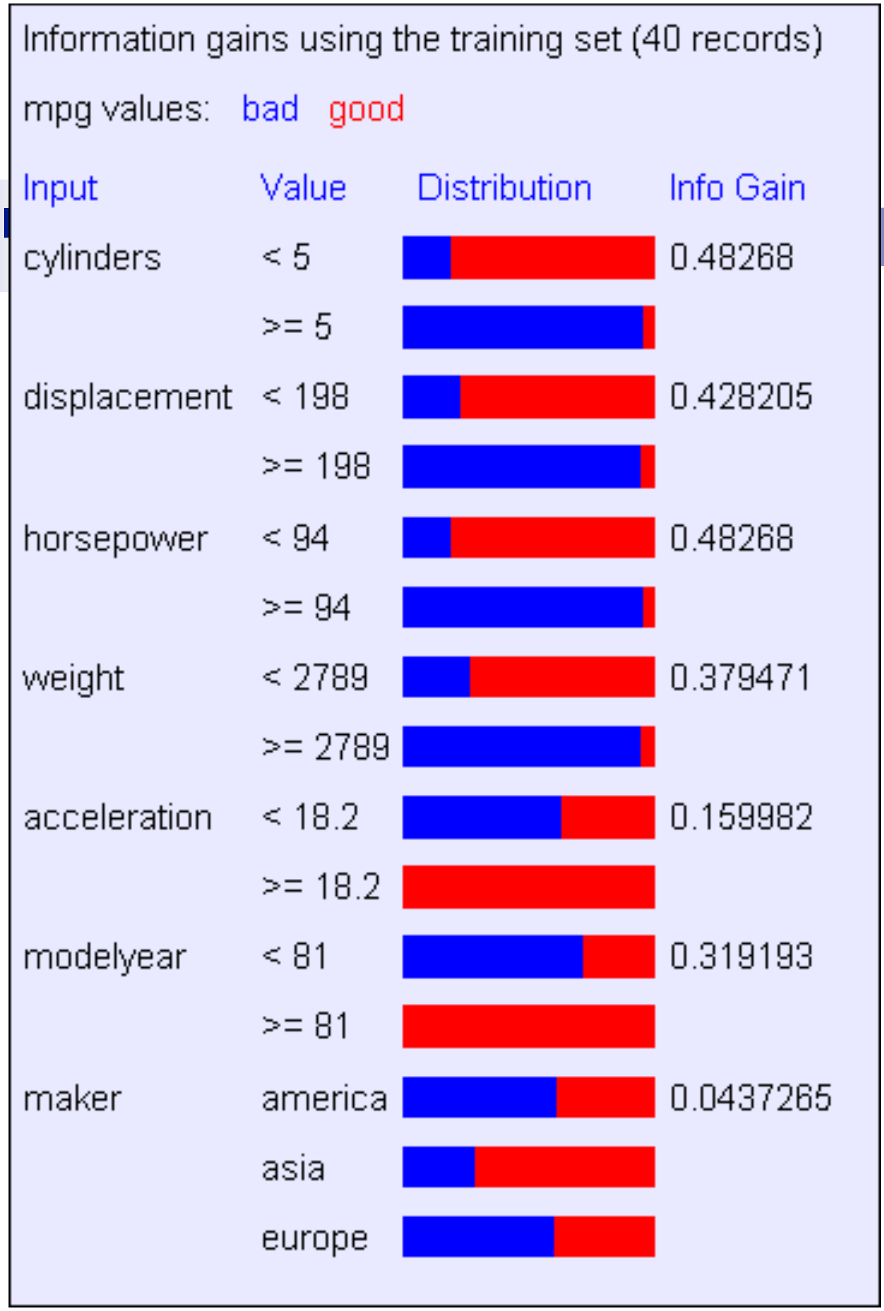
A better idea: thresholded splits

- Suppose X is real valued
- Define $IG(Y|X:t)$ as $H(Y) - H(Y|X:t)$
- Define $H(Y|X:t) =$

  $$H(Y|X < t)\ P(X < t) + H(Y|X >= t)\ P(X >= t)$$

  - $IG(Y|X:t)$ is the information gain for predicting Y if all you know is whether X is greater than or less than t
- Then define $IG^*(Y|X) = \max_t IG(Y|X:t)$
- For each real-valued attribute, use $IG^*(Y|X)$ for assessing its suitability as a split
- Note, may split on an attribute multiple times, with different thresholds

Example with MPG

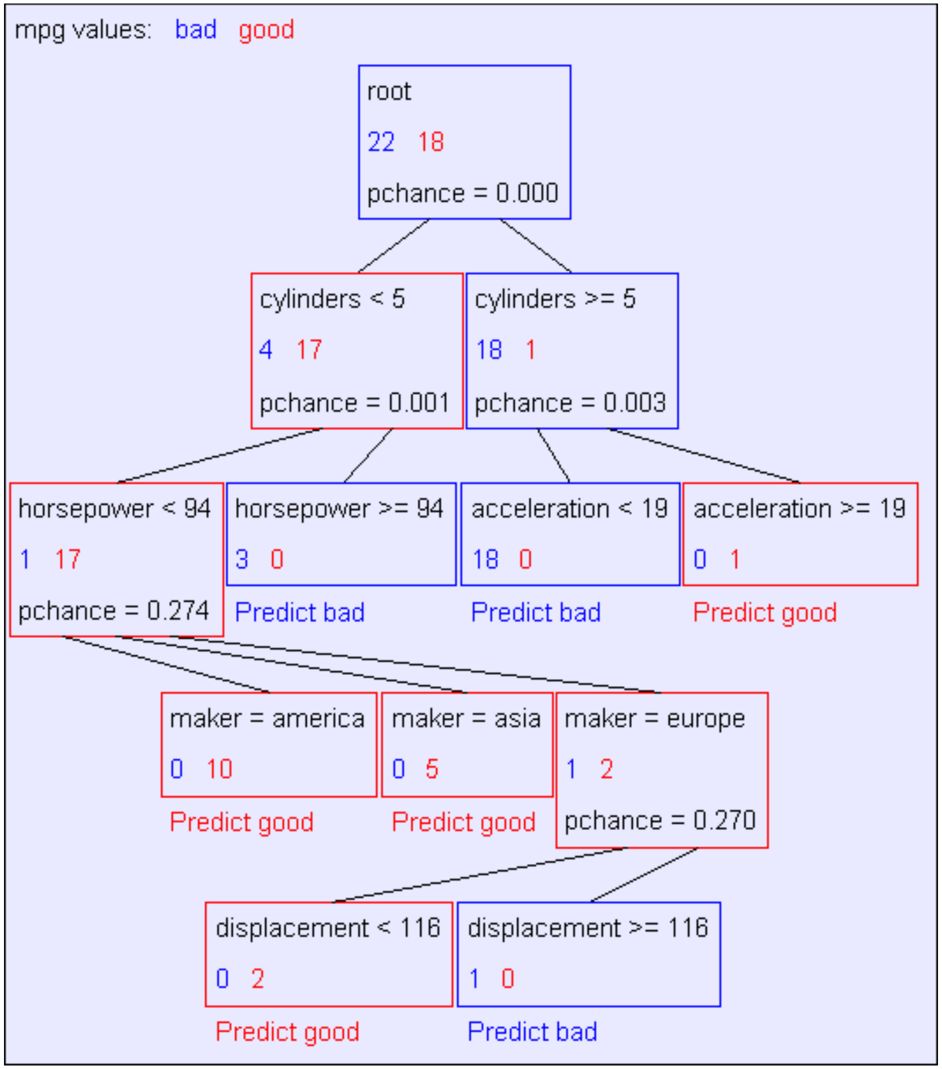


Information gains using the training set (40 records)

mpg values: bad good

Input	Value	Distribution	Info Gain
cylinders	< 5		0.48268
	>= 5		
displacement	< 198		0.428205
	>= 198		
horsepower	< 94		0.48268
	>= 94		
weight	< 2789		0.379471
	>= 2789		
acceleration	< 18.2		0.159982
	>= 18.2		
modelyear	< 81		0.319193
	>= 81		
maker	america		0.0437265
	asia		
	europe		

Example tree using reals



What you need to know about decision trees

- Decision trees are one of the most popular data mining tools
  - Easy to understand
  - Easy to implement
  - Easy to 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!!!
  - Zero bias classifier ! Lots of variance
  - Must use tricks to find “simple trees”, e.g.,
    - Fixed depth/Early stopping
    - Pruning
    - Hypothesis testing

