DS 5220

Supervised Machine Learning and Learning Theory

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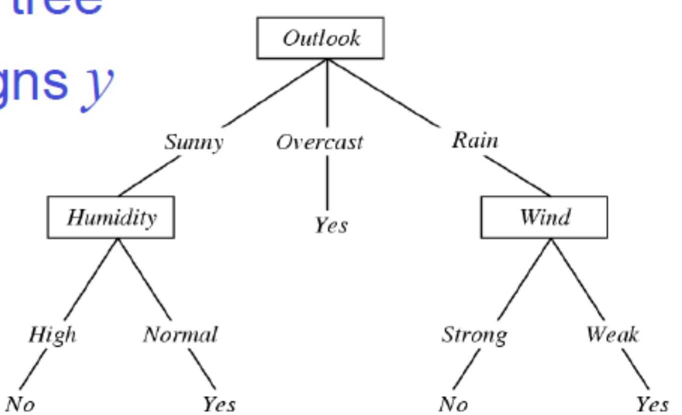
Methods for Feature Selection

- 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)

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 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

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:

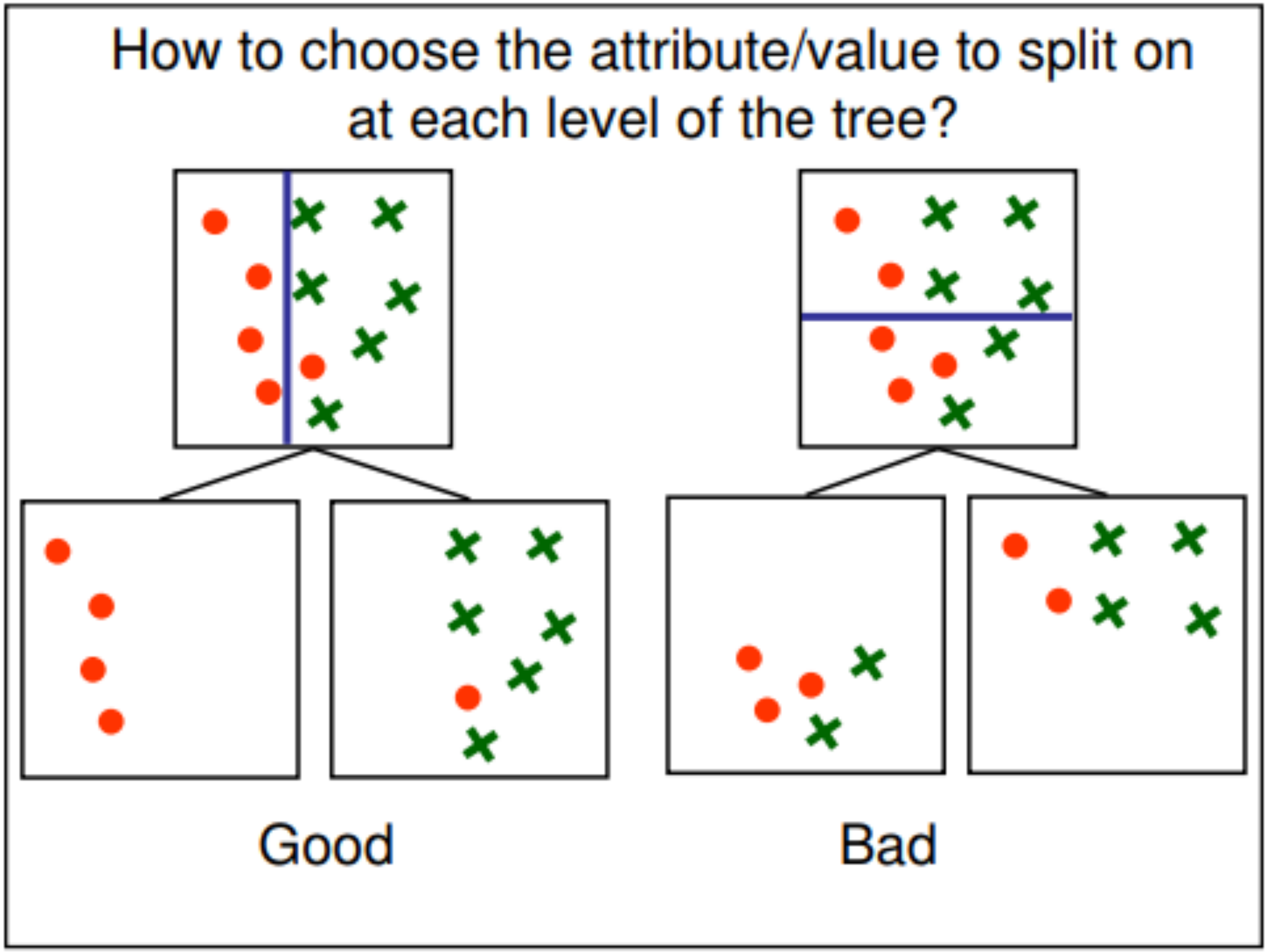
$IG(Y|X)$ = **I must transmit** Y. **How many bits on average would it save me if both ends of the line knew** X**?**

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

Example:

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

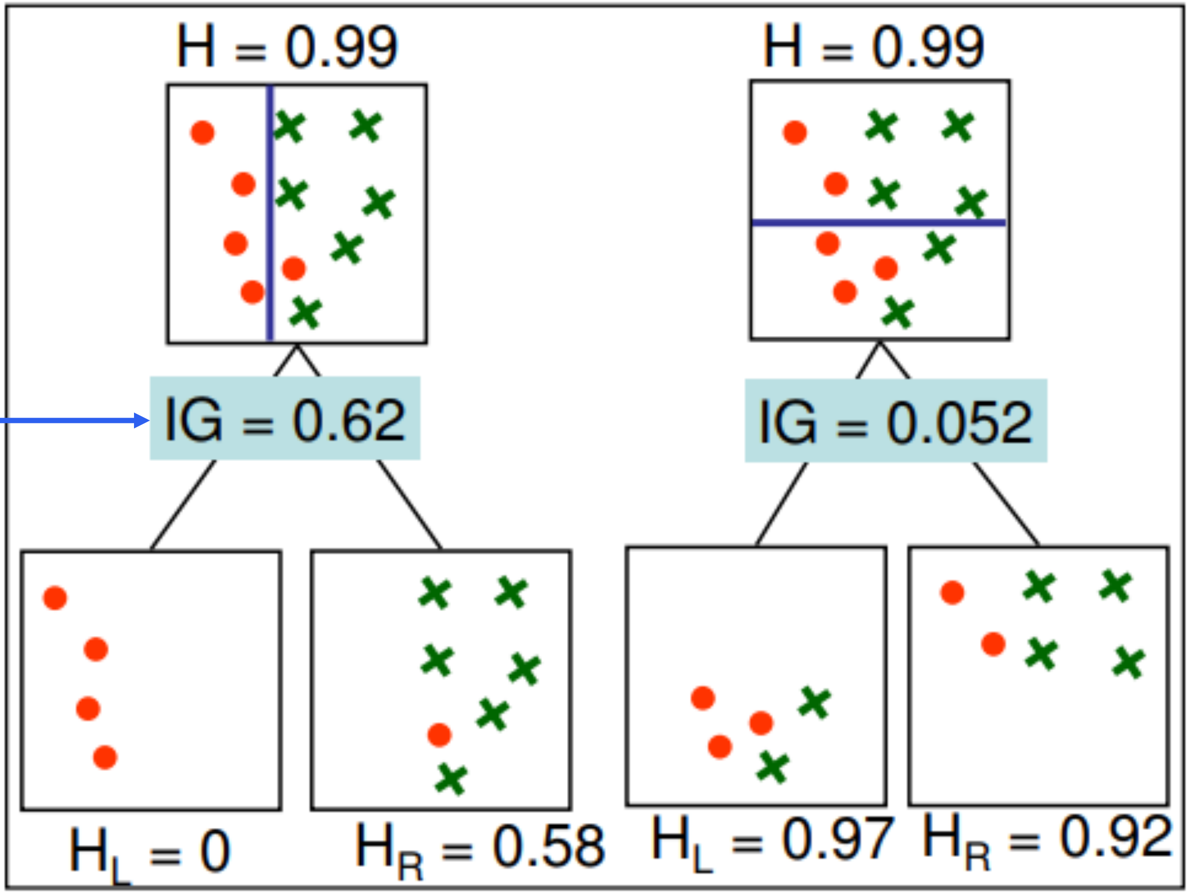
Example


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

Impurity Metrics

- Split a node according to max reduction of impurity
- Properties
  - Impurity measure should be maximum when labels are split evenly among classes: $I\left(\frac{1}{2}, \frac{1}{2}\right) = 1$
  - Impurity measure should be minimum for pure node: $I(1,0) = I(0,1\ ) = 0$
  - Impurity measure should be symmetric
    - $I(p_0, p_1) = I(p_1, p_0)$

