DS 4400

Machine Learning and Data Mining I
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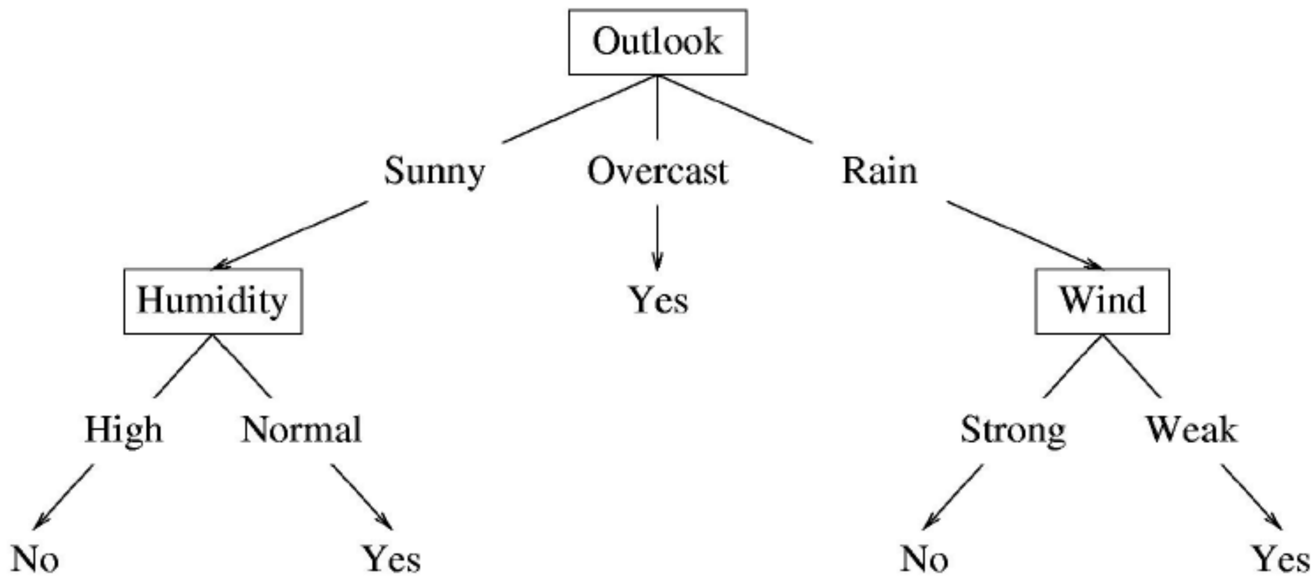
Outline

- Decision trees
  - Information gain / entropy measures
  - Training algorithm
  - Example
- Ensemble models
  - Bagging
  - Boosting

Decision Tree

- A possible decision tree for the data:

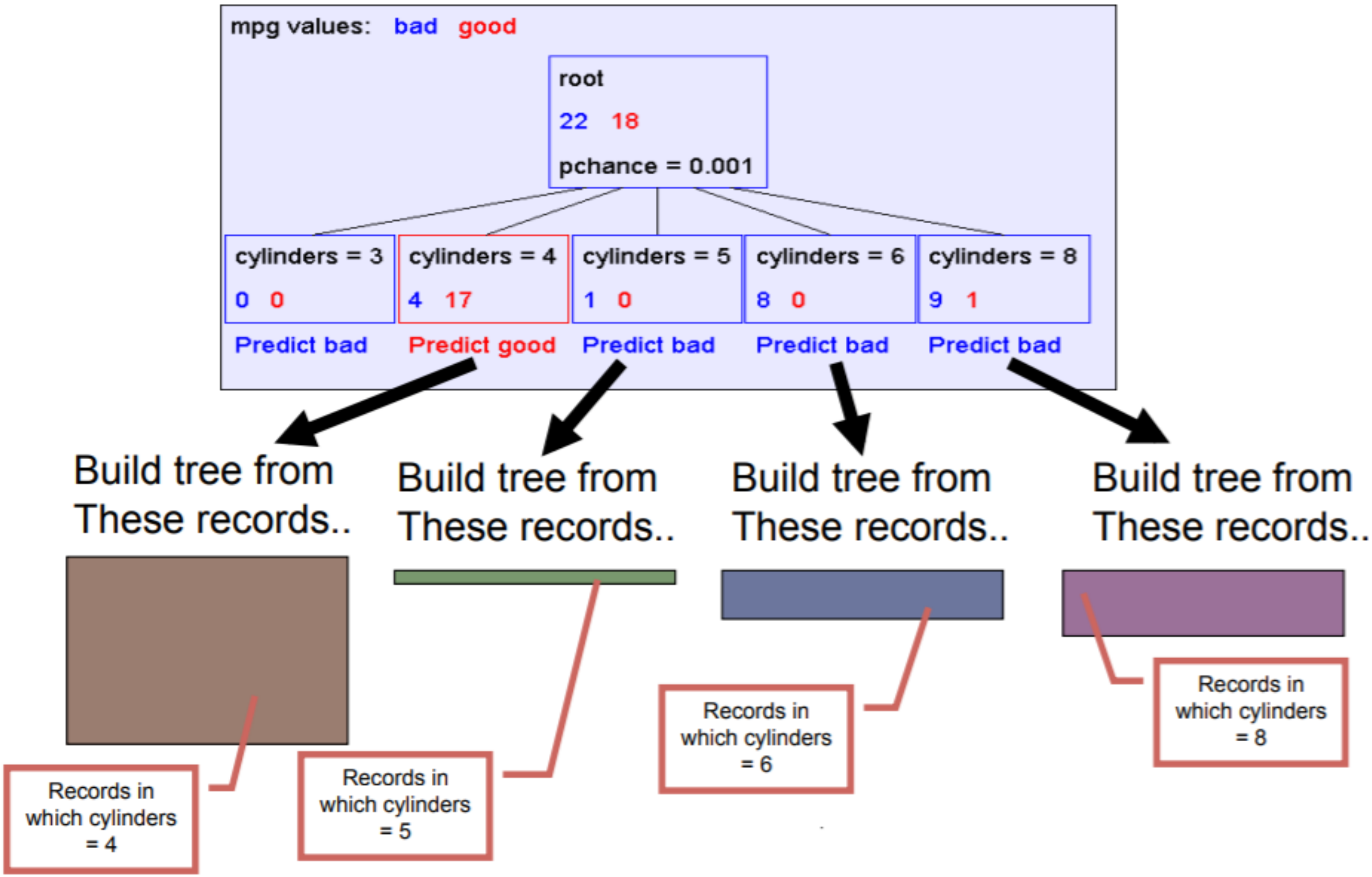


- Each internal node: test one attribute X_i
- Each branch from a node: selects one value for X_i
- Each leaf node: predict Y (or $p(Y \mid x \in \mathrm{leaf})$)

