DM & ML
Basic Methods

Gergely Lukács
Pázmány Péter Catholic University
Faculty of Information Technology and Bionics
Budapest, Hungary
lukacs@itk.ppke.hu

Simplicity first

- Different kinds of simple structures/algorithms exist:
  - One attribute
  - All attributes independently
  - A linear combination
  - An instance-based representation
- Simple algorithms often work surprisingly well
- Useful for understanding data
- Basis for more complicated algorithms

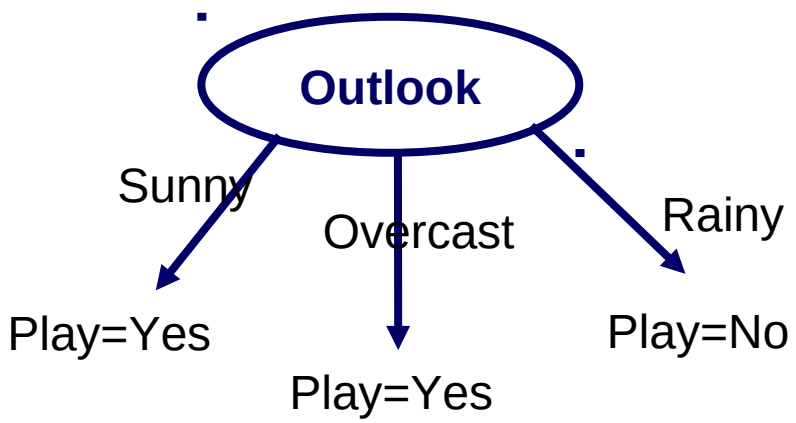
1R
(One Rule: decision tree with only one level)

1R: Output format

- 1R: „one rule”
  - for classification
  - set of „*rules*” that all test one particular attribute
    (== 1-level „decision tree” – see later; „decision stump”)

X				Y (class)
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

IF outlook=sunny THEN play=yes
IF outlook=overcast THEN play=yes
IF outlook=rainy THEN play=no



1R: Algorithm

- Basic version (assuming nominal attributes)
  - Create a ruleset for each of the attributes
    - One branch for each of the attribute's values
    - 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 and the corresponding ruleset with lowest error rate

1R Example: 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	
Temperature	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	

