# Machine Learning
# Chapter 4. Algorithms

# 4 Algorithms: The basic methods

- Simplicity first: 1R
- Use all attributes: Naïve Bayes
- Decision trees: ID3
- Covering algorithms: decision rules: PRISM
- Association rules
- Linear models
- Instance-based learning

# Simplicity first

- Simple algorithms often work very well!
- There are many kinds of simple structure, eg:
  - One attribute does all the work
  - All attributes contribute equally & independently
  - A weighted linear combination might do
  - Instance-based: use a few prototypes
  - Use simple logical rules
- Success of method depends on the domain

# Inferring rudimentary rules

- 1R: learns a 1-level decision tree
  - I.e., rules that all test one particular attribute
- Basic version
  - One branch for each value
  - Each branch assigns most frequent class
  - Error rate: proportion of instances that don't belong to the majority class of their corresponding branch
  - Choose attribute with lowest error rate

(*assumes nominal attributes*)

# 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
```

- Note: “missing” 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

- Discretize numeric attributes
- Divide each attribute's range into intervals
  - Sort instances according to attribute's values
  - Place breakpoints where the class changes (the majority class)
  - This minimizes the total 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
```

# Dealing with numeric attributes

- Discretize numeric attributes
- Divide each attribute's range into intervals
  - Sort instances according to attribute's values
  - Place breakpoints where the class changes (the majority class)
  - This r
- Example

| 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 |
| ... | ... | ... | ... | ... |

```
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
```

# The problem of overfitting

- This procedure is very sensitive to noise
  - One instance with an incorrect class label will probably produce a separate interval
- Also: *time stamp* attribute will have zero errors
- Simple solution:
  *enforce minimum number of instances in majority class per interval*
- Example (with min = 3):

```
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
```

```
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
```

# With overfitting avoidance

- Resulting rule set:

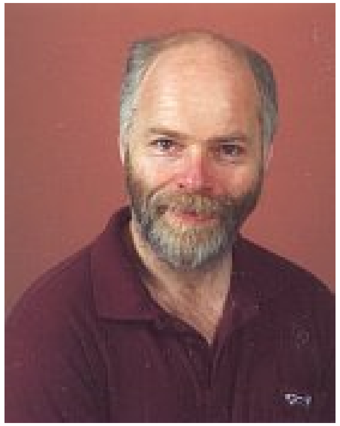
| Attribute | Rules | Errors | Total errors |
|---|---|---|---|
| Outlook | Sunny $\rightarrow$ No | 2/5 | 4/14 |
| | Overcast $\rightarrow$ Yes | 0/4 | |
| | Rainy $\rightarrow$ Yes | 2/5 | |
| Temperature | $\leq$ 77.5 $\rightarrow$ Yes | 3/10 | 5/14 |
| | > 77.5 $\rightarrow$ No* | 2/4 | |
| Humidity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

# Discussion of 1R

- 1R was described in a paper by Holte (1993)
  - Contains an experimental evaluation on 16 datasets (using *cross-validation* so that results were representative of performance on future data)
  - Minimum number of instances was set to 6 after some experimentation
  - 1R's simple rules performed not much worse than much more complex decision trees
- Simplicity first pays off!

**Very Simple Classification Rules Perform Well on Most Commonly Used Datasets**

Robert C. Holte, Computer Science Department, University of Ottawa



# Discussion of 1R: Hyperpipes

- Another simple technique: build one rule for each class
  - Each rule is a conjunction of tests, one for each attribute
  - For numeric attributes: test checks whether instance's value is inside an interval
    - Interval given by minimum and maximum observed in training data
  - For nominal attributes: test checks whether value is one of a subset of attribute values
    - Subset given by all possible values observed in training data
- Class with most matching tests is predicted

# Statistical modeling

- "Opposite" of 1R: use all the attributes
- Two assumptions: Attributes are
  - *equally important*
  - *statistically independent* (given the class value)
    - I.e., knowing the value of one attribute says nothing about the value of another
      (if the class is known)
- Independence assumption is never correct!
- But … this scheme works well in practice

# 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 | | | | | | | | |

# 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 | | | | | | |
| Overcast | 4/9 | 0/5 | Mild | 4/9 | 2/5 | Normal | 6/9 | | | | | | |
| 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 | 9/14 | 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 | | | | | | | | |

- 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

# Bayes's rule

- Probability of event *H* given evidence *E* :

$$\Pr[H \mid E] = \frac{\Pr[E \mid H]\Pr[H]}{\Pr[E]}$$

- *A priori* probability of *H* : $\Pr[H]$
  - Probability of event *before* evidence is seen
- *A posteriori* probability of *H* : $\Pr[H \mid E]$
  - Probability of event *after* evidence is seen

**Thomas Bayes**

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

# Naïve Bayes for classification

- Classification learning: what's the probability of the class given an instance?
  - Evidence $E$ = instance
  - Event $H$ = class value for instance
- Naïve assumption: evidence splits into parts (i.e. attributes) that are *independent*

$$\Pr[H \mid E] = \frac{\Pr[E_1 \mid H]\Pr[E_2 \mid H]\ldots\Pr[E_n \mid H]\Pr[H]}{\Pr[E]}$$

# Weather data example

| Outlook | Temp. | Humidity | Windy | Play |
|---|---|---|---|---|
| Sunny | Cool | High | True | ? |

← *Evidence E*

$$\begin{aligned}\Pr[yes \mid E] = {} & \Pr[Outlook = Sunny \mid yes] \\ & \times \Pr[Temperature = Cool \mid yes] \\ & \times \Pr[Humidity = High \mid yes] \\ & \times \Pr[Windy = True \mid yes] \\ & \times \frac{\Pr[yes]}{\Pr[E]}\end{aligned}$$

