Algorithms: The Basic Methods

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INSTITUTE FOR ARTIFICIAL INTELLIGENCE

Algorithms: The basic methods

- Inferring rudimentary rules
- Simple probabilistic modeling
- Constructing decision trees
- Constructing rules
- Association rule learning
- Linear models
- Instance-based learning
- Clustering
- Multi-instance learning

Simplicity first

- Simple algorithms often work very well!
- There are many kinds of simple structure, e.g.:
  - One attribute does all the work
  - All attributes contribute equally & independently
  - Logical structure with a few attributes suitable for tree
  - A set of simple logical rules
  - Relationships between groups of attributes
  - A weighted linear combination of the attributes
  - Strong neighborhood relationships based on distance
  - Clusters of data in unlabeled data
  - Bags of instances that can be aggregated
- Success of method depends on the domain

Inferring rudimentary rules

- 1R 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
    - 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

```
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

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	

* indicates a tie

Dealing with numeric attributes

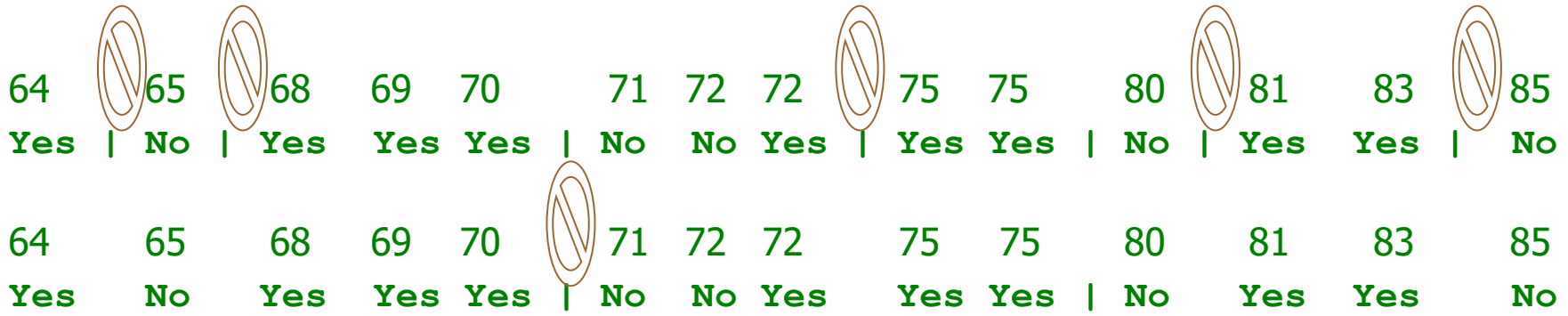
- Idea: discretize numeric attributes into sub ranges (intervals)
- How to divide each attribute's overall range into intervals?
  - Sort instances according to attribute's values
  - Place breakpoints where (majority) class changes
  - This minimizes the total classification error
- Example: *temperature* from weather data

64	65	68	69	70	71	72	72	75	75	80	81	83	85
Yes	No	Yes	Yes	Yes	No	No	Yes	Yes	Yes	No	Yes	Yes	No

Outlook	Temperature	Humidity	Windy	Play
Sunny	85	85	False	No
Sunny	80	90	True	No
Overcast	83	86	False	Yes
Rainy	75	80	False	Yes
...	...	...	...	...

The problem of overfitting

- Discretization procedure is very sensitive to noise
  - A single instance with an incorrect class label will probably produce a separate interval
- Also, something like a time stamp attribute will have zero errors
- Simple solution:
  enforce minimum number of instances in majority class per interval
- Example: temperature attribute with required minimum number of instances in majority class set to three:



Results with overfitting avoidance

Resulting rule sets for the four attributes in the weather data, with only two rules for the temperature attribute:

Attribute	Rules	Errors	Total errors
Outlook	Sunny → No	2/5	4/14
	Overcast → Yes	0/4	
	Rainy → Yes	2/5	
Temperature	≤ 77.5 → Yes	3/10	5/14
	> 77.5 → No*	2/4	
Humidity	≤ 82.5 → Yes	1/7	3/14
	> 82.5 and ≤ 95.5 → No	2/6	
	> 95.5 → Yes	0/1	
Windy	False → Yes	2/8	5/14
	True → No*	3/6	

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)
    - This means knowing the value of one attribute tells us nothing about the value of another takes on (if the class is known)
- 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*

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	2/9	3/5	Hot	2/9	2/5	High	3/9	4/5	False	6/9	2/5	9/	5/
Overcast	4/9	0/5	Mild	4/9	2/5	Normal	6/9	1/5	True	3/9	3/5	14	14
Rainy	3/9	2/5	Cool	3/9	1/5								

A new day:

Outlook	Temp.	Humidity	Windy	Play
Sunny	Cool	High	True	?

Likelihood of the two classes

For "yes" = $2/9 \times 3/9 \times 3/9 \times 3/9 \times 9/14 = 0.0053$

For "no" = $3/5 \times 1/5 \times 4/5 \times 3/5 \times 5/14 = 0.0206$

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* given observed evidence *E:*

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

- *A priori* probability of *H* : $P(H)$
  - Probability of event *before* evidence is seen
- *A posteriori* probability of *H* : $P(H \mid E)$
  - Probability of event *after* evidence is seen

Naïve Bayes for classification

- 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***

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

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

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

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

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

Probability of class "yes"

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

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*

$$\frac{2+\mu/3}{9+\mu} \qquad \frac{4+\mu/3}{9+\mu} \qquad \frac{3+\mu/3}{9+\mu}$$

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" = $3/9 \times 3/9 \times 3/9 \times 9/14 = 0.0238$

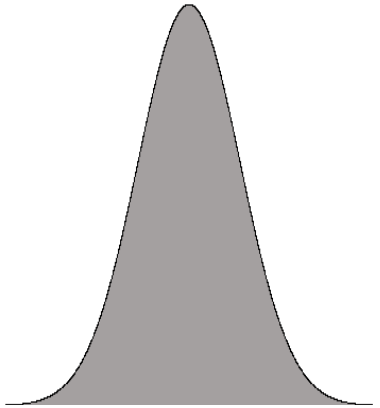
Likelihood of "no" = $1/5 \times 4/5 \times 3/5 \times 5/14 = 0.0343$

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

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

Numeric attributes

- Usual assumption: attributes have a normal or Gaussian probability distribution (given the class)
- The probability density function for the normal distribution is defined by two parameters:
  - *Sample mean* $\mu = \frac{1}{N}\sum_{i=1}^{N} x_i$
  - *Standard deviation* $\sigma = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(x_i-\mu)^2}$
  - Then the density function *f(x) is* $f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$



Statistics for weather data

Outlook			Temperature		Humidity		Windy			Play	
	Yes	*No*	*Yes*	*No*	*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	3	64, 68,	65,71,	65, 70,	70, 85,	False	6	2	9	5
Overcast	4	0	69, 70,	72,80,	70, 75,	90, 91,	True	3	3		
Rainy	3	2	72, …	85, …	80, …	95, …					
Sunny	2/9	3/5	μ =73	μ =75	μ =79	μ =86	False	6/9	2/5	9/ 14	5/ 14
Overcast	4/9	0/5	σ =6.2	σ =7.9	σ =10.2	σ =9.7	True	3/9	3/5		
Rainy	3/9	2/5									

Example density value:

$$f(temperature = 66|yes) = \frac{1}{\sqrt{2\pi}\cdot 6.2} e^{-\frac{(66-73)^2}{2\cdot 6.2^2}} = 0.0340$$

Classifying a new day

- A new day:

Outlook	Temp.	Humidity	Windy	Play
Sunny	66	90	true	?

Likelihood of "yes" = $2/9 \times 0.0340 \times 0.0221 \times 3/9 \times 9/14 = 0.000036$

Likelihood of "no" = $3/5 \times 0.0221 \times 0.0381 \times 3/5 \times 5/14 = 0.000108$

P("yes") = 0.000036 / (0.000036 + 0. 000108) = 25%

P("no") = 0.000108 / (0.000036 + 0. 000108) = 75%

- Missing values during training are not included in calculation of mean and standard deviation

Probability densities

- Probability densities $f(x)$ can be greater than 1; hence, they are not probabilities
  - However, they must integrate to 1: the area under the probability density curve must be 1
- Approximate relationship between probability and probability density can be stated as

$$P(x - \varepsilon/2 \leq X \leq x + \varepsilon/2) \approx \varepsilon f(x)$$

  assuming ε is sufficiently small
- When computing likelihoods, we can treat densities just like probabilities

Multinomial naïve Bayes I

- Version of naïve Bayes used for document classification using *bag of words* model
- $n_1, n_2, \ldots, n_k$: number of times word *i* occurs in the document
- $P_1, P_2, \ldots, P_k$: probability of obtaining word *i* when sampling from documents in class *H*
- Probability of observing a particular document *E* given probabilities class *H* (based on *multinomial distribution*):

$$P(E|H) = N! \times \prod_{i=1}^{k} \frac{P_i^{n_i}}{n_i!}$$

- Note that this expression ignores the probability of generating a document of the right length
  - This probability is assumed to be constant for all classes

Multinomial naïve Bayes II

- Suppose dictionary has two words, *yellow* and *blue*
- Suppose P(*yellow* | *H*) = 75% and P(*blue* | *H*) = 25%