**** A random choice is made between 2 equal outcomes***

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
```

- “missing” is treated as a separate attribute value

Dealing with numeric attributes

- Numeric attributes are discretized: the range of the attribute is divided into a set of intervals:
  - Instances are sorted according to attribute's values
  - Breakpoints are placed where the class changes (so that the total error is minimized)
    - Equal values, different classes: majority class
- 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

The problem of **overfitting**

- Discretization procedure is very sensitive to noise
  - A single instance with an incorrect class label will most likely result in a separate interval
- Simple solution: **enforce minimum number of instances in majority class per interval**
- Weather data example (with minimum set to 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

Result of overfitting avoidance

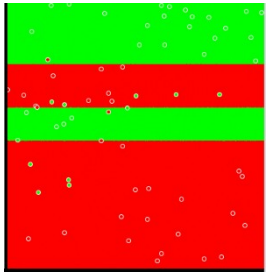
- Resulting rule sets:

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	

**** A random choice is made between 2 equal outcomes***

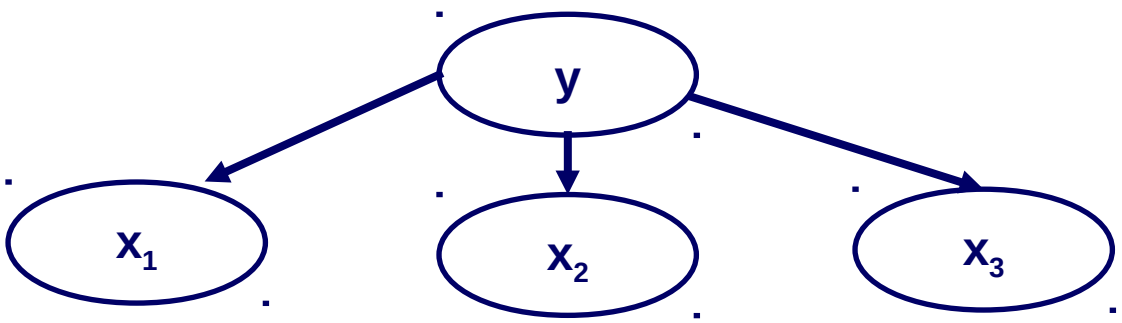
Discussion of 1R

- 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)
  - After some experimentation the minimum number of instances in majority class was set to 6
- Simplicity first …
- Data investigation …
  how important individual attributes are
- Part of more complexe algorithms
  (ensemble learning)
- Decision boundary
  - illustration with 2 input variables (two axes), binary classification (class: colour)



Naïve Bayes

NB: The model

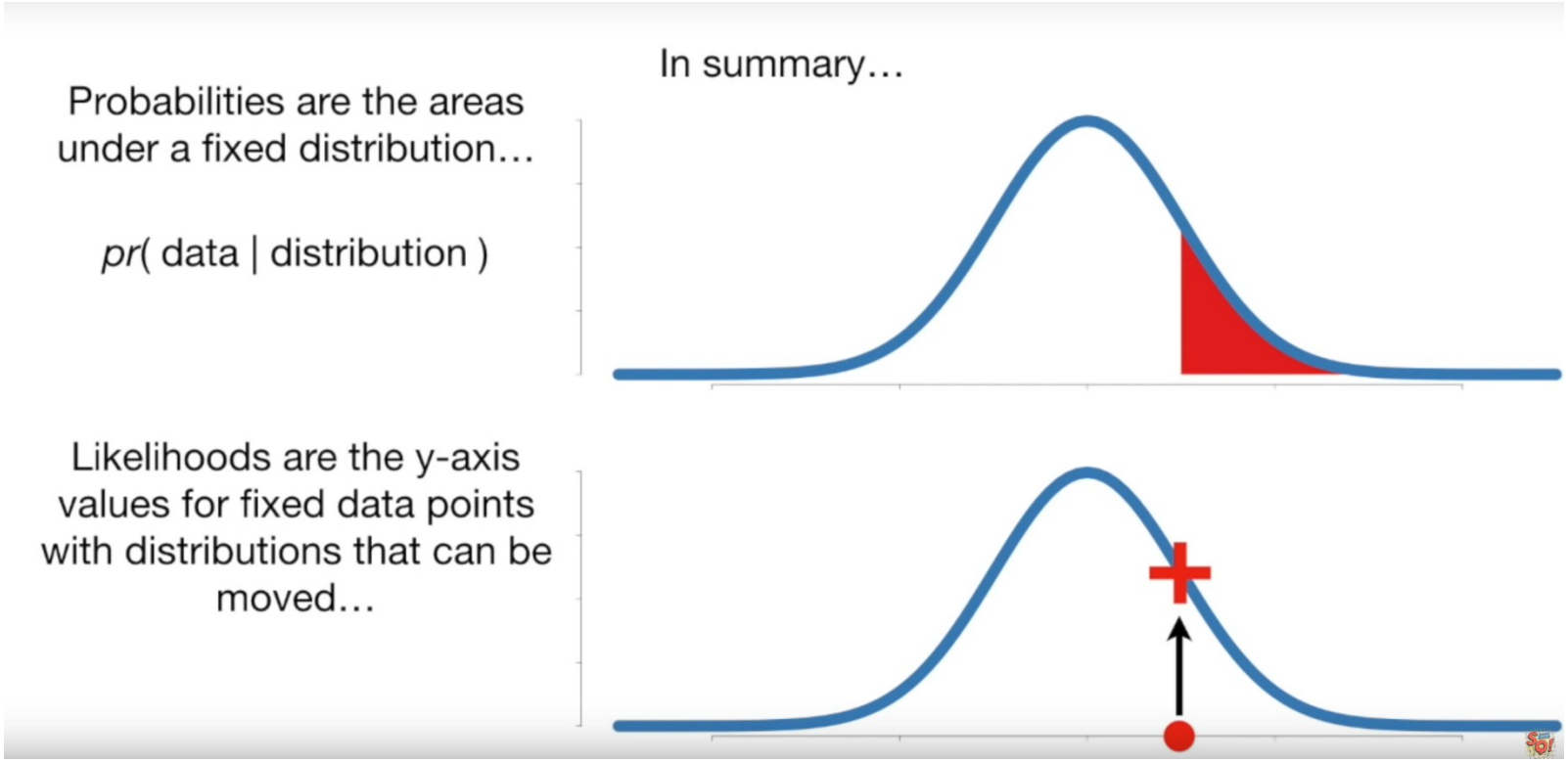


(class attribute,
y, dependent/output variable)

(x, independent/input variables)

- "Opposite" of 1R: use all attributes
- Assumption: Attributes are *statistically independent*, **given the class value**
  - This means that knowledge about the value of a particular attribute doesn't tell us anything about the value of another attribute -- **if the class is known**
  -
  - Fixed $$P(x|y) = P(x_1, x_2, \ldots|y) = P(x_1|y)P(x_2|y)\ldots = \prod_{i=1}^{n} P(x_i|y)$$
- Although assumption almost never (entirely) correct, this scheme works quite often well in practice!

Likelihood vs probability



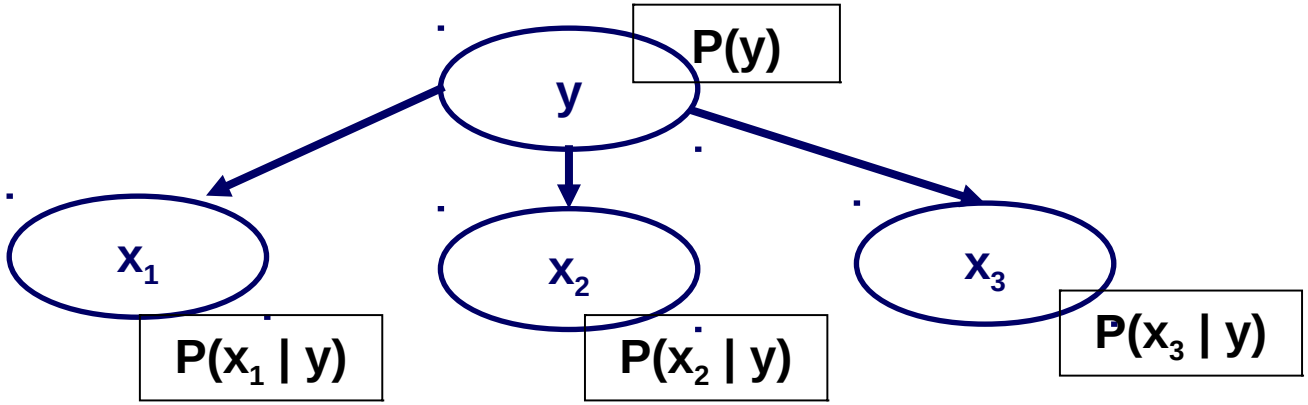
- **StatQuest: Probability vs Likelihood**
  https://www.youtube.com/watch?v=pYxNSUDSFH4

Maximum Likelihood Estimation

- **maximum likelihood estimation** (**MLE**) of parameters given observations. MLE attempts to find the parameter values that maximize the likelihood function, given the observations

- Naive Bayes: learning: estimating parameter values of the model given data, based on the MLE
  (Details: http://www.datasciencecourse.org/notes/mle/)

Naive Bayes: learning (training)



- **(Relative) frequencies of values in training data**
  - For binary classifier:

$$P(y=k) = \frac{1}{m} \times \#\{j | y^{(j)} = k\} \quad \text{and} \quad P(x_i = l | y = k) = \frac{\#\{j | y^{(j)} = k \text{ and } x_i^{(j)} = l\}}{\#\{j | y^{(j)} = k\}}$$

$$k \in \{0, 1\}, l \in [\![1, L]\!]$$

x_1			x_4	y
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 the weather data: Frequencies of cases

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								

Probabilities for the weather data: probability estimations

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

P(Outlook=Sunny| Play=Yes)

(Outlook: X1, E)

P(Play=Yes)

(Play: Y, class, H)

Can you draw the Naive Bayes network,
including the (conditional and apriori) probabilites?

NB: prediction (new/unknown instances)

- Classification learning: what's the probability of the class given the input attributes?

Probabilities for the weather data: Prediction task

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	?

The weather data example

Outlook	Temp.	Humidity	Windy	Play
Sunny	Cool	High	True	?

Evidence E (== X)

$$\Pr[yes \mid E] = \Pr[Outlook = Sunny \mid yes] \times$$
$$\Pr[Temperature = Cool \mid yes] \times$$
$$\Pr[Humdity = High \mid yes] \times$$
$$\Pr[Windy = True \mid yes] \times \frac{\Pr[yes]}{\Pr[E]}$$

Cond. probability for class "yes"
P(Play=yes\|Outlook=Sunny ^ ....)

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

Probabilities for the 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	?

Numerator

For “yes” = 2/9 × 3/9 × 3/9 × 3/9 × 9/14 = 0.0053

For “no” = 3/5 × 1/5 × 4/5 × 3/5 × 5/14 = 0.0206

Conversion into a probability by normalization (instead of by calculating the denominator, P(X)):

P(“yes”) = 0.0053 / (0.0053 + 0.0206) = 0.205

P(“no”) = 0.0206 / (0.0053 + 0.0206) = 0.795

The “zero-frequency problem”

- What if an attribute value doesn’t occur with every class value (e.g. “Outlook = Overcast” for class “no”)?
  - Probability will be zero!
  - *A posteriori* probability will also be zero!
    (No matter how likely the other values are!)
- Remedy: add 1 to the count of **every** value-class combination for such problematic attribute („*Laplace estimator”)*
- Result: probabilities will never be zero

$$\Pr[Outlook = Overcast \mid no] = 0$$

$$\Pr[no \mid E] = 0$$

Applying Laplace estimator

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			Temperature		Humidity			Windy		Play	
	Yes	*No*		*Yes*	*No*		*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	4	Hot	2	2	High	3	4	False	6	2	9	5
Overcast	4	1	Mild	4	2	Normal	6	1	True	3	3		
Rainy	3	3	Cool	3	1								
Sunny	2/9	4/8	Hot	2/9	2/5	High	3/9	4/5	False	6/9	2/5	9/14	5/14
Overcast	4/9	1/8	Mild	4/9	2/5	Normal	6/9	1/5	True	3/9	3/5		
Rainy	3/9	3/8	Cool	3/9	1/5								

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	?

Numerator for “yes” = 3/9 × 3/9 × 3/9 × 9/14 = 0.0238

Numerator for “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%