Learning Decision Trees

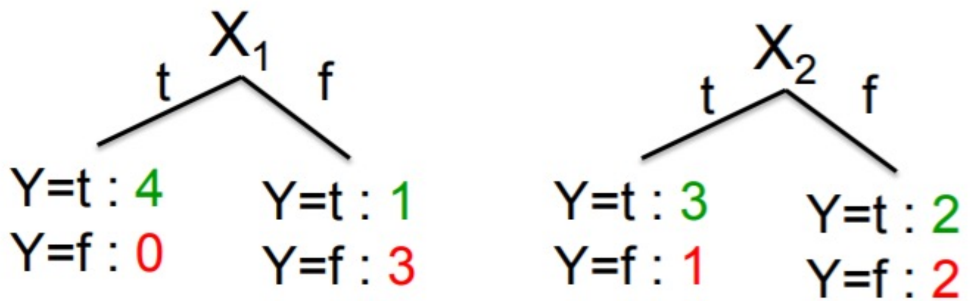
- Learning the simplest (smallest) decision tree is an NP-complete problem [Hyafil & Rivest '76]
- Resort to a greedy heuristic:
  - Start from empty decision tree
  - Split on **next best attribute (feature)**
  - Recurse

Key Idea: Use Recursion Greedily



Splitting

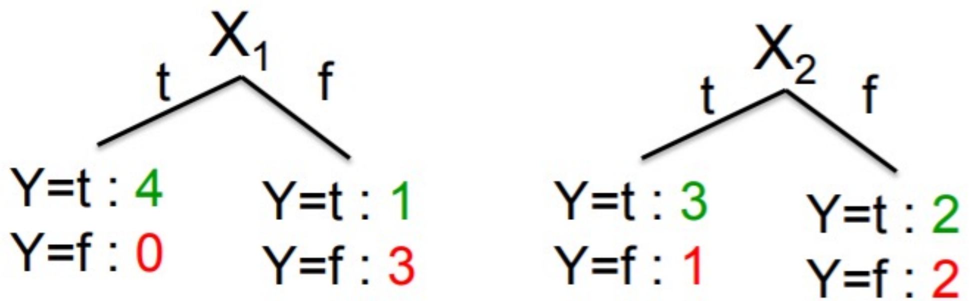
Would we prefer to split on X_1 or X_2?



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

Splitting

Would we prefer to split on X_1 or X_2?



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

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

Use entropy-based measure (Information Gain)

Entropy

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

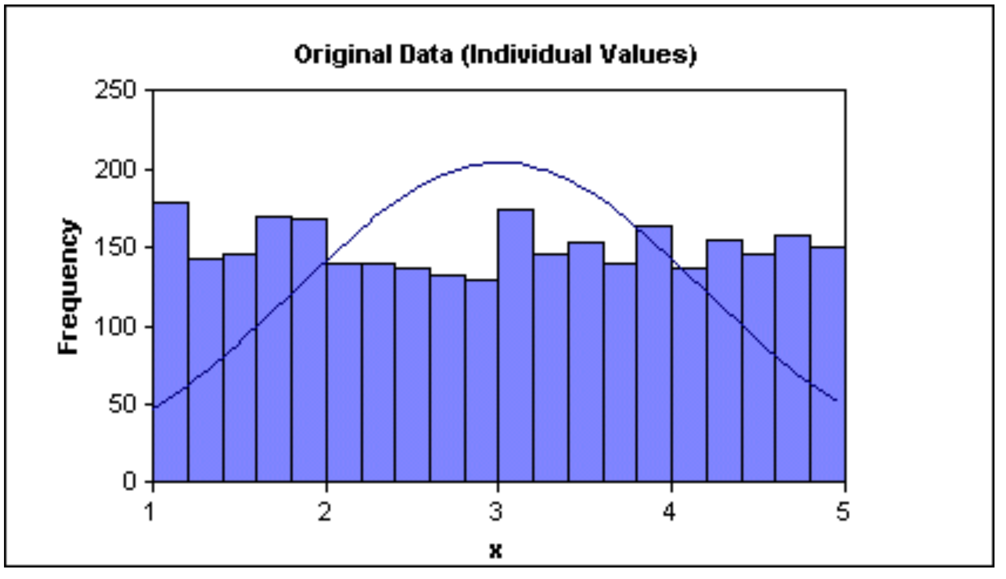
$$H(X) = -p_1 \log_2 p_1 - p_2 \log_2 p_2 - \ldots - p_m \log_2 p_m$$
$$= -\sum_{j=1}^{m} p_j \log_2 p_j$$

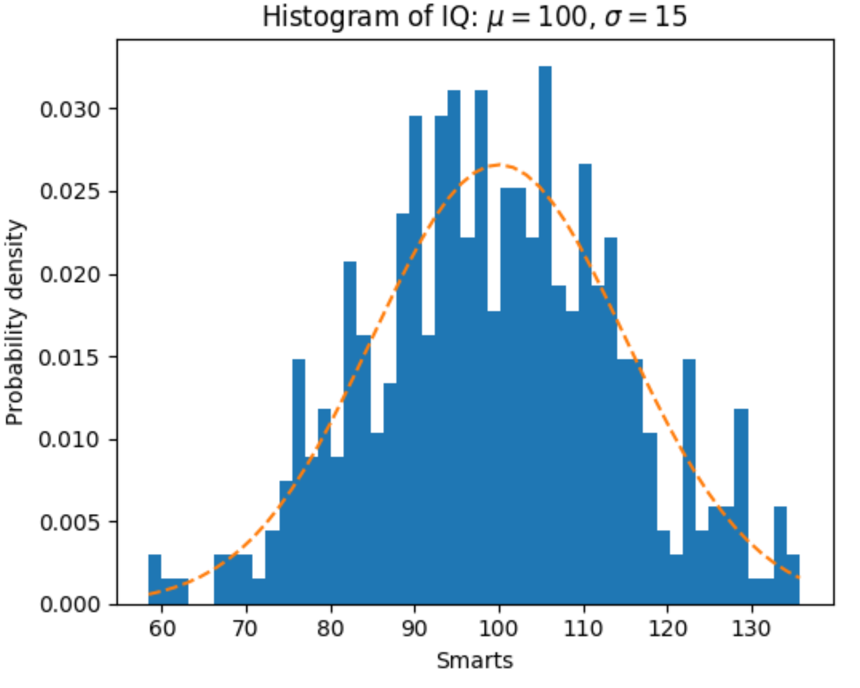
H(X) = The entropy of X

- "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?





