Applied Machine Learning

Course number: W207

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Applied Machine Learning

Lecture 4 …

- *OneR, ZeroR, Frequency table, Confusion matrix*
- *Laplace smoothing*
- *Bias, Variance*
- *Decision trees*
- *Entropy, Information gain*

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Evaluation: the key to success

- How predictive is the model we have learned?
- Error on the training data is *not* a good indicator of performance on future data
- Simple solution that can be used if a large amount of (labeled) data is available:
  - Split data into training and test set
- However: (labeled) data is usually limited
  - More sophisticated techniques need to be used

Training and testing I

- Natural performance measure for classification problems: *error rate*
    - *Success*: instance's class is predicted correctly
    - *Error*: instance's class is predicted incorrectly
    - Error rate: proportion of errors made over the whole set of instances
- *Resubstitution error:* error rate obtained by evaluating model on training data
- Resubstitution error is (hopelessly) optimistic!

Training and testing II

- *Test set*: independent instances that have played no part in formation of classifier
  - Assumption: both training data and test data are representative samples of the underlying problem

- Test and training data may differ in nature
  - Example: classifiers built using customer data from two different towns *A* and *B*
  - To estimate performance of classifier from town *A* in completely new town, test it on data from *B*

Inferring rudimentary rules

- ZeroR rule learner: simplest classifier of them all
- It focuses only on the target (class) and ignores all other attributes
- So it predicts the majority category
- Hence its predictability strength is none
- Used for benchmarking / baseline for other classifiers (can’t go lower)
- Hence huge error in results
- It is dependent on constructing a *frequency table* for the target and choses its most frequent value

Dealing with numeric attributes

- Simple Examples:
  - The Weather Problem: *Weather Data with Some Nominal Attributes*

Outlook	Temperature	Humidity	Windy	Play
Sunny	hot	high	false	no
Sunny	hot	high	true	no
Overcast			false	yes
Rainy			false	yes
Rainy			false	yes
Rainy			true	no
Overcast	cool	normal	true	yes
Sunny	mild	high	false	no
Sunny	cool	normal	false	yes
Rainy	mild	normal	false	yes
Sunny	mild	normal	true	yes
Overcast	mild	high	true	yes
Overcast	hot	normal	false	yes
Rainy	mild	high	true	no

frequency table

Play	
Yes	No
9	5

Dealing with numeric attributes

- Simple Examples:
  - The Weather Problem: *Weather Data with Some Numeric Attributes*

actual values

true positives

false positives

Confusion matrix		Play		Outcome	
		Yes	No		
ZeroR	Yes	9	5	Positive predictive value	0.64
	No	0	0	Negative predictive value	0.00
		Sensitivity 1.00	Specificity 0.00	Accuracy = 0.64	

predicted values

false negatives

true negatives

Inferring rudimentary rules

- OneR rule learner: learns a 1-level decision tree
  - A set of rules that all test one particular attribute that has been identified as the one that yields the lowest classification error
- Basic version for finding the rule set from a given training set (assumes nominal attributes):
  - For each attribute
    - Make one branch for each value of the attribute
      (… or one rule for each predictor)
    - To each branch, assign the most frequent class value of the instances pertaining to that branch
    - Error rate: proportion of instances that do not belong to the majority class of their corresponding branch
  - Choose attribute with lowest error rate

Pseudo-code for 1R

- 1R method at work

```
For each attribute,
  For each value of the attribute, make a rule as follows:
    count how often each class appears
    find the most frequent class
    make the rule assign that class to this attribute-value
  Calculate the error rate of the rules
Choose the rules with the smallest error rate
```

- 1R's handling of missing values:

  a missing value is treated as a separate attribute value

- If the value is numerical it must be converted to categorical before we proceed

Evaluating the weather attributes

Outlook	Temp	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

Attribute	Rules	Errors	Total errors
Outlook	Sunny → No	2/5	4/14
	Overcast → Yes	0/4	
	Rainy → Yes	2/5	
Temp	Hot → No	2/4	5/14
	Mild → Yes	2/6	
	Cool → Yes	1/4	
Humidity	High → No	3/7	4/14
	Normal → Yes	1/7	
Windy	False → Yes	2/8	5/14
	True → No	3/6	

Results with overfitting avoidance

- Let's focus on *Outlook* for a moment:
  - Lets create a *frequency table* for Outlook
  - Then lets construct a confusion matrix for it