Dealing with numeric attributes

- Usual assumption: attributes have a *normal/Gaussian* probability distribution (given the class)
- The *probability density function* for the normal distribution is defined by two parameters:
  - The *sample mean* μ:

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

  - The *standard deviation* σ:

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

  - The density function *f(x)*:

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Statistics for the weather data

Outlook				Temperature			Humidity			Windy			Play	
	Yes	*No*		*Yes*	*No*		*Yes*	*No*		*Yes*	*No*	*Yes*	*No*
Sunny	2	3		83	85		86	85	False	6	2	9	5
Overcast	4	0		70	80		96	90	True	3	3		
Rainy	3	2		68	65		80	70					
				64	72		65	95					
				69	71		70	91					
				....			....						
Sunny	2/9	3/5	*mean*	73	74.6	*mean*	79.1	86.2	False	6/9	2/5	9/14	5/14
Overcast	4/9	0/5	*std dev*	6.2	7.9	*std dev*	10.2	9.7	True	3/9	3/5		
Rainy	3/9	2/5											

- Example density value:

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

Probability densities

- Relationship between probability and density:

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

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

- But: this doesn't change calculation of *a posteriori* probabilities because ε cancels out

Classifying a new day

- A new day:

Outlook	Temp.	Humidity	Windy	Play
Sunny	66	90	true	?

Numerator of "yes" = 2/9 × 0.0340 × 0.0221 × 3/9 × 9/14 = 0.000036

Numerator of "no" = 3/5 × 0.0291 × 0.0380 × 3/5 × 5/14 = 0.000136

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

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

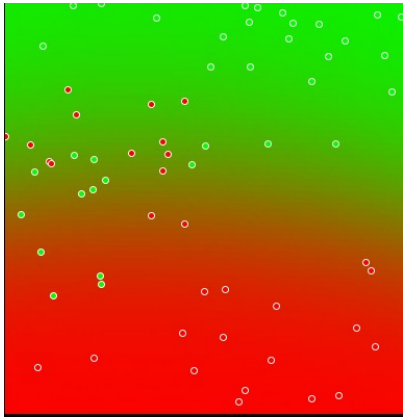
- Note also: many numeric attributes are not normally distributed
  - Known distribution: work with it
  - Unknown distribution: *kernel density estimators*
- Missing values during training: not included in calculation of mean and standard deviation

Discussion of Naïve Bayes

- Naïve Bayes works surprisingly well (even if independence assumption is clearly violated)
- Too many ***redundant attributes*** (e.g. identical attributes) will cause problems
- ***Irrelevant attributes*** are OK, they are filtered out
- Fast to train, fast to classify
  - even for large number of attributes
  - incremental model building possible (streamed data)
- Outputs probability (?) distribution, not just a single class (+)
- (Does not learn training data perfectly (+/-))
- Typical application: text/spam detection

Discussion of Naïve Bayes, 2

- Decision boundary….

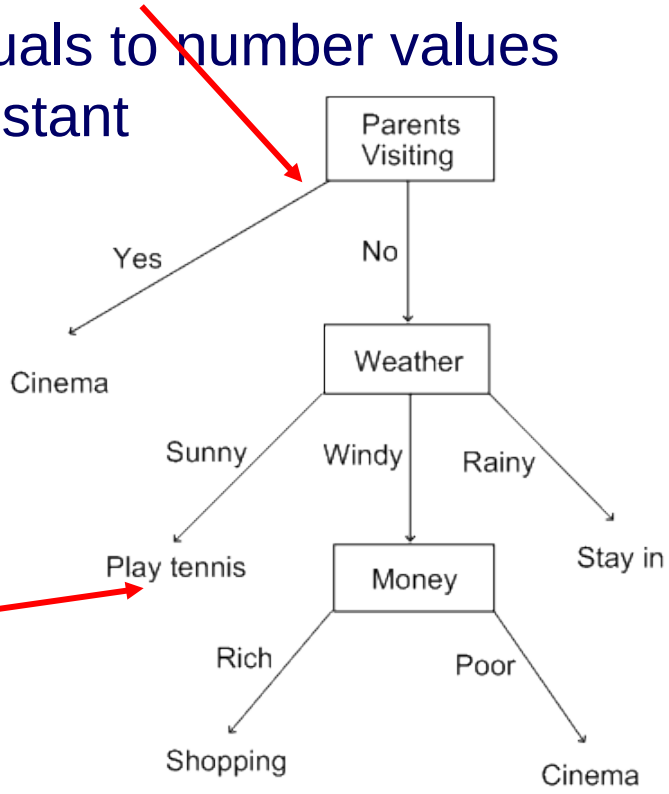


Divide-and-conquer
Decision tree
ID3

DECISION TREE – AS KNOWLEDGE REPRESENTATION

Decision trees
(for **classification**)

- Nodes involve testing a particular attribute
  Nominal attributes:
  - number of children (branches) equals to number values
  - attribute value is compared to constant

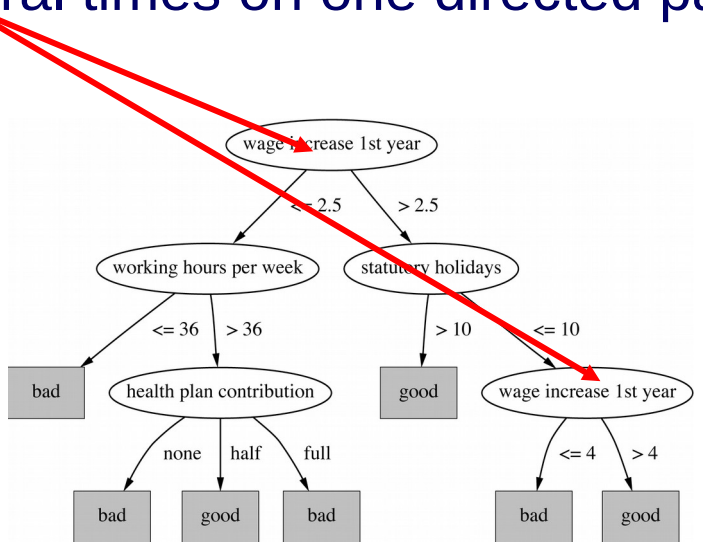


- Leaves assign
  - a class value to instances

(Parameters of decision tree?)

Testing numeric attributes

- Numeric attribute
  - test whether value is greater or less than constant
  - attribute may get tested several times on one directed path



(Parameters of decision tree?)

Missing values (for prediction!)

- ***Does absence of value have some significance?***
- Yes ⇒ “missing” is a separate value
- No ⇒ “missing” must be treated in a special way
  - Solution A: assign instance to ***most popular branch***
  - Solution B: split instance into pieces
    - Pieces receive ***weight according to fraction of training instances*** that go down each branch
  - For both, we need statistics on the training data

Extensions to Decision Trees

- Testing nominal attributes
  - division into subsets of values
  - comparing values of two attributes
  - using a function of one or more attributes
- Testing numeric attributes
  - three/multi-way split)
- Leaf nodes
  - probability distribution
  - set of class values

LEARNING A DECISION TREE – ID 3 ALGORITHM

Constructing decision trees

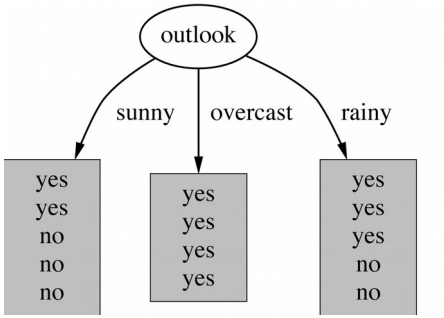
- Preferred: small decision tree (== small number of levels/attributes tested)
- Normal procedure: greedy algorithm, top down in recursive *divide-and-conquer* fashion
  - Attribute is selected for root node and branch is created for each possible attribute value
  - Instances are split into subsets (one for each branch extending from the node)
  - Procedure is repeated recursively for each branch, using only instances that reach the branch
- Process stops if all instances have the same class
  - or no further split makes them purer

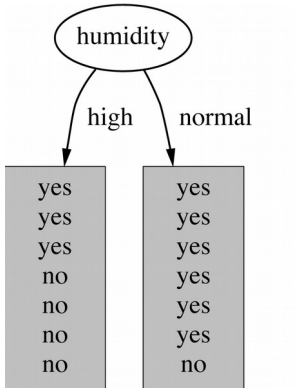
Example

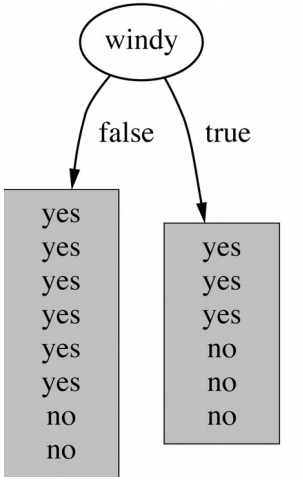
Which attribute for the root?

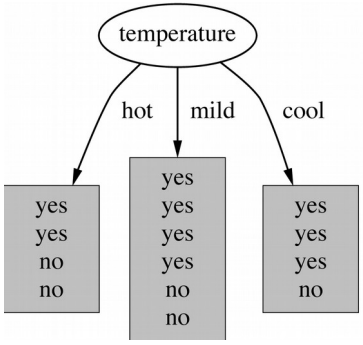
(class attr, y)

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









A criterion for attribute selection

- Which is the best attribute?
  - Greedy algorithm for small 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 that an attribute produces
- Strategy: choose attribute that results in greatest information gain

- „purity": entropy (arguments later…)

Example: attribute *Outlook*

- *Outlook = Sunny* :

  Info([2,3]) = entropy(2/5,3/5)=
  = $-2/5\log_2(2/5)-3/5\log_2(3/5)$=0.971 bits

- *Outlook = Overcast* :

  Info([4,0]) = entropy(1,0)= 0 bits

- *Outlook = Rainy* :

  Info([3,2]) = entropy(3/5,2/5)=
  = $-3/5\log_2(3/5)-2/5\log_2(2/5)$=0.971 bits

- Expected information for attribute
  (weighed sum, weighs: number of instances):

  Info([2,3], [4,0], [3,2]) = 5/14 * 0.971 + 4/14 * 0 + 5/14 * 0.971 =
  = 0.693 bits

Computing information gain

- Information gain:

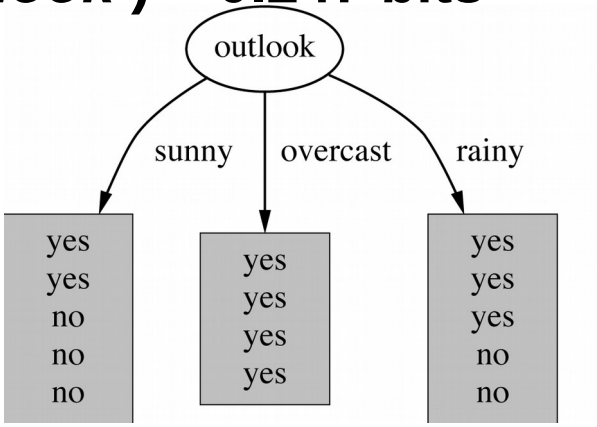