Impurity Metrics

Split a node according to max reduction of impurity

1. Entropy
2. Gini Index for binary class (class 0 and class 1)
   – $I(p_0, p_1) = 4p_0p_1 = 4p_0(1 - p_0)$
3. Resubstitution error
   – Fraction of data points mis-classified if we assigned the majority label at the node

Impurity Metrics

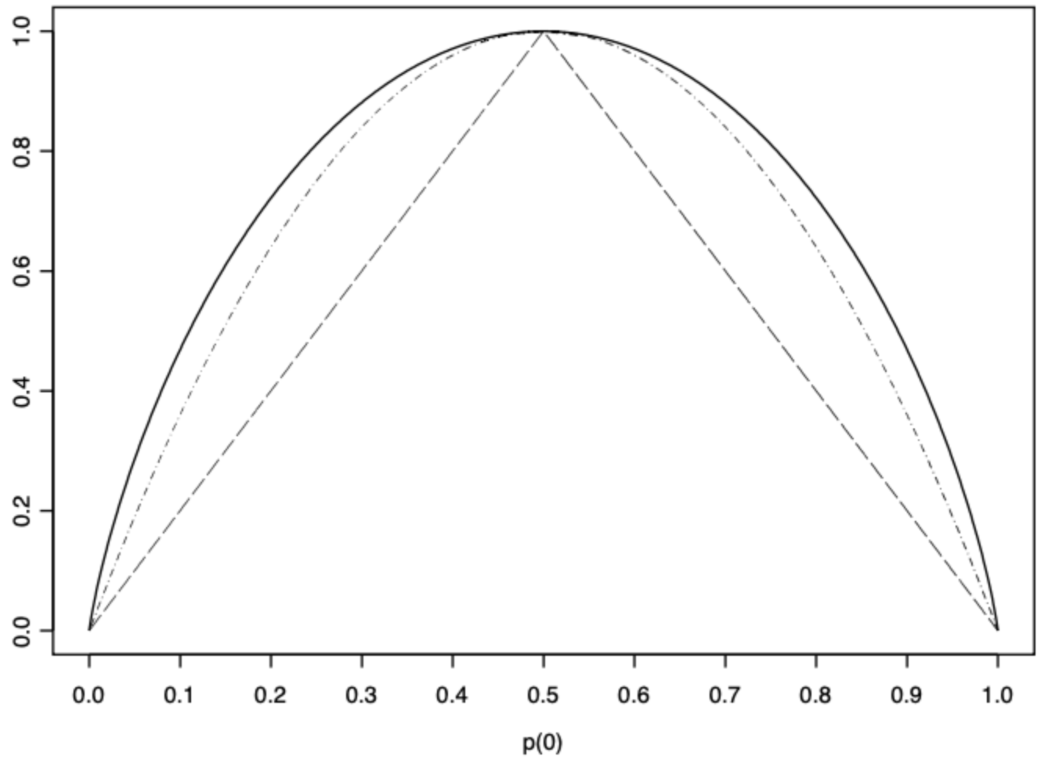
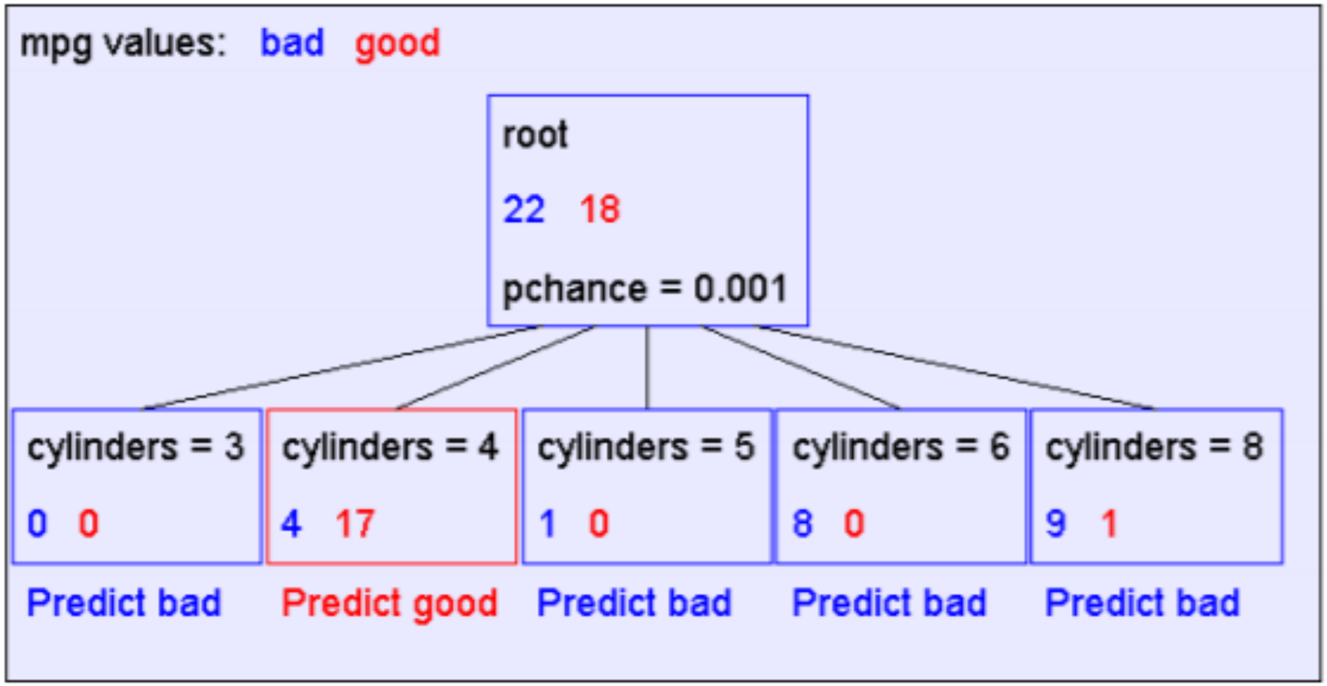