***Probability of class "yes"***

$$= \frac{\frac{2}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{9}{14}}{\Pr[E]}$$

# The “zero-frequency problem”

- What if an attribute value doesn’t occur with every class value?
  (e.g. “Humidity = high” for class “yes”)
  - Probability will be zero! $\Pr[Humidity = High \mid yes] = 0$
  - *A posteriori* probability will also be zero! $\Pr[yes \mid E] = 0$
    (No matter 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!
  (also: stabilizes probability estimates)

# 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 × 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%

# 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* $\mu$

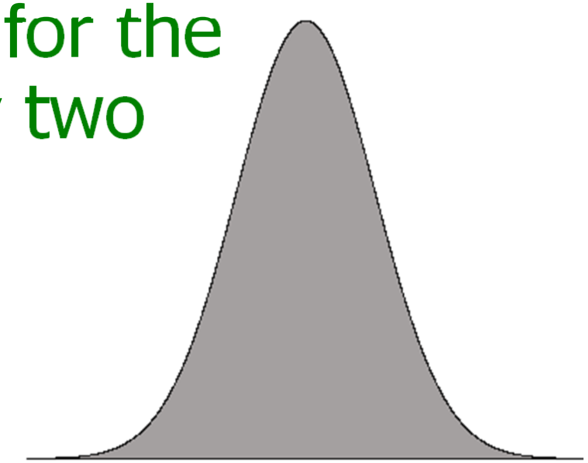
$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$$

  - *Standard deviation* $\sigma$

$$\sigma = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \mu)^2$$

  - 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 | $\mu$ =73 | $\mu$ =75 | $\mu$ =79 | $\mu$ =86 | False | 6/9 | 2/5 | 9/14 | 5/14 |
| Overcast | 4/9 | 0/5 | $\sigma$ =6.2 | $\sigma$ =7.9 | $\sigma$ =10.2 | $\sigma$ =9.7 | True | 3/9 | 3/5 | | |
| Rainy | 3/9 | 2/5 | | | | | | | | | |

- Example density value:

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

# 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" = $3/5 \times 0.0291 \times 0.0380 \times 3/5 \times 5/14 = 0.000136$

P("yes") = 0.000036 / (0.000036 + 0. 000136) = 20.9%

P("no") = 0.000136 / (0.000036 + 0. 000136) = 79.1%

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

# Probability densities

- Relationship between probability and density:

$$\Pr[c - \frac{\varepsilon}{2} < x < c + \frac{\varepsilon}{2}] \approx \varepsilon * f(c)$$

- But: this doesn't change calculation of *a posteriori* probabilities because $\varepsilon$ cancels out
- Exact relationship:

$$\Pr[a \le x \le b] = \int_a^b f(t)dt$$

# Multinomial naïve Bayes I

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

$$\Pr[E \mid H] \approx N! \times \prod_{i=1}^{k} \frac{P_i^{n_i}}{n_i!} \qquad N = n_1 + n_2 + \ldots + n_k$$

- Ignores probability of generating a document of the right length (prob. assumed constant for each class)

# Multinomial naïve Bayes II

- suppose dictionary has two words, *yellow* and *blue*
- suppose $\Pr[yellow \mid H] = 75\%$ and $\Pr[blue \mid H] = 25\%$
- suppose E is the document "*blue yellow blue*"
- Probability of observing document:

$$\Pr[\{blue\ yellow\ blue\} \mid H] \approx 3! \times \frac{0.75^1}{1!} \times \frac{0.25^2}{2!} = \frac{9}{64} \approx 0.14$$

Suppose there is another class H' that has $\Pr[yellow \mid H'] = 10\%$ and $\Pr[blue \mid H'] = 90\%$:

$$\Pr[\{blue\ yellow\ blue\} \mid H'] \approx 3! \times \frac{0.1^1}{1!} \times \frac{0.9^2}{2!} = 0.24$$

- Need to take prior probability of class into account to make final classification
- Factorials don't actually need to be computed
- Underflows can be prevented by using logarithms