  information before splitting – information after splitting

  gain(*Outlook*) = info([9,5]) – info([2,3],[4,0],[3,2])

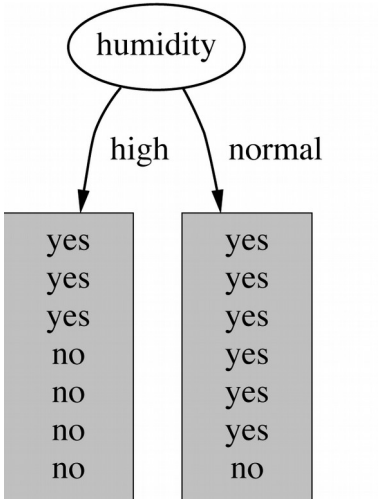
  = 0.940 – 0.693 = 0.247 bits

Which attribute to select?

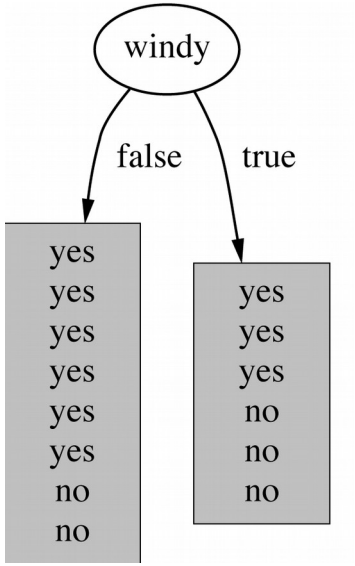
gain(*Outlook*) = 0.247 bits



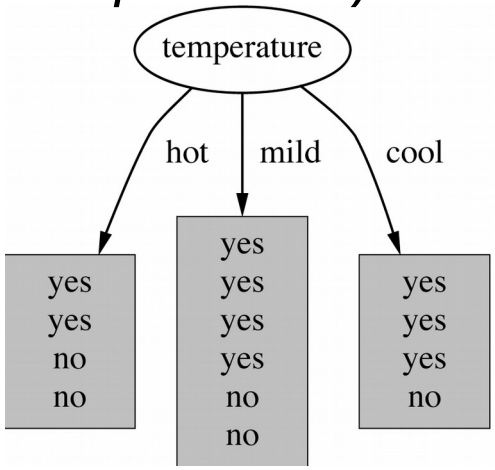
gain(*Humidity*) = 0.152 bits



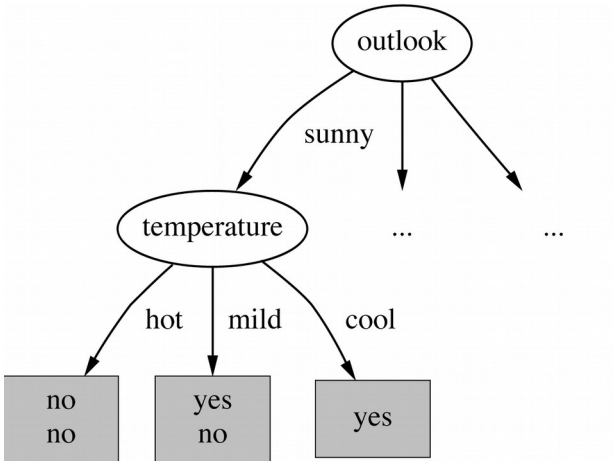
gain(*Windy*) = 0.048 bits

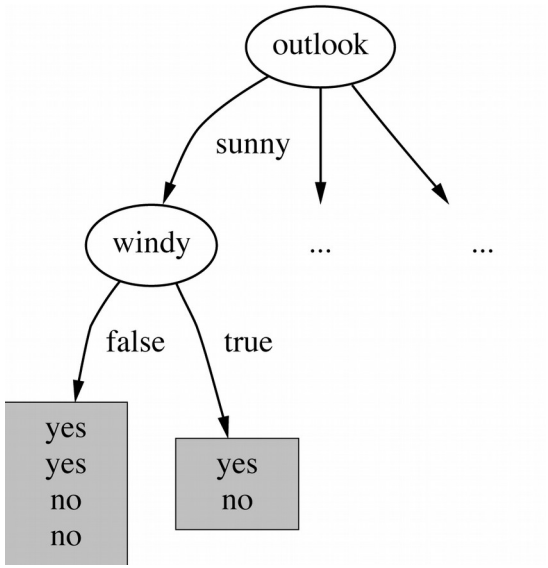


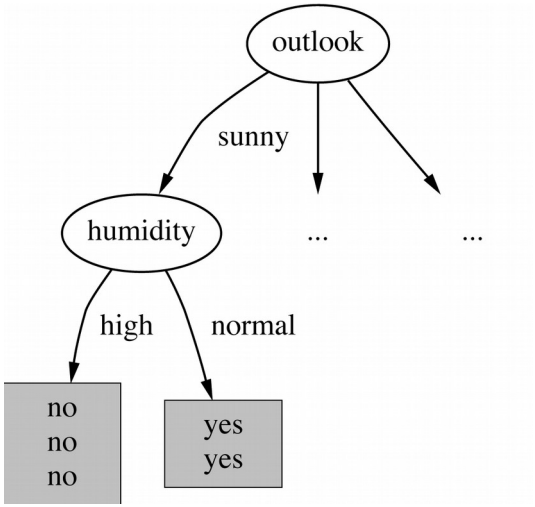
gain(*Temperature*) = 0.029 bits



Continuing to split





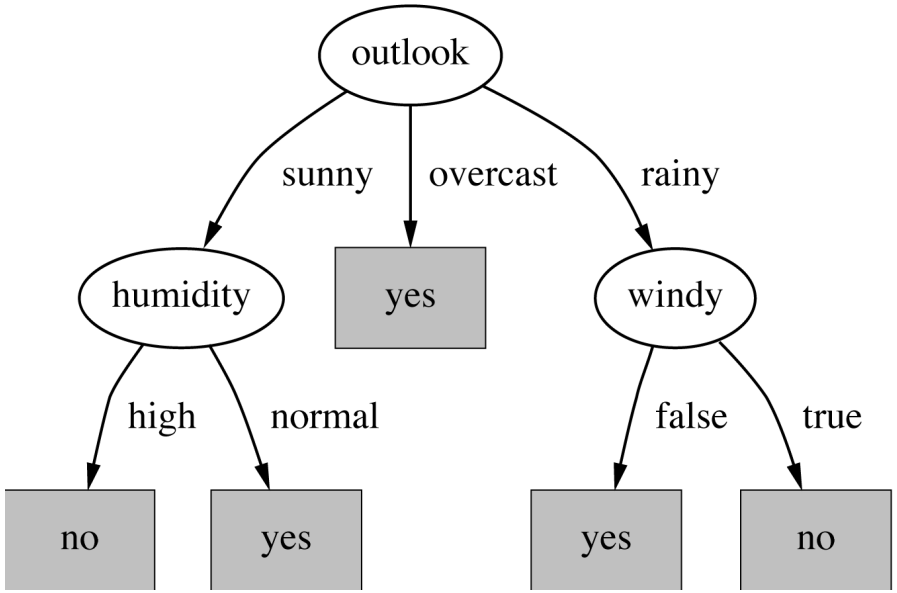


gain("Temperature") = 0.571 bits

gain("Windy") = 0.019 bits

gain("Humidity") = 0.971 bits

The final decision tree



- Note: *not* all leaves need to be pure; sometimes identical instances have different classes
  ⇒ Splitting stops when data can't be split any further

Wish list for a purity measure

- Properties we require from a purity measure
  - Pure node: zero
  - Impurity is maximal (i.e. all classes equally likely): maximal (e.g., binary case: 1)
  - ***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!

Entropy

- Information is measured 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 (this can involve fractions of bits!)
- Formula for computing the entropy:

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

- The multistage property:
-

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

(where p+q+r = 1)

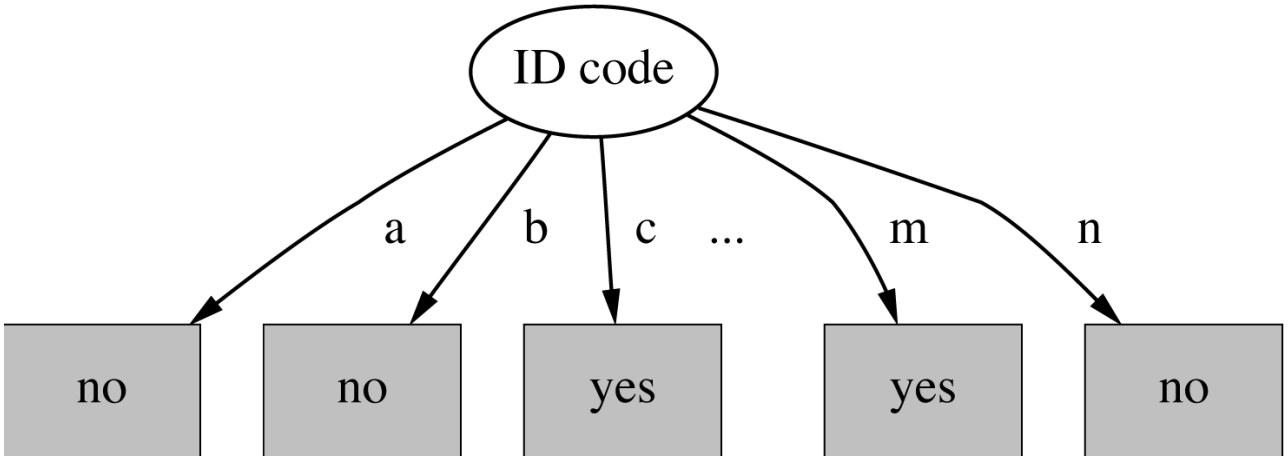
Highly-branching attributes

- 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)

The weather data with ID code (extreme example)

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:

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

⇒Information gain is maximal for ID code (namely 0.940 bits)

The gain ratio

- *Gain ratio*: a modification of the information gain that reduces its bias towards highly branching attributes
- Gain ratio takes the number and the size of branches into account when choosing an attribute (disregarding the class values!)
  - It corrects the information gain by taking the *intrinsic information* of a split into account
- Intrinsic information: entropy of distributing 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:

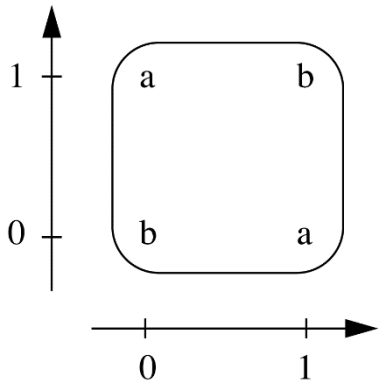
$$\text{gain\_ratio}(\text{"Attribute"}) = \frac{\text{gain}(\text{"Attribute"})}{\text{intrinsic\_info}(\text{"Attribute"})}$$

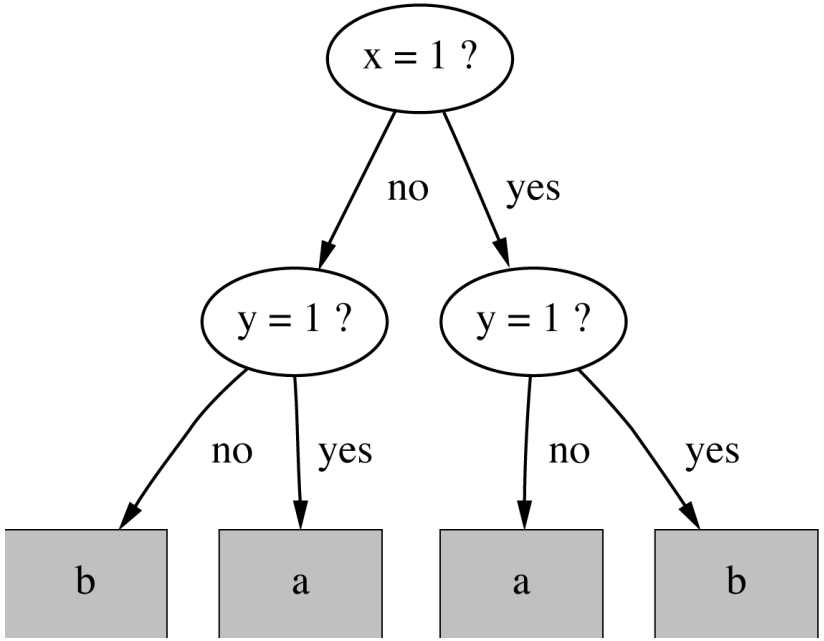
- Example: $\text{gain\_ratio}(\text{"ID\_code"}) = \frac{0.940 \text{ bits}}{3.807 \text{ bits}} = 0.246$

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: 0.029/1.362	0.021
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

Knowledge representation: decision tree (extension): XOR





- awkward representation
- hard to learn
- XOR problem fortunately rare

Discussion

- Algorithm for top-down induction of decision trees (“ID3”) was developed by Ross Quinlan
  - Led to development of C4.5, which can deal with numeric attributes, missing values, and noisy data
- Similar approach: Regression tree (CART: Classification and Regression Tree)
- There are many other attribute selection criteria! (But almost no difference in accuracy of result.)
- Decision Tree: „white box”
- Decision Trees: traditionally most widely used ML models!

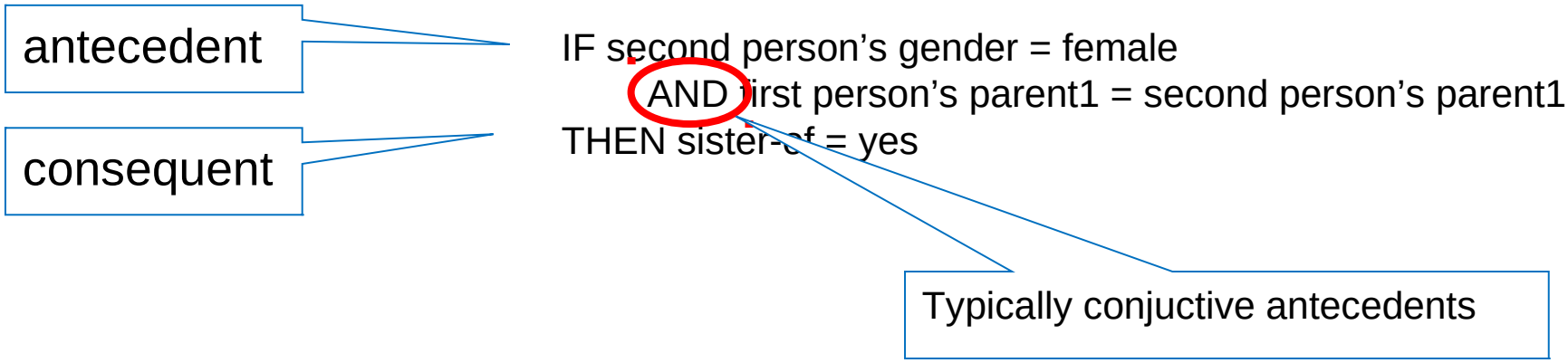
Classification Rule (learning)

Knowlege Representation: Classification rules

- Popular alternative to decision trees

- *Antecedent* (pre-condition): a series of tests (just like the tests at the nodes of a decision tree)
  - tests are usually logically AND-ed together
  - but may also be general logical expressions
- *Consequent* (conclusion):
  - classes, or
  - set of classes, or
  - probability distribution assigned by rule
- Individual rules are often logically OR-ed together…

Classification rule - example



“Nuggets” of knowledge

- Are rules independent pieces of knowledge? (It seems easy to add a rule to an existing rule base.)
- Problem: ignores how rules are executed
- Two ways of executing a rule set:
  - Ordered set of rules (“decision list”)
    - Order is important for interpretation
  - Unordered set of rules
    - Rules may overlap and lead to different conclusions for the same instance

Interpreting rules

- What if two or more rules conflict?
  - Give no conclusion at all?
  - Go with rule that is most popular on training data?
  - …
- What if no rule applies to an instance?
  - Give no conclusion at all?
  - Go with class that is most frequent in training data?
  - …

From trees to rules

- Easy: converting a tree into a set of rules
  - one rule for each leaf:
    - antecedent contains a condition for every node on the path from the root to the leaf
    - consequent is class assigned by the leaf
- Produces rules that are unambiguous
  - doesn't matter in which order they are executed
- But: resulting rules are unnecessarily complex

From rules to trees

- More difficult: transforming a rule set into a tree
  - tree cannot easily express disjunction between rules

Linear models for „regression” (=predicting numeric value)

Linear regression Knowledge Representation

- Inputs (attribute values) and output are all numeric
- Output is the sum of weighted attribute values (linear combination)
  - $x = w_0 + w_1 a_1 + w_2 a_2 + \ldots + w_k a_k$

The trick is to find good values for the weights

(Parameters of linear regression?)

Example: Predicting CPU performance

209 different computer configurations

	Cycle time (ns)	Main memory (Kb)		Cache (Kb)	Channels		Performance
	MYCT	MMIN	MMAX	CACH	CHMIN	CHMAX	PRP
1	125	256	6000	256	16	128	198
2	29	8000	32000	32	8	32	269
...							
208	480	512	8000	32	0	0	67
209	480	1000	4000	0	0	0	45