Frequency table		Play	
		yes	*no*
Outlook	Sunny	2	3
	Overcast	4	0
	Rainy	3	2

Rules:

if Outlook = Sunny THEN Play = No

if Outlook = Overcast THEN Play = Yes

if Outlook = Rainy THEN Play = Yes

majority

Results with overfitting avoidance

- Let's focus on *Outlook* for a moment:
  - Lets create a frequency table for Outlook
  - Then lets construct a *confusion matrix* for it

actual values

true positives

false positives

Confusion matrix		Play		Outcome	
		Yes	No		
OneR	Yes	7	2	Positive predictive value	0.78
	No	2	3	Negative predictive value	0.60
		Sensitivity 0.78	Specificity 0.60	Accuracy = 0.71	

predicted values

false negatives

true negatives

Discussion of 1R

- 1R was described in a paper by Holte (1993):

  Very Simple Classification Rules Perform Well on Most Commonly Used Datasets,
  Robert C. Holte, Computer Science Department, University of Ottawa

  - Contains an experimental evaluation on 16 datasets (using *cross-validation* to estimate classification accuracy on fresh data)
  - Required minimum number of instances in majority class was set to 6 after some experimentation
  - 1R's simple rules performed not much worse than much more complex decision trees
- **Lesson**: simplicity first can pay off on practical datasets
- Note that 1R does not perform as well on more recent, more sophisticated benchmark datasets

Simple probabilistic modeling

- "Opposite" of 1R: use all the attributes
- Two assumptions: Attributes are
  - *equally important*
  - *statistically independent* (given the class value)
- Independence assumption is almost never correct!
- But … this scheme often works surprisingly well in practice
- The scheme is easy to implement in a program and very fast
- It is known as *naïve Bayes*

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Probabilities for weather data

Outlook			Temperature			Humidity			Windy			Play	
	Yes	*No*		*Yes*	*No*		*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	3	Hot	2	2	High	3	4	False	6	2	9	5
Overcast	4	0	Mild	4	2	Normal	6	1	True	3	3		
Rainy	3	2	Cool	3	1								
Sunny	2/9	3/5	Hot	2/9	2/5	High	3/9	4/5	False	6/9	2/5	9/14	5/14
Overcast	4/9	0/5	Mild	4/9	2/5	Normal	6/9	1/5	True	3/9	3/5		
Rainy	3/9	2/5	Cool	3/9	1/5								

Outlook	Temp	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

Probabilities for weather data

Outlook			Temperature			Humidity			Windy			Play	
	Yes	*No*		*Yes*	*No*		*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	3	Hot	2	2	High	3	4	False	6	2	9	5
Overcast	4	0	Mild	4	2	Normal	6	1	True	3	3		
Rainy	3	2	Cool	3	1								
Sunny	$\boxed{2/9}$	3/5	Hot	2/9	2/5	High	$\boxed{3/9}$	4/5	False	6/9	2/5	$\boxed{9/14}$	5/14
Overcast	4/9	0/5	Mild	4/9	2/5	Normal	6/9	1/5	True	$\boxed{3/9}$	3/5		
Rainy	3/9	2/5	Cool	$\boxed{3/9}$	1/5								

- A new day:

Outlook	Temp.	Humidity	Windy	Play
Sunny	Cool	High	True	?

Likelihood of the two classes

For "yes" = 2/9 × 3/9 × 3/9 × 3/9 × 9/14 = 0.0053

For "no" = 3/5 × 1/5 × 4/5 × 3/5 × 5/14 = 0.0206

Conversion into a probability by normalization:

P("yes") = 0.0053 / (0.0053 + 0.0206) = 0.205

P("no") = 0.0206 / (0.0053 + 0.0206) = 0.795

Can combine probabilities using Bayes's rule

- Famous rule from probability theory due to

  Thomas Bayes

  Born: 1702 in London, England
  Died: 1761 in Tunbridge Wells, Kent, England

- Probability of an event *H (class)* given observed evidence *E (data, predictor, attribute):*

$$P(H \mid E) = P(E \mid H)P(H) / P(E)$$

- A posteriori probability of the class *H* given the data *E*: $P(H \mid E)$
  - Probability of event *after* evidence is seen
- A priori probability of *H (class prior probability)*: $P(H)$
  - Probability of event *before* evidence is seen
- Marginal likelihood *E (predictor prior probability)*: $P(E)$
  - Probability of the attribute *before* class is seen
- Probability of the data *E* given the class *H (likelihood)*: $P(E \mid H)$

Naïve Bayes for classification

- It is a supervised classification learning:

  what is the probability of the class given an instance?