Conditional Entropy

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

X = College Major

Y = Likes "Gladiator"

Let's assume this reflects the true probabilities

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

Conditional Entropy

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

X = College Major

Y = Likes "Gladiator"

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Math	Yes
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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:

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

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		
History		
CS		

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) =**
- **H(Y|X) =**
- **Thus IG(Y|X) =**

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:

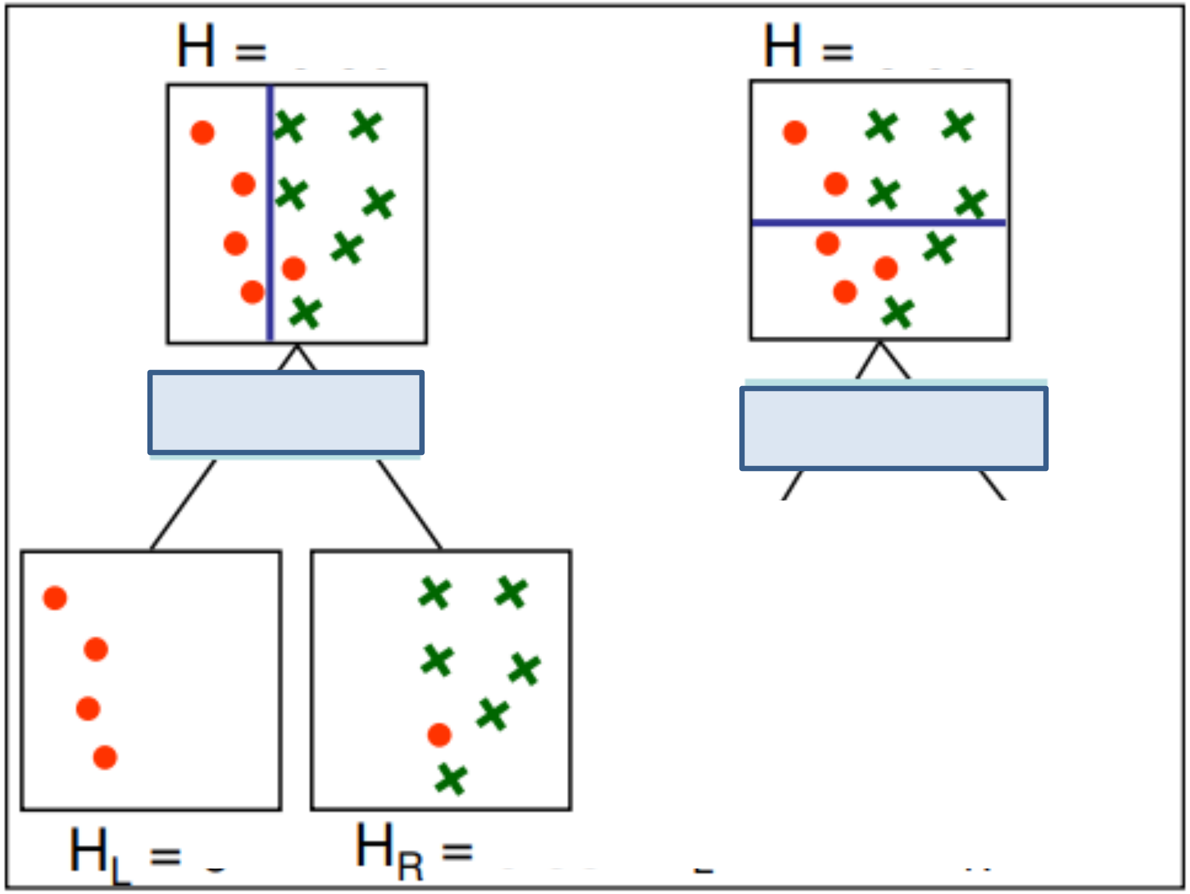
- **H(Y) = 1**
- **H(Y|X) = 0.5**
- **Thus IG(Y|X) = 1 – 0.5 = 0.5**