```
PRP =
    - 56.1
     + 0.049 MYCT
     + 0.015 MMIN
     + 0.006 MMAX
     + 0.630 CACH
     - 0.270 CHMIN
     + 1.46 CHMAX
```

Linear regression – Training

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

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

- Error, squared error for single training instance
- Mean Squared Error (MSE), or L2 loss

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

- Coefficients/weights (k+1) are chosen so that MSE the training data is minimized
- Assumptions …
  - Error: Normal distribution

Linear Regression: Training 2

- Can be done if there are more instances than attributes

- Coefficients can be derived using matrix inversion (expensive, for small datasets)
- Iterative solution -- gradient decent -- computationally less expensive

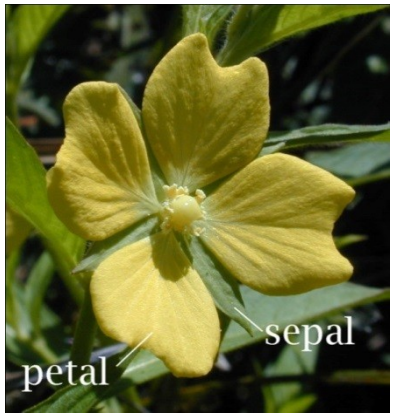
Linear Regression: Training 3

- MSE sensitive to outliers!
- Minimization of *absolute error* is more difficult!

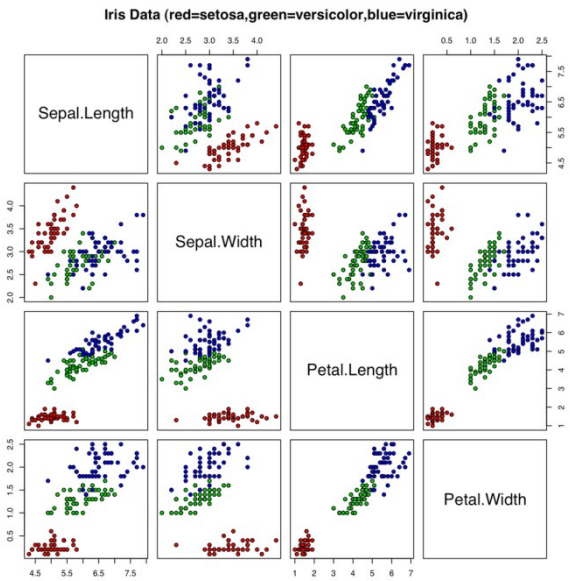
Linear models for binary classification

- Binary classification
- Prediction is made by plugging in observed values of the attributes into the expression
  - Predict one class if output > 0 (or 0.5, …), and the other class if output < 0 (or 0.5, …)
- Decision boundary
  - defines where the decision changes from one class value to the other
  - hyperplane (high-dimensional plane)

Example: Classifying iris flowers

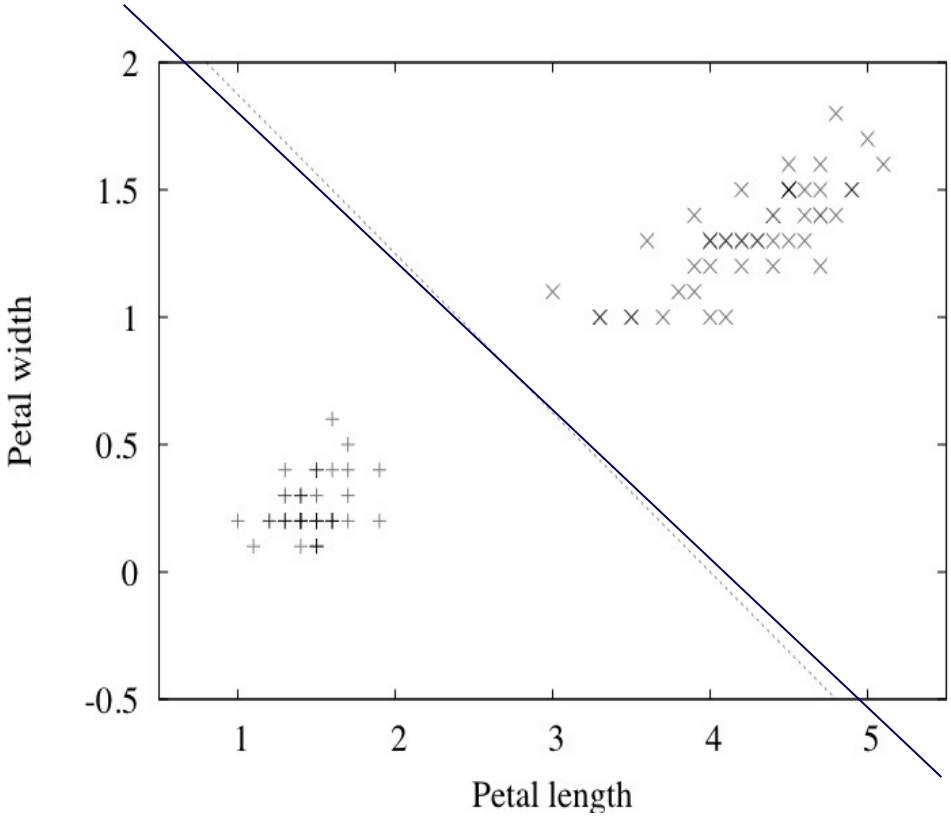


	Sepal length	Sepal width	Petal length	Petal width	Type
1	5.1	3.5	1.4	0.2	Iris setosa
2	4.9	3.0	1.4	0.2	Iris setosa
…					
51	7.0	3.2	4.7	1.4	Iris versicolor
52	6.4	3.2	4.5	1.5	Iris versicolor
…					
	6.3	3.3	6.0	2.5	Iris virginica
	5.8	2.7	5.1	1.9	Iris virginica



http://en.wikipedia.org/wiki/Iris_flower_data_set

Separating setosas from versicolors



- **2.0 – 0.5PETAL-LENGTH – 0.8PETAL-WIDTH = 0 (2 input attributes)**

Classification

- Problems
  - membership values are not in [0,1] range, so aren't proper probability estimates
  - assumptions used in least-square regression
    - normal distribution with same standard deviation for 0 -1 values ??!!

Linear models: logistic regression

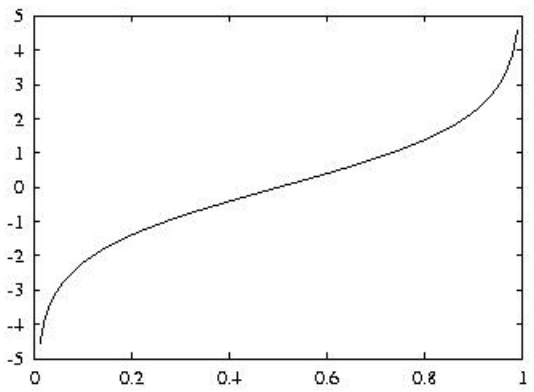
- Linear model for a transformed target variable
- Assume we have two classes
- Logistic regression replaces the target

$$P[1|a_1, a_2, \ldots, a_k]$$

- by this target

$$\log\left(\frac{P[1|a_1, a_2, \ldots, a_k]}{(1-P[1|a_1, a_2, \ldots, a_k])}\right)$$

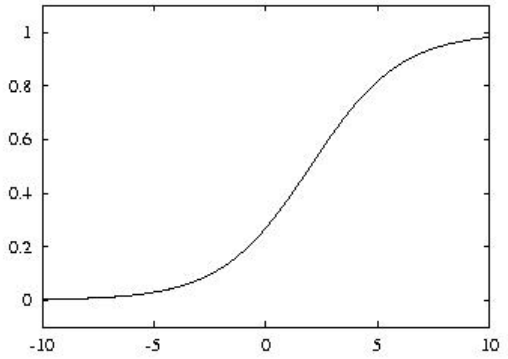
- Logit transformation maps [0,1] to (-oo , +oo) (Inverse function of logit: sigmoid function)



Logit transformation (Sigmoid function): Resulting model

$$Pr[1|a_1, a_2, \ldots, a_k] = \frac{1}{(1+e^{-w_0-w_1a_1-\ldots-w_ka_k})}$$

- Example
  - Model with
    - w_0 = 0.5 (moves curve left-right) and
    - w_1 = 1 (steepness)



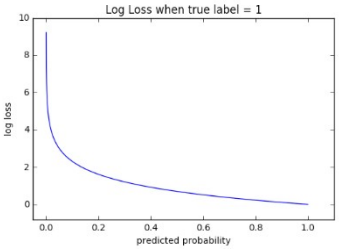
Maximum likelihood

- Parameters are found from training data using *maximum likelihood*
- Aim: choosing parameters to maximize probability of training data („maximum likelihood”)
  - Independence: probabilities multiplied
  - Maximizing multiplied probabilites : maximizing sum of logarithms 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 $x^{(i)}$ are either 0 or 1

Log loss $\sum -y_i z_i + \log(1 + e^{z_i})$



Logistic regression 2

- The independent variables should be independent of each other. That is, the model should have little or no multicollinearity.
- The independent variables are linearly related to logit function - probability.
- Logistic regression requires quite large sample sizes.

Linear models are hyperplanes

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

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

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

Linear models: the perceptron

- Don't actually need probability estimates if all we want to do is classification
- Different approach: learn separating hyperplane
- Assumption: data is *linearly separable*
- Hyperplane: $$0 = w_0 a_0 + w_1 a_1 + w_2 a_2 + \ldots + w_k a_k$$

  where we again assume that there is a constant attribute with value 1 (a0, *bias*)
- If sum is greater than zero we predict the first class, otherwise the second class

Perceptron learning rule