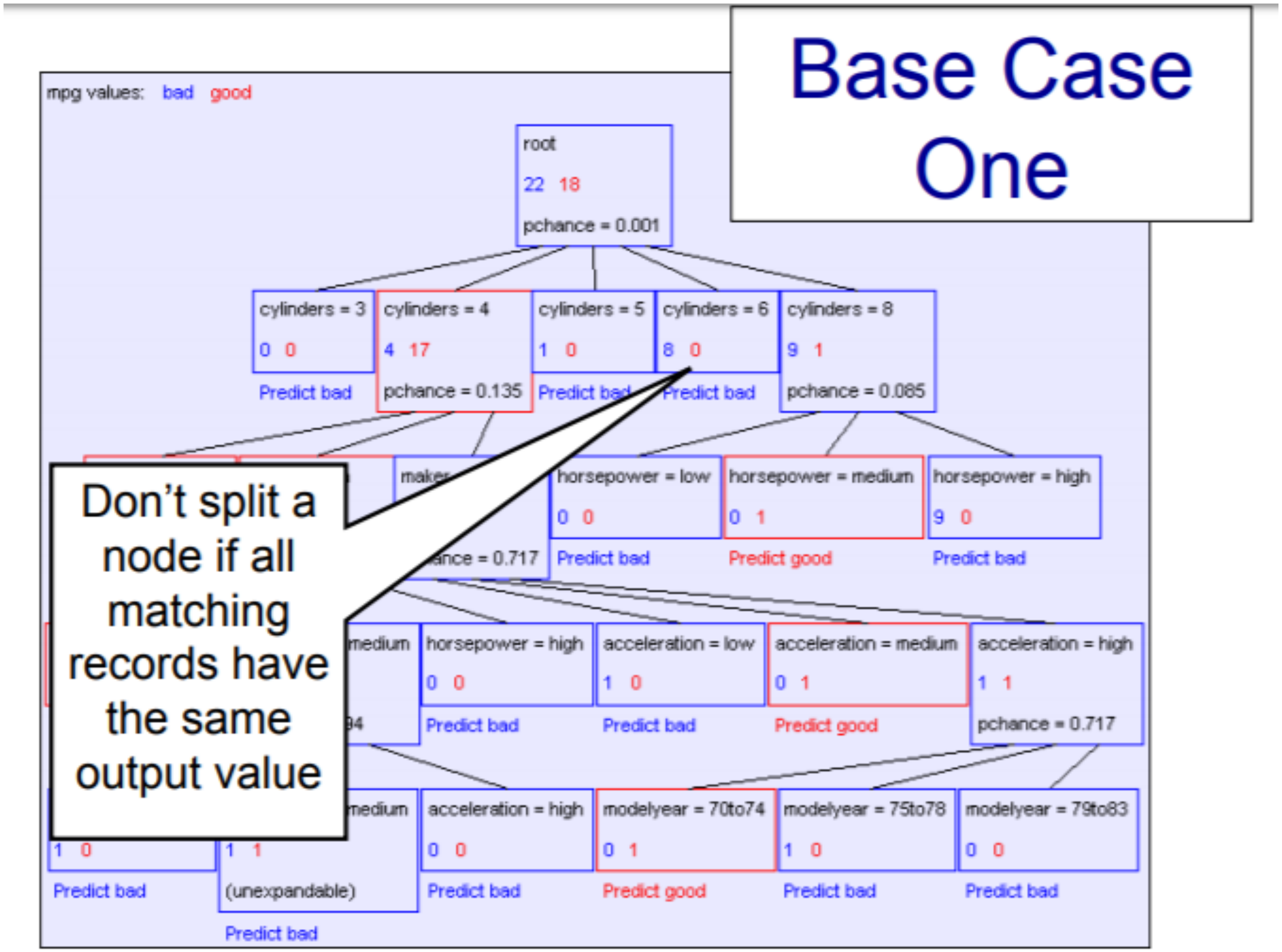
Figure 4: Graph of entropy (solid line), gini-index (dot-dash) and resubstitution error (dashed line) for two-class problem.

When to stop?



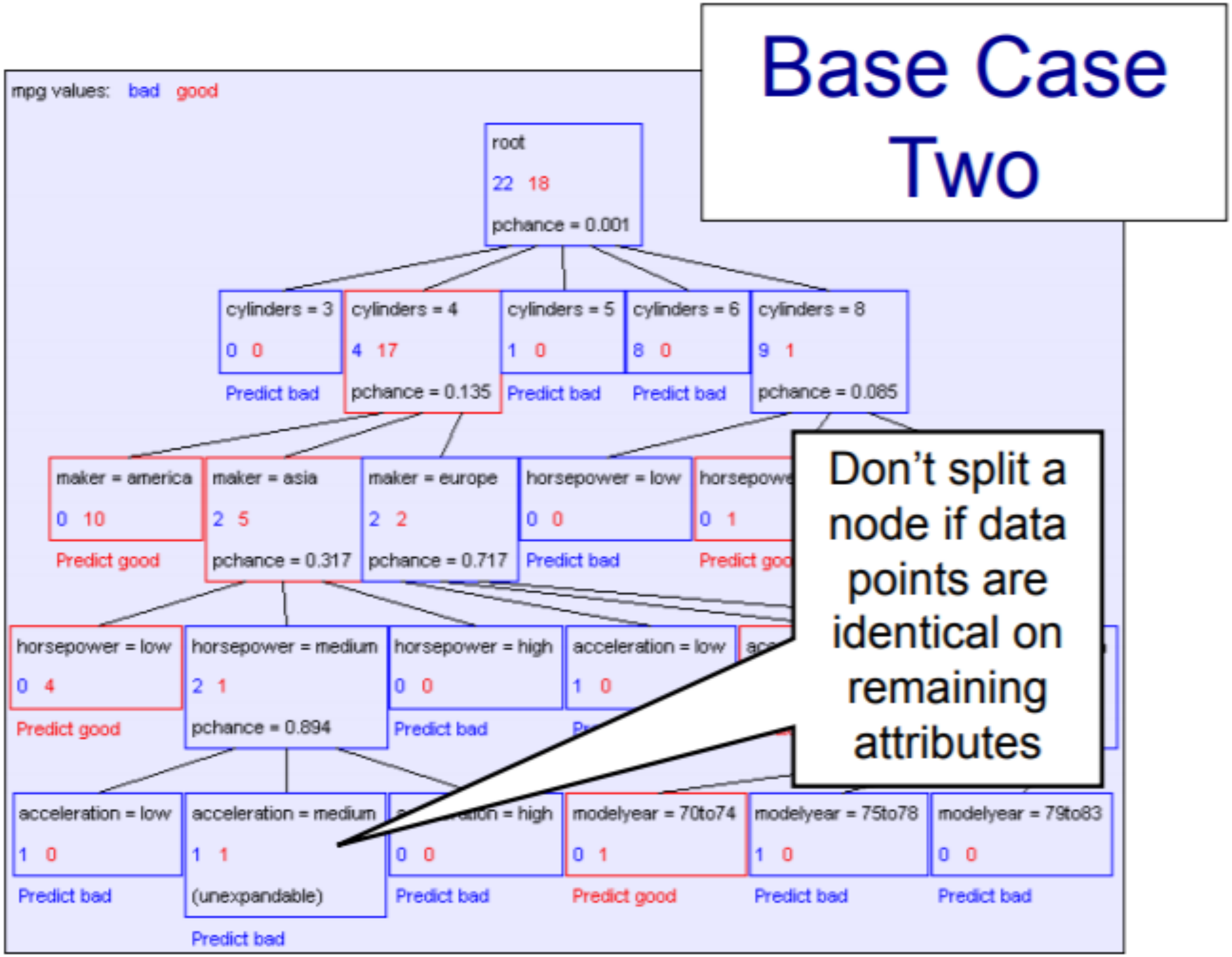
First split looks good! But, when do we stop?