- Suppose *E* is the document "*blue yellow blue*"
- Probability of observing document:

  P({blue yellow blue} |H) =3! x (0.75^1/1!) x (0.25^2/2!)=0.28125/2 or 9/64.

- Suppose there is another class *H*' that has P(*yellow* | *H'*) = 10% and P(*blue*| *H'*) = 90%:

$$P(\{blue\ yellow\ blue\} \mid H) = 3! \times \frac{0.1^1}{1!} \times \frac{0.9^2}{2!} = \frac{243}{1000}$$

- Need to take prior probability of class into account to make the final classification using Bayes' rule
- Factorials do not actually need to be computed: they drop out
- Underflows can be prevented by using logarithms

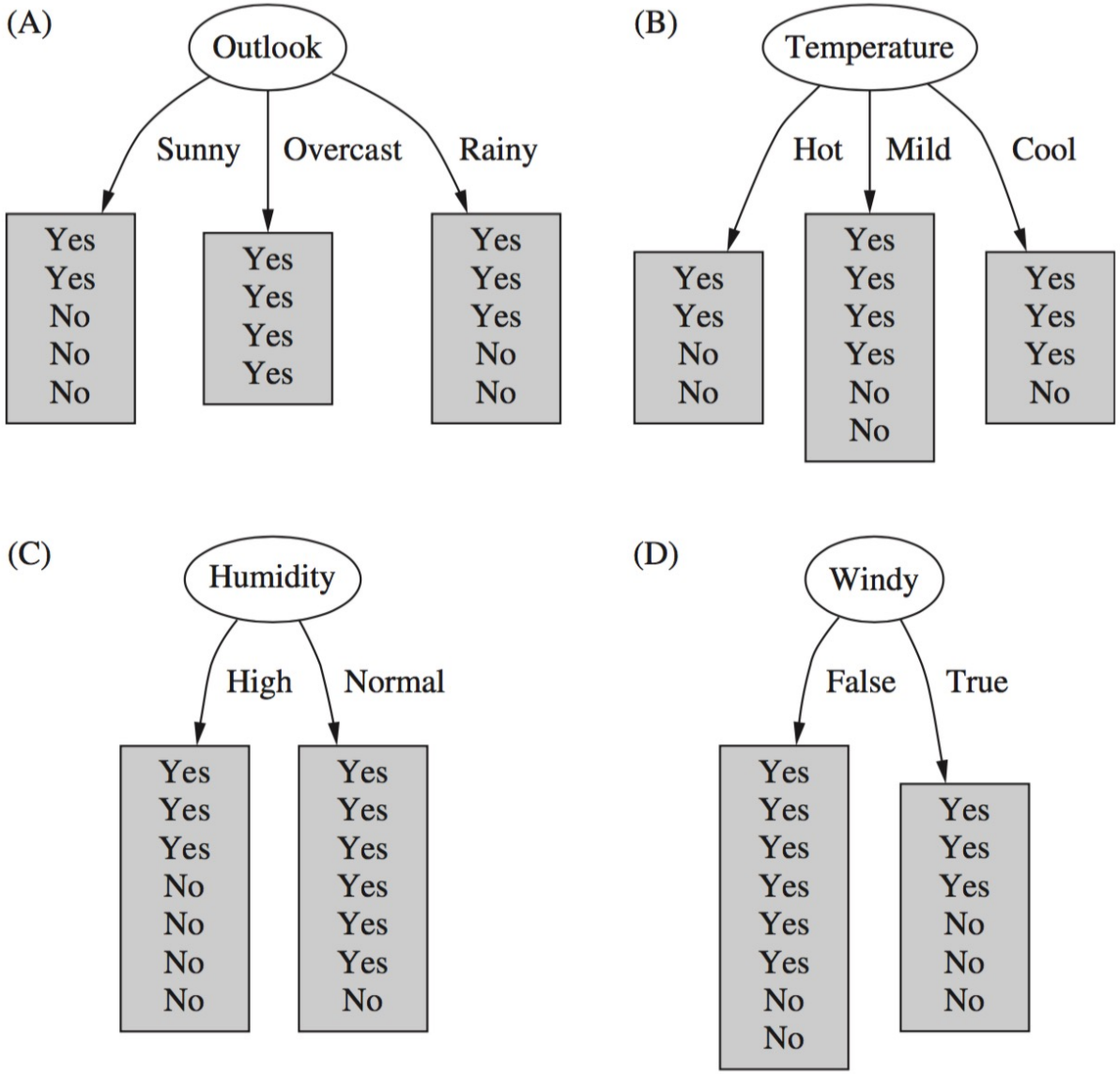
Naïve Bayes: discussion

- Naïve Bayes works surprisingly well even if independence assumption is clearly violated
- Why? Because classification does not require accurate probability estimates *as long as maximum probability is assigned to the correct class*
- However: adding too many redundant attributes will cause problems (e.g., identical attributes)
- Note also: many numeric attributes are not normally distributed (*kernel density estimators* can be used instead)

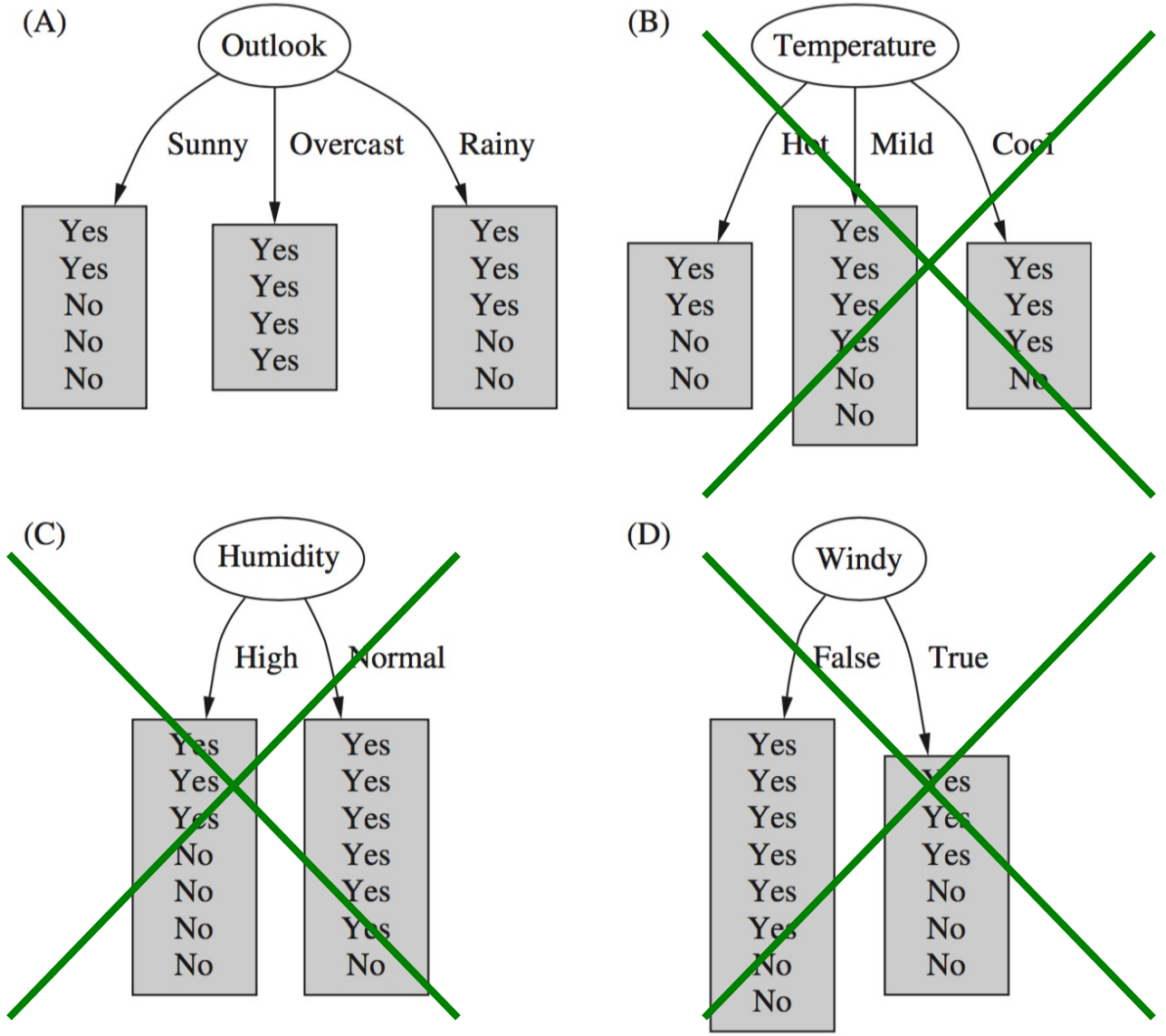
Constructing decision trees

- Strategy: top down learning using recursive *divide-and-conquer* process
  - First: select attribute for root node
    Create branch for each possible attribute value
  - Then: split instances into subsets
    One for each branch extending from the node
  - Finally: repeat recursively for each branch, using only instances that reach the branch
- Stop if all instances have the same class

Which attribute to select?



Which attribute to select?



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 criterion: *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

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* $\log_2(x) = \log_{10}(x) / \log_{10}(2).$
- Entropy is maximal when all classes are equally likely and minimal when one of the classes has probability 1

Example: attribute *Outlook*

- *Outlook* = *Sunny* :

$$\text{Info}([2, 3]) = 0.971 \text{ bits}$$

- *Outlook* = *Overcast* :

$$\text{Info}([4, 0]) = 0.0 \text{ bits}$$

- *Outlook* = *Rainy* :

$$\text{Info}([3, 2]) = 0.971 \text{ bits}$$

- 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

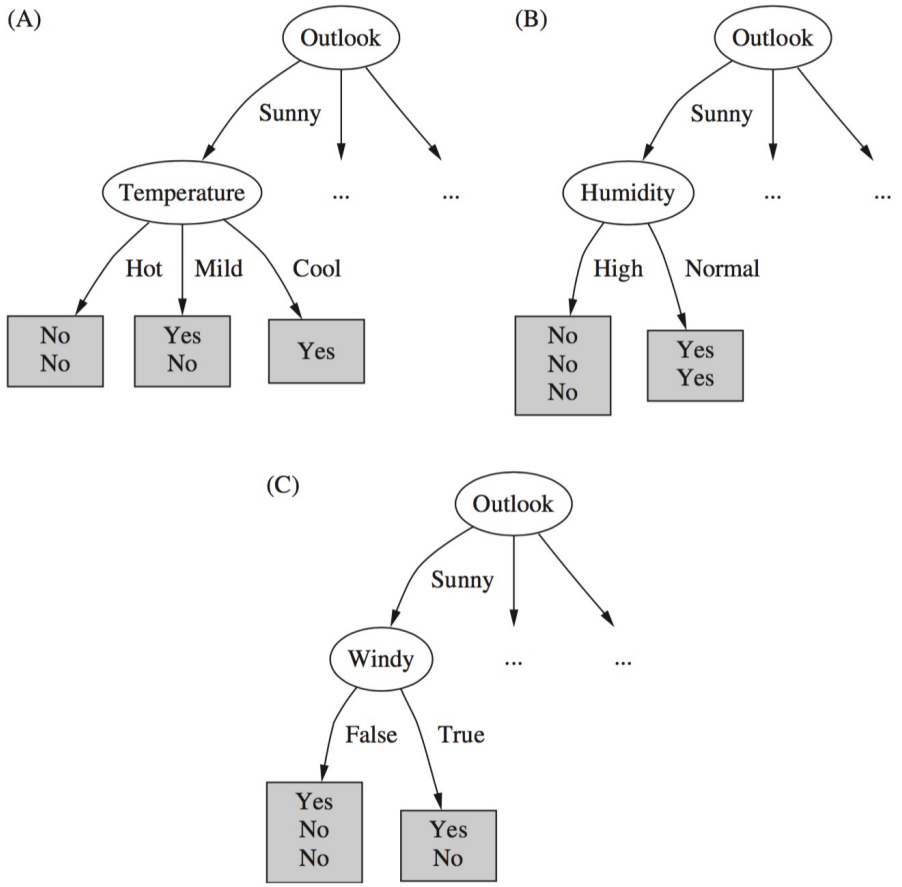
- Information gain: information before splitting – information after splitting

  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

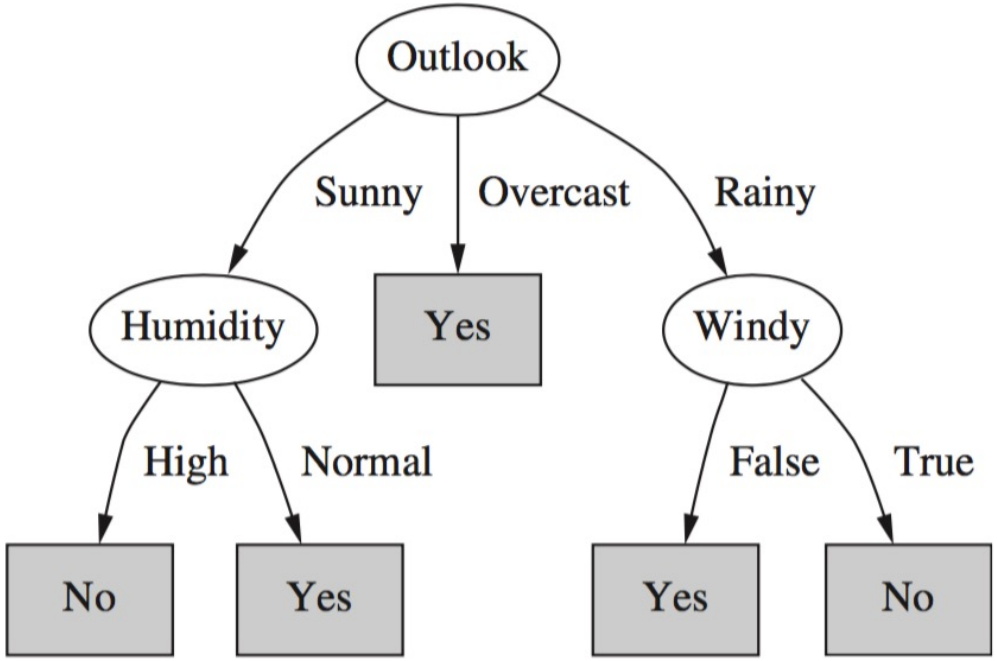


Gain(*Temperature*) = 0.571 bits

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
  - Splitting stops when data cannot be split any further

Wishlist for an impurity measure

- Properties we would like to see in an impurity measure:
  - When node is pure, measure should be zero
  - When impurity is maximal (i.e., all classes equally likely), measure should be maximal
  - Measure should ideally obey *multistage property* (i.e., decisions can be made in several stages):

$$\text{Entropy}(p,q,r) = \text{entropy}(p,q+r) + (q+r)\cdot\text{entropy}\left(\frac{q}{q+r},\frac{r}{q+r}\right)$$

- It can be shown that entropy is the only function that satisfies all three properties!
- Note that the multistage property is intellectually pleasing but not strictly necessary in practice

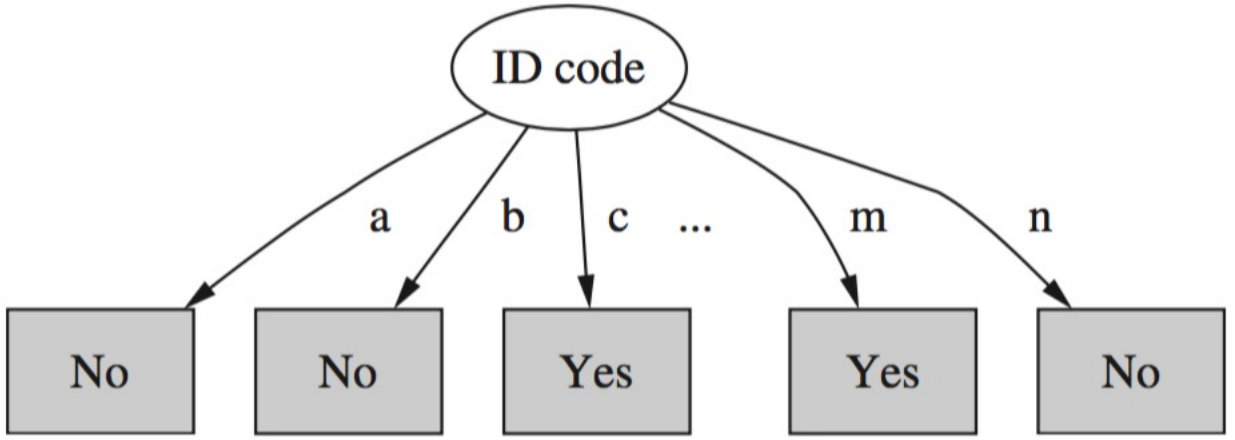
Highly-branching attributes

- Problematic: attributes with a large number of values (extreme case: ID code)
- Subsets are more likely to be pure if there is a large number of values
  - Information gain is biased towards choosing attributes with a large number of values
  - This may result in *overfitting* (selection of an attribute that is non-optimal for prediction)
- An additional problem in decision trees is data *fragmentation*

Weather data with *ID code*

ID code	Outlook	Temp.	Humidity	Windy	Play
A	Sunny	Hot	High	False	No
B	Sunny	Hot	High	True	No
C	Overcast	Hot	High	False	Yes
D	Rainy	Mild	High	False	Yes
E	Rainy	Cool	Normal	False	Yes
F	Rainy	Cool	Normal	True	No
G	Overcast	Cool	Normal	True	Yes
H	Sunny	Mild	High	False	No
I	Sunny	Cool	Normal	False	Yes
J	Rainy	Mild	Normal	False	Yes
K	Sunny	Mild	Normal	True	Yes
L	Overcast	Mild	High	True	Yes
M	Overcast	Hot	Normal	False	Yes
N	Rainy	Mild	High	True	No

Tree stump for *ID code* attribute



- All (single-instance) subsets have entropy zero!
- This means the information gain is maximal for this ID code attribute (namely 0.940 bits)

Gain ratio

- *Gain ratio* is a modification of the information gain that reduces its bias towards attributes with many values
- Gain ratio takes number and size of branches into account when choosing an attribute
  - It corrects the information gain by taking the *intrinsic information* of a split into account
- Intrinsic information: entropy of the distribution of instances into branches
- Measures how much info do we need to tell which branch a randomly chosen instance belongs to

Computing the gain ratio

- Example: intrinsic information of ID code

$$\frac{1}{14}(\text{info}([0,1]) + \text{info}([0,1]) + \text{info}([1,0]) + \cdots + \text{info}([1,0]) + \text{info}([0,1]))$$

- Value of attribute should decrease as intrinsic information gets larger
- The *gain ratio* is defined as the information gain of the attribute divided by its intrinsic information
- Example (*outlook* at root node):

Gain: 0.940–0.693	0.247
Split info: info([5,4,5])	1.577
Gain ratio: 0.247/1.577	0.156

All gain ratios for the weather data

Outlook		Temperature	
Info:	0.693	Info:	0.911
Gain: 0.940-0.693	0.247	Gain: 0.940-0.911	0.029
Split info: info([5,4,5])	1.577	Split info: info([4,6,4])	1.557
Gain ratio: 0.247/1.577	0.157	Gain ratio: 0.029/1.557	0.019
Humidity		Windy	
Info:	0.788	Info:	0.892
Gain: 0.940-0.788	0.152	Gain: 0.940-0.892	0.048
Split info: info([7,7])	1.000	Split info: info([8,6])	0.985
Gain ratio: 0.152/1	0.152	Gain ratio: 0.048/0.985	0.049

More on the gain ratio

- "Outlook" still comes out top
- However: "ID code" has greater gain ratio
  - Standard fix: *ad hoc* test to prevent splitting on that type of identifier attribute
- Problem with gain ratio: it may overcompensate
  - May choose an attribute just because its intrinsic information is very low
  - Standard fix: only consider attributes with greater than average information gain
- Both tricks are implemented in the well-known C4.5 decision tree learner

Knowledge Check

Gain Ratio is helpful for:

A. Continuous attributes

B. When all attributes have the same number of values

C. For nominal attributes

D. For nominal attributes with different numbers of values

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)

Covering algorithms

- Can convert decision tree into a rule set
  - Straightforward, but rule set overly complex
  - More effective conversions are not trivial and may incur a lot of computation
- Instead, we can generate rule set directly
  - One approach: for each class in turn, find rule set that covers all instances in it
    (excluding instances not in the class)
- Called a *covering* approach:
  - At each stage of the algorithm, a rule is identified that “covers” some of the instances

Knowledge Check

Gain ratio helps because:

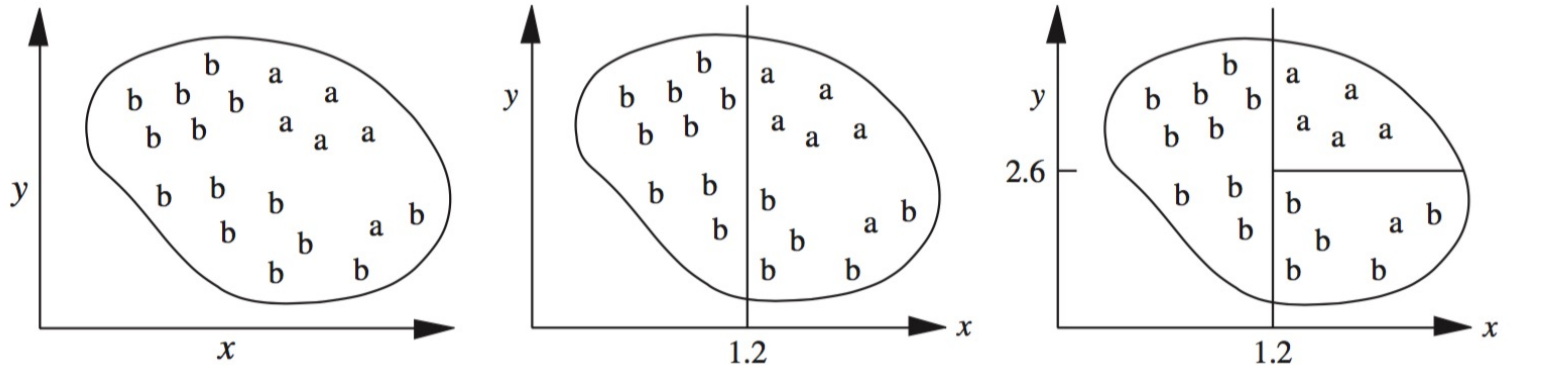
A. There are not enough attributes.

B. An attribute with lots of values is more likely to create homogeneous groups.

C. It it more accurate than information gain.

D. There is a chance it will mitigate spurious attributes.

Example: generating a rule