Acknowledgements

- Some of the material in the decision trees presentation is courtesy of Andrew Moore, from his excellent collection of ML tutorials:
  - http://www.cs.cmu.edu/~awm/tutorials

Instance-based Learning

Nearest Neighbors/Non-Parametric Methods

Machine Learning – CSEP546

Carlos Guestrin

University of Washington

February 3, 2014

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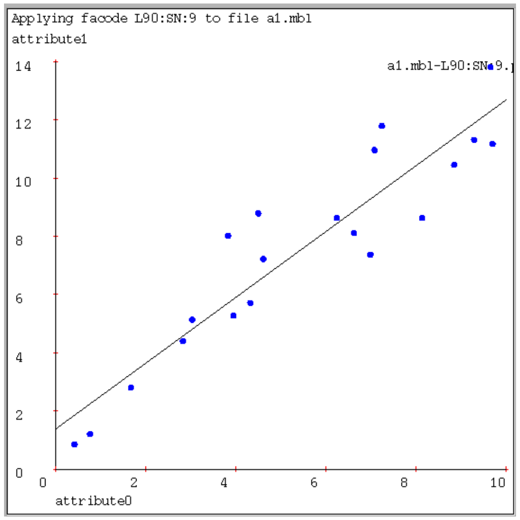
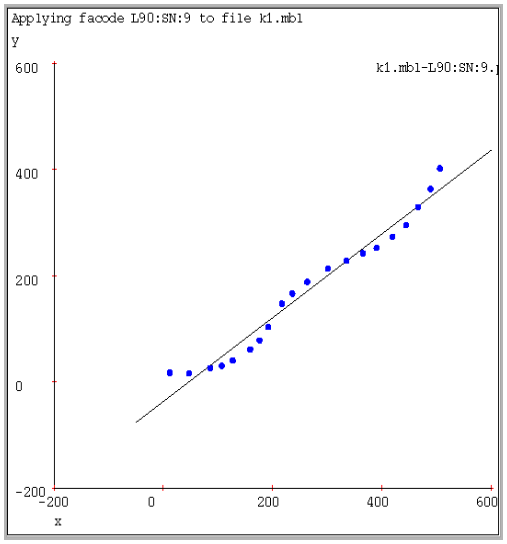
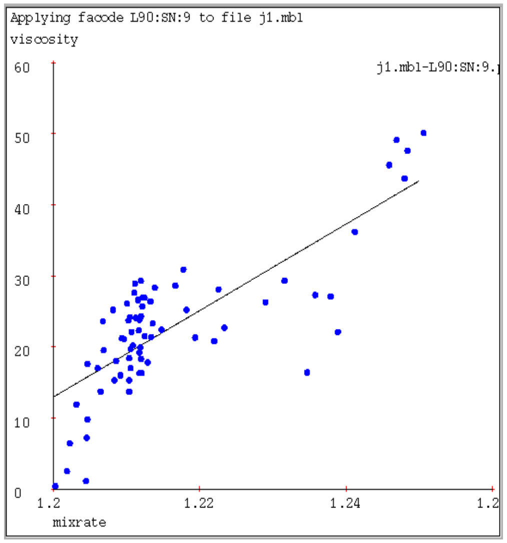
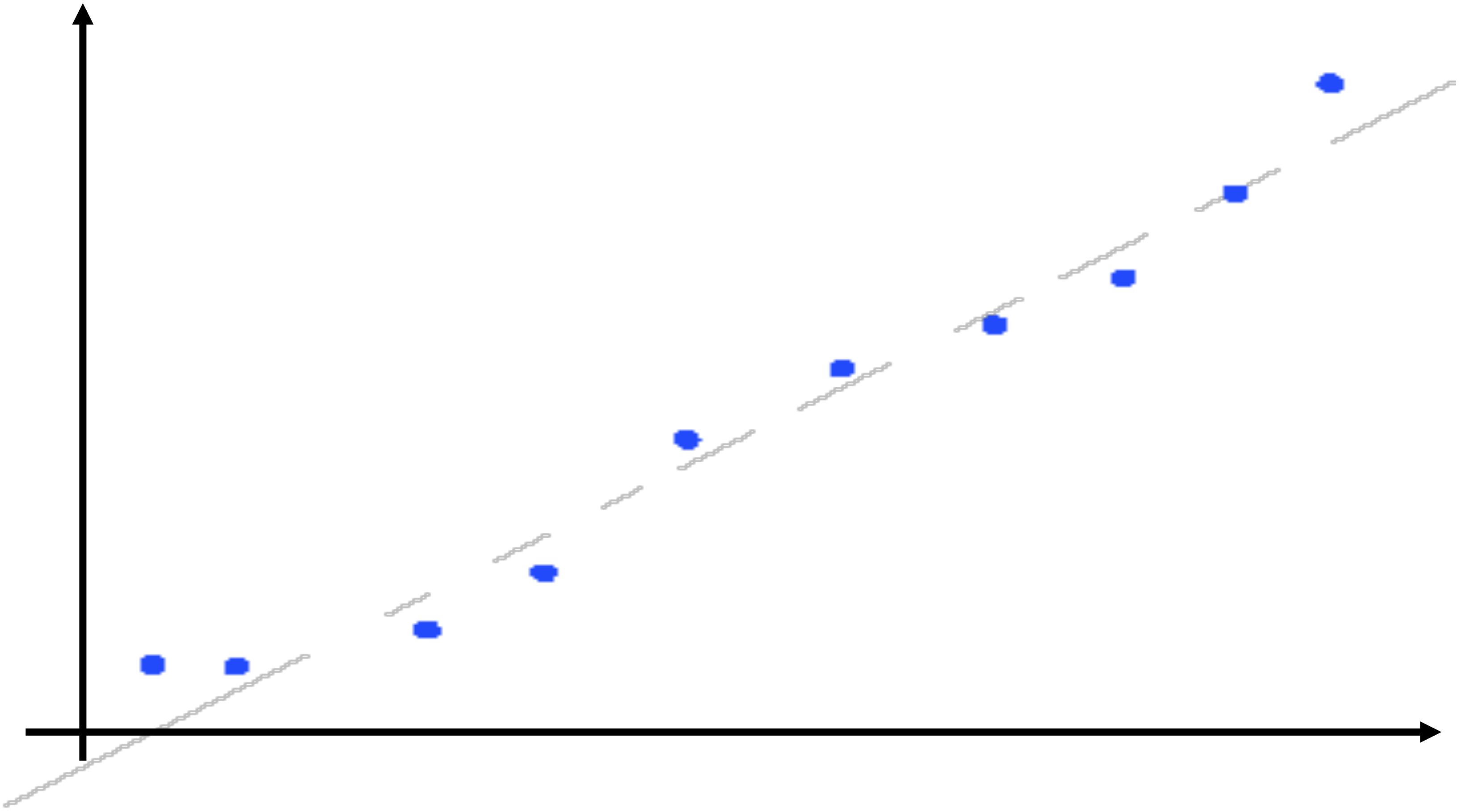
Why not just use Linear Regression?







