#### Data Mining and Knowledge Discovery: Practice Notes

dr. Petra Kralj Novak <u>Petra.Kralj.Novak@ijs.si</u> 2014/11/11

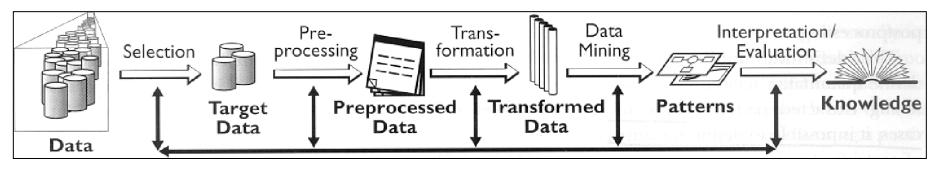
1



- Prof. Nada Lavrač:
  - Data mining overview
  - Advanced topics
- Dr. Petra Kralj Novak
   Data mining basis



## Keywords



- Data
  - Attribute, example, attribute-value data, target variable, class, discretization
- Data mining
  - Heuristics vs. exhaustive search, decision tree induction, entropy, information gain, overfitting, Occam's razor, model pruning, naïve Bayes classifier, KNN, association rules, support, confidence, predictive vs. descriptive DM, numeric prediction, regression tree, model tree
- Evaluation
  - Train set, test set, accuracy, confusion matrix, cross validation, true positives, false positives, ROC space, error, precision, recall



## Practice plan

- 2014/11/11: Predictive data mining
  - Decision trees
  - Naïve Bayes classifier
  - Evaluating classifiers 1: separate test set, confusion matrix, classification accuracy
  - Hands on Weka: Predictive data mining
- 2014/12/9: Numeric prediction and descriptive data mining
  - Discussion on classification
  - Numeric prediction and evaluation in Weka
  - Association rules
  - Hands on Weka: Numeric prediction
  - Hands on Weka: Descriptive data mining
  - Discussion about seminars and exam
- 2014/12/16: Written exam, seminar proposal discussion
- 2014/1/21: Clowdflows platform and data mining seminar presentations



## Decision tree induction

#### Given

- Attribute-value data with nominal target variable Induce
- A decision tree and estimate its performance on new data



Attri	ibu	te-va	alue d	data	(r	ominal) target	
			attributes		V	variable	
						Ţ	
	Doroon	A 70	Dropprintion	Actiomotic	Toor Data		
	Person	Age	Prescription	Astigmatic	Tear_Rate	Lenses	
examples	P1	young	myope	no	normal		> classes
	P2	young	myope	no	reduced	NO	
	P3	young	hypermetrope	no	normal	YES	=
	P4	young	hypermetrope	no	reduced	NO	
	P5	young	myope	yes	normal	YES	values of
	P6	young	myope	yes	reduced	NO	the
•	P7	young	hypermetrope	yes	normal	YES	
	P8	young	hypermetrope	yes	reduced	NO	(nominal)
•	P9	pre-presbyopic	myope	no	normal	YES	target
	P10	pre-presbyopic	myope	no	reduced	NO	•
	P11	pre-presbyopic	hypermetrope	no	normal	YES	variable
	P12	pre-presbyopic	hypermetrope	no	reduced	NO	
	P13	pre-presbyopic	myope	yes	normal	YES	
	P14	pre-presbyopic	myope	yes	reduced	NO	
	P15	pre-presbyopic	hypermetrope	yes	normal	NO	
	P16	pre-presbyopic	hypermetrope	yes	reduced	NO	
	P17	presbyopic	myope	no	normal	NO	12/01/
	P18	presbyopic	myope	no	reduced	NO	
	P19	presbyopic	hypermetrope	no	normal	YES	
	P20	presbyopic	hypermetrope	no	reduced	NO	
	P21	presbyopic	myope	yes	normal	YES	
	P22	presbyopic	myope	yes	reduced	NO	APHED C
DERARTMENT OF	P23	presbyopic	hypermetrope	yes	normal	NO	6
TECHNOLOGIES Jožef Stefan Institute	P24	presbyopic	hypermetrope	yes	reduced	NO	

# Decision tree induction (ID3)

Given:

Attribute-value data with nominal target variable Divide the data into training set (S) and test set (T)

Induce a decision tree on training set S:

- 1. Compute the entropy E(S) of the set S
- 2. **IF** E(S) = 0
- 3. The current set is "clean" and therefore a leaf in our tree
- 4. **IF** E(S) > 0
- 5. Compute the information gain of each attribute Gain(S, A)
- 6. The attribute A with the highest information gain becomes the root
- 7. Divide the set S into subsets S<sub>i</sub> according to the values of A
- 8. Repeat steps 1-7 on each Si