```
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 situation where instance *a* pertaining to the first class has been added:

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

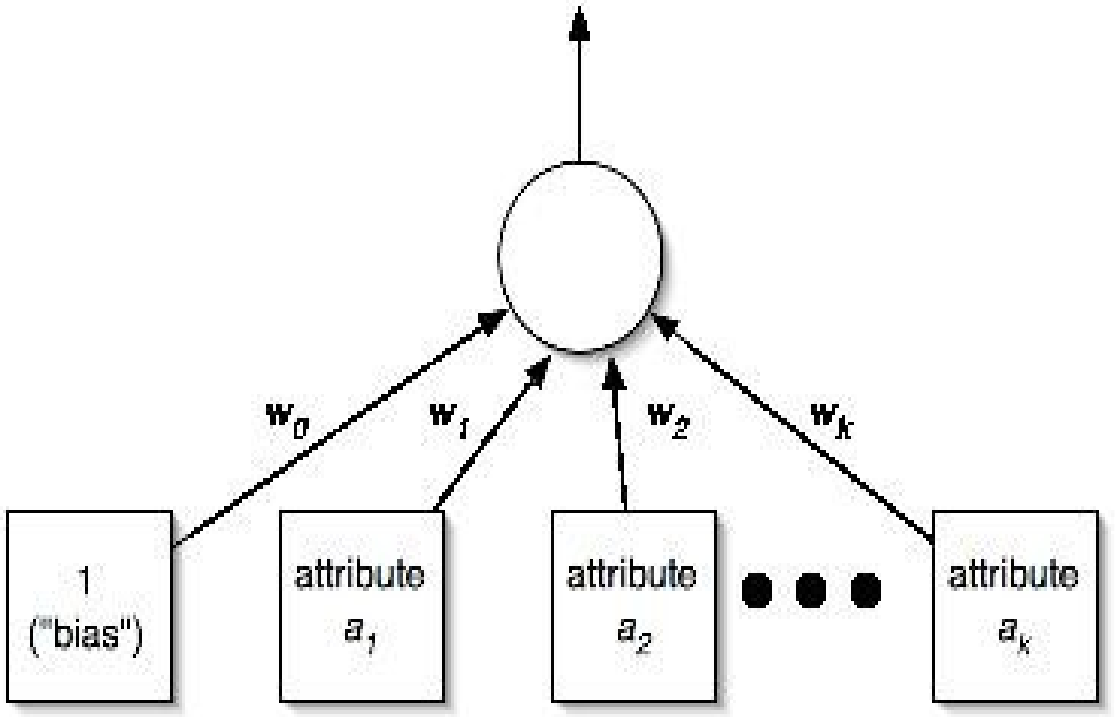
  This means output for *a* has increased by:

  $$a_0a_0+a_1a_1+a_2a_2+\ldots+a_ka_k$$

  This number is [illegible] has moved into the correct direction (and we can show output decreases for instances of other class)
- Convergence guaranteed -- if data linearly separable --, upper bound on number of steps