Case 1



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
(unexpandable)
Predict bad
Base Case One
Don't split a node if all matching records have the same output value

Case 2



mpg values: bad good
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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
0 1
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
0 0
Predict bad
modelyear = 70to74
0 1
Predict good
modelyear = 75to78
1 0
Predict bad
modelyear = 79to83
0 0
Predict bad
Base Case Two
Don't split a node if data points are identical on remaining attributes

Decision Trees

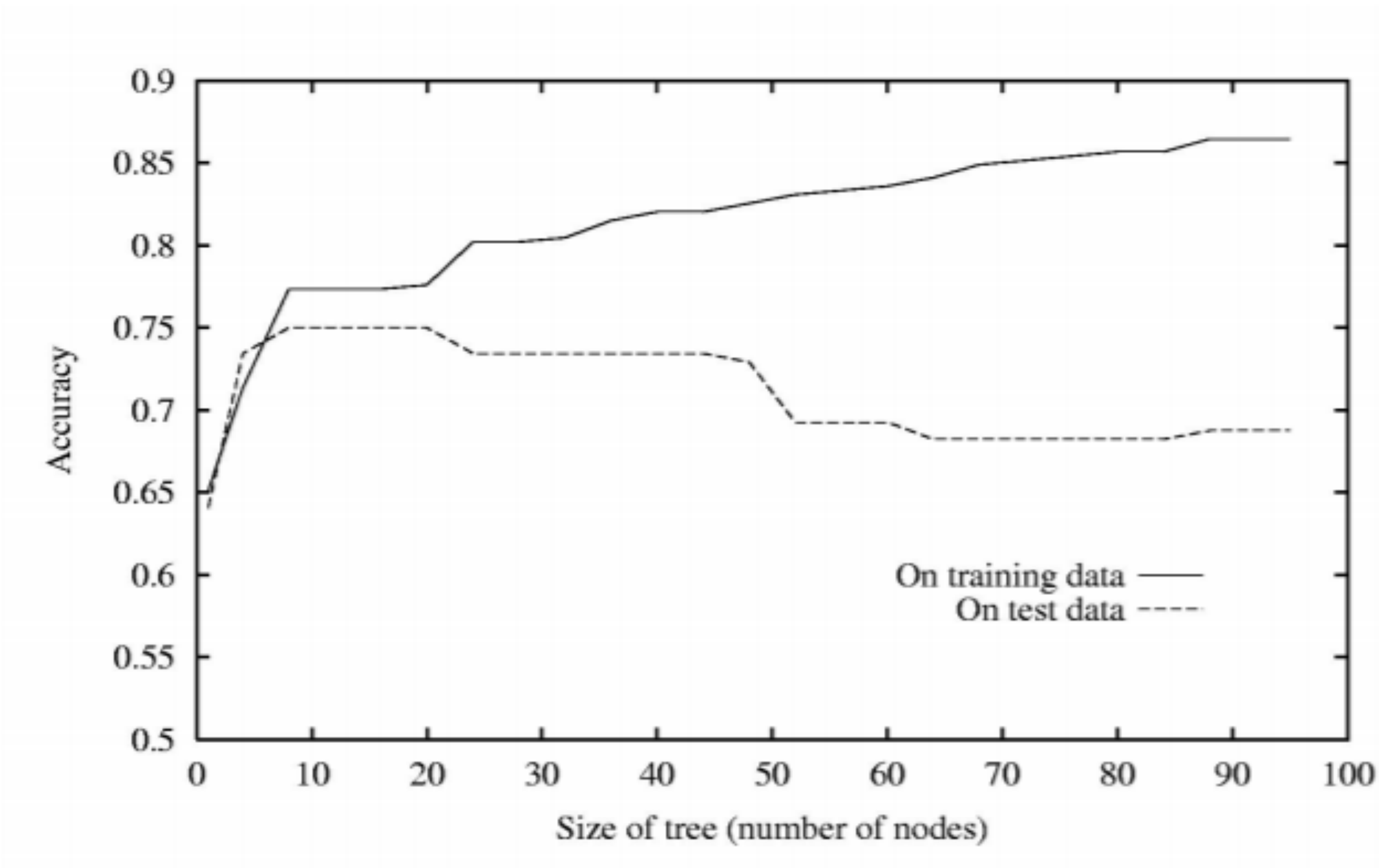
BuildTree(*DataSet,Output*)

- 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

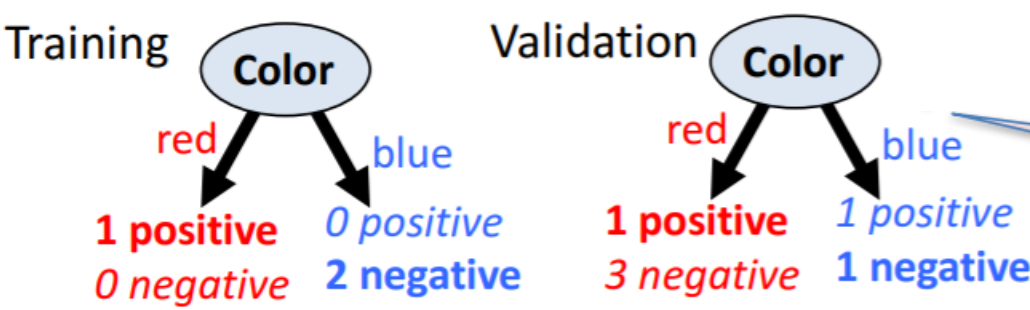
Grow tree based on *training set*

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,



If we had simply predicted the majority class (negative), we make 2 errors instead of 4.

Pruned!

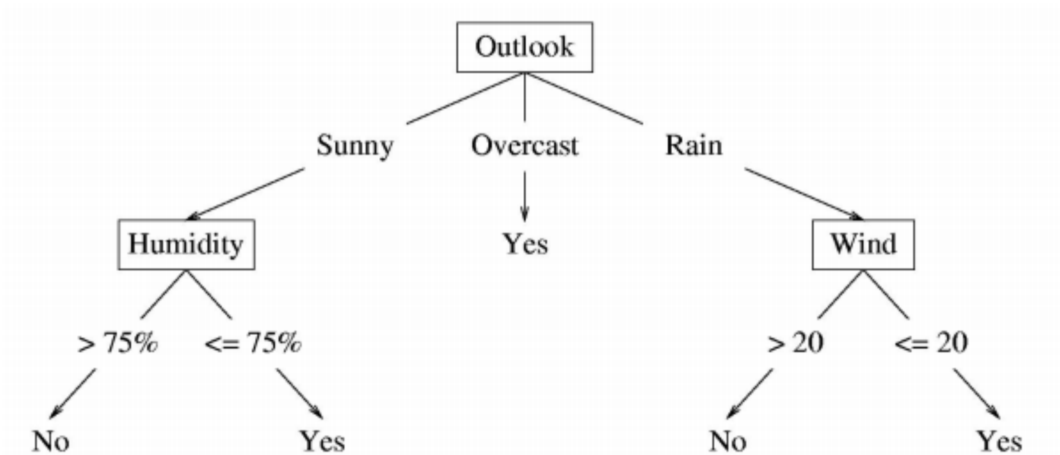
Real-Valued Inputs

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

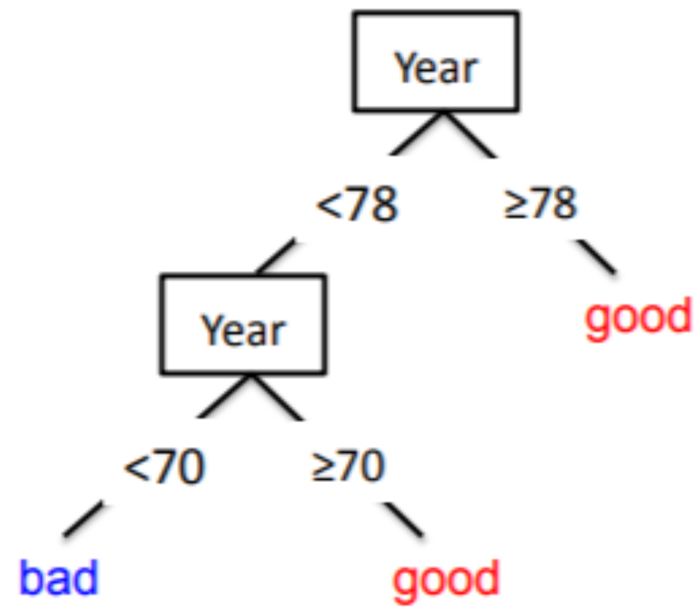
candidate splits

  - Choose among splits by InfoGain()