Relevance for decision trees

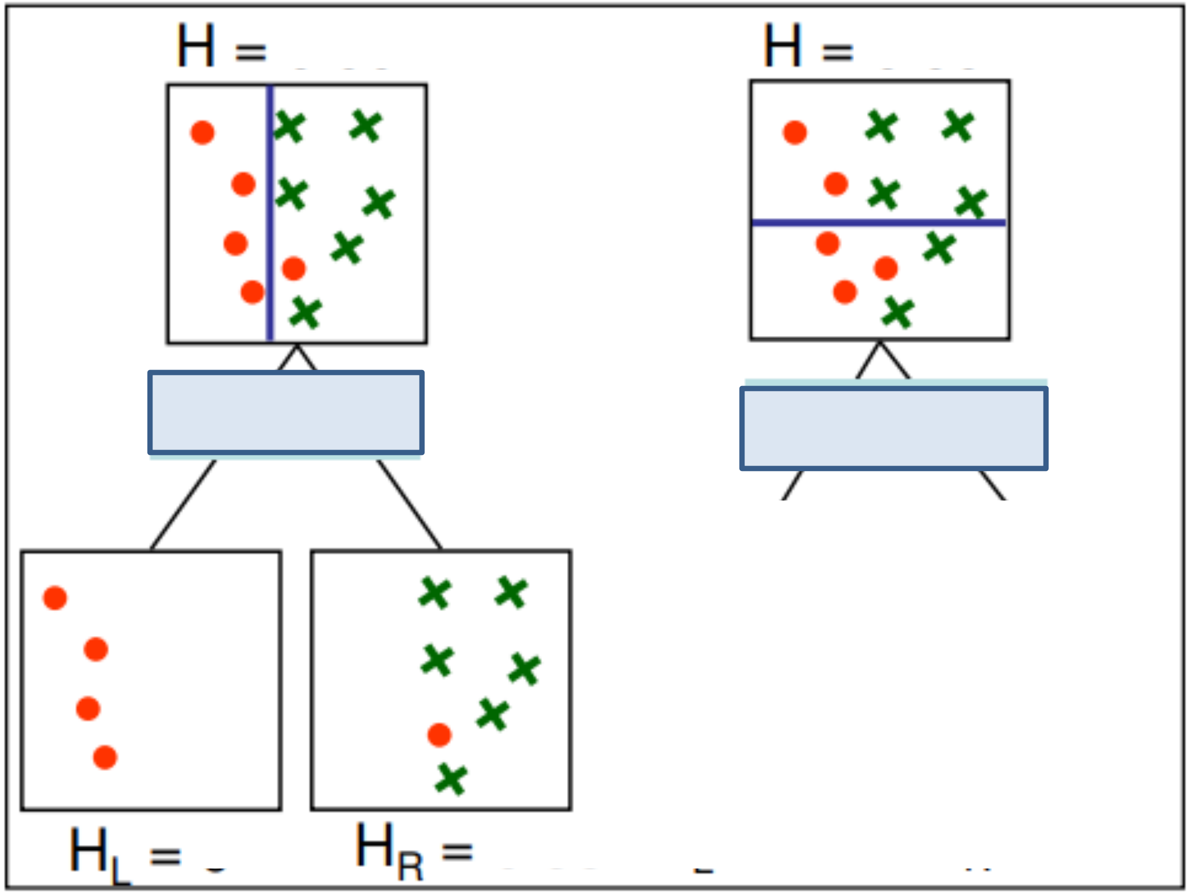
- Multiple features $X_1, \dots, X_d$
- Label Y: Initial entropy $H(Y)$
- How much each feature X_i helps explain uncertainty in Y
  - Compute Information gain