Perceptron as a neural network

Output layer



Input layer

Linear models: Winnow

- Binary classification
- Mistake-driven
- **Multiplicative updates** (perceptron: additive updates):
  - Weights are multiplied (or divided) by a user-specified parameter (alpha > 1)
- User-specific threshold (perceptron: 0)
  - Predict first class, if: $w_0 a_0 + w_1 a_1 + w_2 a_2 + \ldots + w_k a_k > \theta$

Winnow learning rule

```
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)
```

- Effectively focuses on relevant features

Instance-based learning

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
    - ***Lazy learning!***
  - Also called *instance-based* learning
- Similarity function

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: typically Euclidean distance is used and attributes are **normalized**

- Taking the square root is not required when comparing distances
- Other popular metric: *city-block metric*
  - Adds differences without squaring them

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

The distance function

- 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

Discussion of nearest-neighbor learning

- Statisticians have used *k*-NN since early 1950s
- Often very accurate

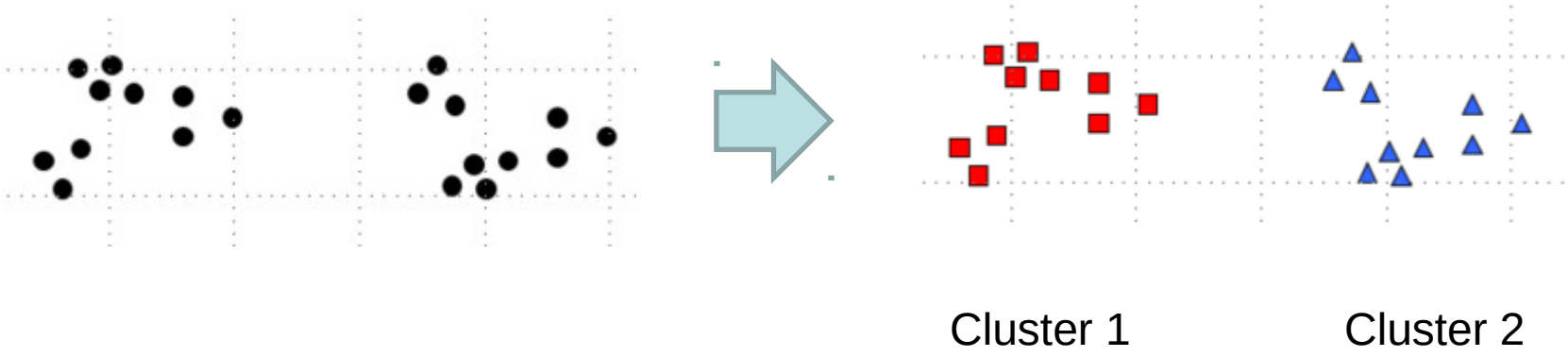
Limitations (of the basic algorithm)

- White box, generalisation ?!
- Speed (of prediction!!)
  - E.g. 1E6 instances, 100 attributes (dimensions)
- Noisy data ?!
- Domains of attributes different ?!
  - comparing e.g. [0,1] with [-5000,5000] ?
- Irrelevant attributes (only noise, with no relevance)

Clustering

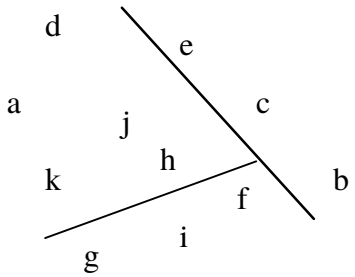
Clustering: Knowledge Representation

- Divide instances into “natural” groups (clusters)
  - Instances in a group (cluster) similar to each other, in some or the other way
  - No class attribute, unlabelled data
  - Unsupervised learning

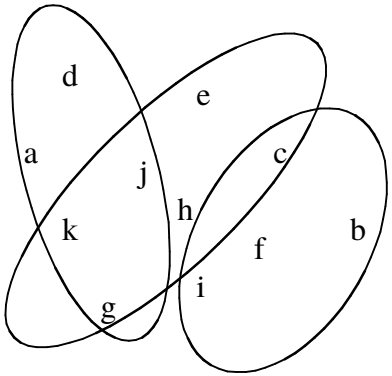


Representing clusters I

Simple 2-D representation



Venn diagram



disjoint vs. overlapping

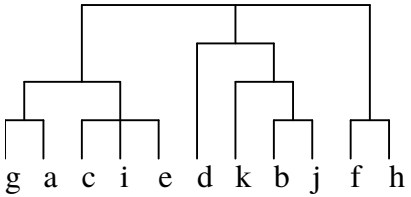
Representing clusters II

Probabilistic assignment

	1	2	3
a	0.4	0.1	0.5
b	0.1	0.8	0.1
c	0.3	0.3	0.4
d	0.1	0.1	0.8
e	0.4	0.2	0.4
f	0.1	0.4	0.5
g	0.7	0.2	0.1
h	0.5	0.4	0.1
…			

probabilistic (vs. deterministic)

Dendrogram



NB: dendron is the Greek word for tree

hierarchical (vs. flat)

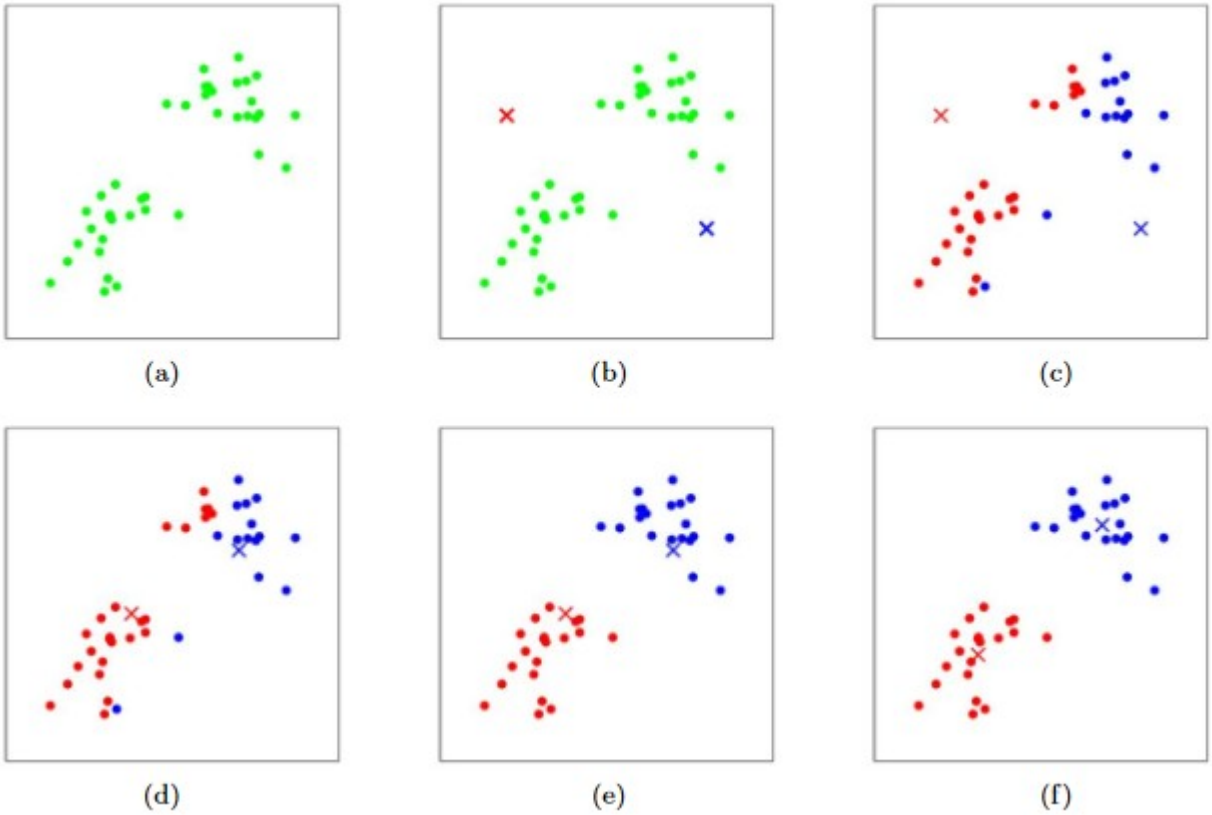
The *k* -means algorithm

- disjoint, deterministic, and flat clusters
- number of clusters (k) preselected

1. Choose *k* cluster centers (e.g. randomly)
2. Repeat until convergence
   1. assign instances to clusters (based on distance; closest cluster center)
   2. compute *centroids* of clusters