Threshold Splits

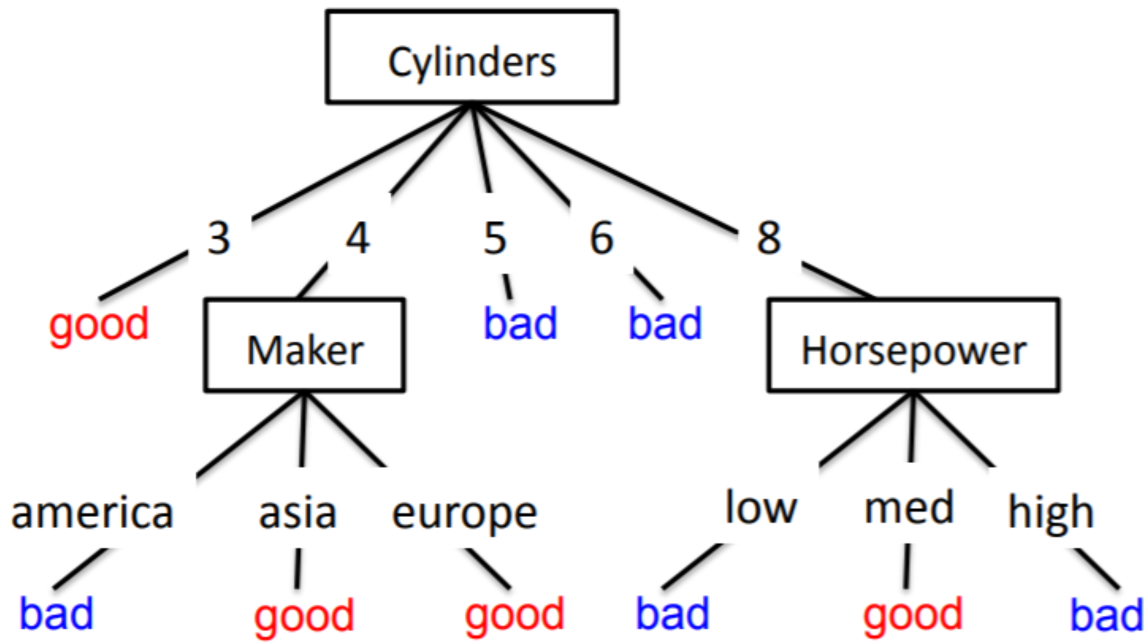
- Binary tree: split on attribute X at value t
  - One branch: $X < t$
  - Other branch: $X \geq t$

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



Interpretability

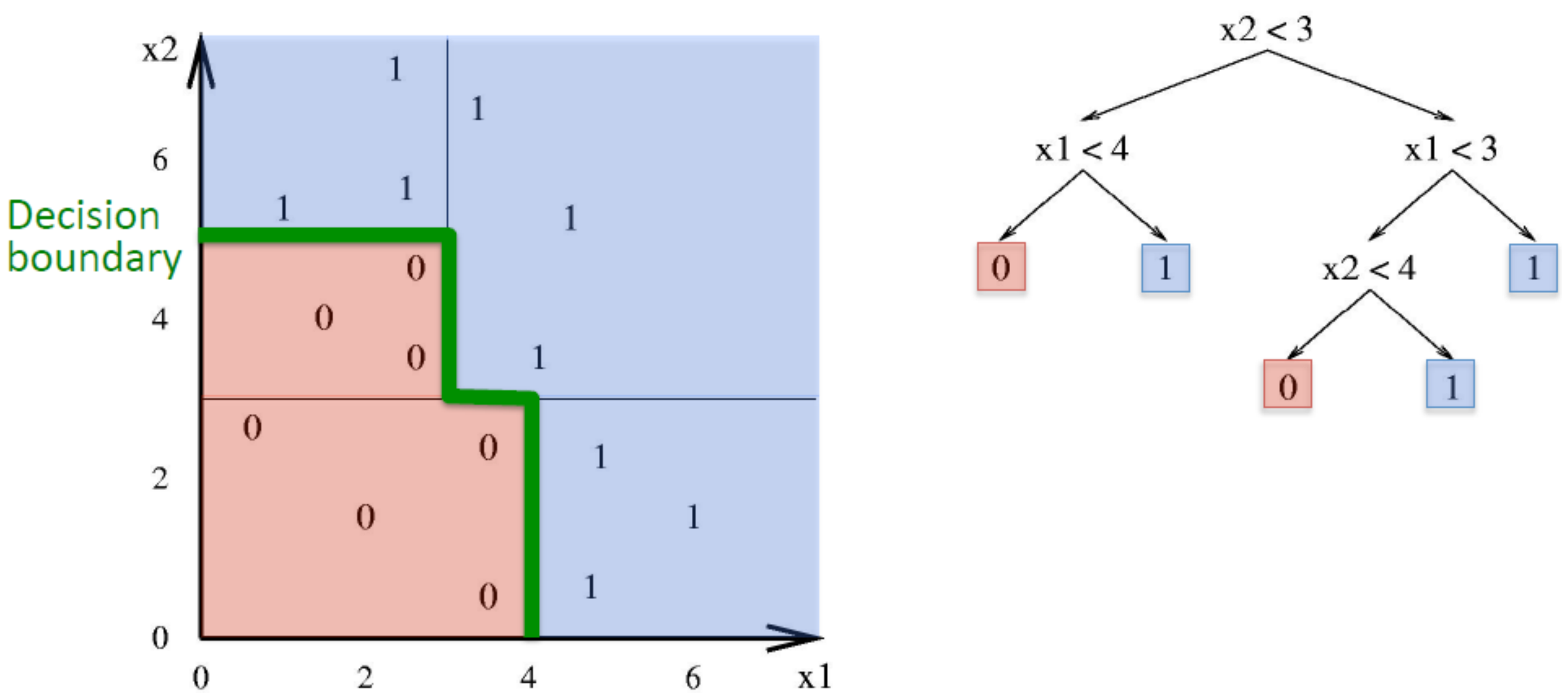
- Each internal node tests an attribute x_i
- One branch for each possible attribute value $x_i=v$
- Each leaf assigns a class y
- To classify input x: traverse the tree from root to leaf, output the labeled y