  - Evidence *E* = instance's non-class attribute values
  - Event *H* = class value of instance

- Naïve assumption: evidence splits into parts (i.e., attributes) that are conditionally *independent*
- This means, given *n* attributes, we can write Bayes' rule using a product of per-attribute probabilities:

$$P(H \mid E) = P(E_1 \mid H)P(E_3 \mid H)\ldots P(E_n \mid H)P(H) / P(E)$$

Weather data example

Outlook	Temp.	Humidity	Windy	Play
Sunny	Cool	High	True	?

← ***Evidence E***

$$P(yes \mid E) = P(Outlook = Sunny \mid yes)$$

$$P(Temperature = Cool \mid yes)$$

$$P(Humidity = High \mid yes)$$

$$P(Windy = True \mid yes)$$

$$P(yes) / P(E)$$

$$= \frac{2/9 \times 3/9 \times 3/9 \times 3/9 \times 9/14}{P(E)}$$

Probability of class "yes"

Probabilities for weather data

Outlook			Temperature			Humidity			Windy			Play	
	Yes	*No*		*Yes*	*No*		*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	3	Hot	2	2	High	3	4	False	6	2	9	5
Overcast	4	0	Mild	4	2	Normal	6	1	True	3	3		
Rainy	3	2	Cool	3	1								
Sunny	2/9	3/5	Hot	2/9	2/5	High	3/9	4/5	False	6/9	2/5	9/14	5/14
Overcast	4/9	0/5	Mild	4/9	2/5	Normal	6/9	1/5	True	3/9	3/5		
Rainy	3/9	2/5	Cool	3/9	1/5								

$P (E \mid H) = P (Sunny \mid Yes) = 2 / 9 = 0.22$

Likelihood matrix		Play: *Yes*	Play: *No*	Outcome
Outlook	Sunny	2/9	3/5	5/14
	Overcast	4/9	0/5	4/14
	Rainy	3/9	2/5	5/14
		9/14	5/14	

$P (E) = P (Sunny) = 5 / 14 = 0.36$

$P (H) = P (Yes) = 9 / 14 = 0.64$

***Posterior probability*:**

$P (H \mid E) = P (Yes \mid Sunny)$

$P (H \mid E) = P (Sunny \mid Yes) * P (Yes) / P (Sunny) = 0.22*0.64/0.36 = 0.39$

The “zero-frequency problem”

- What if an attribute value does not occur with every class value? (e.g., “Humidity = high” for class “yes”)

  - Probability will be zero: $P(Humidity = High \mid yes) = 0$
  - *A posteriori* probability will also be zero: $P(yes \mid E) = 0$
    (Regardless of how likely the other values are!)

- Remedy: add 1 to the count for every attribute value-class combination (*Laplace estimator*)
- Result: probabilities will never be zero
- Additional advantage: stabilizes probability estimates computed from small samples of data

Modified probability estimates

- In some cases adding a constant different from 1 might be more appropriate
- Example: attribute *outlook* for class *yes*

$\frac{2+\mu/3}{9+\mu}$	$\frac{4+\mu/3}{9+\mu}$	$\frac{3+\mu/3}{9+\mu}$
Sunny	***Overcast***	***Rainy***

- Weights don't need to be equal (but they must sum to 1)

$$\frac{2+\mu p_1}{9+\mu} \qquad \frac{4+\mu p_2}{9+\mu} \qquad \frac{3+\mu p_3}{9+\mu}$$

Missing values

- Training: instance is not included in frequency count for attribute value-class combination
- Classification: attribute will be omitted from calculation
- Example:

Outlook	Temp.	Humidity	Windy	Play
?	Cool	High	True	?