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

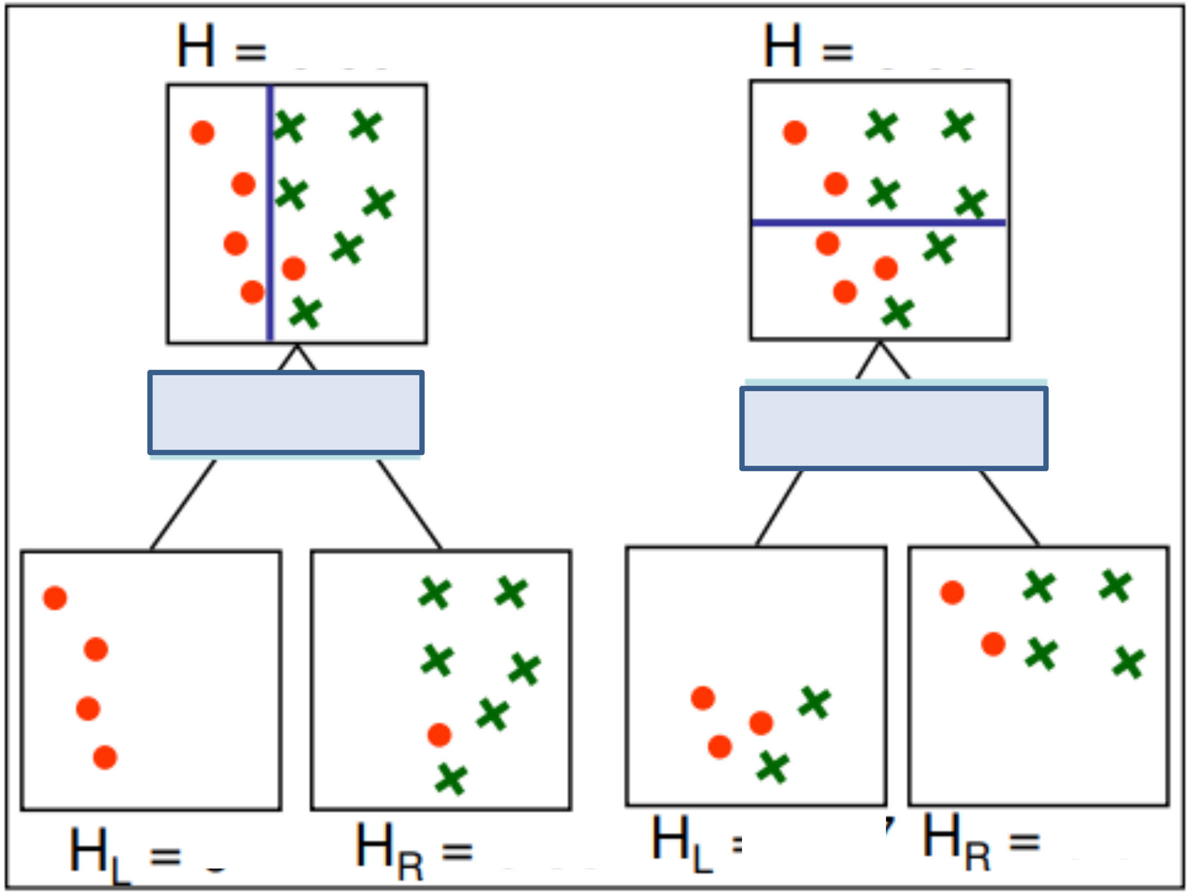
Example Information Gain



Example Information Gain



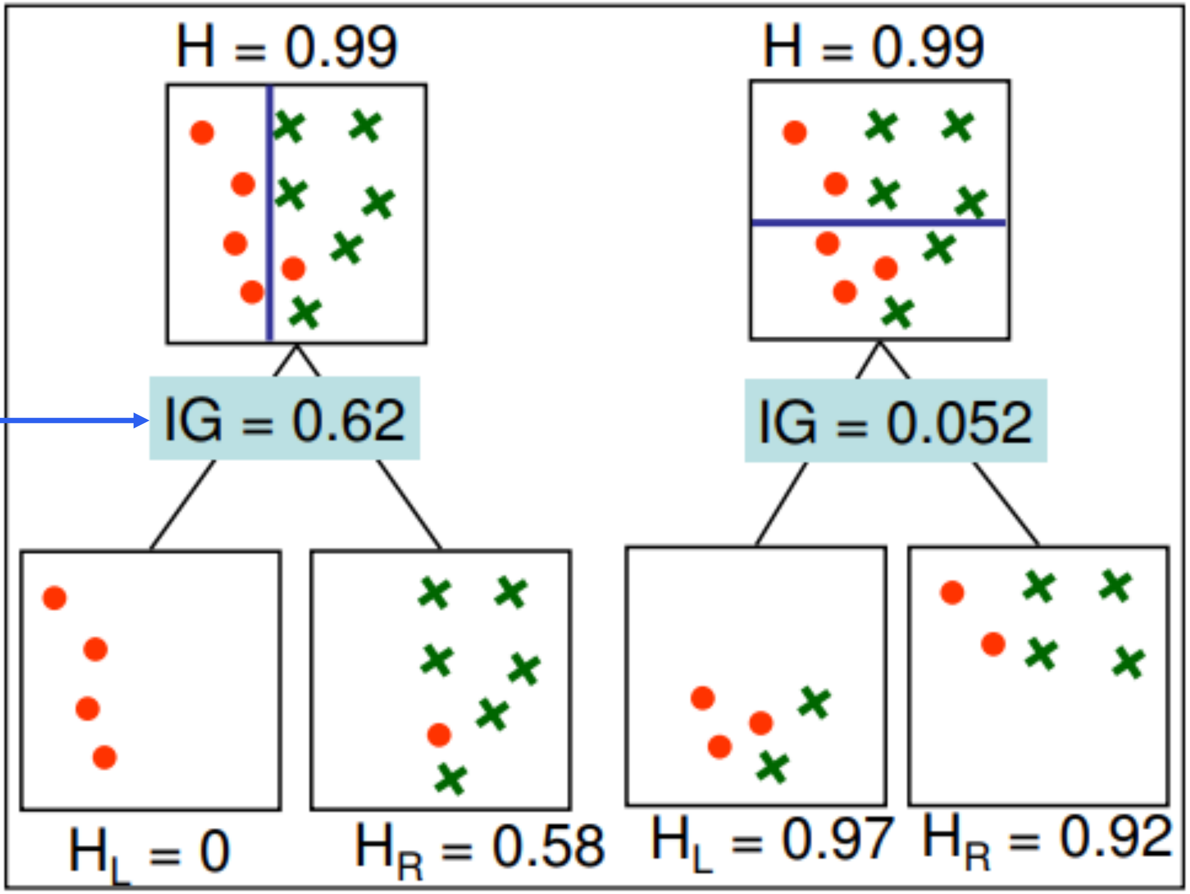
Example Information Gain



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

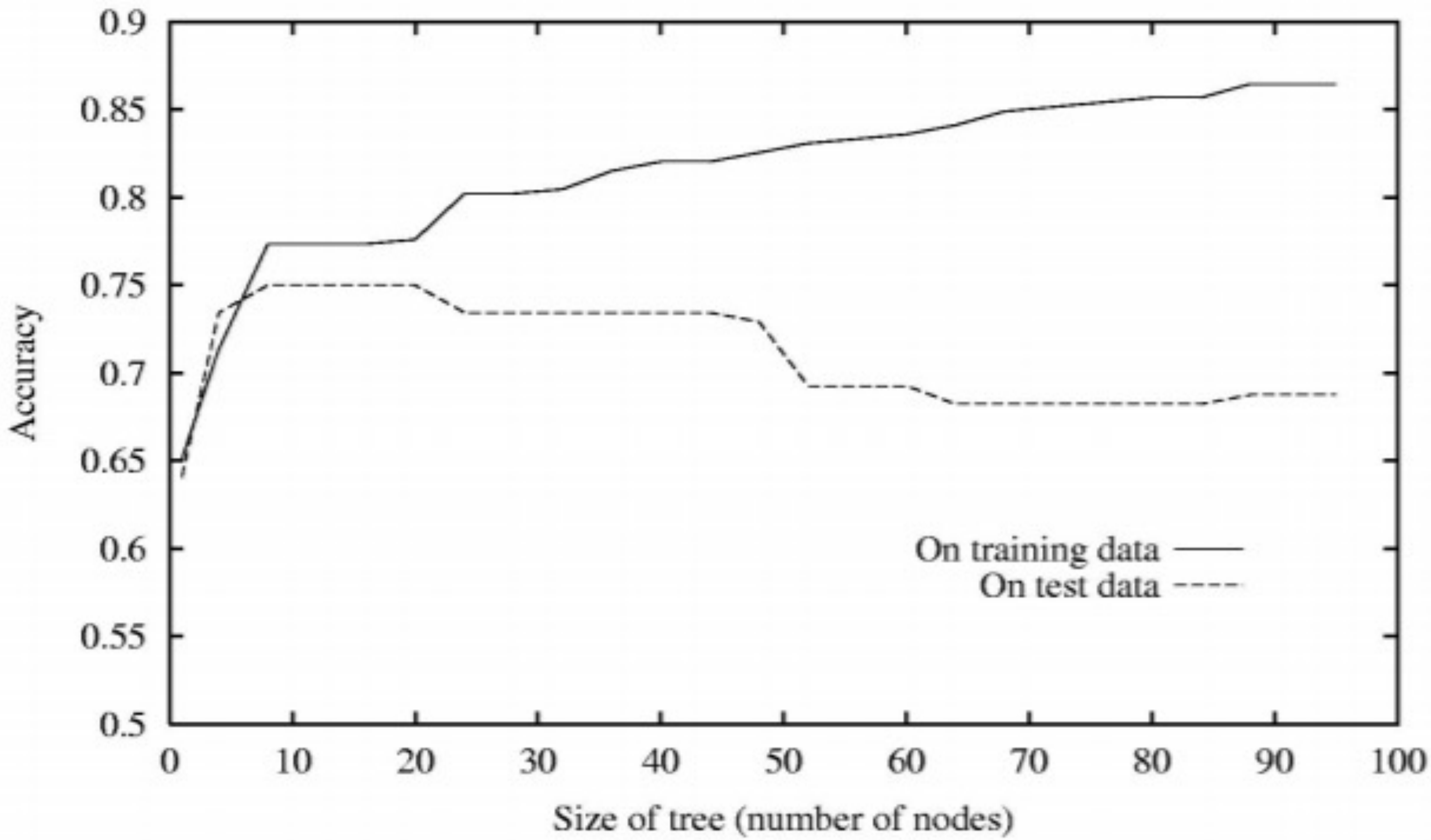
Impurity Metrics

Split a node according to max reduction of impurity

1. Entropy
2. Gini Index
   - For binary case with prob p_0, p_1:
     $$I(p_0, p_1) = 2p_0p_1 = 2p_0(1 - p_0)$$
   - For multi-class with prob $p_1, \dots, p_K$:
     $$I(p_1, \dots p_K\ ) = \sum_{i=1}^{K} p_i\ \ (1 - p_i)$$

- Properties
  - Impurity metrics have value 0 for pure nodes
  - Impurity metrics are maximized for uniform distribution (nodes with most uncertainty)

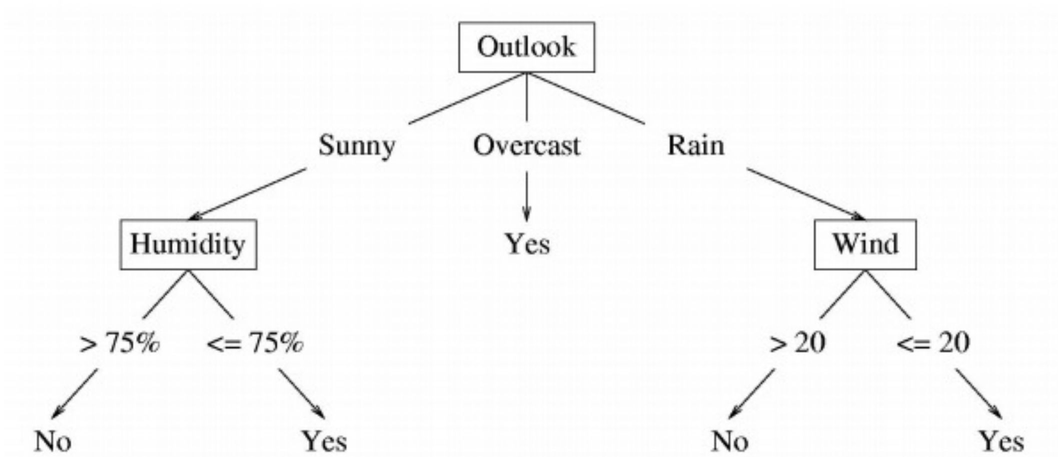
Overfitting



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
  - Remove branches of the tree that increase error using cross-validation

Real-valued Features



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

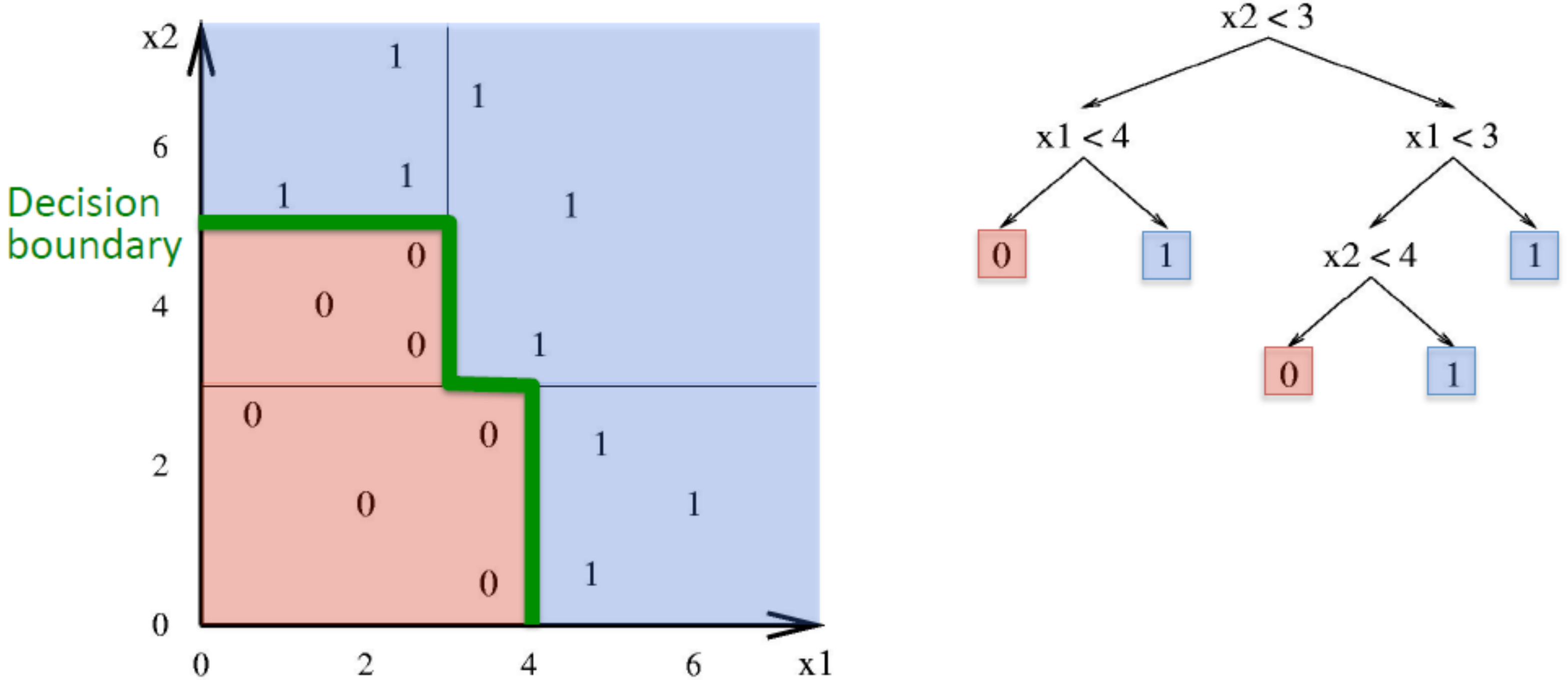
Humidity	40	48	60	72	80	90
PlayTennis:	No	No	Yes	Yes	Yes	No