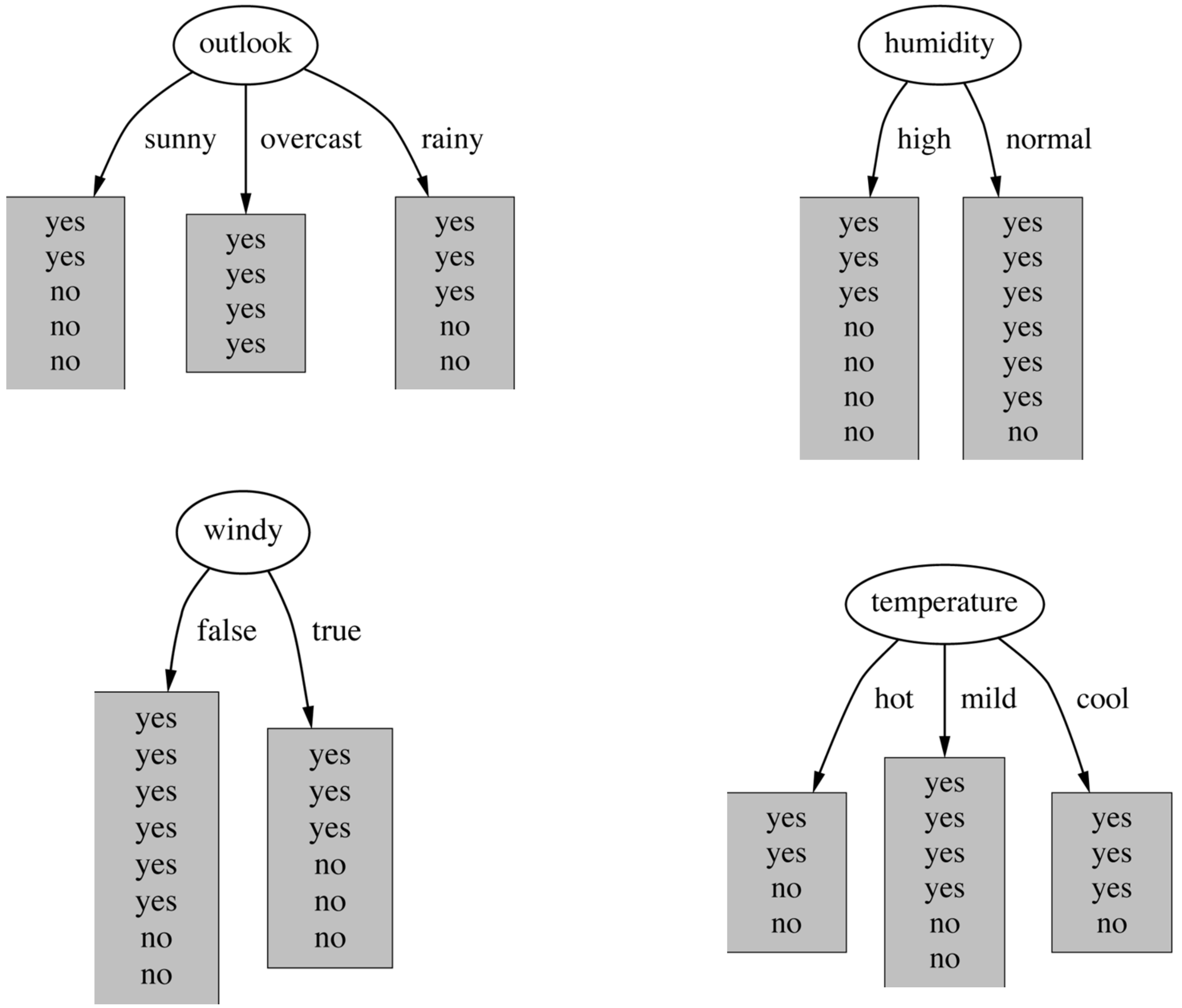
# Naïve Bayes: discussion

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

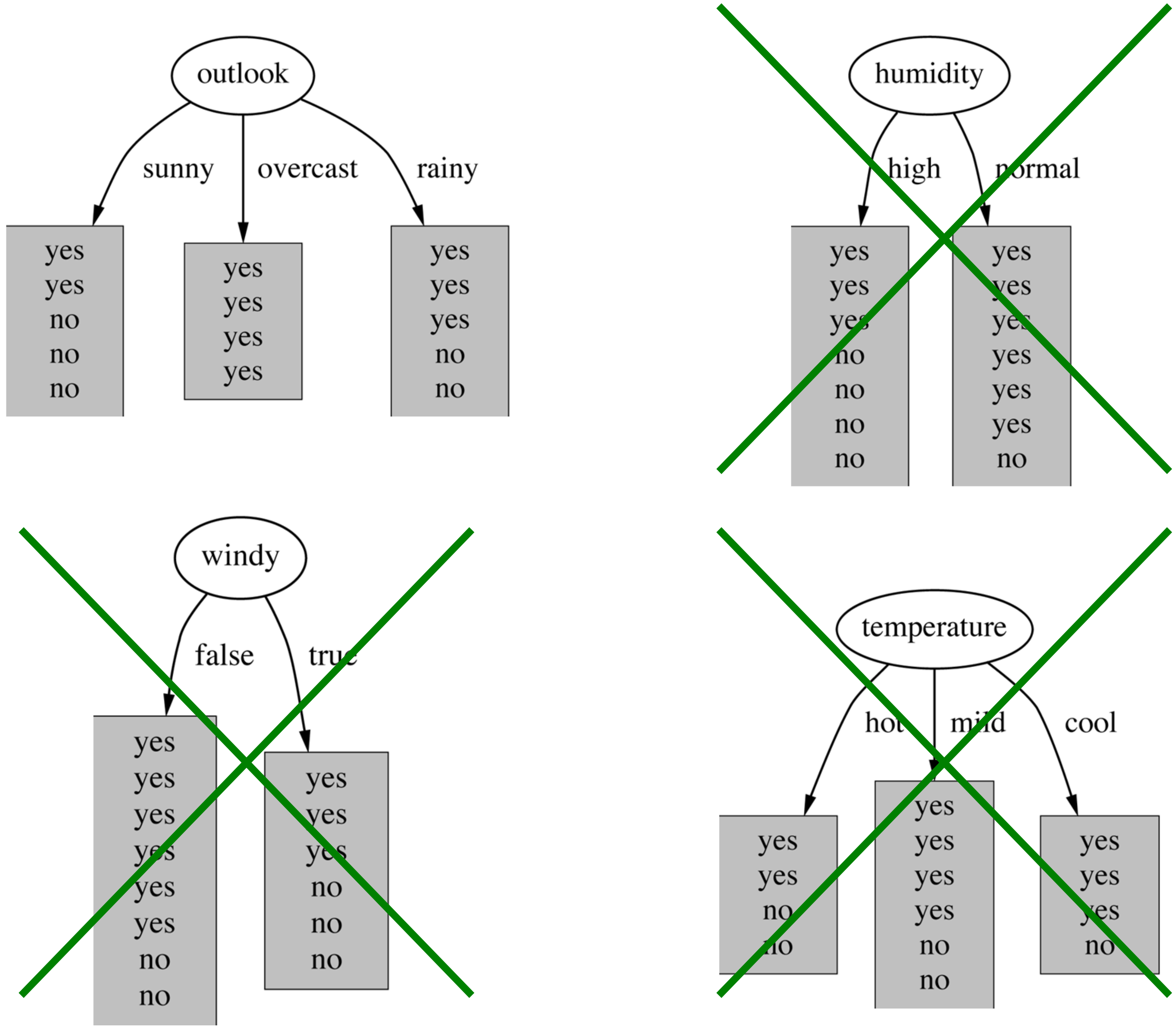
# Constructing decision trees

- Strategy: top down
  Recursive *divide-and-conquer* fashion
  - 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 *impurity criterion*: *information gain*
  - Information gain increases with the average purity of the subsets
- Strategy: choose attribute that gives greatest information gain