```
If true
   then class = a
```

```
If x > 1.2
   then class = a
```

```
If x > 1.2 and y > 2.6
   then class = a
```

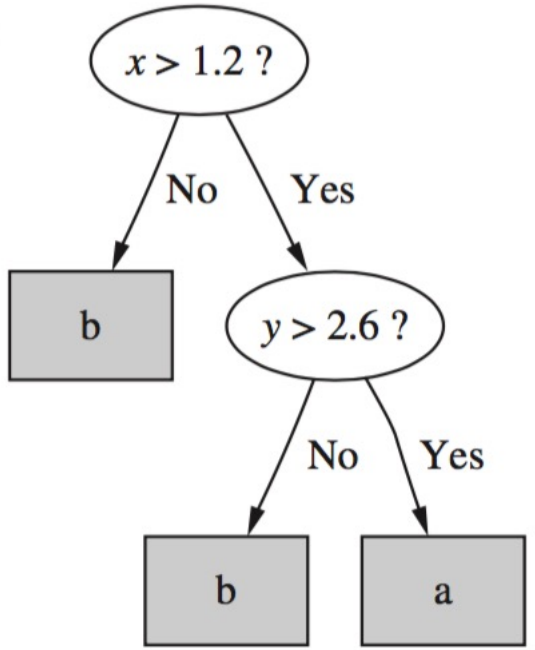
- Possible rule set for class “b”:

```
If x ≤ 1.2 then class = b
If x > 1.2 and y ≤ 2.6 then class = b
```

- Could add more rules, get “perfect” rule set

Rules vs. trees

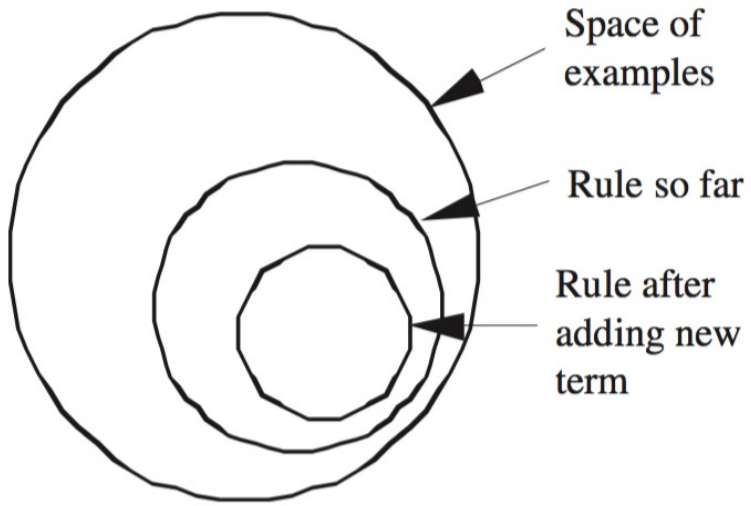
- Corresponding decision tree:
- (produces exactly the same
- predictions)



- But: rule sets *can* be more perspicuous when decision trees suffer from replicated subtrees
- Also: in multiclass situations, covering algorithm concentrates on one class at a time whereas decision tree learner takes all classes into account

Simple covering algorithm

- Basic idea: generate a rule by adding tests that maximize the rule's accuracy
- Similar to situation in decision trees: problem of selecting an attribute to split on
  - But: decision tree inducer maximizes overall purity
- Each new test reduces rule's coverage:



Selecting a test

- Goal: maximize accuracy
  - t total number of instances covered by rule
  - p positive examples of the class covered by rule
  - t – p number of errors made by rule
  - Select test that maximizes the ratio p/t
- We are finished when p/t = 1 or the set of instances cannot be split any further

Example: contact lens data

- Rule we seek:

```
If ?
    then recommendation = hard
```

- Possible tests:

Age = Young	2/8
Age = Pre-presbyopic	1/8
Age = Presbyopic	1/8
Spectacle prescription = Myope	3/12
Spectacle prescription = Hypermetrope	1/12
Astigmatism = no	0/12
Astigmatism = yes	4/12
Tear production rate = Reduced	0/12
Tear production rate = Normal	4/12

Modified rule and resulting data

- Rule with best test added:

```
If astigmatism = yes
    then recommendation = hard
```

- Instances covered by modified rule:

Age	Spectacle prescription	Astigmatism	Tear production rate	Recommended lenses
Young	Myope	Yes	Reduced	None
Young	Myope	Yes	Normal	Hard
Young	Hypermetrope	Yes	Reduced	None
Young	Hypermetrope	Yes	Normal	hard
Pre-presbyopic	Myope	Yes	Reduced	None
Pre-presbyopic	Myope	Yes	Normal	Hard
Pre-presbyopic	Hypermetrope	Yes	Reduced	None
Pre-presbyopic	Hypermetrope	Yes	Normal	None
Presbyopic	Myope	Yes	Reduced	None
Presbyopic	Myope	Yes	Normal	Hard
Presbyopic	Hypermetrope	Yes	Reduced	None
Presbyopic	Hypermetrope	Yes	Normal	None

Further refinement

- Current state:

```
If astigmatism = yes
    and ?
  then recommendation = hard
```

- Possible tests:

Age = Young	2/4
Age = Pre-presbyopic	1/4
Age = Presbyopic	1/4
Spectacle prescription = Myope	3/6
Spectacle prescription = Hypermetrope	1/6
Tear production rate = Reduced	0/6
Tear production rate = Normal	4/6

Modified rule and resulting data

- Rule with best test added:

```
If astigmatism = yes
    and tear production rate = normal
then recommendation = hard
```

- Instances covered by modified rule:

Age	Spectacle prescription	Astigmatism	Tear production rate	Recommended lenses
Young	Myope	Yes	Normal	Hard
Young	Hypermetrope	Yes	Normal	hard
Pre-presbyopic	Myope	Yes	Normal	Hard
Pre-presbyopic	Hypermetrope	Yes	Normal	None
Presbyopic	Myope	Yes	Normal	Hard
Presbyopic	Hypermetrope	Yes	Normal	None

Further refinement

- Current state:

```
If astigmatism = yes
     and tear production rate = normal
     and ?
   then recommendation = hard
```

- Possible tests:

Age = Young	2/2
Age = Pre-presbyopic	1/2
Age = Presbyopic	1/2
Spectacle prescription = Myope	3/3
Spectacle prescription = Hypermetrope	1/3

- Tie between the first and the fourth test
  - We choose the one with greater coverage

The final rule

- Final rule:

```
If astigmatism = yes
   and tear production rate = normal
   and spectacle prescription = myope
   then recommendation = hard
```

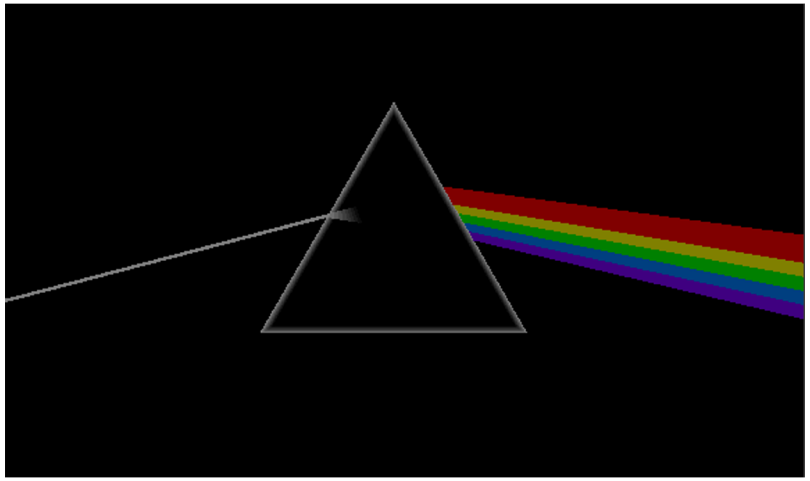
- Second rule for recommending “hard lenses”:
  (built from instances not covered by first rule)

```
If age = young and astigmatism = yes
   and tear production rate = normal
   then recommendation = hard
```

- These two rules cover all “hard lenses”:
  - Process is repeated with other two classes

Pseudo-code for PRISM

```
For each class C
  Initialize E to the instance set
  While E contains instances in class C
    Create a rule R with an empty left-hand side that predicts class C
    Until R is perfect (or there are no more attributes to use) do
      For each attribute A not mentioned in R, and each value v,
        Consider adding the condition A = v to the left-hand side of R
        Select A and v to maximize the accuracy p/t
          (break ties by choosing the condition with the largest p)
      Add A = v to R
    Remove the instances covered by R from E
```



Rules vs. decision lists

- PRISM with outer loop removed generates a decision list for one class
  - Subsequent rules are designed for rules that are not covered by previous rules
  - But: order does not matter because all rules predict the same class so outcome does not change if rules are shuffled
- Outer loop considers all classes separately
  - No order dependence implied
- Problems: overlapping rules, default rule required

Separate and conquer rule learning

- Rule learning methods like the one PRISM employs (for each class) are called separate-and-conquer algorithms:
  - First, identify a useful rule
  - Then, separate out all the instances it covers
  - Finally, “conquer” the remaining instances
- Difference to divide-and-conquer methods:
  - Subset covered by a rule does not need to be explored any further

Mining association rules

- Naïve method for finding association rules:
  - Use separate-and-conquer method
  - Treat every possible combination of attribute values as a separate class
- Two problems:
  - Computational complexity
  - Resulting number of rules (which would have to be pruned on the basis of support and confidence)
- It turns out that we can look for association rules with high support and accuracy directly

Knowledge Check

Rules might outperform decision trees because

A. They have more attribute values.

B. They are simpler.

C. They are able to better fit complex data.

D. They are more flexible in creation focusing on 2 classes for instance.

Item sets: the basis for finding rules

- Support: number of instances correctly covered by association rule
  - The same as the number of instances covered by all tests in the rule (LHS and RHS!)
- Item: one test/attribute-value pair
- Item set : all items occurring in a rule
- Goal: find only rules that exceed pre-defined support
- Do it by finding all item sets with the given minimum support and generating rules from them!

Weather data

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

Item sets for weather data

One-item sets	Two-item sets	Three-item sets	Four-item sets
Outlook = Sunny (5)	Outlook = Sunny Temperature = Hot (2)	Outlook = Sunny Temperature = Hot Humidity = High (2)	Outlook = Sunny Temperature = Hot Humidity = High Play = No (2)
Temperature = Cool (4)	Outlook = Sunny Humidity = High (3)	Outlook = Sunny Humidity = High Windy = False (2)	Outlook = Rainy Temperature = Mild Windy = False Play = Yes (2)
…	…	…	…

Total number of item sets with a minimum support of at least two instances: 12 one-item sets, 47 two-item sets, 39 three-item sets, 6 four-item sets and 0 five-item sets

Generating rules from an item set

- Once all item sets with the required minimum support have been generated, we can turn them into rules
- Example 3-item set with a support of 4 instances:

```
Humidity = Normal, Windy = False, Play = Yes (4)
```

- Seven (2N-1) potential rules:

```
If Humidity = Normal and Windy = False then Play = Yes    4/4
If Humidity = Normal and Play = Yes then Windy = False    4/6
If Windy = False and Play = Yes then Humidity = Normal    4/6
If Humidity = Normal then Windy = False and Play = Yes    4/7
If Windy = False then Humidity = Normal and Play = Yes    4/8
If Play = Yes then Humidity = Normal and Windy = False    4/9
If True then Humidity = Normal and Windy = False
   and Play = Yes                                         4/14
```

Rules for weather data

- All rules with support > 1 and confidence = 100%:

	Association rule			Sup.	Conf.
1	Humidity=Normal Windy=False	⇒	Play=Yes	4	100%
2	Temperature=Cool	⇒	Humidity=Normal	4	100%
3	Outlook=Overcast	⇒	Play=Yes	4	100%
4	Temperature=Cold Play=Yes	⇒	Humidity=Normal	3	100%
	...	...		...	...
58	Outlook=Sunny Temperature=Hot	⇒	Humidity=High	2	100%

- In total:
  3 rules with support four
  5 with support three
  50 with support two

Example rules from the same item set

- Item set:

```
Temperature = Cool, Humidity = Normal, Windy = False, Play = Yes (2)
```

- Resulting rules (all with 100% confidence):

```
Temperature = Cool, Windy = False ⇒ Humidity = Normal, Play = Yes
Temperature = Cool, Windy = False, Humidity = Normal ⇒ Play = Yes
Temperature = Cool, Windy = False, Play = Yes ⇒ Humidity = Normal
```

- We can establish their confidence due to the following “frequent” item sets:

```
Temperature = Cool, Windy = False                      (2)
Temperature = Cool, Humidity = Normal, Windy = False   (2)
Temperature = Cool, Windy = False, Play = Yes          (2)
```

Knowledge Check

High support rules:

A. Are most useful if they are also high confidence rules.

B. Prevalent.

C. Not necessarily interesting.

D. Likely to apply quite often.

Generating item sets efficiently

- How can we efficiently find all frequent item sets?
- Finding one-item sets easy
- Idea: use one-item sets to generate two-item sets, two-item sets to generate three-item sets, …
  - If (A B) is a frequent item set, then (A) and (B) have to be frequent item sets as well!
  - In general: if X is a frequent k-item set, then all (k-1)-item subsets of X are also frequent
  - Compute k-item sets by merging (k-1)-item sets

Example

- Given: five frequent three-item sets
- (A B C), (A B D), (A C D), (A C E), (B C D)
- Lexicographically ordered!
- Candidate four-item sets:
- (A B C D)OK because of (A,B,C), (A,B,D) (A C D) (B C D)
- (A C D E) Not OK because of lack of (C D E)
- To establish that these item sets are really frequent, we need to perform a final check by counting instances
- For fast look-up, the (k –1)-item sets are stored in a hash table

Algorithm for finding item sets

```
Set k to 1
Find all k-item sets with sufficient coverage and store them in hash table #1
While some k-item sets with sufficient coverage have been found
    Increment k
    Find all pairs of (k–1)-item sets in hash table #(k–1) that differ only in
    their last item
    Create a k-item set for each pair by combining the two (k–1)-item sets
    that are paired
    Remove all k-item sets containing any (k–1)-item sets that are not in the
    #(k–1)hash table
    Scan the data and remove all remaining k-item sets that do not have
    sufficient coverage
    Store the remaining k-item sets and their coverage in hash table #k,
    sorting items in lexical order
```

Generating rules efficiently

- We are looking for all high-confidence rules
  - Support of antecedent can be obtained from item set hash table
  - But: brute-force method is (2N-1) for an N-item set
- Better way: building (c + 1)-consequent rules from c-consequent ones
  - Observation: (c + 1)-consequent rule can only hold if all corresponding c-consequent rules also hold
- Resulting algorithm similar to procedure for large item sets

Example

- 1-consequent rules:

```
If Outlook = Sunny and Windy = False and Play = No
   then Humidity = High (2/2)
```

```
If Humidity = High and Windy = False and Play = No
   then Outlook = Sunny (2/2)
```

- Corresponding 2-consequent rule:

```
If Windy = False and Play = No
   then Outlook = Sunny and Humidity = High (2/2)
```

- Final check of antecedent against item set hash table is required to check that rule is actually sufficiently accurate

Algorithm for finding association rules

```
Set n to 1
Find all sufficiently accurate n-consequent rules for the k-item set and
    store them in hash table #1, computing accuracy using the hash tables
    found for item sets
While some sufficiently accurate n-consequent rules have been found
    Increment n
    Find all pairs of (n–1)-consequent rules in hash table #(n–1) whose
    consequents differ only in their last item
    Create an n-consequent rule for each pair by combining the two (n–1)-
    consequent rules that are paired
    Remove all n-consequent rules that are insufficiently accurate, computing
    accuracy using the hash tables found for item sets
    Store the remaining n-consequent rules and their accuracy in hash table
    #k, sorting items for each consequent in lexical order
```

Association rules: discussion

- Above method makes one pass through the data for each different item set size
  - Another possibility: generate (k+2)-item sets just after (k+1)-item sets have been generated
  - Result: more candidate (k+2)-item sets than necessary will be generated but this requires less passes through the data
  - Makes sense if data too large for main memory
- Practical issue: support level for generating a certain minimum number of rules for a particular dataset
- This can be done by running the whole algorithm multiple times with different minimum support levels
- Support level is decreased until a sufficient number of rules has been found

Other issues

- Standard ARFF format very inefficient for typical market basket data
  - Attributes represent items in a basket and most items are usually missing from any particular basket
  - Data should be represented in sparse format
- Note on terminology: instances are also called transactions in the literature on association rule mining
- Confidence is not necessarily the best measure
  - Example: milk occurs in almost every supermarket transaction
  - Other measures have been devised (e.g., lift)
  - It is often quite difficult to find interesting patterns in the large number of association rules that can be generated

Knowledge Check

It is important to be efficient in creating association rules because:

A. It has a big effect on accuracy.

B. The search space is linear.

C. The search space is very large.

D. All of the above.

Linear models: linear regression

- Work most naturally with numeric attributes
- Standard technique for numeric prediction
  - Outcome is linear combination of attributes

$$x = w_0 + w_1 a_1 + w_2 a_2 + \cdots + w_k a_k$$

- Weights are calculated from the training data
- Predicted value for first training instance a(1)

$$w_0 a_0^{(1)} + w_1 a_1^{(1)} + w_2 a_2^{(1)} + \cdots + w_k a_k^{(1)} = \sum_{j=0}^{k} w_j a_j^{(1)}$$

(assuming each instance is extended with a constant attribute with value 1)

Minimizing the squared error

- Choose k +1 coefficients to minimize the squared error on the training data
- Squared error:

$$\sum_{i=1}^{n}\left(x^{(i)}-\sum_{j=0}^{k}w_j a_j^{(i)}\right)^2$$

- Coefficients can b l matrix operations
- Can be done if there are more instances than attributes (roughly speaking)
- Minimizing the absolute error is more difficult

Classification

- Any regression technique can be used for classification
  - Training: perform a regression for each class, setting the output to 1 for training instances that belong to class, and 0 for those that don't
  - Prediction: predict class corresponding to model with largest output value (membership value)
- For linear regression this method is also known as multi-response linear regression
- Problem: membership values are not in the [0,1] range, so they cannot be considered proper probability estimates
- In practice, they are often simply clipped into the [0,1] range and normalized to sum to 1

Knowledge Check

To predict a value, we can use

A. Decision trees

B. Regression with the squared error loss function

C. Any classifier if we appropriately binarize the data.

D. Regression using the absolute value loss function.

Linear models: logistic regression

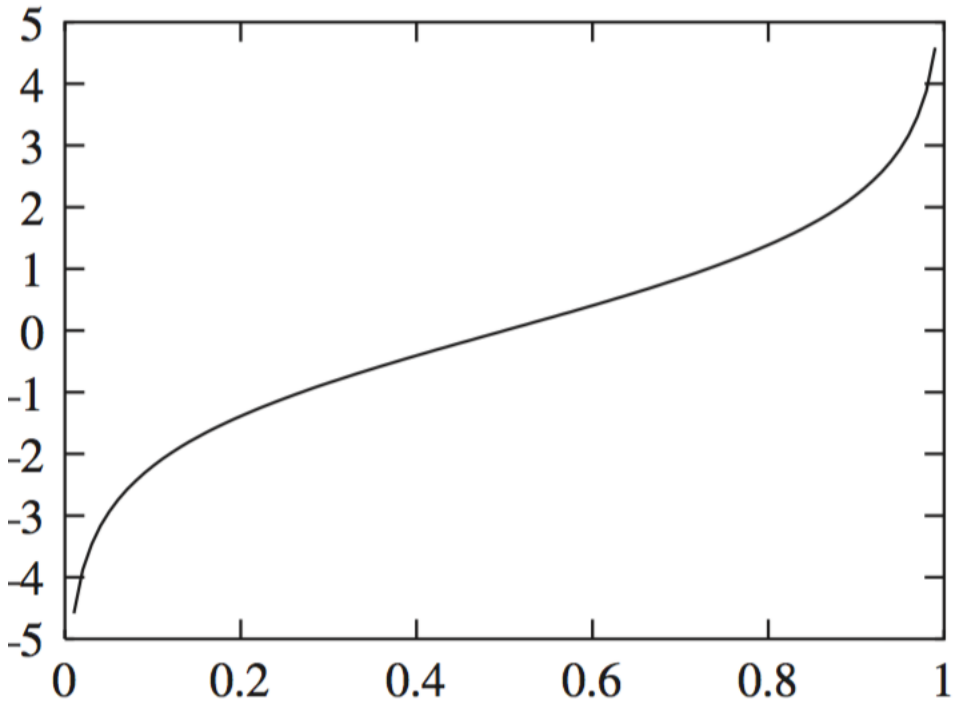
- Can we do better than using linear regression for classification?
- Yes, we can, by applying logistic regression
- Logistic regression builds a linear model for a transformed target variable
- Assume we have two classes
- Logistic regression replaces the target

  by this target $\Pr[1|a_1, a_2, \ldots, a_k]$

  $\log[\Pr[1|a_1, a_2, \ldots, a_k]/(1 - \Pr[1|a_1, a_2, \ldots, a_k])$

- This *logit transformation* maps [0,1] to (-¥ , +¥), i.e., the new target values are no longer restricted to the [0,1] interval

Logit transformation

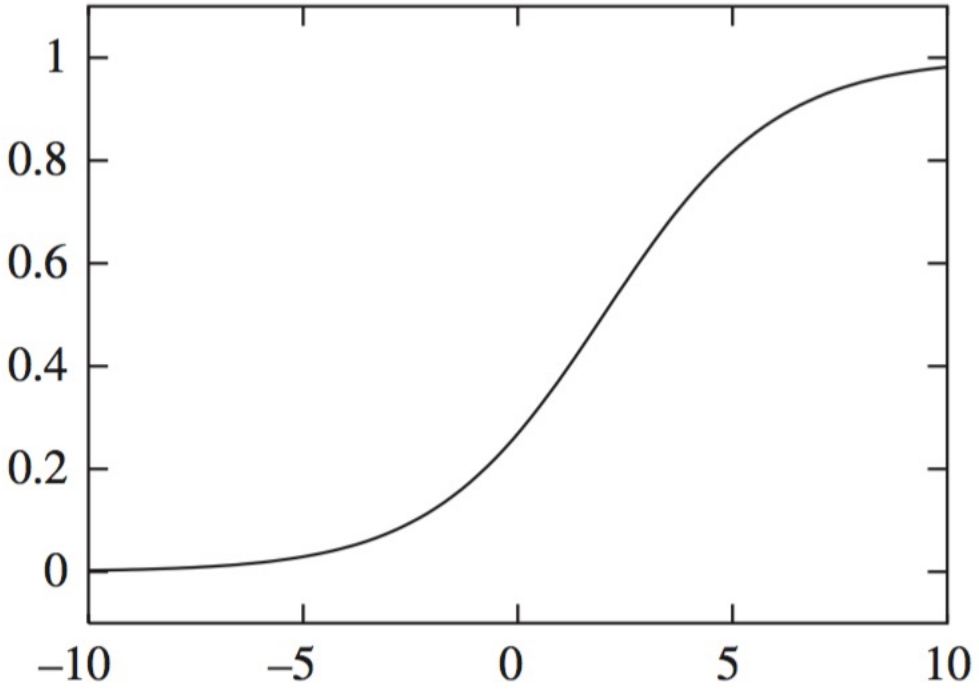


Resulting class probability model:

$$\Pr[1|a_1, a_2, \ldots, a_k] = 1/(1 + \exp(-w_0 - w_1 a_1 - \cdots - w_k a_k))$$

Example logistic regression model

- Model with w_0 = -1.25 and w_1 = 0.5:



- Parameters are found from training data using *maximum likelihood*

Knowledge Check

Logistic regression

A. Uses a linear model.

B. Uses maximum likelihood (a probabilistic approach) to find a set of weights.

C. Builds a line with the normal equation.

D. Requires no learning.

Maximum likelihood

- Aim: maximize probability of observed training data with respect to final parameters of the logistic regression model
- We can use logarithms of probabilities and maximize conditional *log-likelihood* instead of product of probabilities:

$$\sum_{i=1}^{n}(1-x^{(i)})\log(1-\Pr[1|a_1^{(i)},\ a_2^{(i)},\ \ldots,\ a_k^{(i)}])+x^{(i)}\log(\Pr[1|a_1^{(i)},a_2^{(i)},\ldots,a_k^{(i)}])$$

  where the class values $x^{(i)}$ are either 0 or 1
- Weights w_i need to be chosen to maximize log-likelihood
- A relatively simple method to do this is *iteratively re-weighted least squares* but other optimization methods can be used

Multiple classes

- Logistic regression for two classes is also called binomial logistic regression
- What do we do when have a problem with *k* classes?
- Can perform logistic regression independently for each class (like in multi-response linear regression)
- Problem: the probability estimates for the different classes will generally not sum to one
- Better: train *k*-1 coupled linear models by maximizing likelihood over all classes simultaneously
- This is known as multi-class logistic regression, multinomial logistic regression or polytomous logistic regression
- Alternative multi-class approach that often works well in practice: *pairwise classification*

Pairwise classification

- Idea: build model for each pair of classes, using only training data from those classes
- Classifications are derived by voting: given a test instance, let each model vote for one of its two classes
- Problem? Have to train $k(k\text{-}1)/2$ two-class classification models for a k-class problem
- Turns out not to be a problem in many cases because pairwise training sets become small:
  - Assume data evenly distributed, i.e., $2n/k$ instances per learning problem for n instances in total
  - Suppose training time of learning algorithm is linear in n
  - Then runtime for the training process is proportional to $(k(k\text{-}1)/2)\times(2n/k) = (k\text{-}1)n$, i.e., linear in the number of classes and the number of instances
  - Even more beneficial if learning algorithm scales worse than linearly

Linear models are hyperplanes

- Decision boundary for two-class logistic regression is where probability equals 0.5:

$$\Pr[1|a_1, a_2, \ldots, a_k] = 1/(1 + \exp(-w_0 - w_1 a_1 - \cdots - w_k a_k)) = 0.5$$

  which occurs when $-w_0 - w_1 a_1 - \cdots - w_k a_k = 0$.

- Thus logistic regression can only separate data that can be separated by a hyperplane
- Multi-response linear regression has the same problem. Class 1 is assigned if:

$$w_0^{(1)} + w_1^{(1)} a_1 + \cdots + w_k^{(1)} a_k > w_0^{(2)} + w_1^{(2)} a_1 + \cdots + w_k^{(2)} a_k$$

$$(w_0^{(1)} - w_0^{(2)}) + (w_1^{(1)} - w_1^{(2)}) a_1 + \cdots + (w_k^{(1)} - w_k^{(2)}) a_k > 0$$

Linear models: the perceptron

- Observation: we do not actually need probability estimates if all we want to do is classification
- Different approach: learn separating hyperplane directly
- Let us assume the data is *linearly separable*
- In that case there is a simple algorithm for learning a separating hyperplane called the *perceptron learning rule*
- Hyperplane: $w_0 a_0 + w_1 a_1 + w_2 a_2 + \cdots + w_k a_k = 0$
  - where we again assume that there is a constant attribute with value 1 (*bias*)
- If the weighted sum is greater than zero we predict the first class, otherwise the second class

The algorithm