candidate splits

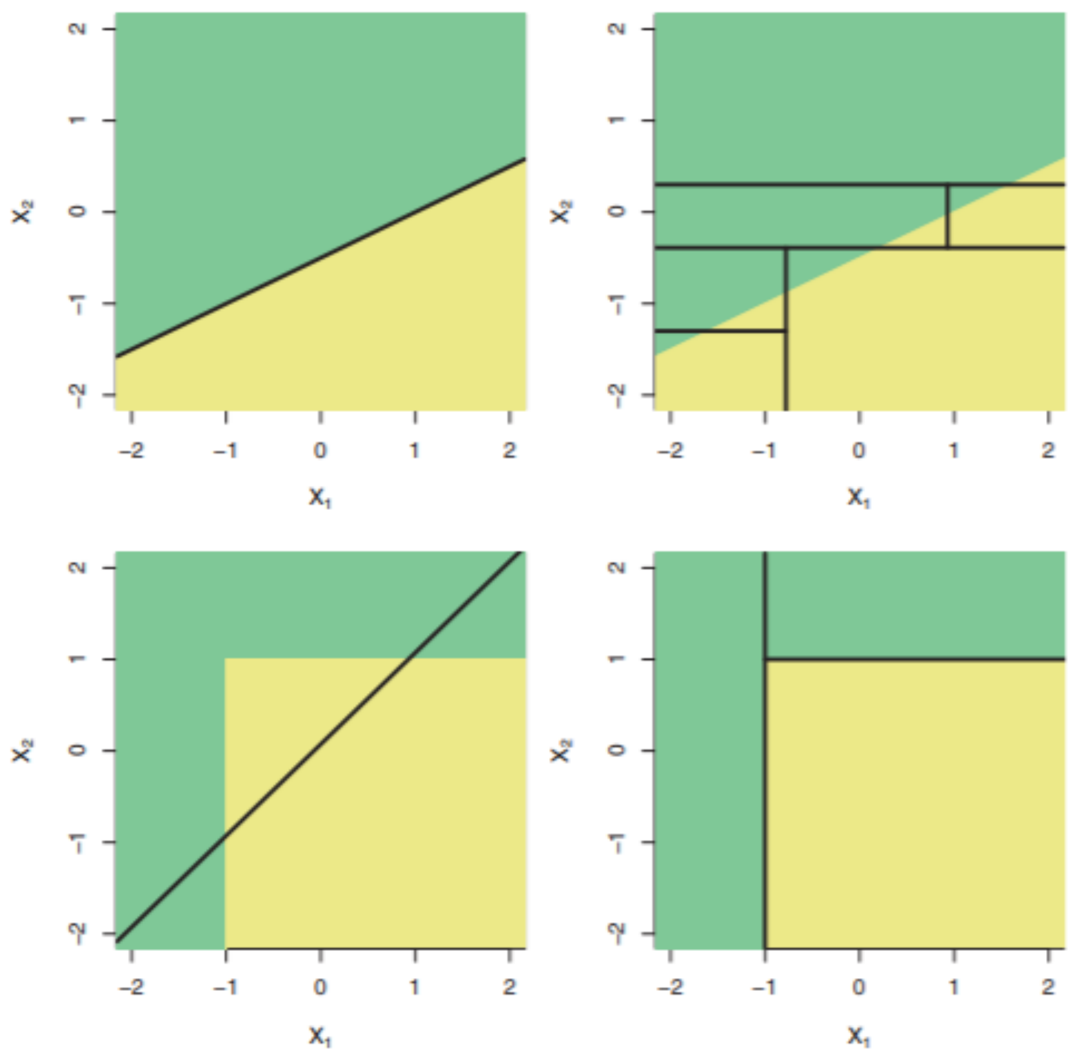
  - Choose among splits by InfoGain()

Decision Boundary

- Decision trees divide the feature space into axis-parallel (hyper-)rectangles
- Each rectangular region is labeled with one label