# Computing information

- Measure information in *bits*
  - Given a probability distribution, the info required to predict an event is the distribution's *entropy*
  - Entropy gives the information required in bits
    (can involve fractions of bits!)
- Formula for computing the entropy:

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

# Claude Shannon

***Born: 30 April 1916***

***Died: 23 February 2001***

***"Father of information theory"***

Claude Shannon, who has died aged 84, perhaps more than anyone laid the groundwork for today's digital revolution. His exposition of information theory, stating that all information could be represented mathematically as a succession of noughts and ones, facilitated the digital manipulation of data without which today's information society would be unthinkable.


Shannon's master's thesis, obtained in 1940 at MIT, demonstrated that problem solving could be achieved by manipulating the symbols 0 and 1 in a process that could be carried out automatically with electrical circuitry. That dissertation has been hailed as one of the most significant master's theses of the 20th century. Eight years later, Shannon published another landmark paper, *A Mathematical Theory of Communication*, generally taken as his most important scientific contribution.

Shannon applied the same radical approach to cryptography research, in which he later became a consultant to the US government.

Many of Shannon's pioneering insights were developed before they could be applied in practical form. He was truly a remarkable man, yet unknown to most of the world.

# Example: attribute *Outlook*

- *Outlook* = *Sunny* :

$$\text{info}([2,3]) = \text{entropy}(2/5,3/5) = -2/5\log(2/5) - 3/5\log(3/5) = 0.971\,\text{bits}$$

- *Outlook* = *Overcast* :

$$\text{info}([4,0]) = \text{entropy}(1,0) = -1\log(1) - 0\log(0) = 0\,\text{bits}$$

***Note: this is normally undefined.***

- *Outlook* = *Rainy* :

$$\text{info}([3,2]) = \text{entropy}(3/5,2/5) = -3/5\log(3/5) - 2/5\log(2/5) = 0.971\,\text{bits}$$

- Expected information for attribute:

$$\begin{aligned}\text{info}([3,2],[4,0],[3,2]) &= (5/14)\times 0.971 + (4/14)\times 0 + (5/14)\times 0.971 \\ &= 0.693\,\text{bits}\end{aligned}$$

# Computing information gain

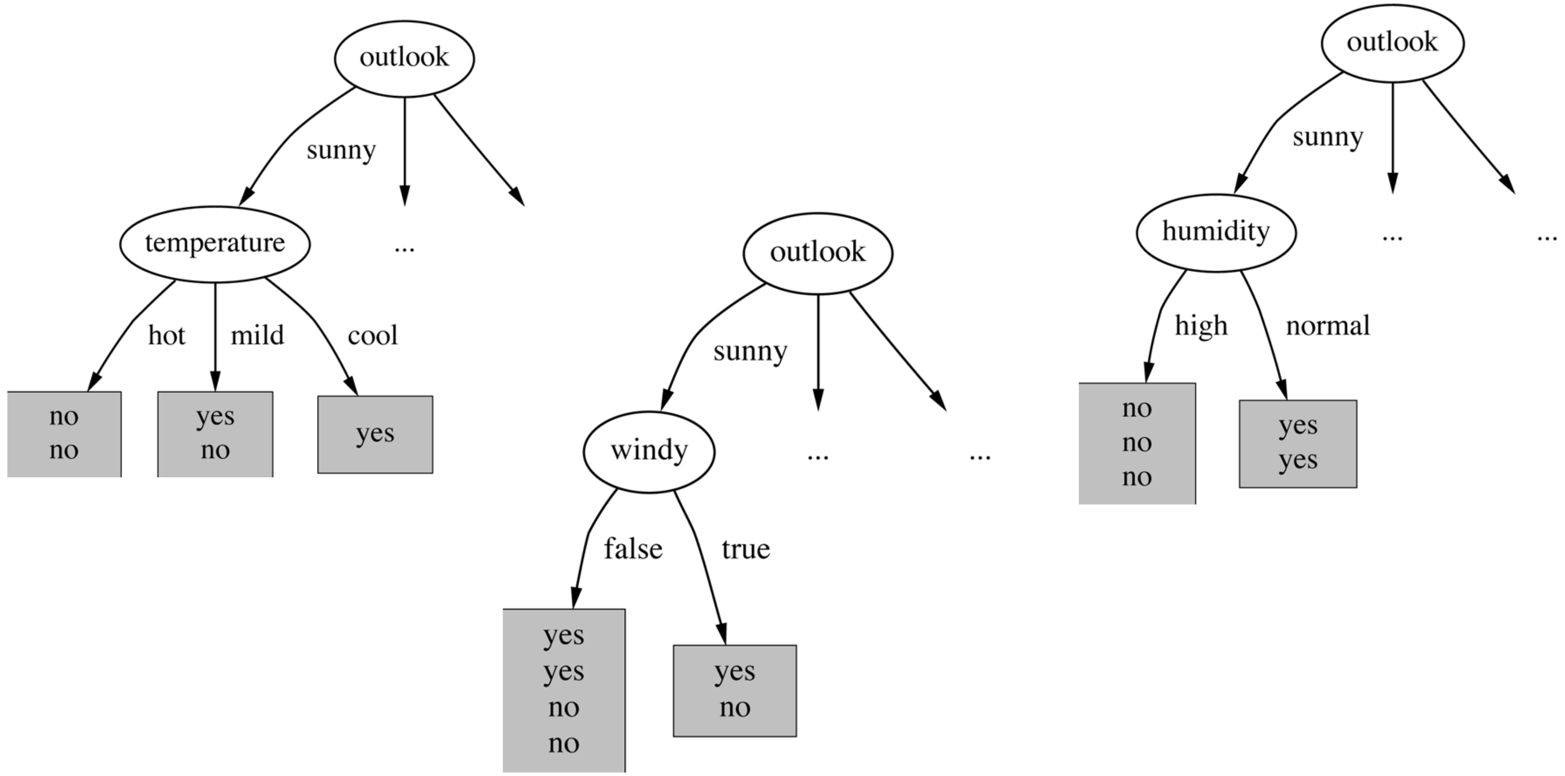
- Information gain: information before splitting – information after splitting