Using data to predict new data



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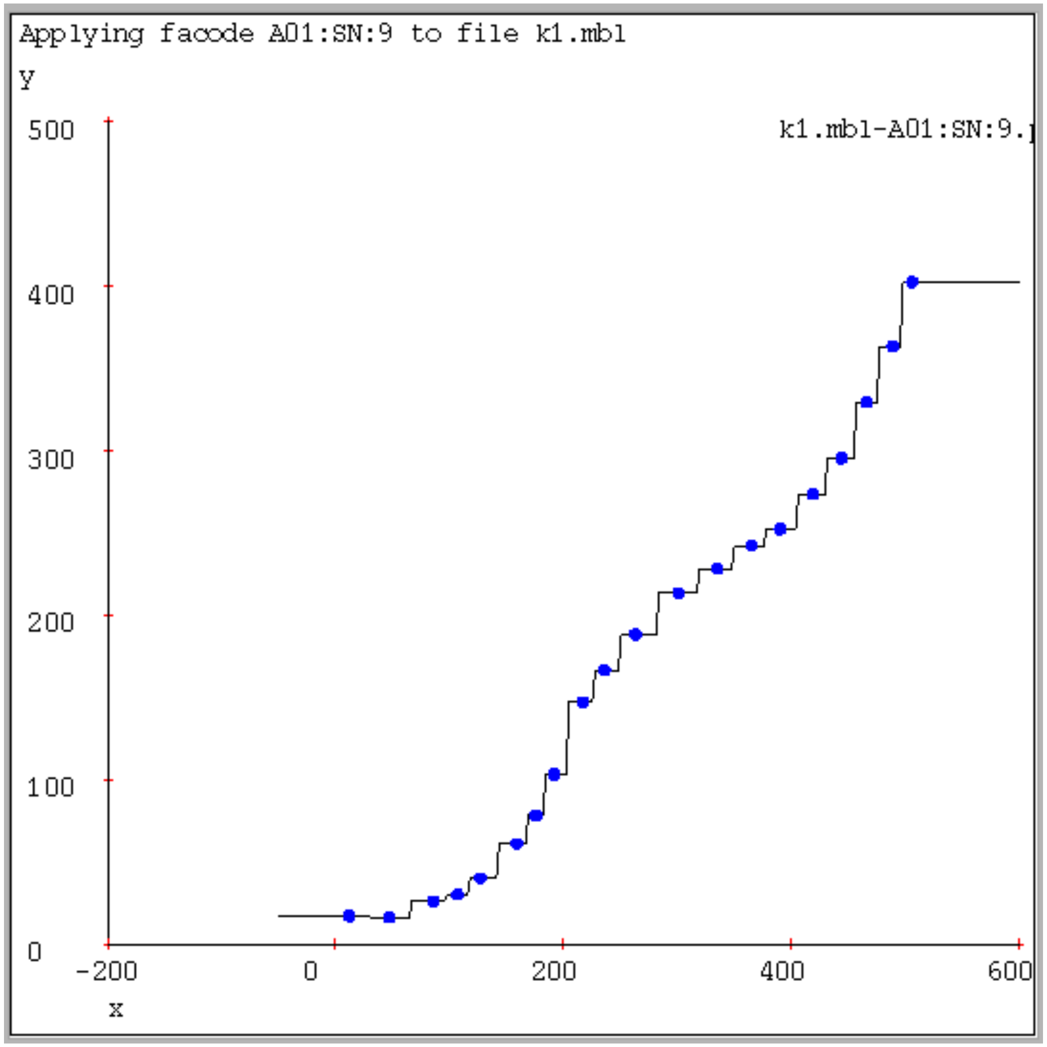
Nearest neighbor



Univariate 1-Nearest Neighbor

Given datapoints (x^1,y^1) (x^2,y^2)..(x^N,y^N),where we assume $y^i=f(x^i)$ for some unknown function f.

Given query point x^q, your job is to predict $\hat{y} \approx f\left(x^q\right)$

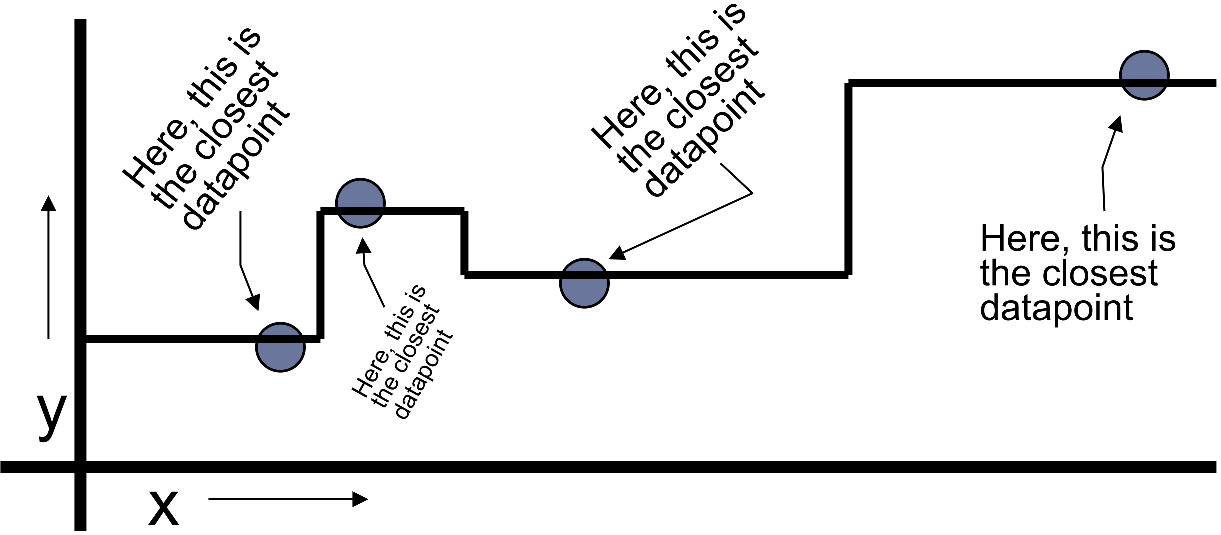
Nearest Neighbor:

1. Find the closest x_i in our set of datapoints

$$j(nn) = \underset{j}{\operatorname{argmin}} \left| x^j - x^q \right|$$

2. Predict $\hat{y} = y^{i(nn)}$

Here's a dataset with one input, one output and four datapoints.

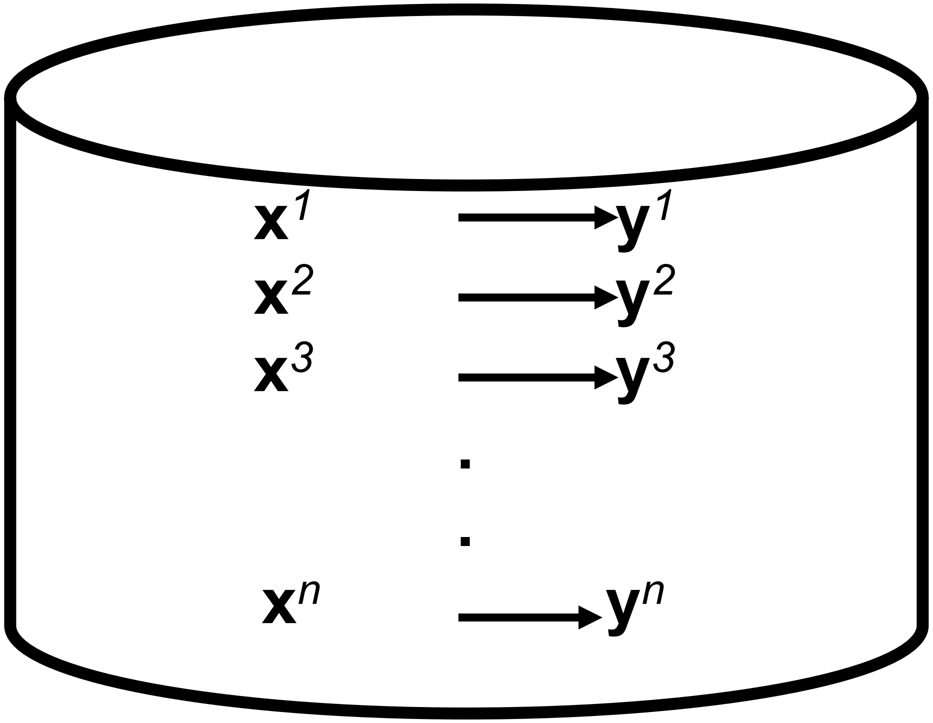


Here, this is the closest datapoint
Here, this is the closest datapoint
Here, this is the closest datapoint
Here, this is the closest datapoint
y
x

1-Nearest Neighbor is an example of…. **Instance-based learning**

A function approximator that has been around since about 1910.

To make a prediction, search database for similar datapoints, and fit with the local points.


$\mathbf{x}^1 \longrightarrow \mathbf{y}^1$
$\mathbf{x}^2 \longrightarrow \mathbf{y}^2$
$\mathbf{x}^3 \longrightarrow \mathbf{y}^3$
.
.
$\mathbf{x}^n \longrightarrow \mathbf{y}^n$

Four things make a memory based learner:

- A distance metric
- How many nearby neighbors to look at?
- A weighting function (optional)
- How to fit with the local points?

1-Nearest Neighbor

Four things make a memory based learner:

1. *A distance metric*

   Euclidian (and many more)

2. *How many nearby neighbors to look at?*

   One

3. *A weighting function (optional)*

   Unused

4. *How to fit with the local points?*

   Just predict the same output as the nearest neighbor.