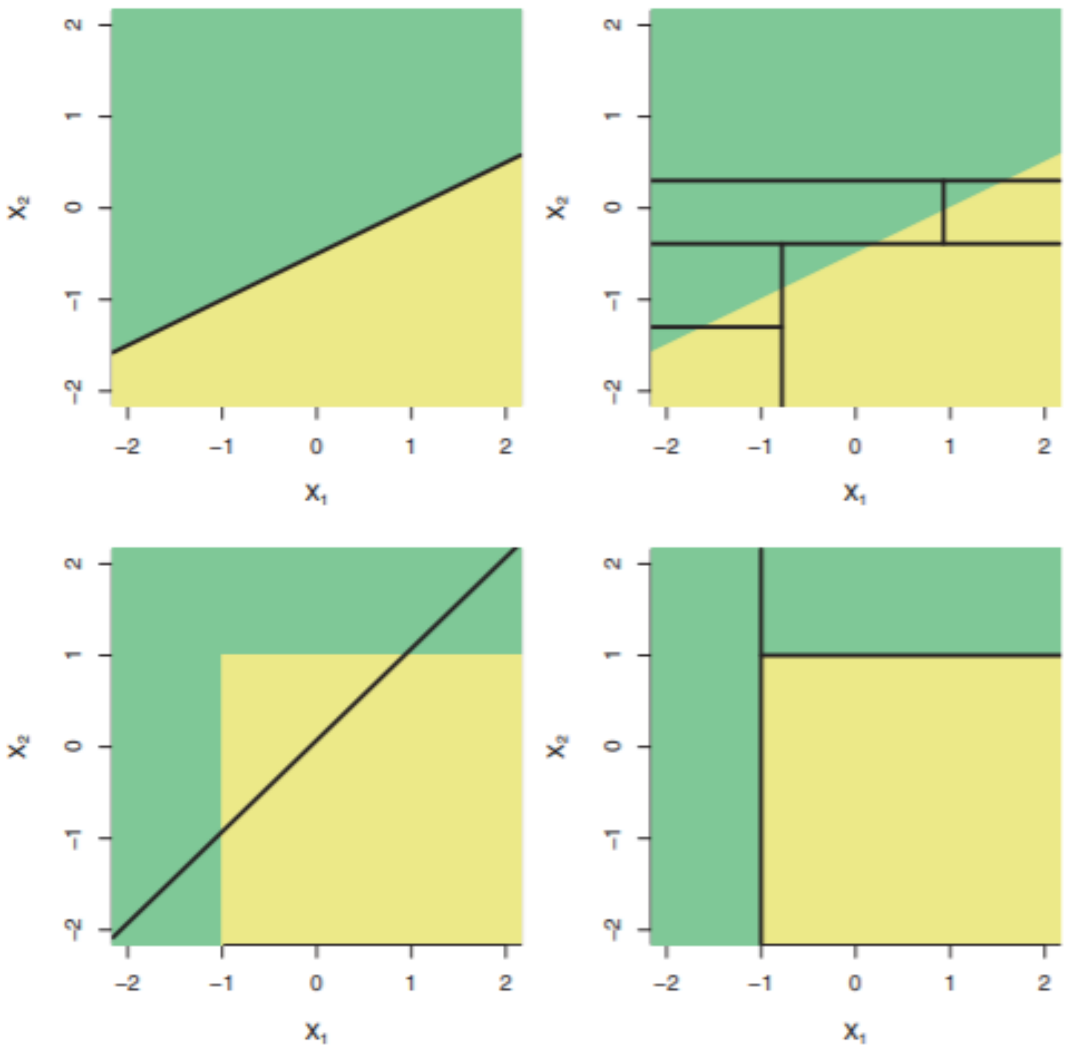
Human interpretable!

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



Decision Trees vs Linear Models



Linear model Decision tree

Lab

```
> library(tree)
> library(ISLR)
> fix(Carseats)
```

	Sales	CompPrice	Income	Advertising	Population	Price	ShelveLoc	Age
1	9.5	138	73	11	276	120	Bad	42
2	11.22	111	48	16	260	83	Good	65
3	10.06	113	35	10	269	80	Medium	59
4	7.4	117	100	4	466	97	Medium	55
5	4.15	141	64	3	340	128	Bad	38
6	10.81	124	113	13	501	72	Bad	78
7	6.63	115	105	0	45	108	Medium	71
8	11.85	136	81	15	425	120	Good	67
9	6.54	132	110	0	108	124	Medium	76
10	4.69	132	113	0	131	124	Medium	76
11	9.01	121	78	9	150	100	Bad	26
12	11.96	117	94	4	503	94	Good	50
13	3.98	122	35	2	393	136	Medium	62
14	10.96	115	28	11	29	86	Good	53
15	11.17	107	117	11	148	118	Good	52

Lab

Add Label “High” is Sales > 8

```
> High=ifelse(Sales<=8,"No","Yes")
> Carseats=data.frame(Carseats,High)
> head(Carseats)
  Sales CompPrice Income Advertising Population Price ShelveLoc Age Education Urban  US High
1  9.50       138     73          11        276   120       Bad  42        17   Yes Yes  Yes
2 11.22       111     48          16        260    83      Good  65        10   Yes Yes  Yes
3 10.06       113     35          10        269    80    Medium  59        12   Yes Yes  Yes
4  7.40       117    100           4        466    97    Medium  55        14   Yes Yes   No
5  4.15       141     64           3        340   128       Bad  38        13   Yes  No   No
6 10.81       124    113          13        501    72       Bad  78        16    No Yes  Yes
> 
```

Lab

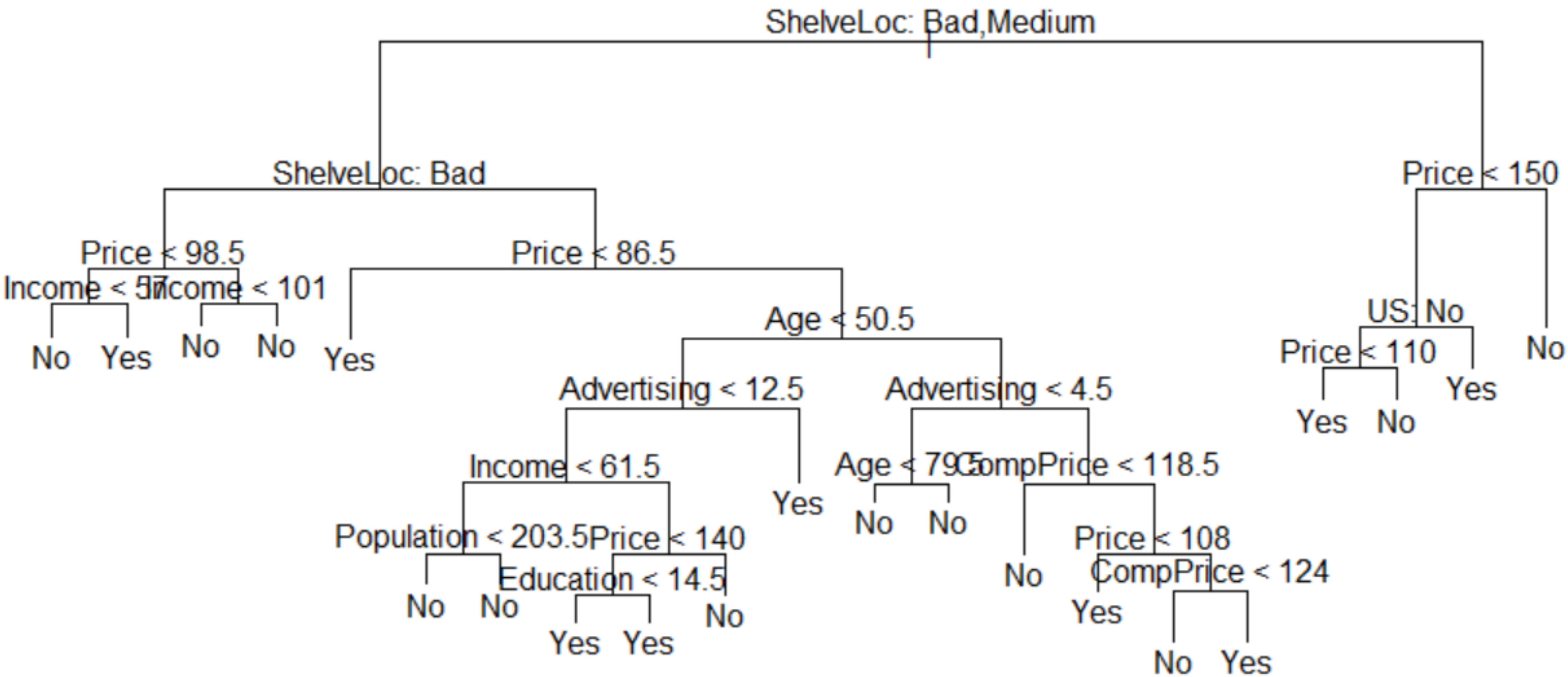
Train and Test

```
> train=sample(1:nrow(Carseats), 200)
> Carseats.test=Carseats[-train,]
> High.test=High[-train]
> tree.carseats=tree(High~.-Sales,Carseats,subset=train)
> tree.pred=predict(tree.carseats,Carseats.test,type="class")
> table(tree.pred,High.test)
         High.test
tree.pred No Yes
      No  85  22
      Yes 34  59
> mean(tree.pred==High.test)
[1] 0.72
>
```