$$\begin{aligned}\text{gain}(\textit{Outlook}) &= \text{info}([9,5]) - \text{info}([2,3],[4,0],[3,2]) \\ &= 0.940 - 0.693 \\ &= 0.247 \text{ bits}\end{aligned}$$

- Information gain for attributes from weather data:

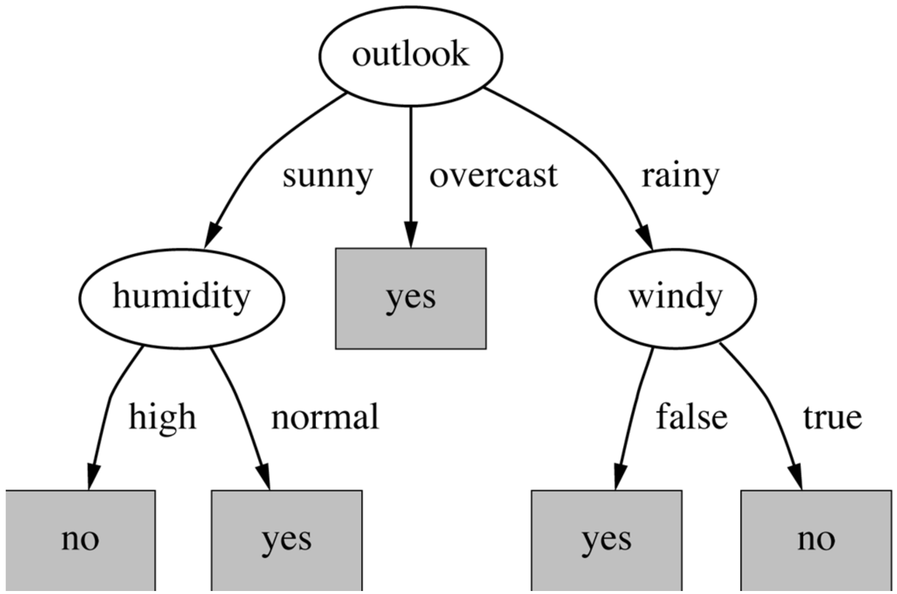
$$\begin{aligned}\text{gain}(\textit{Outlook}) &= 0.247 \text{ bits} \\ \text{gain}(\textit{Temperature}) &= 0.029 \text{ bits} \\ \text{gain}(\textit{Humidity}) &= 0.152 \text{ bits} \\ \text{gain}(\textit{Windy}) &= 0.048 \text{ bits}\end{aligned}$$

# 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 can't be split any further

# Wishlist for a purity measure

- Properties we require from a purity 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 obey *multistage property* (i.e. decisions can be made in several stages):

$$\text{measure}([2,3,4]) = \text{measure}([2,7]) + (7/9) \times \text{measure}([3,4])$$

- Entropy is the only function that satisfies all three properties!

# Properties of the entropy

- The multistage property:

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

- Simplification of computation:

$$\text{info}([2,3,4]) = -2/9 \times \log(2/9) - 3/9 \times \log(3/9) - 4/9 \times \log(4/9)$$
$$= [-2\log 2 - 3\log 3 - 4\log 4 + 9\log 9]/9$$

- Note: instead of maximizing info gain we could just minimize information

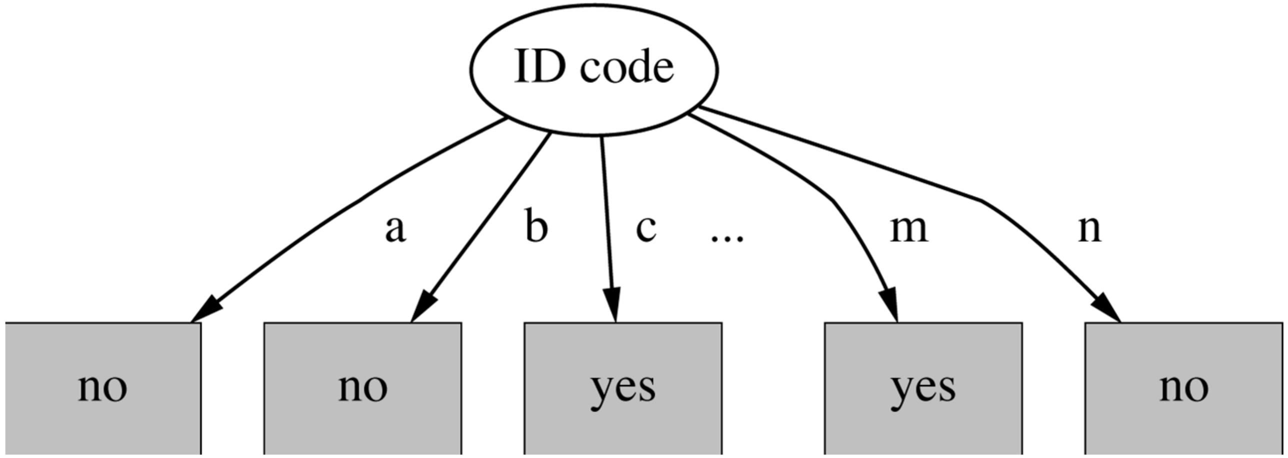
# Highly-branching attributes

- 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
  - $\Rightarrow$ Information gain is biased towards choosing attributes with a large number of values
  - $\Rightarrow$ This may result in *overfitting* (selection of an attribute that is non-optimal for prediction)
- Another problem: *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