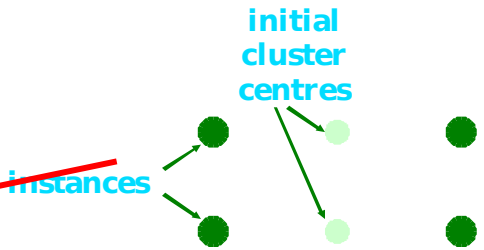
   (convergence: assignment of instances to clusters do not change)

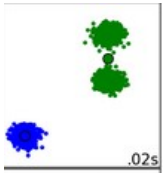
K-means: illustration

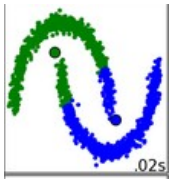


Discussion

- Algorithm minimizes squared distance to cluster centers
- Converges
  - distortion function (==sum of squared errors) converges
  - typically also cluster centers and assignment of instances to clusters)
- Result can vary significantly
  - based on initial choice of seeds
    (restarting with different random seeds)
- Can get trapped in local minimum
  (in practice not typical)
- Number of clusters?
- Distance?
- Speed of distance calculations…
- Probabilistic, hierarchical, overlapping…







Mining Association Rules (Apriori Algorithm)

Association rules (knowledge representation)

- Form of rules
  If a and b and c occurs in the set, then t is also part of the set
  - **if** Milk = true **and**
    Bread = True
    then Eggs = true **and**
    Coke = True

- Typically boolean attributes
  - Compact notation: **if** Milk and Bread **then** Eggs and Coke
- No selected class attribute
- Multiple attributes on consequent side possible/typical
- Rules interpreted individually!
  - **if** Milk **and** True **then** Eggs **and** Coke

Association rule mining, applications

- Application areas
  - Market basket analysis
  - ~Sequence mining

TID	Items
1	Bread, Milk
2	Bread, Diaper, Beer, Eggs
3	Milk, Diaper, Beer, Coke
4	Bread, Milk, Diaper, Beer
5	Bread, Milk, Diaper, Coke

{Diaper} → {Beer},
{Milk, Bread} → {Eggs,Coke},
{Beer, Bread} → {Milk},

Association rule mining

Immense number of potential rules…

Sufficiently **general** rules

Sufficiently **correct/ precise** rules

a,**b,c,d,**e
b,c,d
a,**b,c,d**
a,**b,c,d,**e
a,c,e,f
d,c,e,f
a,**b,c,d,**f

b,c,d co-occur

in 71% of the cases

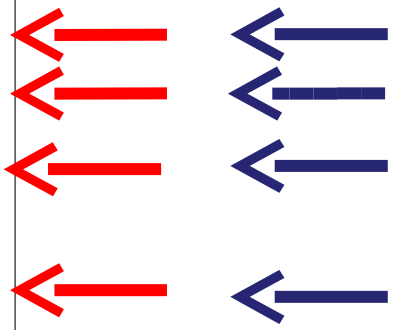
If b and c then d
in 100% of the cases

Support and confidence of a rule

- (Rule: X -> Y)
- *Support/coverage*: number of instances predicted correctly
  - Supp(X and Y) „*Itemset*" – no matter, whether an item (attribute) is on the left or on the right hand side of the rule
  - Can also be calculated as a relative number (relative to the number of all instances)
- *Confidence/accuracy*: number of correct predictions, as proportion of all instances that rule applies to
  - confidence=Supp(X and Y)/Supp(X)
- *Lift*: How popular is Y, when X, **considering also how popular Y is**
  - lift= Confidence of Rule / Relative support of Y
  - 1: no association,
    >1 Y is more likely when X,
    <1 Y is less likely when X

Association rules
Example for support & confidence

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



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

support = 4
confidence = 100%

```
If temperature = cool
then play= yes
```

support = 3
confidence = 75%

Interpreting association rules

Interpretation is not obvious:

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

is *not* the same as the two rules

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

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

It means that the following **also** holds:

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

Why?

Interpreting association rules

Interpretation is not obvious:

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

is *not* the same as the two rules

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

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

It means that the following **also** holds:

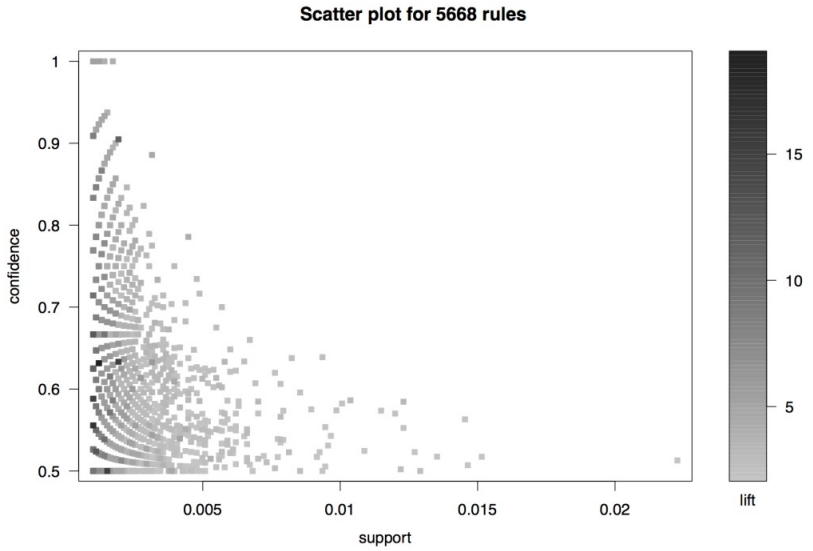
```
If humidity = high
    and windy = false
    and play = no
then outlook = sunny
```

Why?
Support…
Confidence…

ASSOCIATION RULES: APRIORI ALGORITHM

Mining association rules

- Normally: minimum support and confidence pre-specified (e.g. for weather data:
  support $\geq$ 2 and confidence $\geq$ 95%, -> 58 rules)
- Brute force: All rules, filtering on the bases of support and confidence
- Immense number
  of possible associations
- Computational complexity!



Association rules

- But: we can look for high support rules (itemsets) and high confidence rules directly!
- Two steps
  1. High support (frequent item sets)
  2. High confidence

Frequent 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 (that is, attribute-value pair)
- *Item set*: all items occurring in a rule (LHS and RHS !!)
- Goal: only rules that exceed pre-defined support

  ⇒ We can do it by finding all item sets with the given minimum support (=frequent item sets) and generating rules from them!

Frequent Item Sets for weather data

One-item sets	Two-item sets	Three-item sets	Four-item sets
Outlook = Sunny (5)	Outlook = Sunny Temperature = Mild (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)
…	…	…	…

- Number of frequent item sets (with minimum support of two) :
  - 12 with 1 item,
  - 47 with 2 items,
  - 39 with 3 items,
  - 6 with 4 items
  - 0 with 5 items

Generating item sets efficiently

- How can we efficiently find all frequent item sets (item sets with support value higher than the threshold for support)?

- If (A B) is frequent item set, then (A) and (B) have to be frequent item sets as well!
  - Necessary, but not sufficient condition: if (A) and (B) are frequent item sets, (A B) is not necessaryily frequent, too.
- In general: if X is frequent *k*-item set, then all (*k*-1)-item subsets of X are also frequent

Generating item sets efficiently

- Find frequent (support larger than threshold) one-item sets
- Compute candidate frequent *k*-item sets by merging frequent (*k*-1)-item sets
- Check (real) support of candidate frequent k-items sets
  by reading through the whole database

- Remark: The algorithm reduces the number of k-item sets, the support of which has to be checked by reading through the whole database.

An 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 frequent four-item sets:

  `(A B C D)` `candidate`

  `(B C D E)` `no candidate, e.g., because of (C D E)`

- Check real support by counting instances in dataset!

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	4/14

Rules with same itemset: all k-1 consequent rules have at least the same confidence, as k consequent rules

Generating rules efficiently

- We are looking for all high-confidence rules
  - Which items on the RHS of the rule?
  - But: brute-force method is (2^N-1)
- Observation: (c + 1)-consequent rule can only have a confidence above the threshold if all corresponding c-consequent rules also have
- Building (c + 1)-consequent rules from c-consequent ones!

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 candidate 2-consequent rule:

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

- Final check of antecedent against data!

Discussion of association rules

- 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
- Practical issue: generating a certain number of rules (e.g. by incrementally reducing min. support)

Summary/concepts/questions

- 1R
  - Model
  - Algorithm
  - Unknown values
  - Numeric attributes
- Naive Bayes
  - Model
  - Algorithm (Learning, predicting)
  - Laplace estimator
  - Unknown values
  - Numeric attributes
- ID3 decision tree
  - Level of surprise, entropy, information gain, algorithm
- Rules: problem with interpretation

Summary/concepts/questions - 2

- Linear models
  - Form of linear model for regression
  - Form of error to be minimized
- Linear models for classification
  - Logistic regression
  - Perceptron
  - Winnow
  - Instance based (Nearest neighbour) learning
  - „Knowledge representation”
  - Algorithm
  - Problems
- Clustering
  - Knowledge representation
  - K-means: algorithm + limitations
- Association rule mining
  - Knowledge representation
  - Item, itemset, support, confidence, lift
  - Apriori algorithm