```
Set all weights to zero
Until all instances in the training data are classified correctly
  For each instance I in the training data
    If I is classified incorrectly by the perceptron
      If I belongs to the first class add it to the weight vector
      else subtract it from the weight vector
```

- Why does this work?
  Consider a situation where an instance *a* pertaining to the first class has been added:

  This means the output for *a* has increased by:

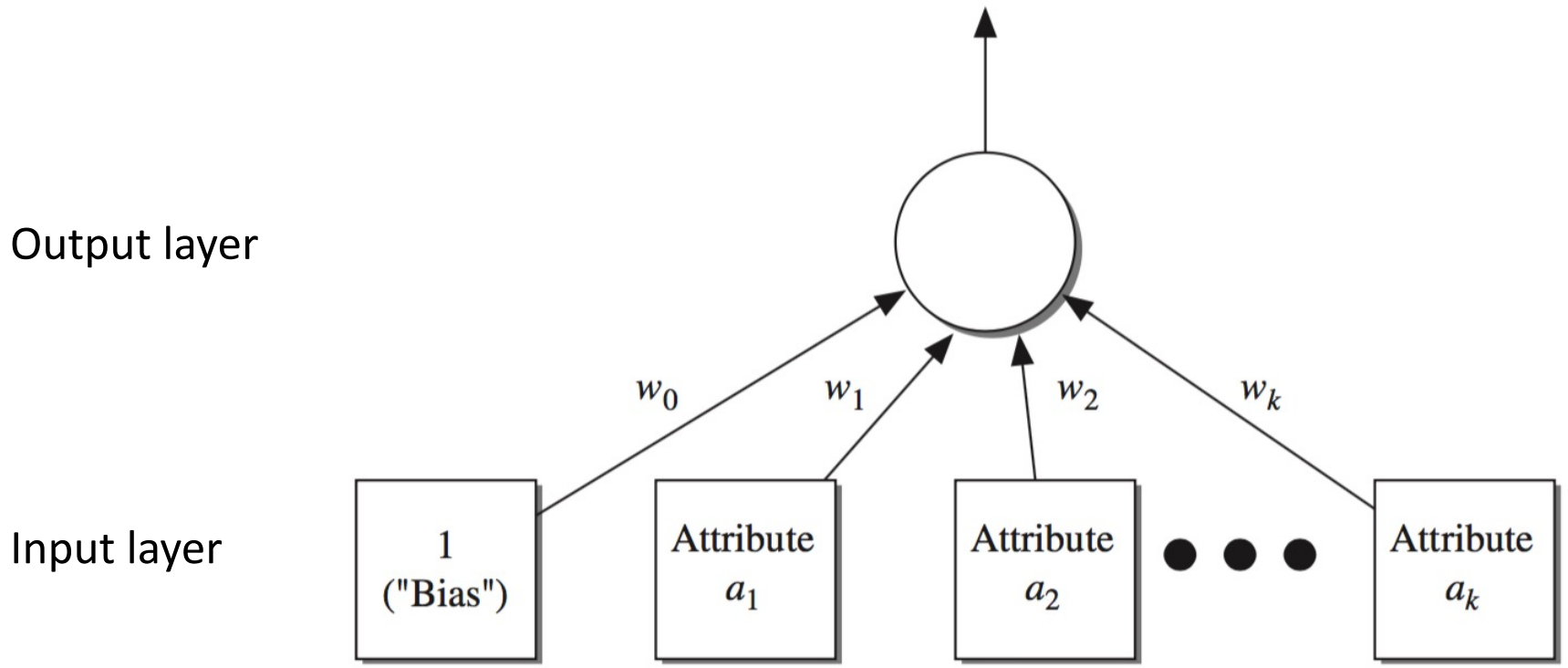
$$(w_0 + a_0)a_0 + (w_1 + a_1)a_1 + (w_2 + a_2)a_2 + \cdots + (w_k + a_k)a_k$$

  This number is always positive, thus the hyperplane has moved into the correct direction (and we can show that output decreases for instances of other class)

$$a_0 \times a_0 + a_1 \times a_1 + a_2 \times a_2 + \cdots + a_k \times a_k$$

- It can be shown that this process converges to a linear separator if the data is linearly separable

Perceptron as a neural network



Knowledge Check

Neural Networks have knowledge:

A. In their rules

B. On the node weights

C. On the weights on the links

D. In the transfer function only

Linear models: Winnow

- The perceptron is driven by mistakes because the classifier only changes when a mistake is made
- Another *mistake-driven* algorithm for finding a separating hyperplane is known as *Winnow*
  - Assumes binary data (i.e., attribute values are either zero or one)
- Difference to perceptron learning rule: *multiplicative* updates instead of *additive* updates
  - Weights are multiplied by a user-specified parameter $a > 1$ (or its inverse)
- Another difference: user-specified threshold parameter q
  - Predict first class if

$$w_0 a_0 + w_1 a_1 + w_2 a_2 + \cdots + w_k a_k > \theta$$

The algorithm

```
while some instances are misclassified
  for each instance a in the training data
    classify a using the current weights
    if the predicted class is incorrect
      if a belongs to the first class
        for each a_i that is 1, multiply w_i by alpha
        (if a_i is 0, leave w_i unchanged)
      otherwise
        for each a_i that is 1, divide w_i by alpha
        (if a_i is 0, leave w_i unchanged)
```

- Winnow is very effective in homing in on relevant features (it is *attribute efficient*)
- Can also be used in an on-line setting in which new instances arrive continuously (like the perceptron algorithm)

Balanced Winnow

- Winnow does not allow negative weights and this can be a drawback in some applications
- Balanced Winnow maintains two weight vectors, one for each class:

```
while some instances are misclassified
  for each instance a in the training data
    classify a using the current weights
    if the predicted class is incorrect
      if a belongs to the first class
        for each a_i that is 1, multiply w_i+ by alpha and divide w_i- by alpha
          (if a_i is 0, leave w_i+ and w_i- unchanged)
      otherwise
        for each a_i that is 1, multiply w_i- by alpha and divide w_i+ by alpha
          (if a_i is 0, leave w_i+ and w_i- unchanged)
```

- Instance is classified as belonging to the first class if:

$$(w_0^+ - w_0^-)a_0 + (w_1^+ - w_1^-)a_1 + \cdots + (w_k^+ - w_k^-)a_k > \theta$$

Instance-based learning

- In instance-based learning the distance function defines what is learned
- Most instance-based schemes use *Euclidean distance*:

$$\sqrt{(a_1^{(1)} - a_1^{(2)})^2 + (a_2^{(1)} - a_2^{(2)})^2 + \cdots + (a_k^{(1)} - a_k^{(2)})^2}$$

- $\mathbf{a}^{(1)}$ and $\mathbf{a}^{(2)}$: two instances with k attributes
- Note that taking the square root is not required when comparing distances
- Other popular metric: *city-block metric*
  - Adds differences without squaring them

Normalization and other issues

- Different attributes are measured on different scales need to be *normalized, e.g., to range* [*0,1*]:

$$a_i = \frac{v_i - \min v_i}{\max v_i - \min v_i}$$

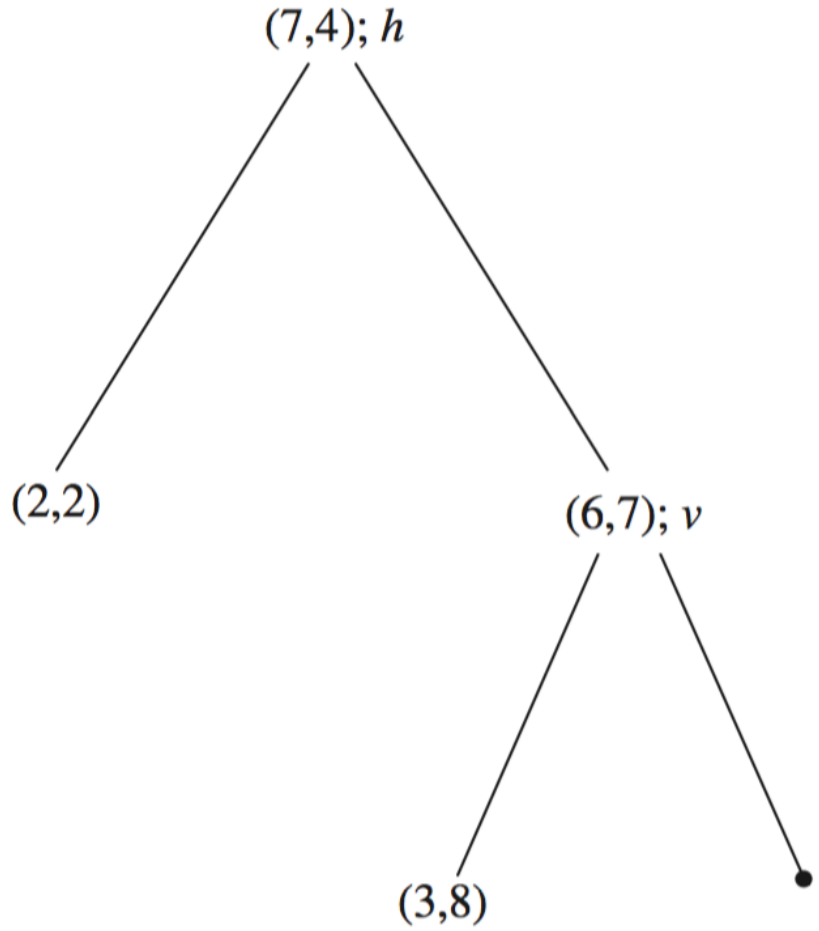
-
- v_i : the actual value of attribute *i*
- Nominal attributes: distance is assumed to be either 0 (values are the same) or 1 (values are different)
- Common policy for missing values: assumed to be maximally distant (given normalized attributes)

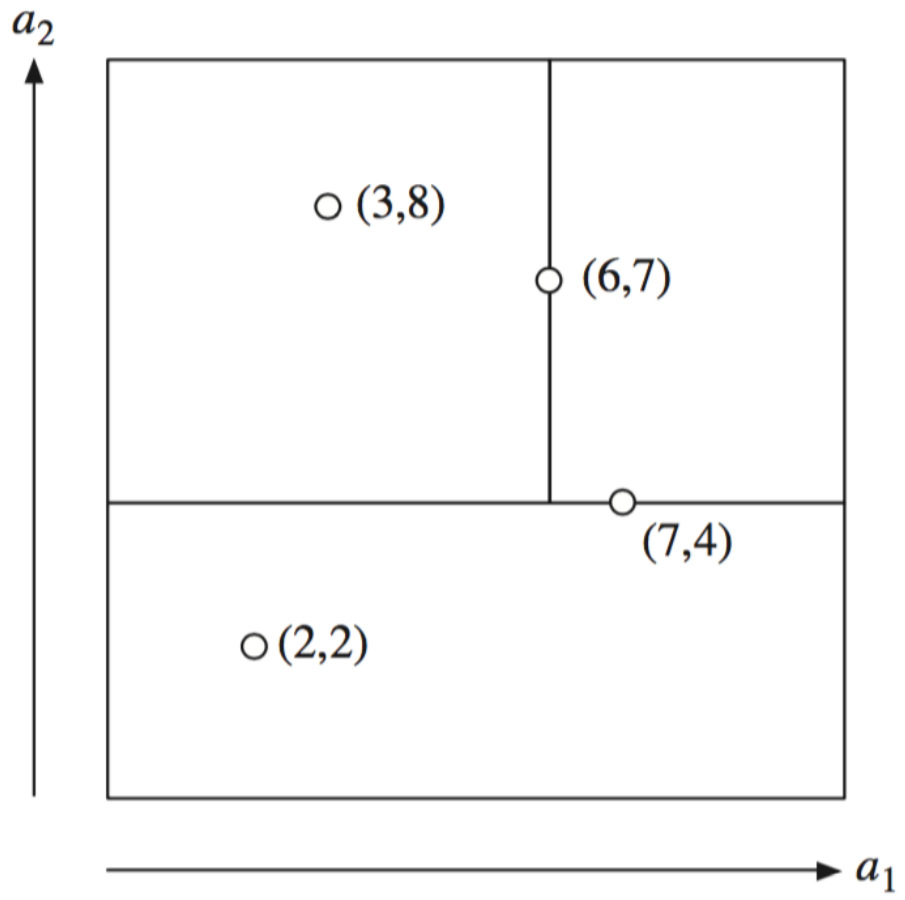
Finding nearest neighbors efficiently

- Simplest way of finding nearest neighbour: linear scan of the data
  - Classification takes time proportional to the product of the number of instances in training and test sets
- Nearest-neighbor search can be done more efficiently using appropriate data structures
- We will discuss two methods that represent training data in a tree structure:

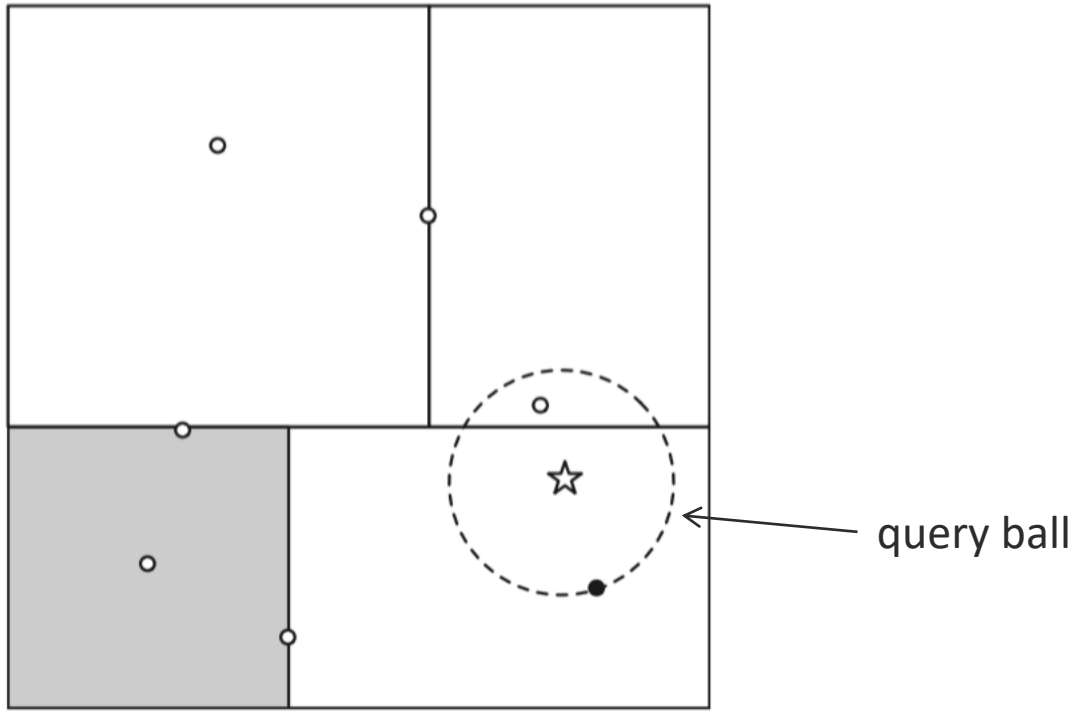
  kD-trees and *ball trees*

*k*D-tree example





Using *k*D-trees: example



More on *k*D-trees

- Complexity depends on depth of the tree, given by the logarithm of number of nodes for a balanced tree
- Amount of backtracking required depends on quality of tree ("square" vs. "skinny" nodes)
- How to build a good tree? Need to find good split point and split direction
  - Possible split direction: direction with greatest variance
  - Possible split point: median value along that direction
- Using value closest to mean (rather than median) can be better if data is skewed
- Can apply this split selection strategy recursively just like in the case of decision tree learning

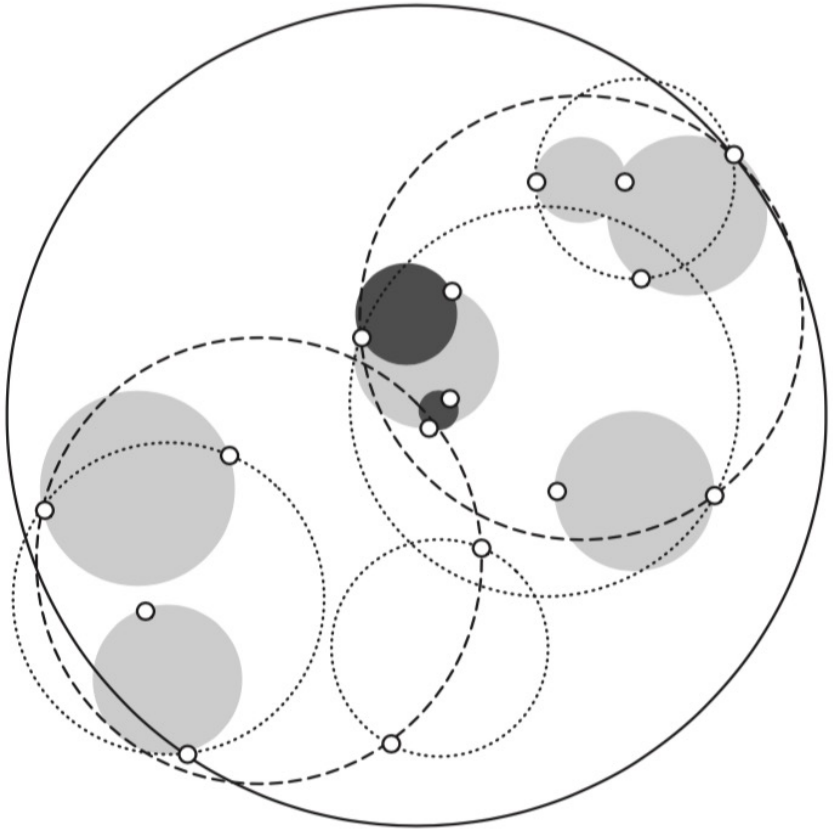
Building trees incrementally

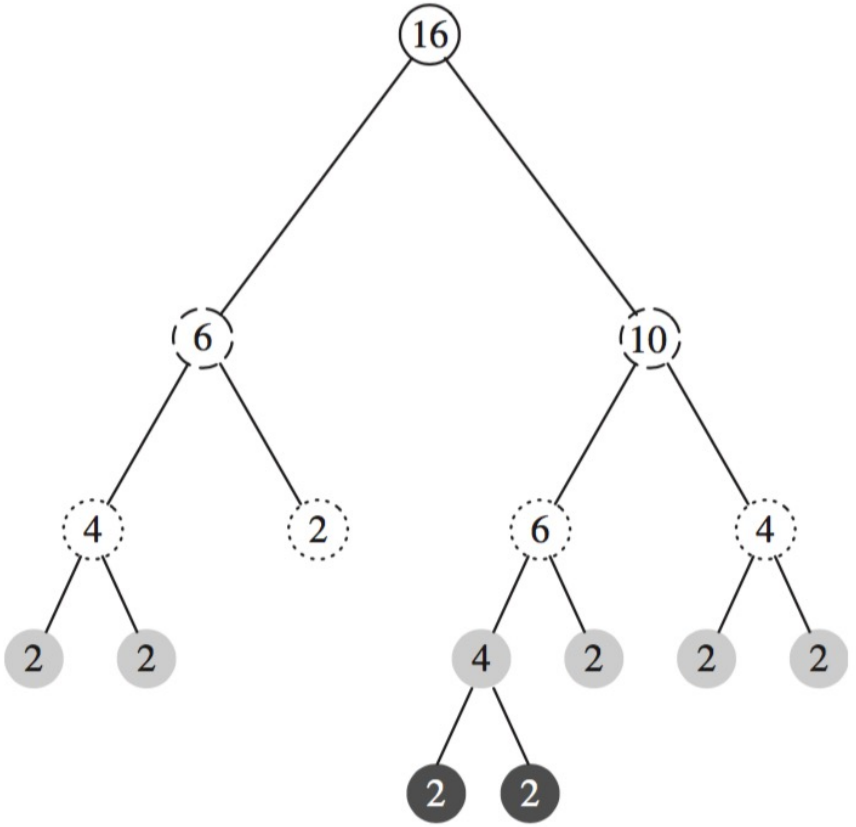
- Big advantage of instance-based learning: classifier can be updated incrementally
  - Just add new training instance!
- Can we do the same with *k*D-trees?
- Heuristic strategy:
  - Find leaf node containing new instance
  - Place instance into leaf if leaf is empty
  - Otherwise, split leaf according to the longest dimension (to preserve squareness)
- Tree should be re-built occasionally (e.g., if depth grows to twice the optimum depth for given number of instances)

Ball trees

- Potential problem in *k*D-trees: corners in high-dimensional space may mean query ball intersects with many regions
- Observation: no need to make sure that regions do not overlap, so they do not need to be hyperrectangles
- Can use balls (hyperspheres) instead of hyperrectangles
  - A *ball tree* organizes the data into a tree of *k*-dimensional hyperspheres
  - Motivation: balls may allow for a better fit to the data and thus more efficient search

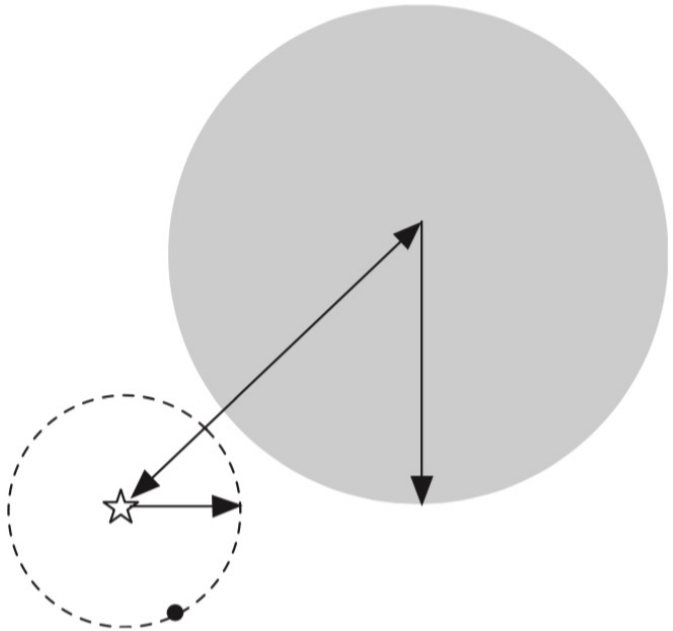
Ball tree example





Using ball trees

- Nearest-neighbor search is done using the same backtracking strategy as in *k*D-trees
- Ball can be ruled out during search if distance from target to ball's center exceeds ball's radius plus radius of query ball



Building ball trees

- Ball trees are built top down, applying the same recursive strategy as in *k*D-trees
- We do not have to continue until leaf balls contain just two points (examples): can enforce minimum occupancy
  (this can also be done for efficiency in *k*D-trees)
- Basic problem: splitting a ball into two
- Simple (linear-time) split selection strategy:
  - Choose point farthest from ball's center
  - Choose second point farthest from first one
  - Assign each example to these two points
  - Compute cluster centers and radii based on the two subsets to get two successor balls

Discussion of nearest-neighbor learning

- Often very accurate
- Assumes all attributes are equally important
  - Remedy: attribute selection, attribute weights, or attribute scaling
- Possible remedies against noisy instances:
  - Take a majority vote over the *k* nearest neighbors
  - Remove noisy instances from dataset (difficult!)
- Statisticians have used *k*-NN since the early 1950s
  - If $n \rightarrow \infty$ and $k/n \rightarrow 0$, classification error approaches minimum
- *k*D-trees can become inefficient when the number of attributes is too large
- Ball trees are instances *may* help; they are instances of *metric trees*

Knowledge Check