Accuracy

Lab

```
> plot(tree.carseats)
> text(tree.carseats,pretty=0)
>
```



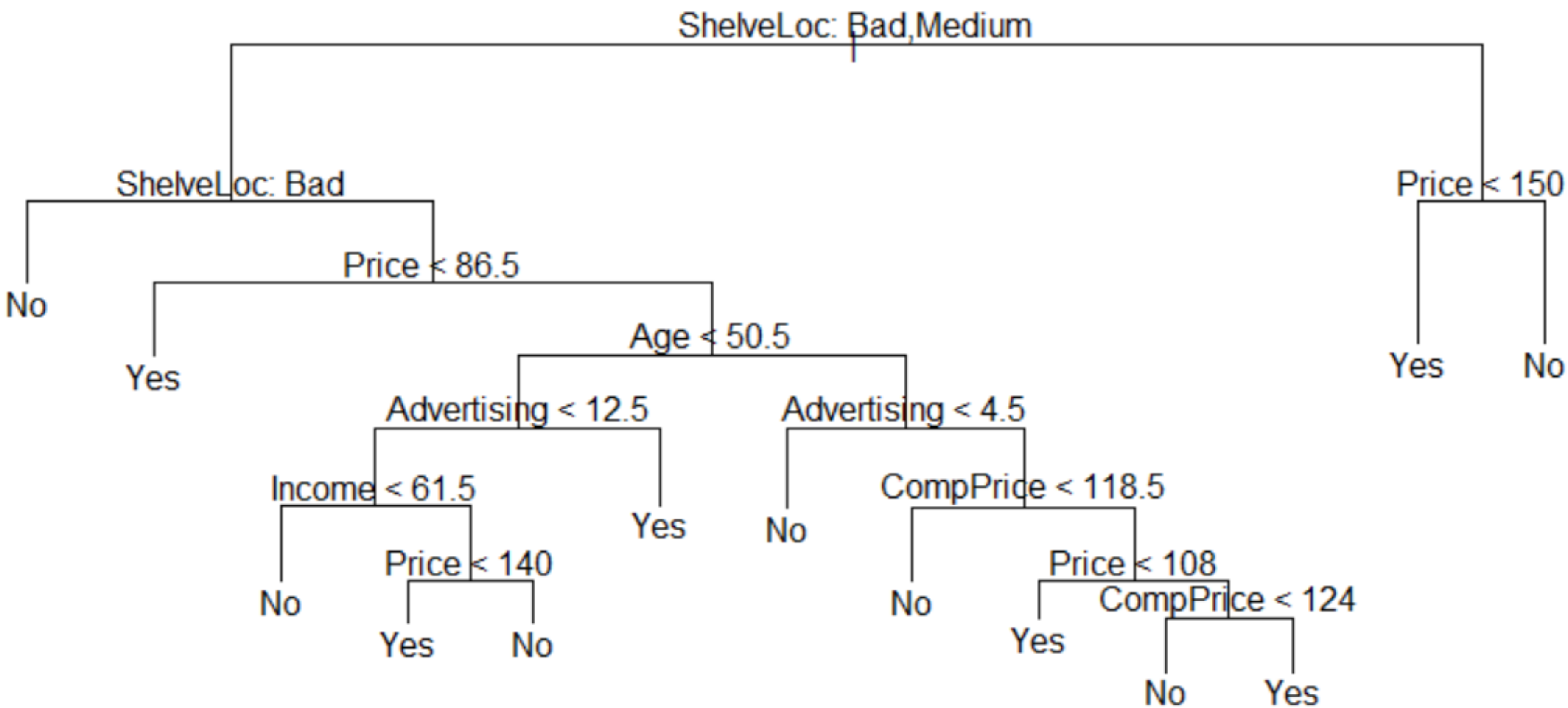
```
> tree.carseats
node), split, n, deviance, yval, (yprob)
      * denotes terminal node

  1) root 200 271.500 No ( 0.58500 0.41500 )
    2) ShelveLoc: Bad,Medium 157 196.500 No ( 0.68153 0.31847 )
      4) ShelveLoc: Bad 46  31.630 No ( 0.89130 0.10870 )
        8) Price < 98.5 13  16.050 No ( 0.69231 0.30769 )
         16) Income < 57 6   0.000 No ( 1.00000 0.00000 ) *
         17) Income > 57 7   9.561 Yes ( 0.42857 0.57143 ) *
        9) Price > 98.5 33   8.962 No ( 0.96970 0.03030 )
         18) Income < 101 28   0.000 No ( 1.00000 0.00000 ) *
         19) Income > 101 5   5.004 No ( 0.80000 0.20000 ) *
      5) ShelveLoc: Medium 111 149.900 No ( 0.59459 0.40541 )
       10) Price < 86.5 7   0.000 Yes ( 0.00000 1.00000 ) *
       11) Price > 86.5 104 136.500 No ( 0.63462 0.36538 )
         22) Age < 50.5 47  64.620 Yes ( 0.44681 0.55319 )
           44) Advertising < 12.5 37  50.620 No ( 0.56757 0.43243 )
             88) Income < 61.5 17  12.320 No ( 0.88235 0.11765 )
              176) Population < 203.5 5   6.730 No ( 0.60000 0.40000 ) *
              177) Population > 203.5 12   0.000 No ( 1.00000 0.00000 ) *
             89) Income > 61.5 20  24.430 Yes ( 0.30000 0.70000 )
              178) Price < 140 15  11.780 Yes ( 0.13333 0.86667 )
                356) Education < 14.5 10   0.000 Yes ( 0.00000 1.00000 )
                357) Education > 14.5 5   6.730 Yes ( 0.40000 0.60000 ) *
              179) Price > 140 5   5.004 No ( 0.80000 0.20000 ) *
           45) Advertising > 12.5 10   0.000 Yes ( 0.00000 1.00000 ) *
         23) Age > 50.5 57  58.670 No ( 0.78947 0.21053 )
           46) Advertising < 4.5 31   8.835 No ( 0.96774 0.03226 )
             92) Age < 79.5 25   0.000 No ( 1.00000 0.00000 ) *
             93) Age > 79.5 6   5.407 No ( 0.83333 0.16667 ) *
           47) Advertising > 4.5 26  35.430 No ( 0.57692 0.42308 )
             94) CompPrice < 118.5 9   0.000 No ( 1.00000 0.00000 ) *
             95) CompPrice > 118.5 17  22.070 Yes ( 0.35294 0.64706 )
```