Likelihood of "yes" = 3/9 × 3/9 × 3/9 × 9/14 = 0.0238

Likelihood of "no" = 1/5 × 4/5 × 3/5 × 5/14 = 0.0343

P("yes") = 0.0238 / (0.0238 + 0.0343) = 41%

P("no") = 0.0343 / (0.0238 + 0.0343) = 59%

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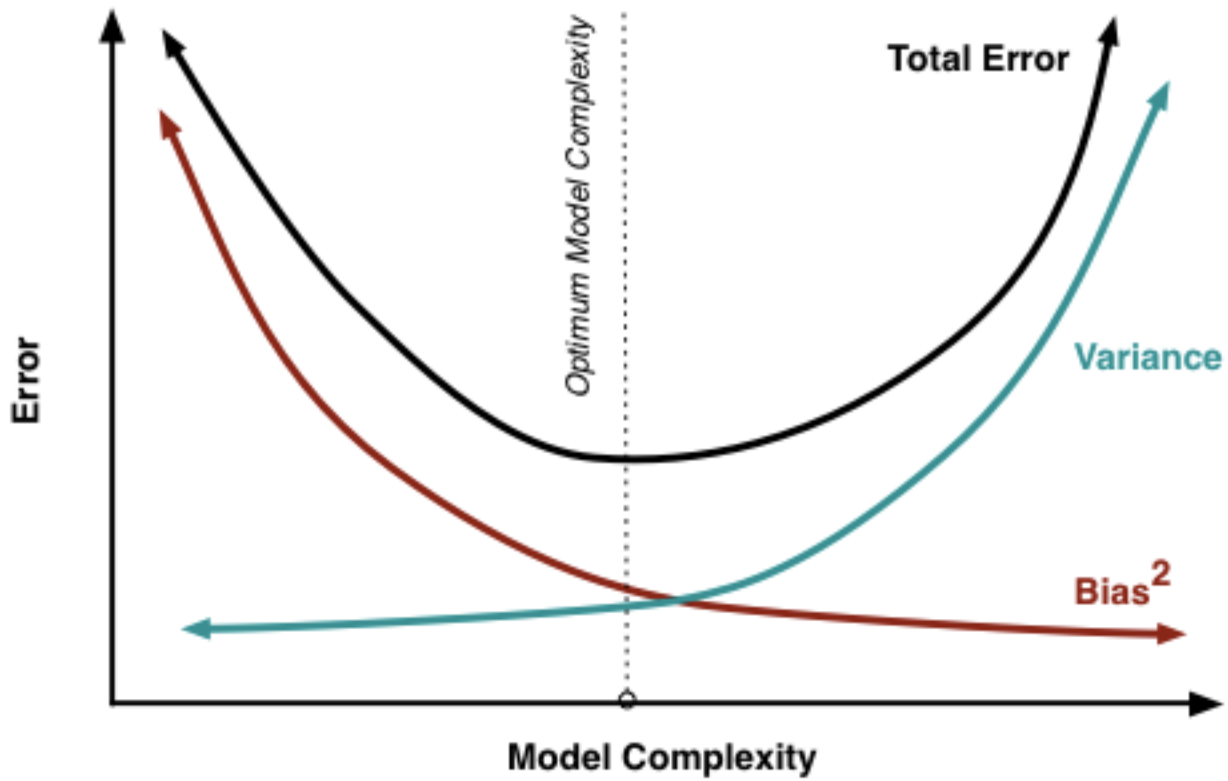

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Weather Data				
Day	Outlook	Humidity	Wind	Play
1	Sunny	High	Weak	No
2	Sunny	High	Strong	No
3	Overcast	High	Weak	Yes
4	Rain	High	Weak	Yes
5	Rain	Normal	Weak	Yes
6	Rain	Normal	Strong	No
7	Overcast	Normal	Strong	Yes
8	Sunny	High	Weak	No
9	Sunny	Normal	Weak	Yes
10	Rain	Normal	Weak	Yes
11	Sunny	Normal	Strong	Yes
12	Overcast	High	Strong	Yes
13	Overcast	Normal	Weak	Yes
14	Rain	High	Strong	No
	New Day			
15	Rain	High	Weak	?

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Criterion for attribute selection

- Which is the best attribute?
  - Want to get the smallest tree
  - Heuristic: choose the attribute that produces the "purest" nodes
- Popular selection criteria: *information gain*
  - Information gain increases with the average purity of the subsets
- Strategy: amongst attributes available for splitting, choose attribute that gives greatest information gain
- Information gain requires measure of *impurity*
- Impurity measure that it uses is the *entropy* of the class distribution, which is a measure from information theory

What is Entropy?