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Multivariate 1-NN examples

Classification

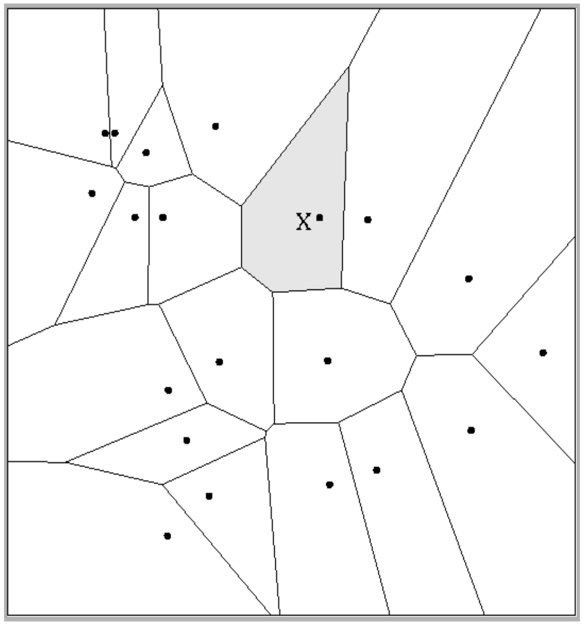
Regression

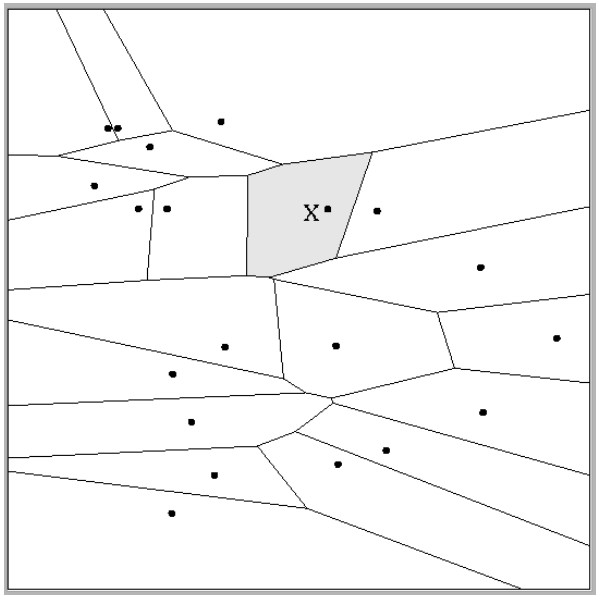
Multivariate distance metrics

Suppose the input vectors $x^1, x^2, \ldots x^N$ are two dimensional:

$\mathbf{x}^1 = (x^1_1 , x^1_2)$, $\mathbf{x}^2 = (x^2_1 , x^2_2)$, $\ldots \mathbf{x}^N = (x^N_1 , x^N_2)$.

One can draw the nearest-neighbor regions in input space.





$Dist(\mathbf{x}^i,\mathbf{x}^j) = (x^i_1 - x^j_1)^2 + (x^i_2 - x^j_2)^2$

$Dist(\mathbf{x}^i,\mathbf{x}^j) = (x^i_1 - x^j_1)^2 + (3x^i_2 - 3x^j_2)^2$

The relative scalings in the distance metric affect region shapes

Euclidean distance metric

$$D(\mathrm{x},\mathrm{x}') = \sqrt{\sum_i \sigma_i^{\,2}\left(x_i - x'_i\right)^2}$$

Or equivalently,

$$D(\mathrm{x},\mathrm{x}') = \sqrt{(\mathrm{x}-\mathrm{x}')^T \sum (\mathrm{x}-\mathrm{x}')}$$

where

$$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & \sigma_N^2 \end{bmatrix}$$

Other Metrics…

- Mahalanobis, Rank-based, Correlation-based,…

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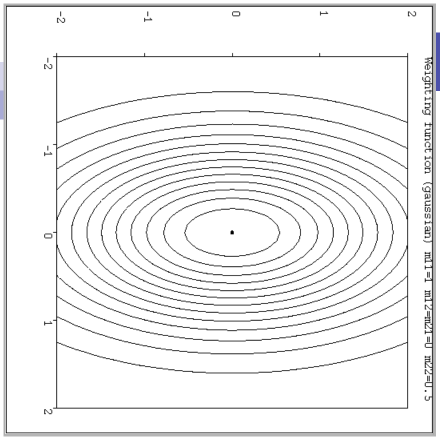
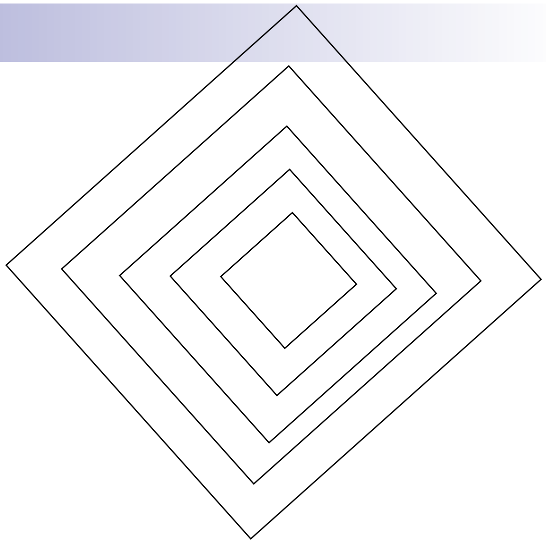
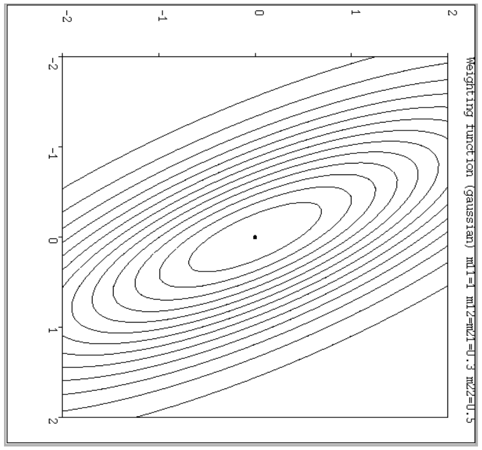
Notable distance metrics (and their level sets)



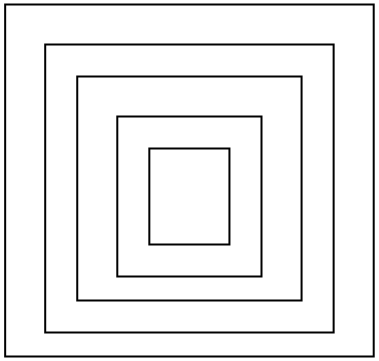
Scaled Euclidian (L_2)



L_1 norm (absolute)



Mahalanobis (here, Σ on the previous slide is not necessarily diagonal, but is symmetric



L1 *(max) norm*

Consistency of 1-NN

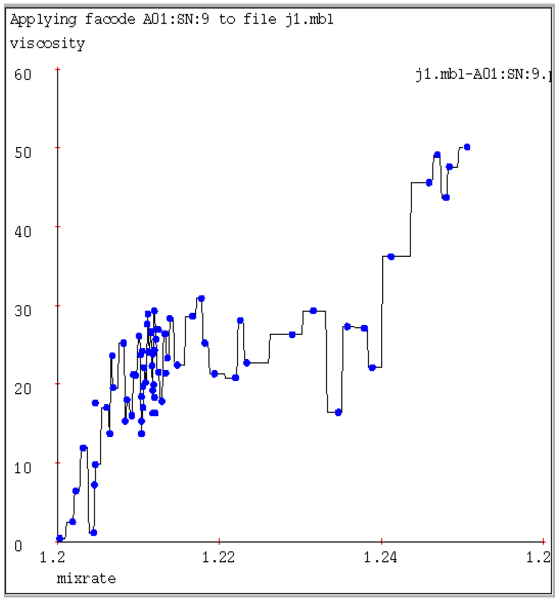
- Consider an estimator f_n trained on n examples
  - e.g., 1-NN, neural nets, regression,...
- Estimator is *consistent* if true error goes to zero as amount of data increases
  - e.g., for no noise data, consistent if:

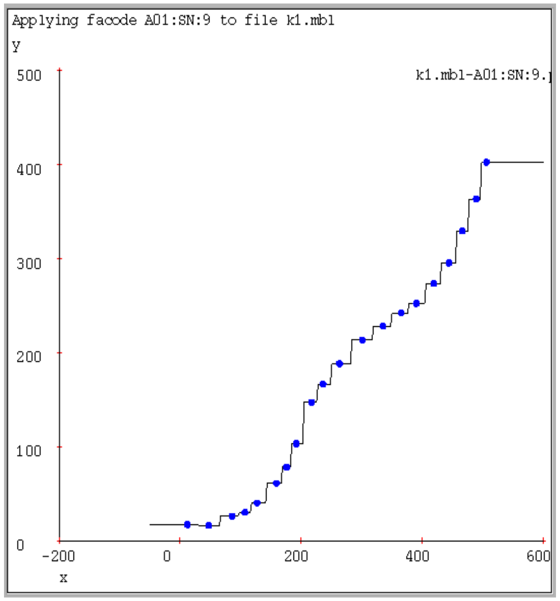
$$\lim_{n \rightarrow \infty} MSE(f_n) = 0$$

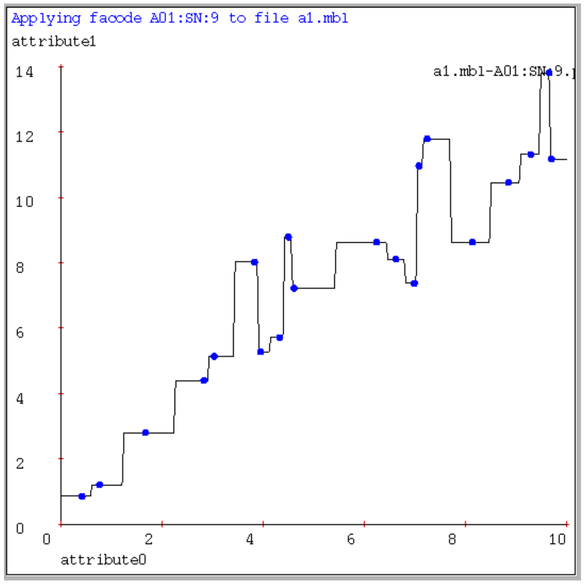
- Regression is not consistent!
  - Representation bias
- **1-NN is consistent** (under some mild fineprint)

What about variance???

1-NN overfits?







k-Nearest Neighbor

Four things make a memory based learner:

1. *A distance metric*

   Euclidian (and many more)

2. *How many nearby neighbors to look at?*

   k

1. *A weighting function (optional)*

   Unused

2. *How to fit with the local points?*

   Just predict the average output among the k nearest neighbors.

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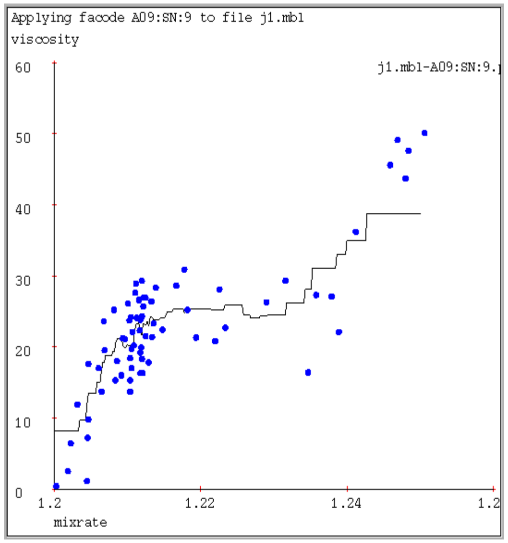
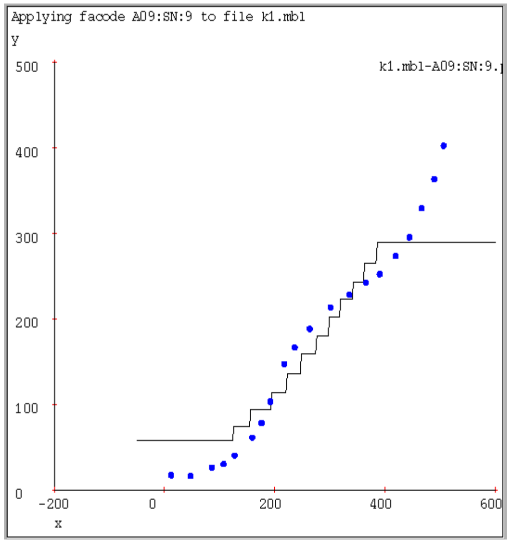
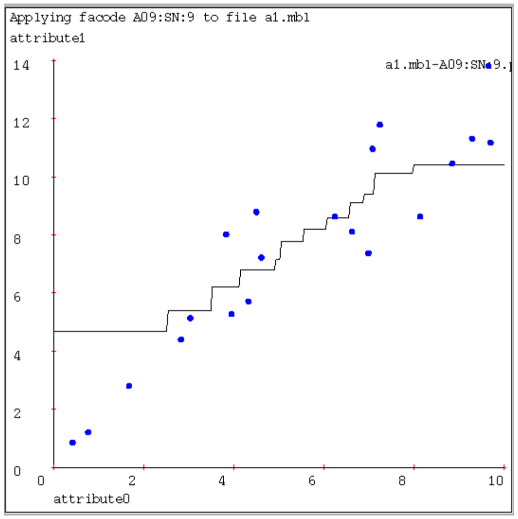
k-Nearest Neighbor (here k=9)







K-nearest neighbor for function fitting smoothes away noise, but there are clear deficiencies.

What can we do about all the discontinuities that k-NN gives us?

Weighted k-NNs

- Neighbors are not all the same

Kernel regression

Four things make a memory based learner:

1. *A distance metric*

   Euclidian (and many more)

2. *How many nearby neighbors to look at?*

   All of them

3. *A weighting function (optional)*

   $\boldsymbol{\pi^i = \exp(-D(x^i, \text{query})^2 / \rho^2)}$

   Nearby points to the query are weighted strongly, far points weakly. The $\boldsymbol{\rho}$ parameter is the **Kernel Width**. Very important.

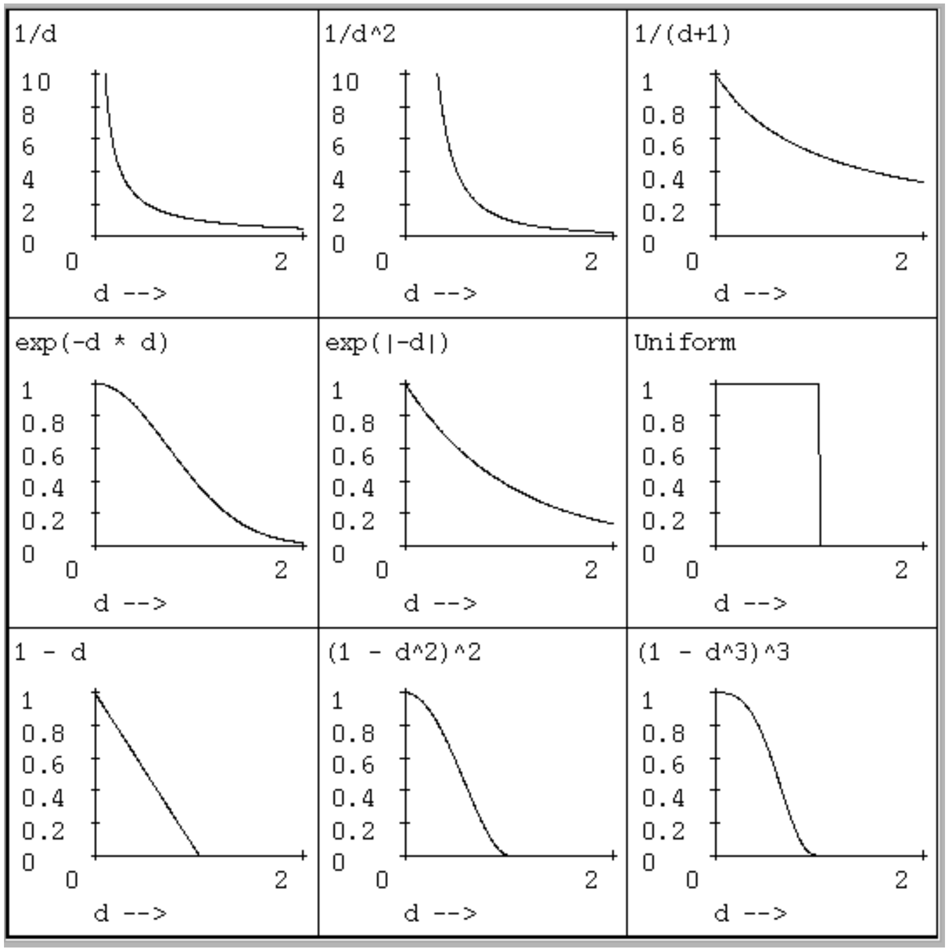
4. *How to fit with the local points?*

   Predict the weighted average of the outputs:

   predict = $\boldsymbol{\Sigma \pi^i y^i / \Sigma \pi^i}$

Weighting functions

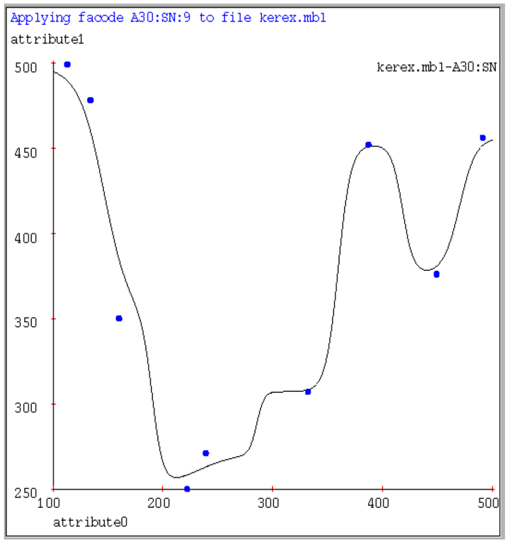
$\pi^i = \exp(-D(x^i, \text{query})^2 / \rho^2)$



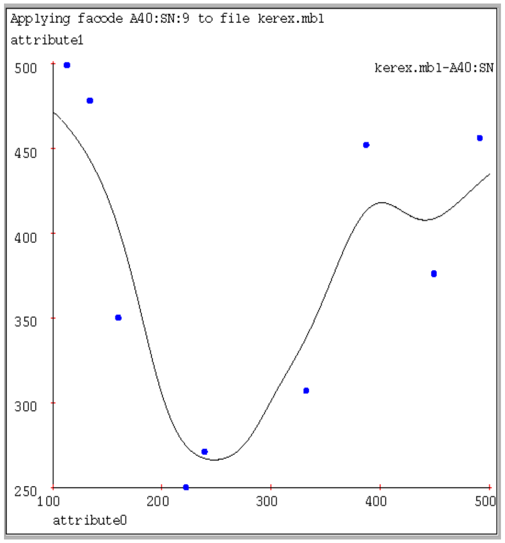
Typically optimize $\boldsymbol{\rho}$ using gradient descent

(Our examples use Gaussian)

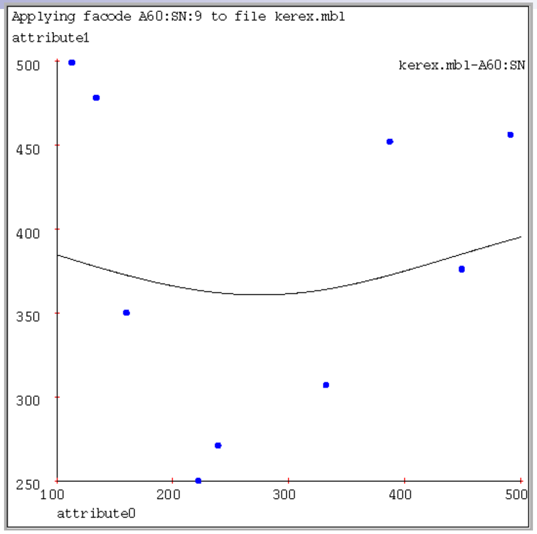
Kernel regression predictions



***ρ*=10**



***ρ*=20**

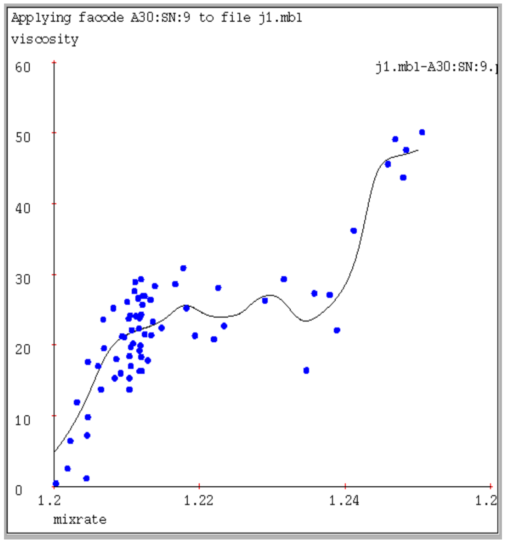


***ρ*=80**

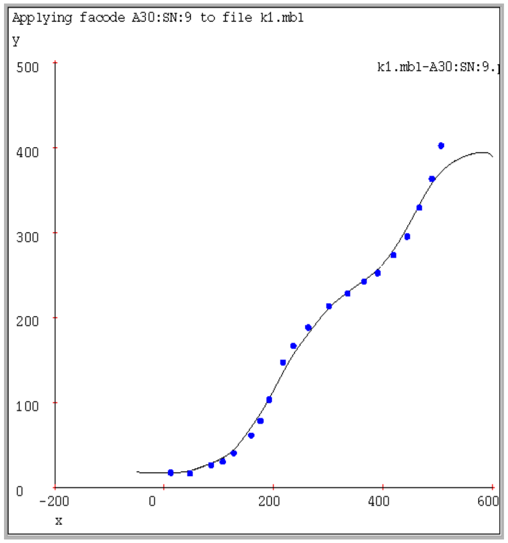
Increasing the kernel width *ρ* means further away points get an opportunity to influence you.

As ***ρ***→∞, the prediction tends to the global average.

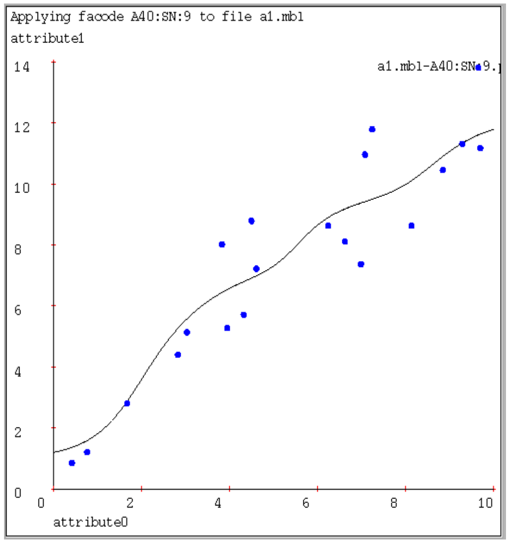
Kernel regression on our test cases



ρ=1/32 of x-axis width.



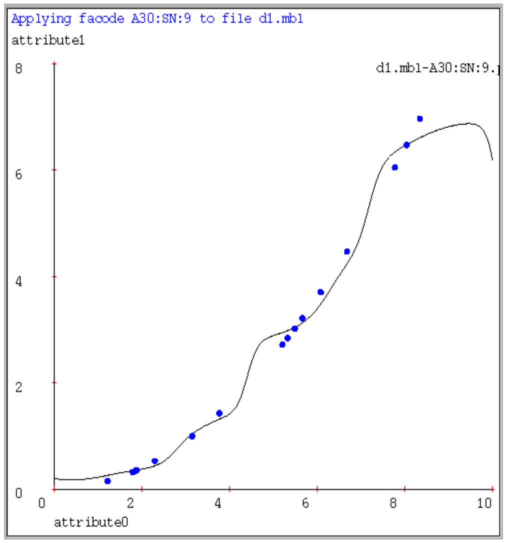
ρ=1/32 of x-axis width.