Pruning

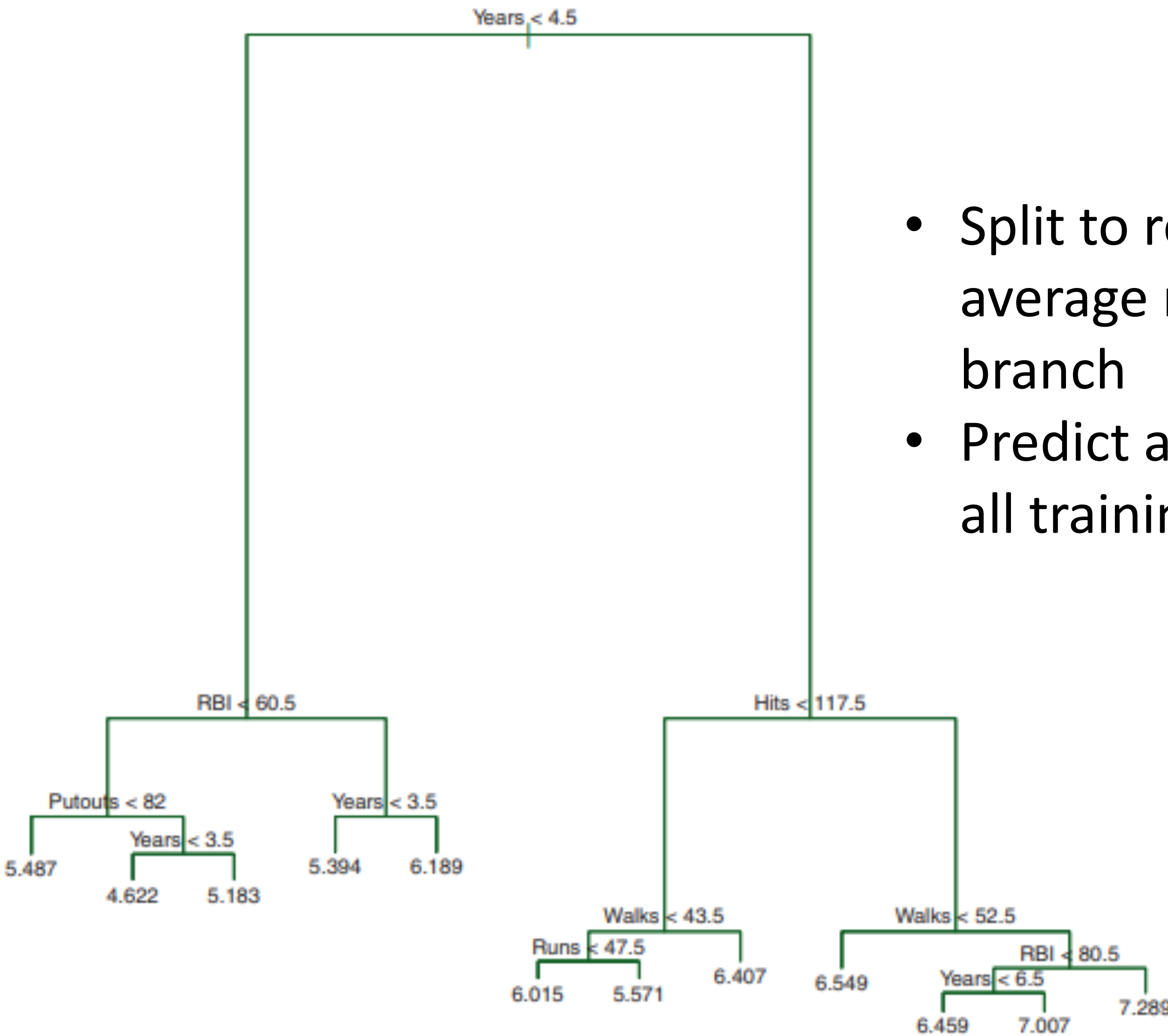
```
> set.seed(3)
> cv.carseats=cv.tree(tree.carseats,FUN=prune.misclass)
> prune.carseats=prune.misclass(tree.carseats,best=12)
> plot(prune.carseats)
> text(prune.carseats,pretty=0)
>
```

- Cross-validation for pruning
- FUN = prune.misclass indicates that classification error is metric to minimize

Pruning


ShelveLoc: Bad,Medium
ShelveLoc: Bad
Price < 150
No
Price < 86.5
Yes
Yes
No
Age < 50.5
Advertising < 12.5
Advertising < 4.5
Income < 61.5
Yes
No
CompPrice < 118.5
No
Price < 140
No
Price < 108
Yes
No
CompPrice < 124
Yes
No
Yes

Regression Trees



- Split to reduce sum of average responses on each branch
- Predict average response of all training data at each leaf

Summary Decision Trees

- Representation: decision trees
- Bias: prefer small decision trees
- Search algorithm: greedy
- Heuristic function: information gain or information content or others
- Overfitting / pruning

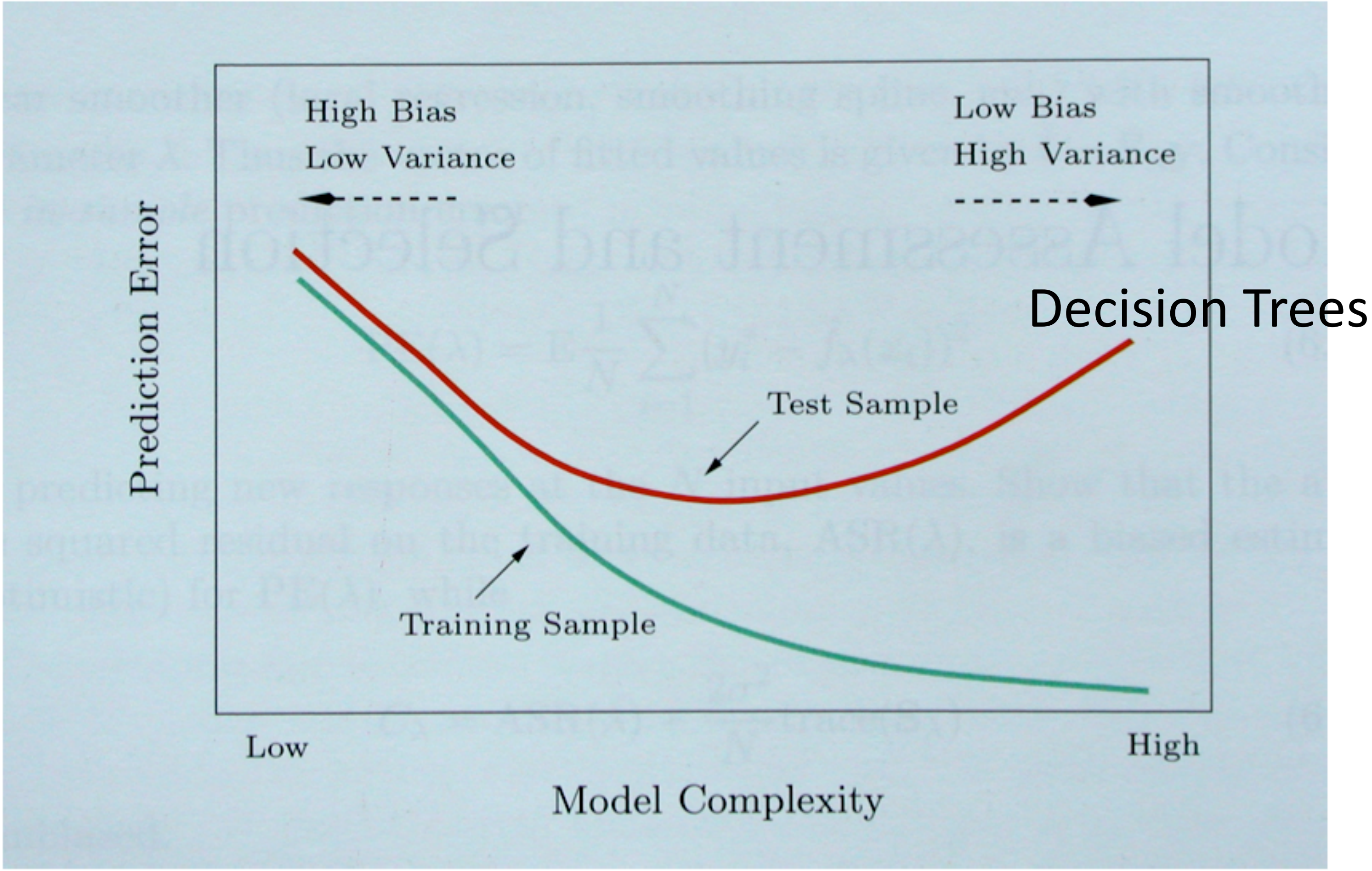
Strengths

- Fast to evaluate
- Interpretable
- Generate rules
- Supports categorical and numerical data

Weaknesses

- Overfitting
- Splitting method might not be optimal
- Accuracy is not always high
- Batch learning

Bias/Variance Tradeoff



Hastie, Tibshirani, Friedman "Elements of Statistical Learning" 2001

How to reduce variance of single decision tree?

Acknowledgements

- Slides made using resources from:
  - Andrew Ng
  - Eric Eaton
  - David Sontag
  - Andrew Moore
- Thanks!