For the nearest neighbor learning KD trees and ball trees:

A. Add time to training

B. KD trees and ball tress reduce accuracy

C. Significantly reduce the time for classification

D. Have the property that ball trees are better for lots attributes

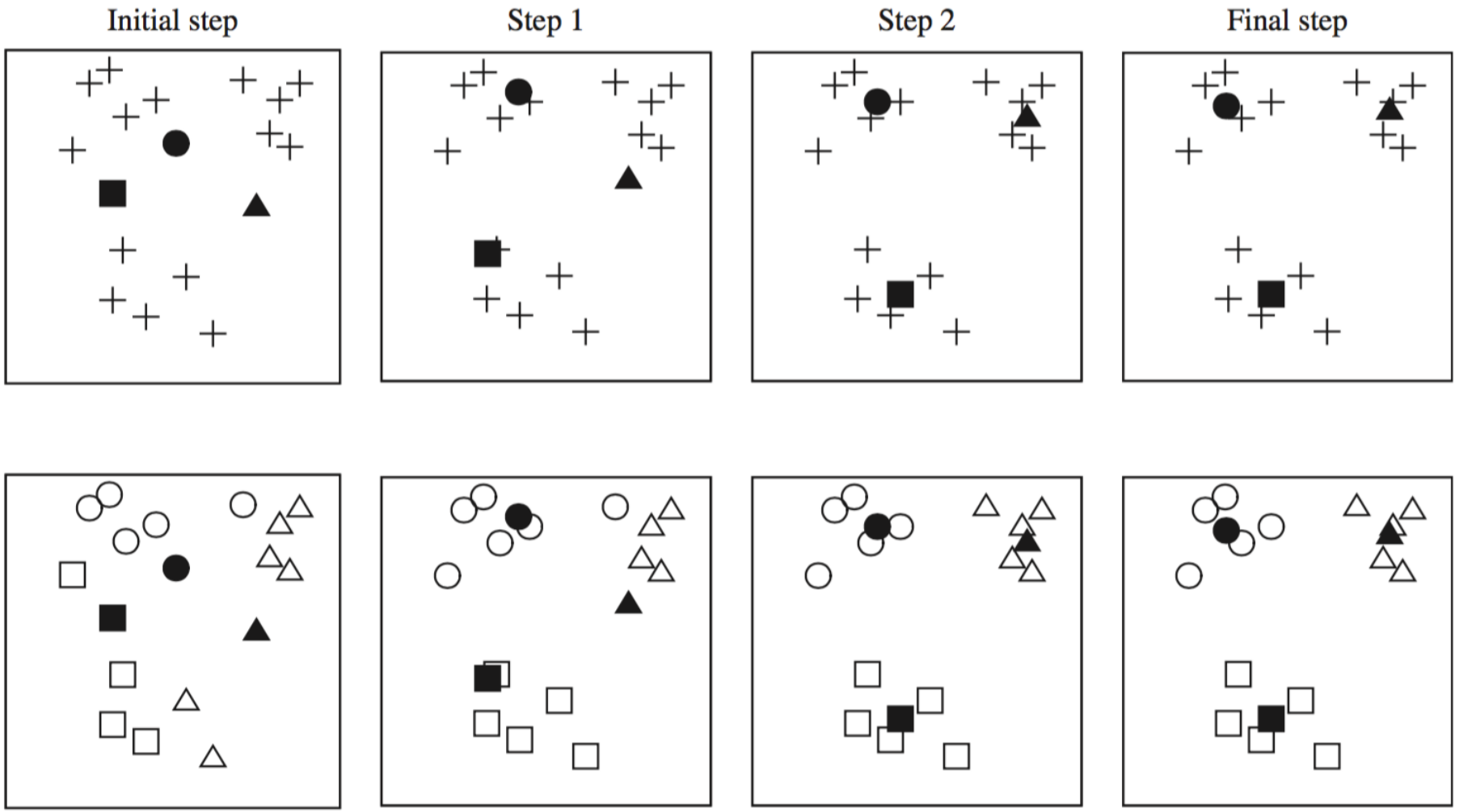
Clustering

- Clustering techniques apply when there is no class to be predicted: they perform unsupervised learning
- Aim: divide instances into “natural” groups
- As we have seen, clusters can be:
  - disjoint vs. overlapping
  - deterministic vs. probabilistic
  - flat vs. hierarchical
- We will look at a classic clustering algorithm called *k-means*
- *k-means* clusters are disjoint, deterministic, and flat

The *k*-means algorithm

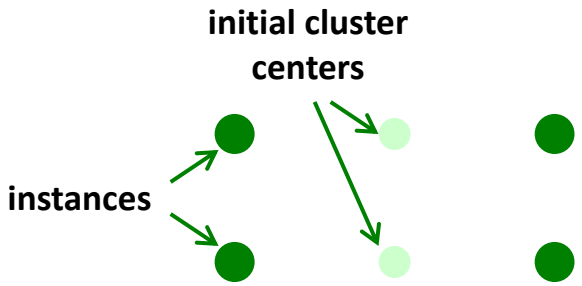
- Step 1: Choose *k* random cluster centers
- Step 2: Assign each instance to its closest cluster center based on Euclidean distance
- Step 3: Recompute cluster centers by computing the average (aka *centroid*) of the instances pertaining to each cluster
- Step 4: If cluster centers have moved, go back to Step 2
- This algorithm minimizes the squared Euclidean distance of the instances from their corresponding cluster centers
  - Determines a solution that achieves a *local* minimum or saddle point of the squared Euclidean distance
- Equivalent termination criterion: stop when assignment of instances to cluster centers has not changed

The *k*-means algorithm: example



Discussion

- Algorithm minimizes squared distance to cluster centers
- Result can vary significantly
  - based on initial choice of seeds
- Can get trapped in local minimum or a saddle point
  - Example:

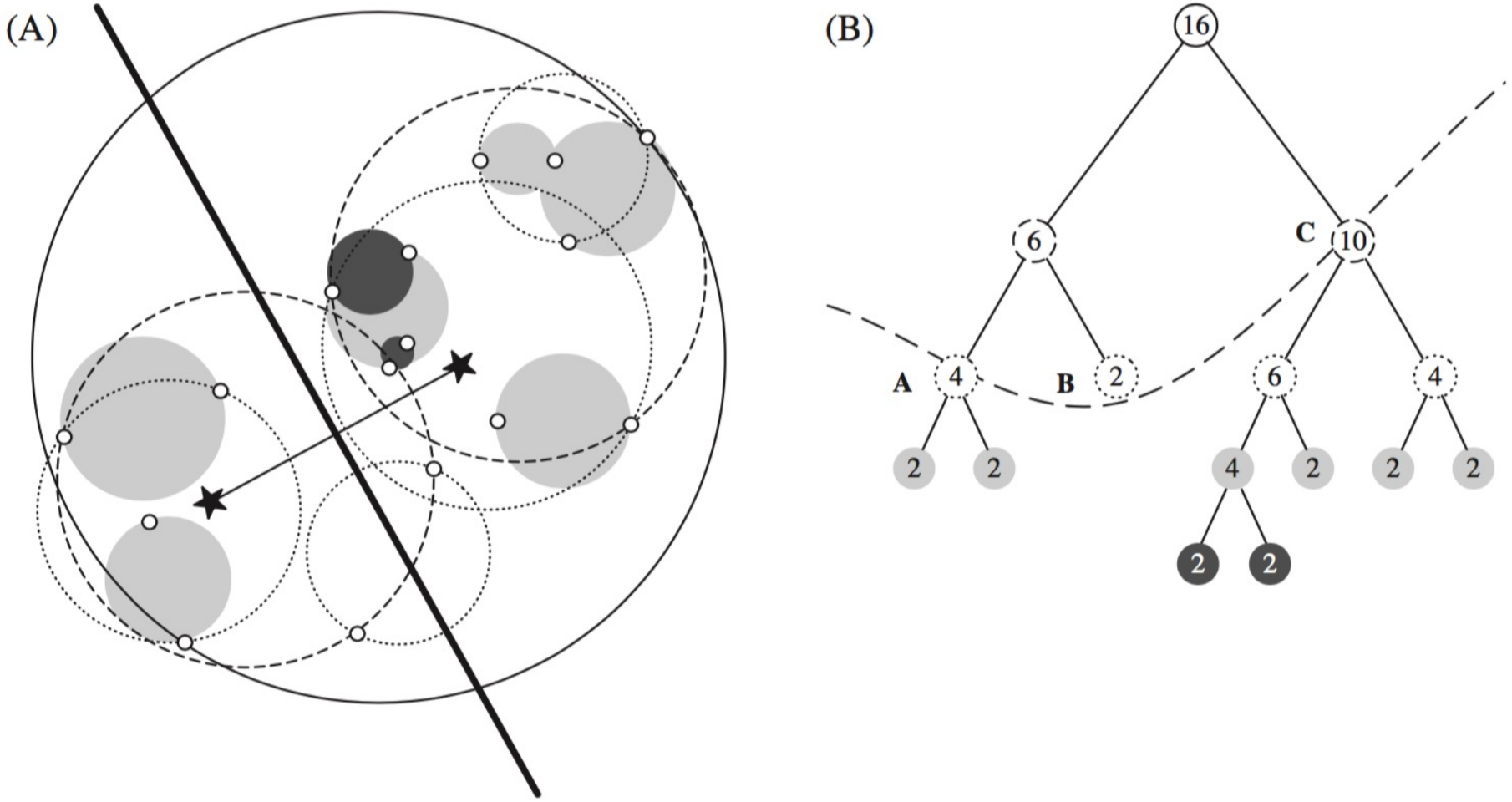


- To increase chance of finding global optimum: restart with different random seeds
- Can be applied recursively with $k = 2$

Faster distance calculations

- Can we use *k*D-trees or ball trees to speed up the process? Yes, we can:
  - First, build the tree data structure, which remains static, for all the data points
  - At each node, store the number of instances and the sum of all instances (summary statistics)
  - In each iteration of *k*-means, descend the tree and find out which cluster each node belongs to
  - Can stop descending as soon as we find out that a node belongs entirely to a particular cluster
  - Use summary statistics stored previously at the nodes to compute new cluster centers

Example scenario (using a ball tree)



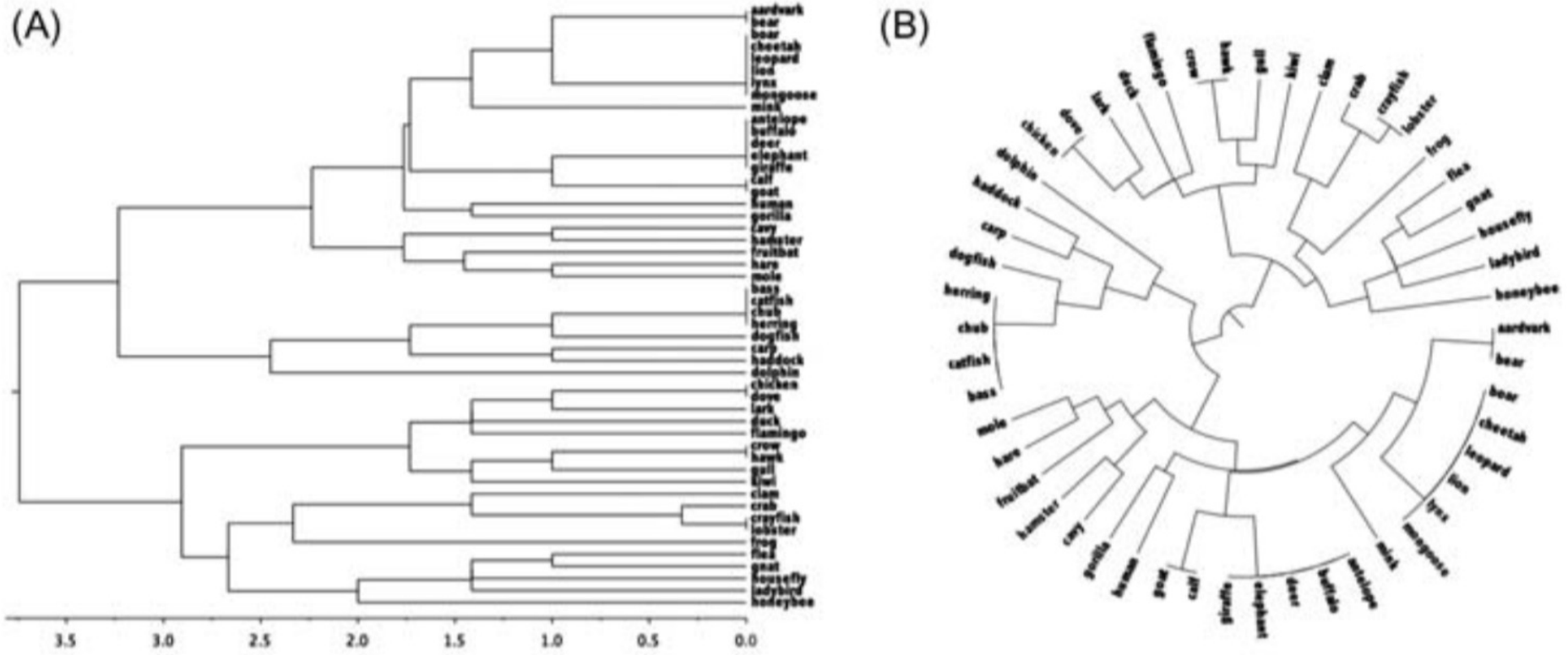
Choosing the number of clusters

- Big question in practice: what is the right number of clusters, i.e., what is the right value for *k*?
- Cannot simply optimize squared distance on training data to choose k
  - Squared distance decreases monotonically with increasing values of *k*
- Need some measure that balances distance with complexity of the model, e.g., based on the MDL principle (covered later)
- Finding the right-size model using MDL becomes easier when applying a recursive version of *k*-means (*bisecting k-means*):
  - Compute A: information required to store data centroid, and the location of each instance with respect to this centroid
  - Split data into two clusters using 2-means
  - Compute B: information required to store the two new cluster centroids, and the location of each instance with respect to these two
  - If A > B, split the data and recurse (just like in other tree learners)

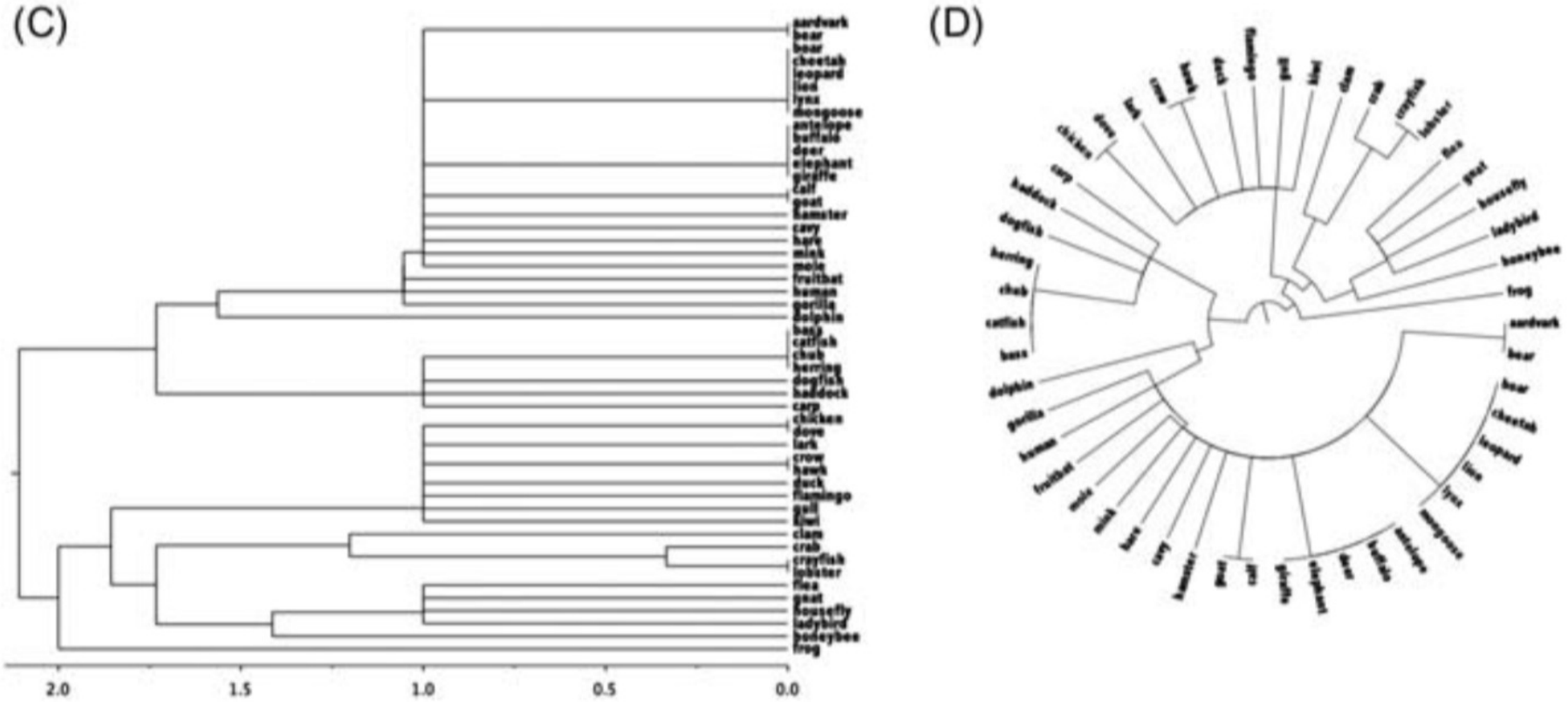
Hierarchical clustering

- Bisecting *k*-means performs hierarchical clustering in a top-down manner
- Standard hierarchical clustering performs clustering in a bottom-up manner; it performs *agglomerative* clustering:
  - First, make each instance in the dataset into a trivial mini-cluster
  - Then, find the two closest clusters and merge them; repeat
  - Clustering stops when all clusters have been merged into a single cluster
- Outcome is determined by the distance function that is used:
  - *Single-linkage* clustering: distance of two clusters is measured by finding the two closest instances, one from each cluster, and taking their distance
  - *Complete-linkage* clustering*:* use the two most distant instances instead
  - *Average-linkage* clustering: take average distance between all instances
  - *Centroid-linkage* clustering: take distance of cluster centroids
  - *Group-average* clustering: take average distance in merged clusters
  - *Ward's method*: optimize *k-means* criterion (i.e., squared distance)

Example: complete linkage



Example: single linkage



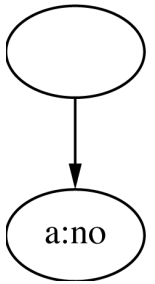
Incremental clustering

- Heuristic approach (COBWEB/CLASSIT)
- Forms a hierarchy of clusters incrementally
- Start:
  - tree consists of empty root node
- Then:
  - add instances one by one
  - update tree appropriately at each stage
  - to update, find the right leaf for an instance
  - may involve restructuring the tree using *merging* or *splitting* of nodes
- Update decisions are based on a goodness measure called *category utility*

Clustering the weather data I

ID	Outlook	Temp.	Humidity	Windy
A	Sunny	Hot	High	False
B	Sunny	Hot	High	True
C	Overcast	Hot	High	False
D	Rainy	Mild	High	False
E	Rainy	Cool	Normal	False
F	Rainy	Cool	Normal	True
G	Overcast	Cool	Normal	True
H	Sunny	Mild	High	False
I	Sunny	Cool	Normal	False
J	Rainy	Mild	Normal	False
K	Sunny	Mild	Normal	True
L	Overcast	Mild	High	True
M	Overcast	Hot	Normal	False