- *Various definitions same meaning:*
  - *Entropy*: lack of order or predictability; gradual decline into disorder
  - *Entropy*: (in information theory) a logarithmic measure of the rate of transfer of information in a particular message or language
  - *Entropy* may be understood as a measure of disorder within a macroscopic system
  - *Entropy* is the measure of the level of disorder in a closed but changing system, a system in which energy can only be transferred in one direction from an ordered state to a disordered state
  - The higher the *entropy*, the higher the disorder and the system's energy to do useful work is lower

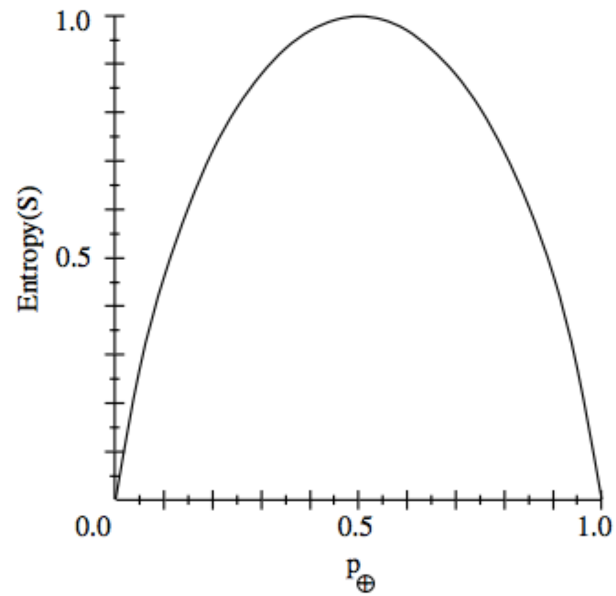
Computing information

- We have a probability distribution: the class distribution in a subset of instances
- The expected information required to determine an outcome (i.e., class value), is the distribution's *entropy*
- Formula for computing the entropy:

$$\text{Entropy}(p_1, p_2, \ldots, p_n) = -p_1 \log p_1 - p_2 \log p_2 \ldots - p_n \log p_n$$

- Using base-2 logarithms, entropy gives the information required in expected *bits*
- *Entropy is maximal when all classes are equally likely and minimal when one of the classes has probability 1*

Entropy



- S is a sample of training examples
- $p_\oplus$ is the proportion of positive examples in S
- $p_\ominus$ is the proportion of negative examples in S
- Entropy measures the impurity of S

$$Entropy(S) \equiv -p_\oplus \log_2 p_\oplus - p_\ominus \log_2 p_\ominus$$

Example: attribute *Outlook*

- *Outlook* = *Sunny* :

$$\text{Info}([2,3]) = 0.971 \text{ bits} \qquad Entropy(S_{sunny}) = -\frac{2}{5}\log_2\left(\frac{2}{5}\right) - \frac{3}{5}\log_2\left(\frac{3}{5}\right)$$

- *Outlook* = *Overcast* :

$$\text{Info}([4,0]) = 0.0 \text{ bits} \qquad Entropy(S_{overcast}) = -\frac{4}{4}\log_2\left(\frac{4}{4}\right) - 0\log_2(0)$$

- *Outlook* = *Rainy* :

$$\text{Info}([3,2]) = 0.971 \text{ bits} \qquad Entropy(S_{rain}) = -\frac{3}{5}\log_2\left(\frac{3}{5}\right) - \frac{2}{5}\log_2\left(\frac{2}{5}\right)$$

- Expected information for attribute:

$$\text{Info}([2,3],[4,0],[3,2]) = (5/14) \times 0.971 + (4/14) \times 0 + (5/14) \times 0.971$$

$$= 0.693 \text{ bits}$$

Computing information gain

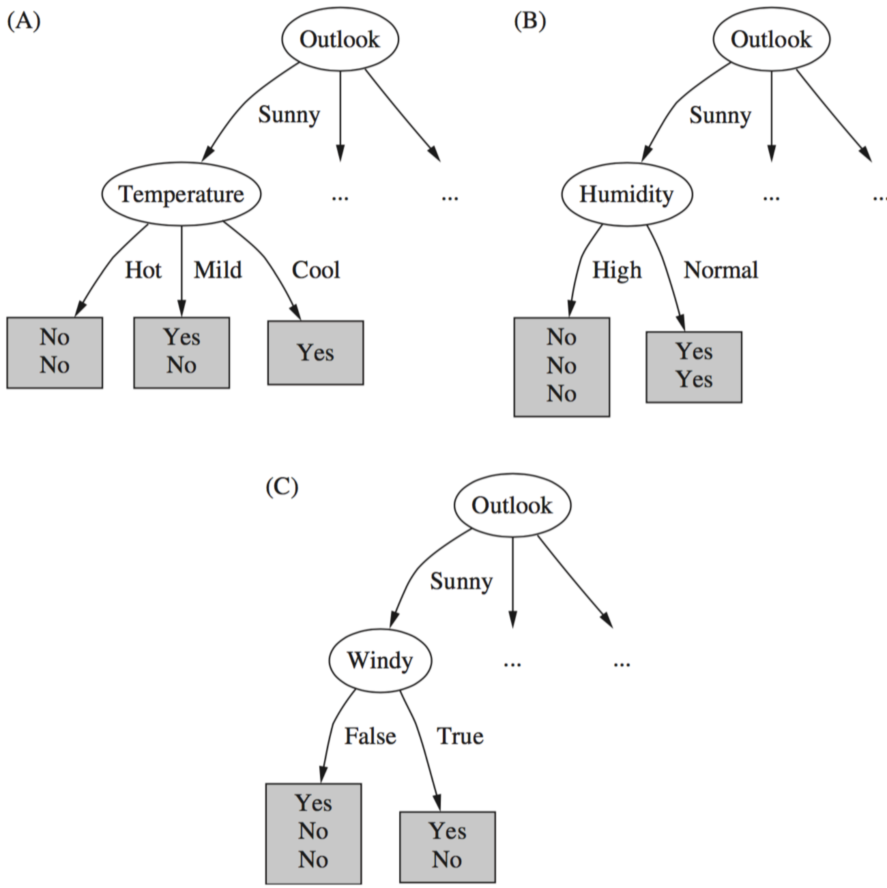
- Information gain: information before splitting – information after splitting