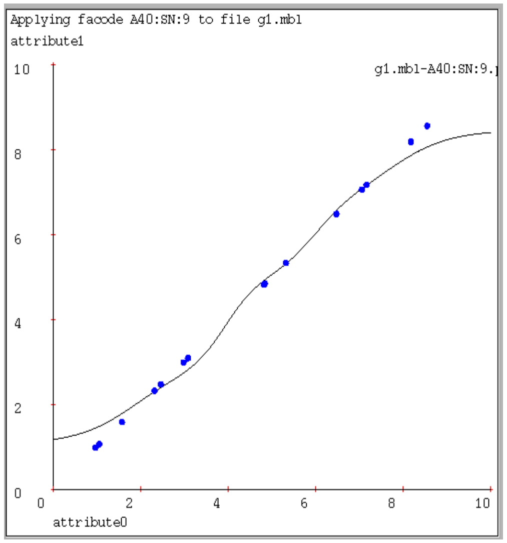
ρ=1/16 axis width.

Choosing a good ***ρ*** is important. Not just for Kernel Regression, but for all the locally weighted learners we're about to see.

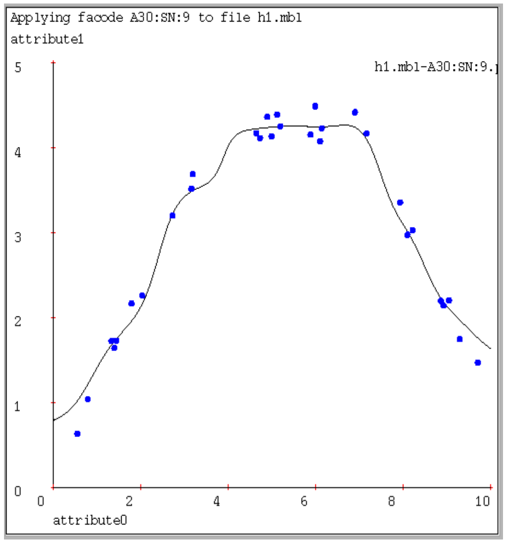
Kernel regression can look bad



ρ = Best.



ρ = Best.



ρ = Best.

Time to try something more powerful…

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Locally weighted regression

Kernel regression:

Take a very very conservative function approximator called AVERAGING. Locally weight it.

Locally weighted regression:

Take a conservative function approximator called LINEAR REGRESSION. Locally weight it.

Locally weighted regression

- **Four things make a memory based learner:**
- *A distance metric*

  Any
- *How many nearby neighbors to look at?*

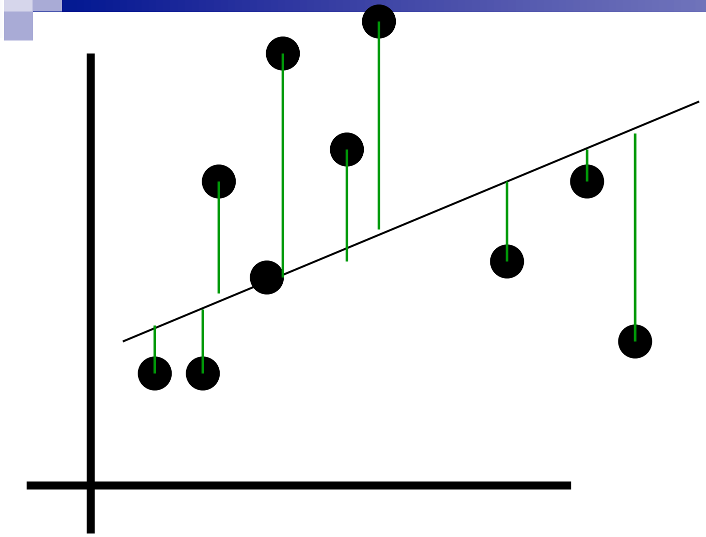
  All of them
- *A weighting function (optional)*

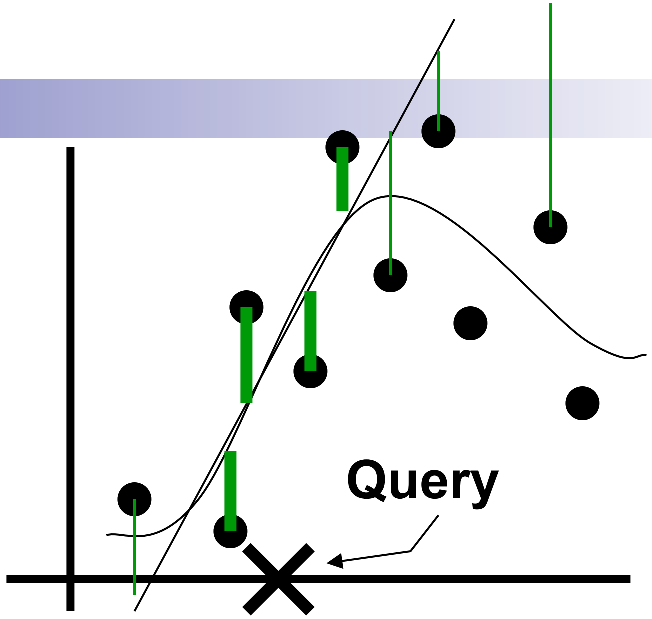
  Kernels
  - ***$\pi^i = \exp(-D(x^i, \text{query})^2 / \rho^2)$***
- *How to fit with the local points?*

  General weighted regression:

$$\hat{w}^q = \underset{w}{\operatorname{argmin}} \sum_{k=1}^{N} \pi_q^k \left(y^k - w^T x^k \right)^2$$

How LWR works





Linear regression

- Same parameters for all queries

$$\hat{w} = \left(X^T X\right)^{-1} X^T Y$$

Locally weighted regression

- Solve weighted linear regression for each query

$$w^q = \left((\Pi X)^T \Pi X\right)^{-1} (\Pi X)^T \Pi Y$$

$$\Pi = \begin{pmatrix} \pi_1 & 0 & 0 & 0 \\ 0 & \pi_2 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \pi_n \end{pmatrix}$$

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Another view of LWR

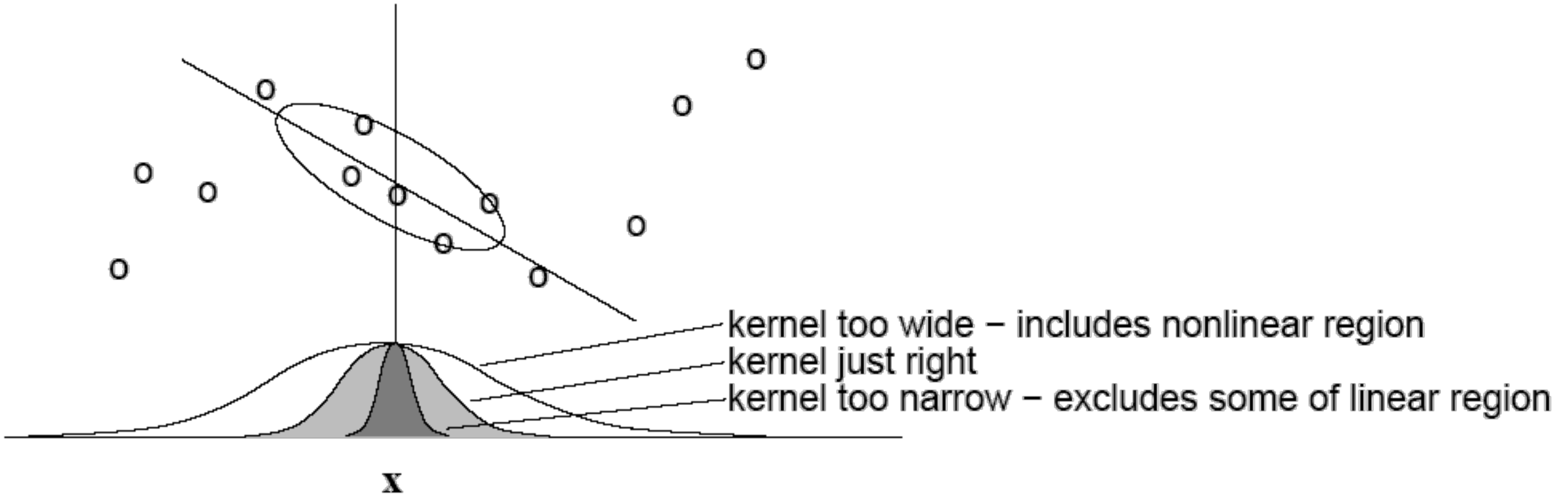
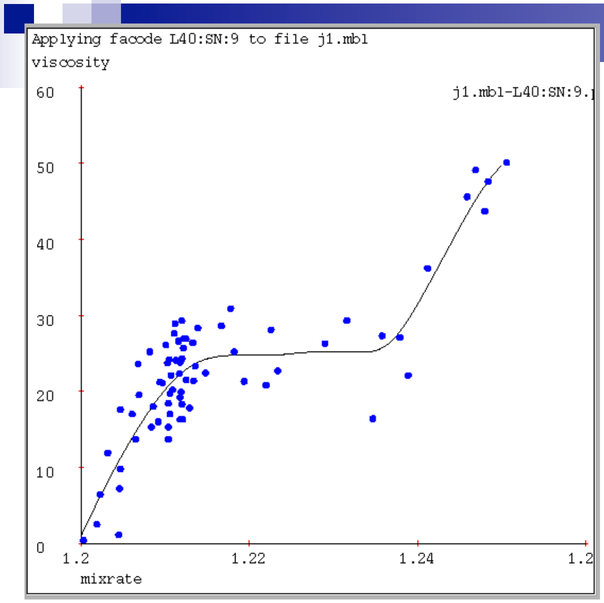