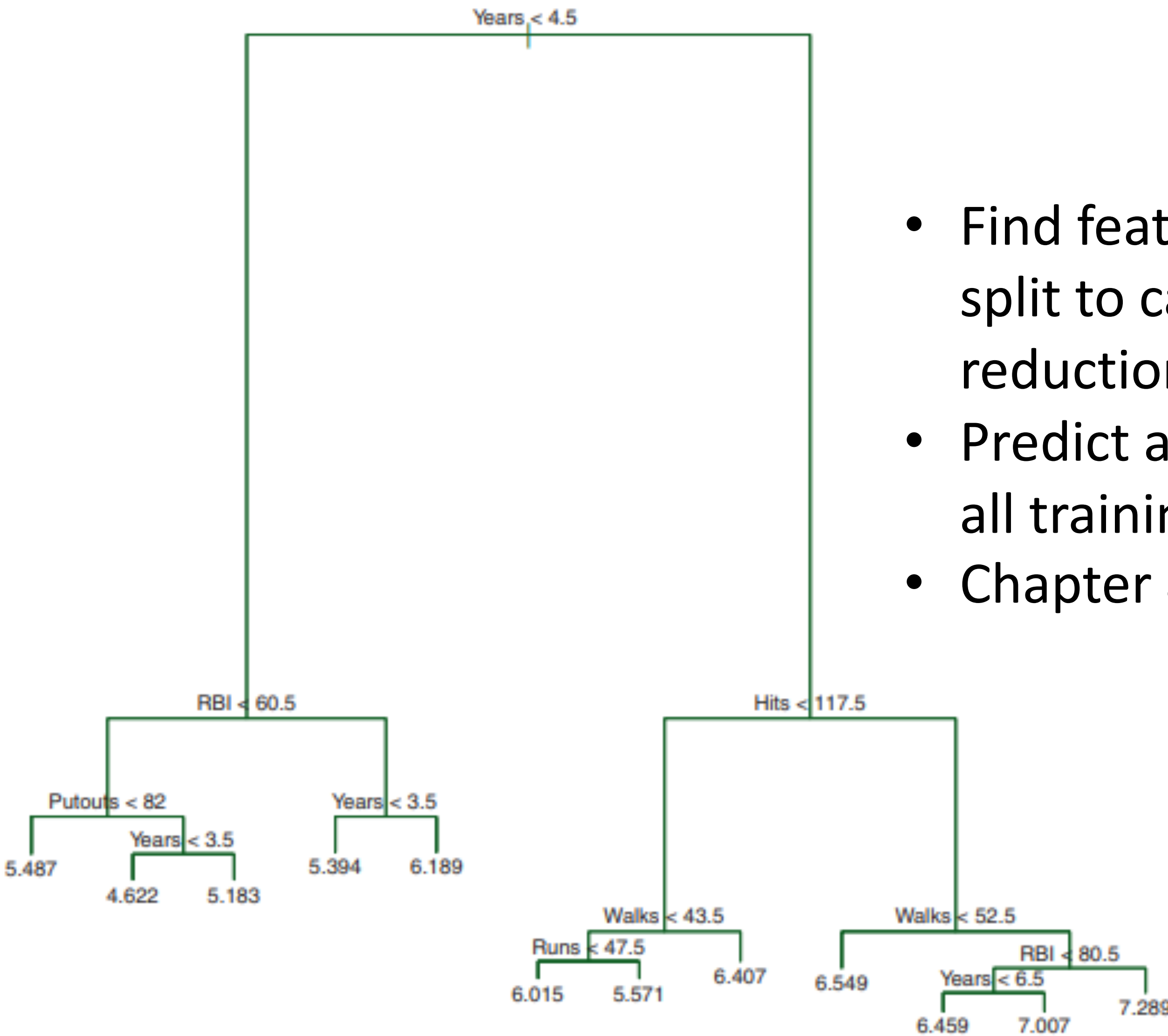


Decision Trees vs Linear Models



Linear model Decision tree

Regression Trees

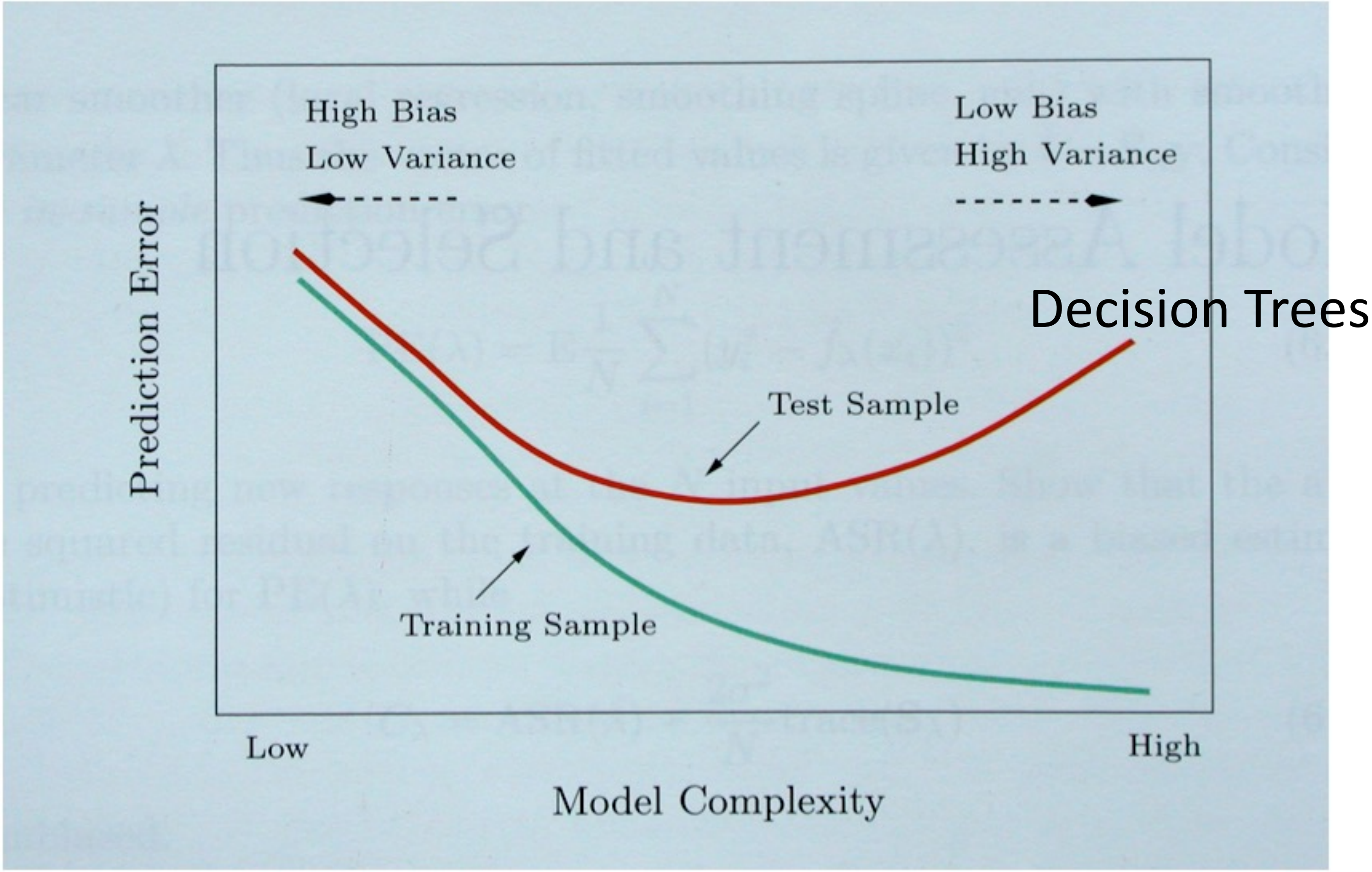


- Find feature and value to split to cause the maximum reduction in MSE
- Predict average response of all training data at each leaf
- Chapter 8.1 from textbook

Summary Decision Trees

- Greedy method for training
  - Not based on optimization or probabilities
- Uses impurity metric (e.g., information gain or Gini index) for splitting
- Advantages
  - Interpretability of decisions
- Limitations
  - Decision trees are prone to overfitting
  - Can be addressed by pruning or using ensembles of decision trees

Bias/Variance Tradeoff



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

How to reduce variance of single decision tree?