Gain (*Outlook*) = Info([9,5]) – info([2,3],[4,0],[3,2])
= 0.940 – 0.693
= 0.247 bits

- Information gain for attributes from weather data:

Gain (*Outlook*)	= 0.247 bits
Gain (*Temperature*)	= 0.029 bits
Gain (*Humidity*)	= 0.152 bits
Gain (*Windy*)	= 0.048 bits

Continuing to split

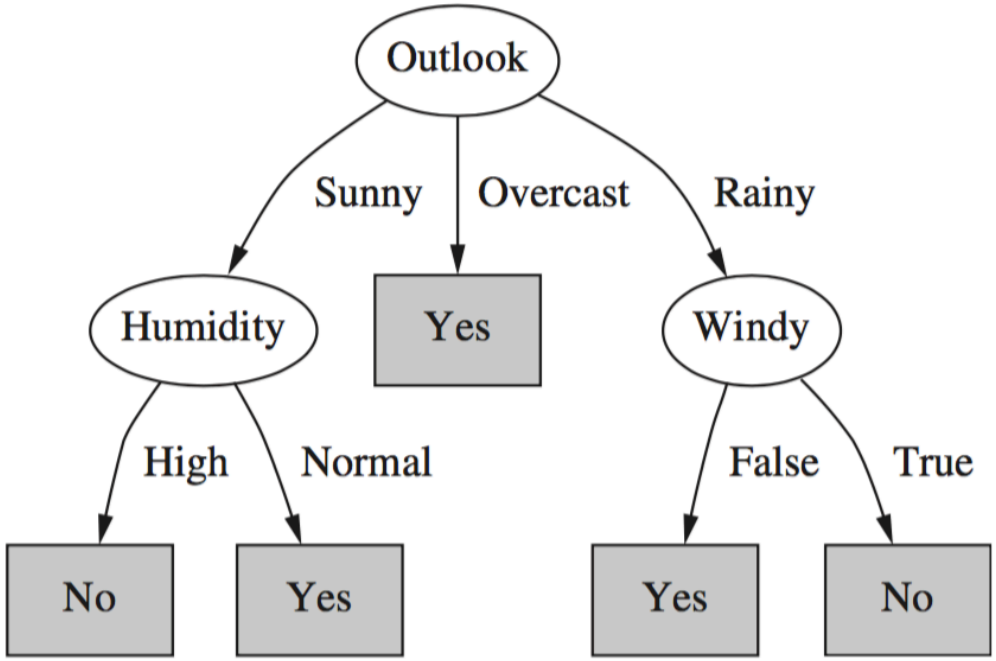


Gain (*Temperature*) = 0.571 bits

Gain (*Humidity*) = 0.971 bits

Gain (*Windy*) = 0.020 bits

Final decision tree



- Note: not all leaves need to be pure; sometimes identical instances have different classes
  - $\Rightarrow$ Splitting stops when data cannot be split any further

Discussion

- Top-down induction of decision trees: ID3, algorithm developed by Ross Quinlan
  - Gain ratio just one modification of this basic algorithm
  - C4.5 tree learner deals with numeric attributes, missing values, noisy data
- Similar approach: CART tree learner
  - Uses Gini index rather than entropy to measure impurity
- There are many other attribute selection criteria! (But little difference in accuracy of result)