N	Rainy	Mild	High	True

1



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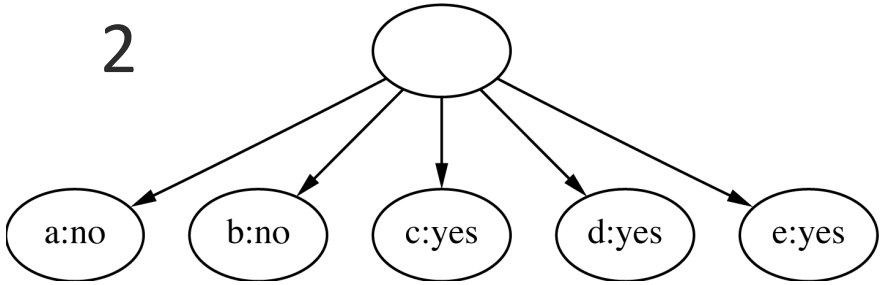

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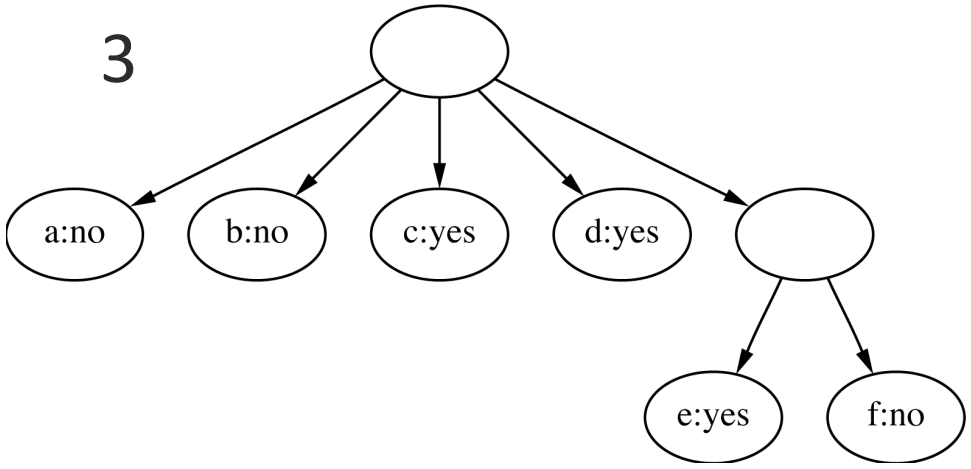
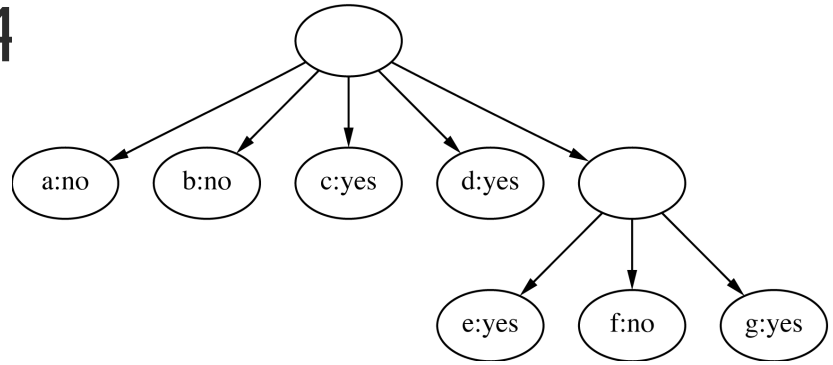


Clustering the weather data II

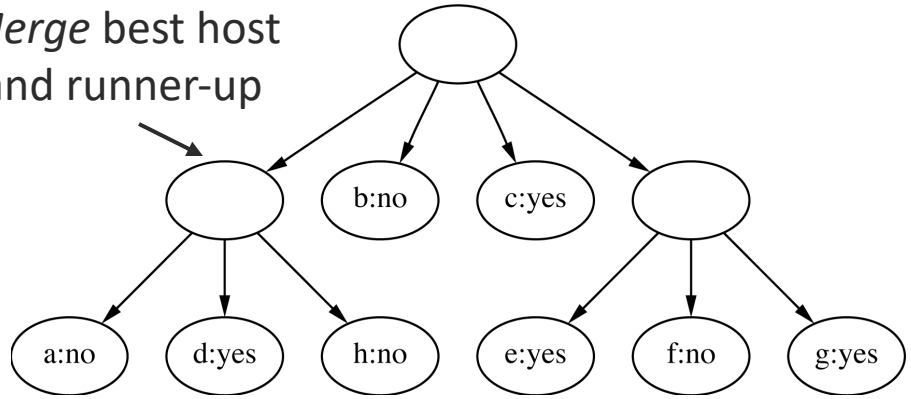
ID	Outlook	Temp.	Humidity	Windy
A	Sunny	Hot	High	False
B	Sunny	Hot	High	True
C	Overcast	Hot	High	False
D	Rainy	Mild	High	False
E	Rainy	Cool	Normal	False
F	Rainy	Cool	Normal	True
G	Overcast	Cool	Normal	True
H	Sunny	Mild	High	False
I	Sunny	Cool	Normal	False
J	Rainy	Mild	Normal	False
K	Sunny	Mild	Normal	True
L	Overcast	Mild	High	True
M	Overcast	Hot	Normal	False
N	Rainy	Mild	High	True

4



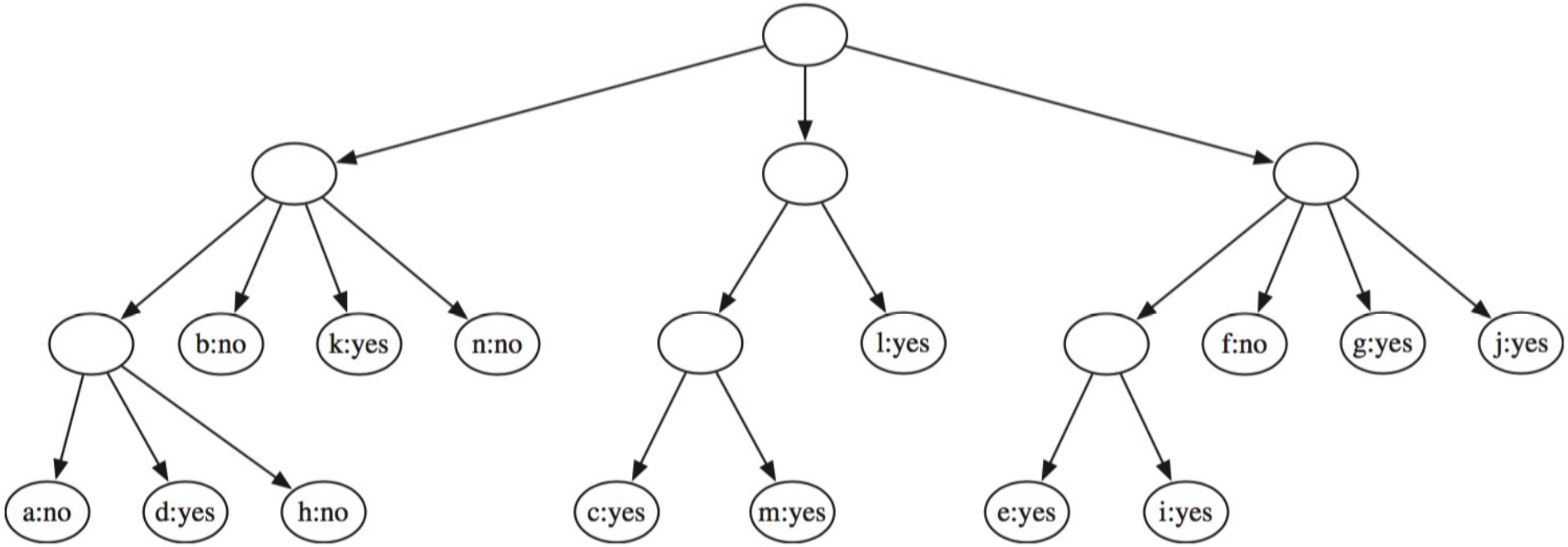
5

Merge best host and runner-up

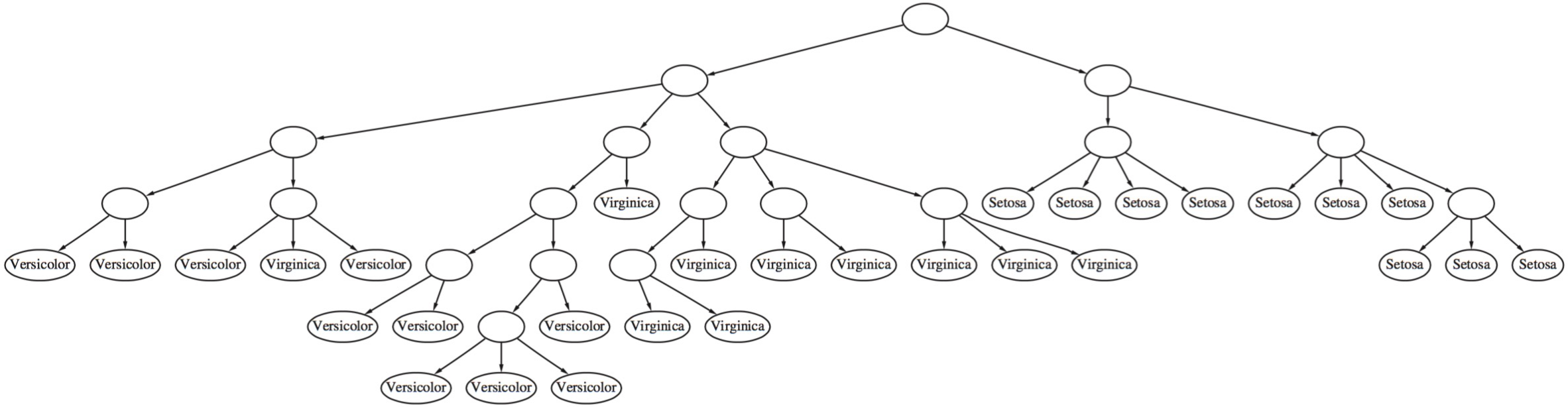


Consider *splitting* the best host if merging does not help

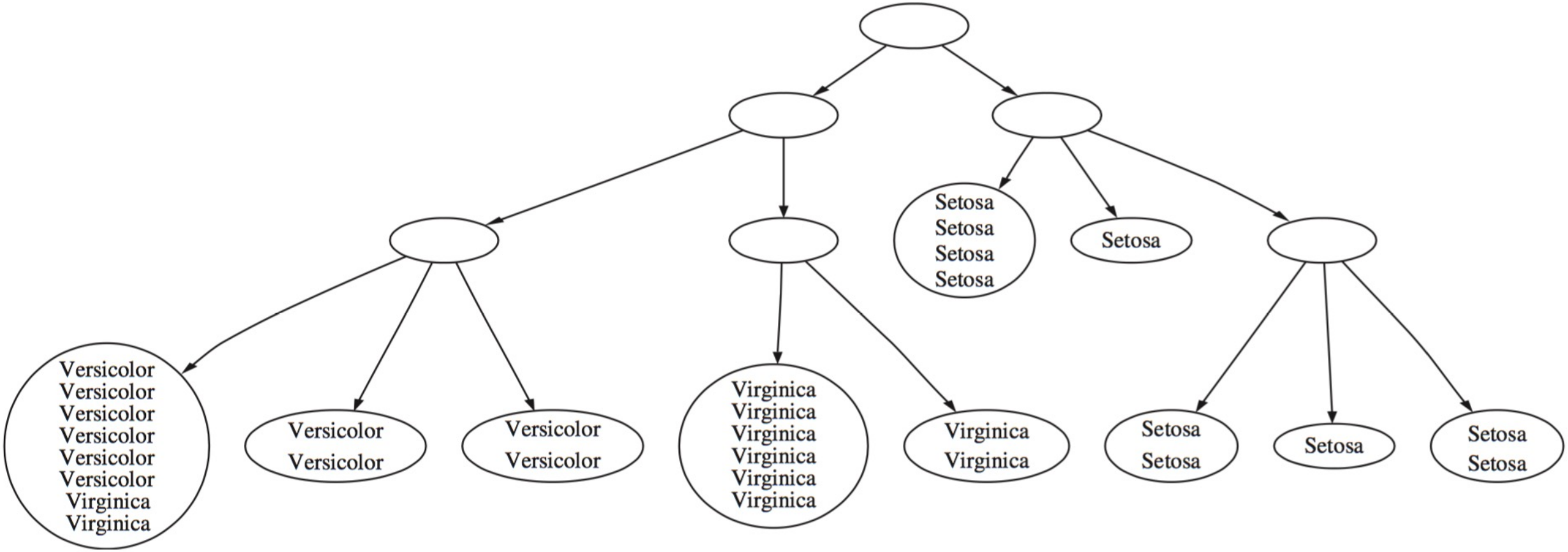
Final clustering



Example: clustering a subset of the iris data



Example: iris data with cutoff



The category utility measure

- Category utility: quadratic loss function defined on conditional probabilities:

$$CU(C_1, C_2, \ldots, C_k) = \frac{\sum_l \mathrm{P}(C_l) \sum_i \sum_j (\mathrm{P}(a_i = v_{ij} \mid C_l)^2 - \mathrm{P}(a_i = v_{ij})^2)}{k}$$

- Every instance in a different category ⇒ numerator becomes

$$m - \mathrm{P}(a_i = v_{ij})^2 \longleftarrow \text{maximum}$$

m: number of attributes

Numeric attributes?

- Assume normal distribution: $$f(a) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(a-\mu)^2}{2\sigma^2}}$$
- Then: $$\sum_j \mathrm{P}(a_i = v_{ij})^2 \Leftrightarrow \int f(a_i)^2 \, da_i = \frac{1}{2\sqrt{\pi}\sigma_i}$$
- Thus $$CU = \frac{\sum_l \mathrm{P}(C_l) \sum_i \sum_j (\mathrm{P}(a_i = v_{ij} \mid C_l)^2 - \mathrm{P}(a_i = v_{ij})^2)}{k}$$

  becomes $$CU = \frac{\sum_l \Pr[C_l] \frac{1}{2\sqrt{\pi}} \sum_i \left(\frac{1}{\sigma_{il}} - \frac{1}{\sigma_i} \right)}{k}$$

- Prespecified minimum variance can be enforced to combat overfitting (called *acuity* parameter)

Multi-instance learning

- Recap: multi-instance learning is concerned with examples corresponding to sets (really, *bags* or *multi-sets*) of instances
  - All instances have the same attributes but the full set of instances is split into subsets of related instances that are not necessarily independent
  - These subsets are the examples for learning
- Example applications of multi-instance learning: image classification, classification of molecules
- Simplicity-first methodology can be applied to multi-instance learning with surprisingly good results
- Two simple approaches to multi-instance learning, both using standard single-instance learners:
  - Manipulate the input to learning
  - Manipulate the output of learning

Knowledge Check

KNN will work best when

A. There is lots of training data.

B. K >2 to help with mislabeled examples.

C. When the data is all nominal attributes.

D. When an effective distance measure is used.

Aggregating the input

- Idea: convert multi-instance learning problem into a single-instance one
  - Summarize the instances in a bag by computing the mean, mode, minimum and maximum, etc., of each attribute as new attributes
  - “Summary” instance retains the class label of its bag
  - To classify a new bag the same process is used
- Any single-instance learning method, e.g., decision tree learning, can be applied to the resulting data
- This approach discards most of the information in a bag of instances but works surprisingly well in practice
- Should be used as a base line when evaluating more advanced approaches to multi-instance learning
- More sophisticated region-based summary statistics can be applied to extend this basic approach

Aggregating the output

- Idea: learn a single-instance classifier directly from the original instances in all the bags
  - Each instance is given the class of the bag it originates from
  - But: bags can contain differing numbers of instances -> give each instance a weight inversely proportional to the bag's size
- To classify a new bag:
  - Produce a prediction for each instance in the bag
  - Aggregate the predictions to produce a prediction for the bag as a whole
  - One approach: treat predictions as votes for the various class labels; alternatively, average the class probability estimates
- This approach treats all instances as independent at training time, which is not the case in true multi-instance applications
- Nevertheless, it often works very well in practice and should be used as a base line

Some final comments on the basic methods

- Bayes' rule stems from his "Essay towards solving a problem in the doctrine of chances" (1763)
  - Difficult bit in general: estimating prior probabilities (easy in the case of naïve Bayes)
- Extension of naïve Bayes: Bayesian networks (which we will discuss later)
- The algorithm for association rules we discussed is called APRIORI; many other algorithms exist
- Minsky and Papert (1969) showed that linear classifiers have limitations, e.g., can't learn a logical XOR of two attributes
  - But: combinations of them can (this yields multi-layer neural nets, which we will discuss later)

You have reached the end of the lecture.

Reference:

I. H. Witten, E. Frank, M. A. Hall and C. J. Pal(2016).*Data Mining: Practical Machine Learning Tools and Techniques.* Morgan Kaufmann