- Entropy of split:

$$\text{info}(\text{"ID code"}) = \text{info}([0,1]) + \text{info}([0,1]) + \ldots + \text{info}([0,1]) = 0 \text{ bits}$$

$\Rightarrow$ Information gain is maximal for ID code (namely 0.940 bits)

# Gain ratio

- *Gain ratio*: a modification of the information gain that reduces its bias
- 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 distribution of instances into branches (i.e. how much info do we need to tell which branch an instance belongs to)

# Computing the gain ratio

- Example: intrinsic information for ID code

$$\text{info}([1,1,\ldots,1]) = 14 \times (-1/14 \times \log 1/14) = 3.807 \text{ bits}$$

- Value of attribute decreases as intrinsic information gets larger
- Definition of gain ratio:

$$\text{gain\_ratio}(\text{"Attribute"}) = \frac{\text{gain}(\text{"Attribute"})}{\text{intrinsic\_info}(\text{"Attribute"})}$$

- Example:

$$\text{gain\_ratio}(\text{"ID\_code"}) = \frac{0.940 \text{ bits}}{3.807 \text{ bits}} = 0.246$$

# Gain ratios for 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]) | 1.362 |
| Gain ratio: 0.247/1.577 | 0.156 | 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 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

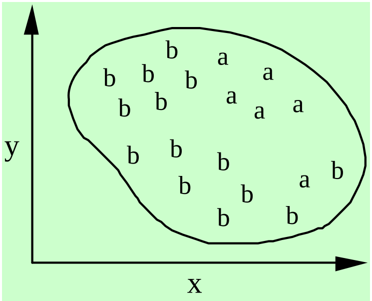
# Discussion

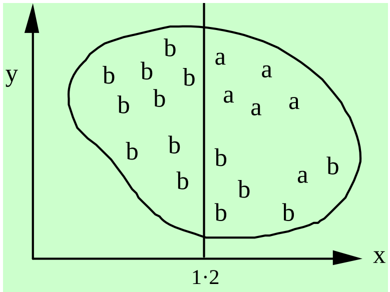
- Top-down induction of decision trees: ID3, algorithm developed by Ross Quinlan
  - Gain ratio just one modification of this basic algorithm
  - $\Rightarrow$ C4.5: deals with numeric attributes, missing values, noisy data
- Similar approach: CART
- There are many other attribute selection criteria!
  (But little difference in accuracy of result)

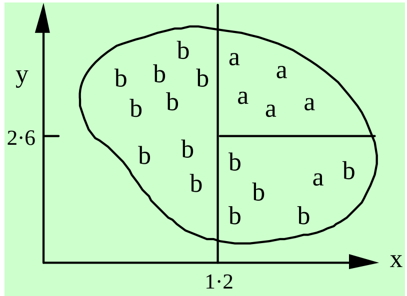
# Covering algorithms

- Convert decision tree into a rule set
  - Straightforward, but rule set overly complex
  - More effective conversions are not trivial
- Instead, can generate rule set directly
  - 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 a rule is identified that “covers” some of the instances

# 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
```

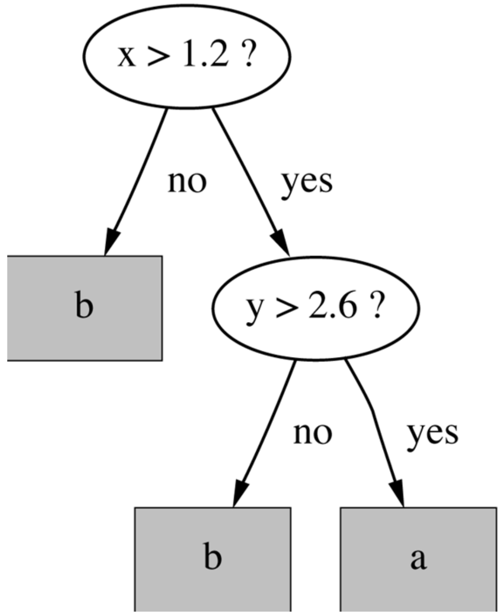
❖ Possible rule set for class “b”:

```
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

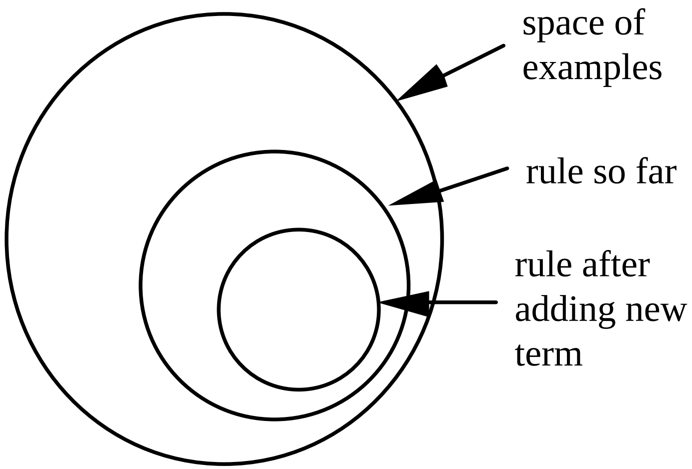
- Corresponding decision tree: (produces exactly the same predictions)