kernel too wide – includes nonlinear region
kernel just right
kernel too narrow – excludes some of linear region
x

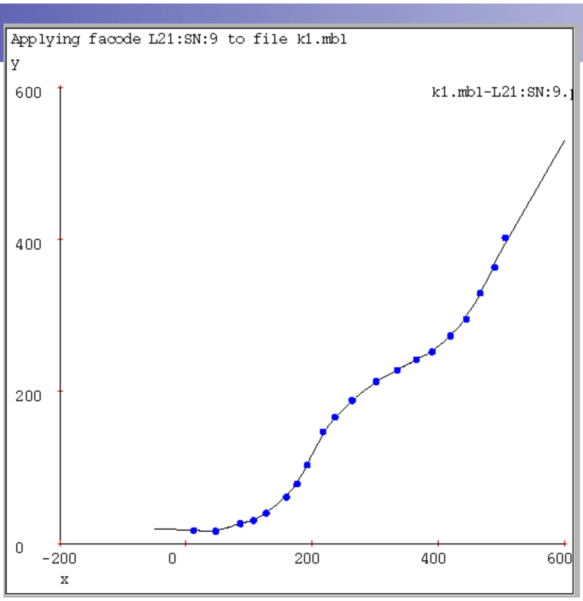
Image from Cohn, D.A., Ghahramani, Z., and Jordan, M.I. (1996) "Active Learning with Statistical Models", JAIR Volume 4, pages 129-145.

LWR on our test cases



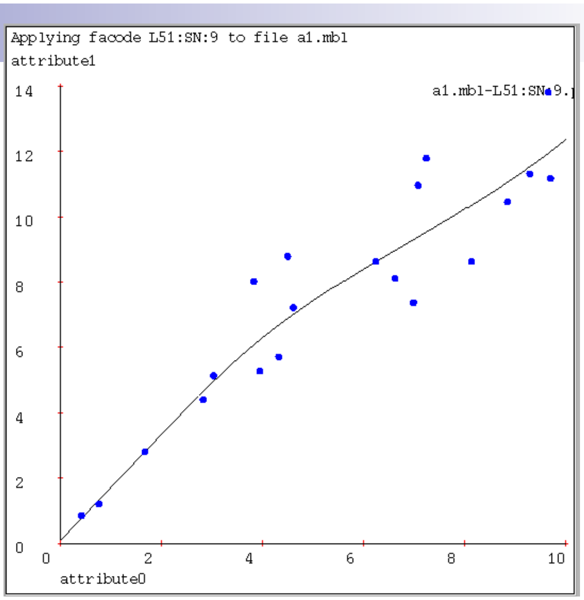
Applying facode L40:SN:9 to file j1.mbl

ρ = 1/16 of x-axis width.



Applying facode L21:SN:9 to file k1.mbl

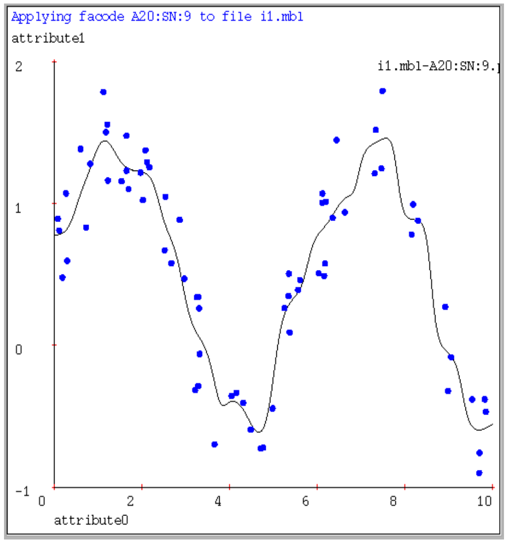
ρ = 1/32 of x-axis width.



Applying facode L51:SN:9 to file a1.mbl

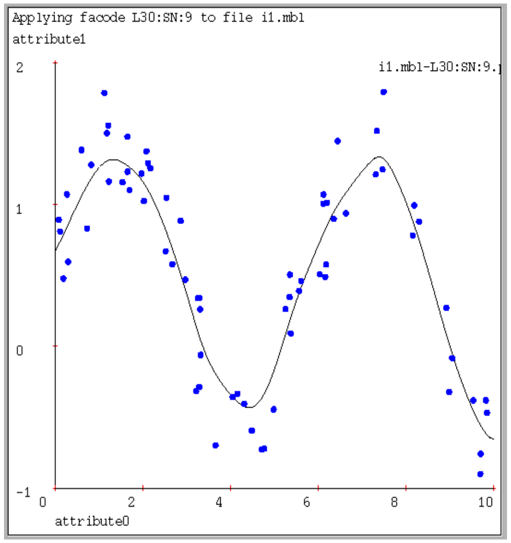
ρ = 1/8 of x-axis width.

Locally weighted polynomial regression



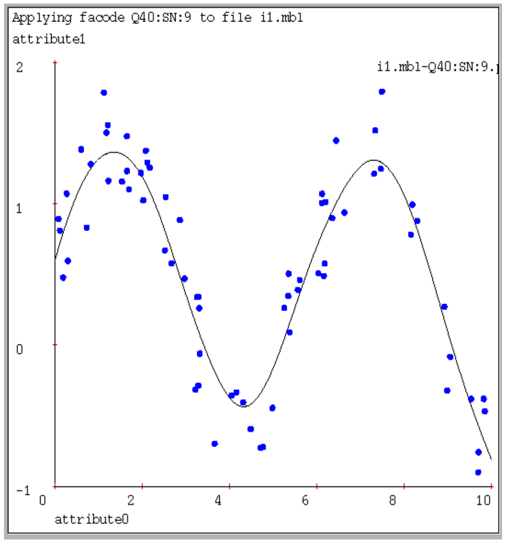
Kernel Regression
Kernel width ρ at optimal level.

ρ = 1/100 x-axis



LW Linear Regression
Kernel width ρ at optimal level.

ρ = 1/40 x-axis



LW Quadratic Regression
Kernel width ρ at optimal level.

ρ = 1/15 x-axis

Local quadratic regression is easy: just add quadratic terms to the X matrix. As the regression degree increases, the kernel width can increase without introducing bias.

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Curse of dimensionality for instance-based learning

- Must store and retreve all data!
  - □ Most real work done during testing
  - □ For every test sample, must search through all dataset – very slow!
  - □ There are (sometimes) fast methods for dealing with large datasets
- Instance-based learning often poor with noisy or irrelevant features

Curse of the irrelevant feature

What you need to know about instance-based learning

- k-NN
  - □ Simplest learning algorithm
  - □ With sufficient data, very hard to beat “strawman” approach
  - □ Picking k?
- Kernel regression
  - □ Set k to n (number of data points) and optimize weights by gradient descent
  - □ Smoother than k-NN
- Locally weighted regression
  - □ Generalizes kernel regression, not just local average
- Curse of dimensionality
  - □ Must remember (very large) dataset for prediction
  - □ Irrelevant features often killers for instance-based approaches

Acknowledgment

- This lecture contains some material from Andrew Moore's excellent collection of ML tutorials:
  - □ http://www.cs.cmu.edu/~awm/tutorials