- 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

- Generates a rule by adding tests that maximize 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
  - $\Rightarrow$ Select test that maximizes the ratio $p/t$
- We are finished when $p/t = 1$ or the set of instances can't 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 result

- Final rule:

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

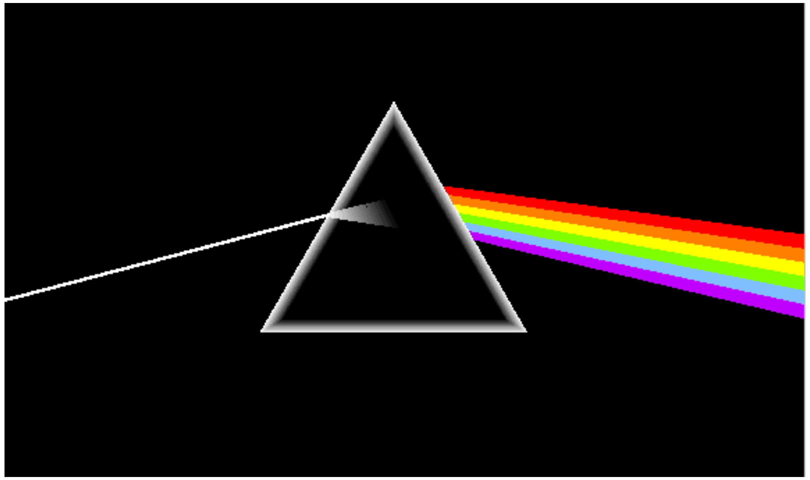
- Second rule for recommending “hard lenses”:
  (built from instances not covered by first rule)

```
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 doesn't matter because all rules predict the same class
- Outer loop considers all classes separately
  - No order dependence implied
- Problems: overlapping rules, default rule required

# Separate and conquer

- Methods like PRISM (for dealing with one class) are *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 rule doesn’t need to be explored any further

# Association rules

- Association rules...
  - ... can predict any attribute and combinations of attributes
  - ... are not intended to be used together as a set
- Problem: immense number of possible associations
  - Output needs to be restricted to show only the most predictive associations $\Rightarrow$ only those with high *support* and high *confidence*

# Support and confidence of a rule

- Support: number of instances predicted correctly
- Confidence: number of correct predictions, as proportion of all instances the rule applies to
- Example: 4 cool days with normal humidity

```
If temperature = cool then humidity = normal
```

$\Rightarrow$ Support = 4, confidence = 100%

- Normally: minimum support and confidence pre-specified (e.g. 58 rules with support $\geq$ 2 and confidence $\geq$ 95% for weather data)

# Support and c... a ru...

| 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 |

- Support: number of i... correctly
- Confidence: number ... proportion of all insta...
- Example: 4 cool days

```
If temperature = cool
```

$\Rightarrow$ Support = 4, confide...

- Normally: minimum s... pre-specified (e.g. 58 rules with support $\geq$ 2 and confidence $\geq$ 95% for weather data)

# Interpreting association rules

- Interpretation is not obvious:

```
If windy = false and play = no
   then outlook = sunny and humidity = high
```

is *not* the same as

```
If windy = false and play = no
   then outlook = sunny
If windy = false and play = no
   then humidity = high
```

- However, it means that the following also holds:

```
If humidity = high and windy = false and play = no
   then outlook = sunny
```

# 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)
- But: we can look for high support rules directly!

# Item sets

- 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: only rules that exceed pre-defined support

  ⇒ Do it by finding all item sets with the given minimum support and generating rules from them!

# Item sets for weather data

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

- In total: 12 one-item sets, 47 two-item sets, 39 three-item sets, 6 four-item sets and 0 five-item sets (with minimum support of two)

# Item sets fo… da…

| 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 |

| One-item sets | Two-item sets |
|---|---|
| Outlook = Sunny (5) | Outlook = Sunny<br>Temperature = Hot (2) |
| Temperature = Cool (4) | Outlook = Sunny<br>Humidity = High (3) |
| … | … |

- In total: 12 one-item sets, 47 two-item sets, 39 three-item sets, 6 four-item sets and 0 five-item sets (with minimum support of two)

# Generating rules from an item set

- Once all item sets with minimum support have been generated, we can turn them into rules
- Example:

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

- Seven ($2^N$-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                                          4/12
```

# Rules for weather data

- 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 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
```

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)
```

# 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 frequent item set, then (A) and (B) have to be frequent item sets as well!
  - In general: if X is frequent *k*-item set, then all (*k*-1)-item subsets of X are also frequent

  $\Rightarrow$ Compute *k*-item set by merging (*k*-1)-item sets

# Example

- Given: five 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 (B C D)`**

  **`(A C D E)        Not OK because of (C D E)`**

- Final check by counting instances in dataset!
- ($k$ –1)-item sets are stored in hash table

# Generating rules efficiently

- We are looking for all high-confidence rules
  - Support of antecedent obtained from hash table
  - But: brute-force method is $(2^N-1)$
- 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 hash table!

# Association rules: discussion

- Above method makes one pass through the data for each different size item set
  - Other possibility: generate ($k$+2)-item sets just after ($k$+1)-item sets have been generated
  - Result: more ($k$+2)-item sets than necessary will be considered but less passes through the data
  - Makes sense if data too large for main memory
- Practical issue: generating a certain number of rules (e.g. by incrementally reducing min. support)

# Other issues

- Standard ARFF format very inefficient for typical *market basket data*
  - Attributes represent items in a basket and most items are usually missing
  - Need way of representing sparse data
- Instances are also called *transactions*
- Confidence is not necessarily the best measure
  - Example: milk occurs in almost every supermarket transaction
  - Other measures have been devised (e.g. lift)

# Linear models

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

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

- Weights are calculated from the training data
- Predicted value for first training instance **a**$^{(1)}$

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

# Minimizing the squared error

- Choose $k+1$ coefficients to minimize the squared error on the training data
- Squared error: $$\sum_{i=1}^{n}\left(x^{(i)}-\sum_{j=0}^{k}w_j a_j^{(i)}\right)^2$$
- Derive coefficients using standard 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 is known as *multi-response linear regression*

# Theoretical justification

*Observed target value (either 0 or 1)*

*Model* *Instance* *The scheme minimizes this*

$$E_y\{(f(X)-Y)^2 \mid X = x\}$$

*True class probability*

$$= E_y\{(f(X)-P(Y=1 \mid X=x)+P(Y=1 \mid X=x)-Y)^2 \mid X = x\}$$

$$= (f(x)-P(Y=1 \mid X=x))^2 + 2\times(f(x)-P(Y=1 \mid X=x))\times$$
$$E_y\{P(Y=1 \mid X=x)-Y \mid X=x\} + E_y\{(P(Y=1 \mid X=x)-Y)^2 \mid X=x\}$$

$$= (f(x)-P(Y=1 \mid X=x))^2 + 2\times(f(x)-P(Y=1 \mid X=x))\times$$
$$(P(Y=1 \mid X=x)-E_y\{Y \mid X=x\}) + E_y\{(P(Y=1 \mid X=x)-Y)^2 \mid X=x\}$$

$$= \underbrace{(f(x)-P(Y=1 \mid X=x))^2}_{\textit{We want to minimize this}} + \underbrace{E_y\{(P(Y=1 \mid X=x)-Y)^2 \mid X=x\}}_{\textit{Constant}}$$

# Pairwise regression

- Another way of using regression for classification:
  - A regression function for every *pair* of classes, using only instances from these two classes
  - Assign output of +1 to one member of the pair, –1 to the other
- Prediction is done by voting
  - Class that receives most votes is predicted
  - Alternative: “don’t know” if there is no agreement
- More likely to be accurate but more expensive

# Logistic regression

- Problem: some assumptions violated when linear regression is applied to classification problems
- *Logistic* regression: alternative to linear regression
  - Designed for classification problems
  - Tries to estimate class probabilities directly
    - Does this using the *maximum likelihood* method
  - Uses this linear model:

$$\log\left(\frac{P}{1-P}\right) = w_0 a_0 + w_1 a_1 + w_2 a_2 + \ldots + w_k a_k$$

***Class probability***

# Discussion of linear models

- Not appropriate if data exhibits non-linear dependencies
- But: can serve as building blocks for more complex schemes (i.e. model trees)
- Example: multi-response linear regression defines a *hyperplane* for any two given classes:

$$(w_0^{(1)} - w_0^{(2)})a_0 + (w_1^{(1)} - w_1^{(2)})a_1 + (w_2^{(1)} - w_2^{(2)})a_2 + \ldots + (w_k^{(1)} - w_k^{(2)})a_k > 0$$

# Instance-based representation

- Simplest form of learning: *rote learning*
  - Training instances are searched for instance that most closely resembles new instance
  - The instances themselves represent the knowledge
  - Also called *instance-based* learning
- Similarity function defines what's "learned"
- Instance-based learning is *lazy* learning
- Methods:
  - *nearest-neighbor*
  - *k-nearest-neighbor*
  - *...*

# The distance function

- Simplest case: one numeric attribute
  - Distance is the difference between the two attribute values involved (or a function thereof)
- Several numeric attributes: normally, Euclidean distance is used and attributes are normalized
- Nominal attributes: distance is set to 1 if values are different, 0 if they are equal
- Are all attributes equally important?
  - Weighting the attributes might be necessary

# Instance-based learning

- Distance function defines what's learned
- Most instance-based schemes use *Euclidean distance*:

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

  $\mathbf{a}^{(1)}$ and $\mathbf{a}^{(2)}$: two instances with $k$ attributes
- 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*:

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

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

# Discussion of 1-NN

- Often very accurate
- ... but slow:
  - simple version scans entire training data to derive a prediction
- Assumes all attributes are equally important
  - Remedy: attribute selection or weights
- Possible remedies against noisy instances:
  - Take a majority vote over the *k* nearest neighbors
  - Removing noisy instances from dataset (difficult!)
- Statisticians have used *k*-NN since early 1950s
  - If $n \to \infty$ and $k/n \to 0$, error approaches minimum

# Clustering

- Clustering techniques apply when there is no class to be predicted
- 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 algorithm called k-means
  - k-means clusters are disjoint, deterministic, and flat

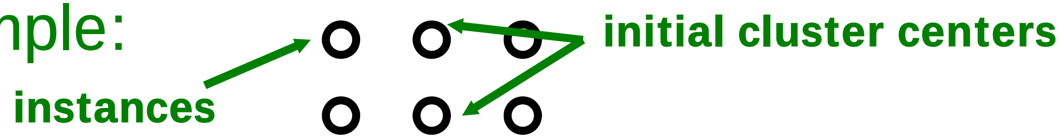
# The k-means algorithm

- To cluster data into k groups: (k is predefined)

1. Choose k cluster centers
   - e.g. at random
2. Assign instances to clusters
   - based on distance to cluster centers
3. Compute *centroids* of clusters
4. Go to step 1
   - until convergence

# Discussion

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




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

# Comments on basic methods

- Bayes' rule stems from his "Essay towards solving a problem in the doctrine of chances" (1763)
  - Difficult bit: estimating prior probabilities
- Extension of Naïve Bayes: Bayesian Networks
- Algorithm for association rules is called APRIORI
- Minsky and Papert (1969) showed that linear classifiers have limitations, e.g. can't learn XOR
  - But: combinations of them can ($\rightarrow$ Neural Nets)