Test the model on the test set T



### Training and test set

	Person	Age	Prescription	Astigmatic	Tear_Rate	Lenses	
	P1	young	myope	no	normal	YES	
	P2	young	myope	no	reduced	NO	
	P3	young	hypermetrope	no	normal	YES	
	P4	young	hypermetrope	no	reduced	NO	
	P5	young	myope	yes	normal	YES	
	P6	young	myope	yes	reduced	NO	
	P7	young	hypermetrope	yes	normal	YES	
	P8	young	hypermetrope	yes	reduced	NO	_
	P9	pre-presbyopic	myope	no	normal	YES	
	P10	pre-presbyopic	myope	no	reduced	NO	
	P11	pre-presbyopic	hypermetrope	no	normal	YES	
	P12	pre-presbyopic	hypermetrope	no	reduced	NO	1
	P13	pre-presbyopic	myope	yes	normal	YES	4
	P14	pre-presbyopic	myope	yes	reduced	NO	
	P15	pre-presbyopic	hypermetrope	yes	normal	NO	*
	P16	pre-presbyopic	hypermetrope	yes	reduced	NO	ł
	P17	presbyopic	myope	no	normal	NO	
	P18	presbyopic	myope	no	reduced	NO	
	P19	presbyopic	hypermetrope	no	normal	YES	
	P20	presbyopic	hypermetrope	no	reduced	NO	
	P21	presbyopic	myope	yes	normal	YES	
	P22	presbyopic	myope	yes	reduced	NO	
	P23	presbyopic	hypermetrope	yes	normal	NO	*
_	P24	presbyopic	hypermetrope	yes	reduced	NO	
DERARTMENT OF	05	· · ·		-			

KNOWI FDGF

ožef Stefan Institute

Put 30% of examples in a separate test set



8

## Test set

Person	Age	Prescription	Astigmatic	Tear_Rate	Lenses
P3	young	hypermetrope	no	normal	YES
P9	pre-presbyopic	myope	no	normal	YES
P12	pre-presbyopic	hypermetrope	no	reduced	NO
P13	pre-presbyopic	myope	yes	normal	YES
P15	pre-presbyopic	hypermetrope	yes	normal	NO
P16	pre-presbyopic	hypermetrope	yes	reduced	NO
P23	presbyopic	hypermetrope	yes	normal	NO

Put these data away and do not look at them in the training phase!



## Training set

Person	Age	Prescription	Astigmatic	Tear_Rate	Lenses
P1	young	myope	no	normal	YES
P2	young	myope	no	reduced	NO
P4	young	hypermetrope	no	reduced	NO
P5	young	myope	yes	normal	YES
P6	young	myope	yes	reduced	NO
P7	young	hypermetrope	yes	normal	YES
P8	young	hypermetrope	yes	reduced	NO
P10	pre-presbyopic	myope	no	reduced	NO
P11	pre-presbyopic	hypermetrope	no	normal	YES
P14	pre-presbyopic	myope	yes	reduced	NO
P17	presbyopic	myope	no	normal	NO
P18	presbyopic	myope	no	reduced	NO
P19	presbyopic	hypermetrope	no	normal	YES
P20	presbyopic	hypermetrope	no	reduced	NO
P21	presbyopic	myope	yes	normal	YES
P22	presbyopic	myope	yes	reduced	NO
P24	presbyopic	hypermetrope	yes	reduced	NO



# Decision tree induction (ID3)

Given:

Attribute-value data with nominal target variable Divide the data into training set (S) and test set (T)

Induce a decision tree on training set S:

- 1. Compute the entropy E(S) of the set S
- 2. **IF** E(S) = 0
- 3. The current set is "clean" and therefore a leaf in our tree
- 4. **IF** E(S) > 0
- 5. Compute the information gain of each attribute Gain(S, A)
- 6. The attribute A with the highest information gain becomes the root

11

- 7. Divide the set S into subsets S<sub>i</sub> according to the values of A
- 8. Repeat steps 1-7 on each Si

Test the model on the test set T



## Information gain

number of examples in the subset  $S_v$ 

(probability of the branch) set S attribute A  $Gain(S, A) = E(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} \cdot E(S_v)$ number of examples in set S





$$E(S) = -\sum_{c=1}^{N} p_c . \log_2 p_c$$

 Calculate the following entropies: E(0,1) =E(1/2, 1/2) =E(1/4, 3/4) =E(1/7, 6/7) =E(6/7, 1/7) =E(0.1, 0.9) =E(0.001, 0.999) =

13



### Entropy

$$E(S) = -\sum_{c=1}^{N} p_c . \log_2 p_c$$

• Calculate the following entropies: E(0,1) = 0E(1/2, 1/2) = 1E(1/4, 3/4) = 0.81E(1/7, 6/7) = 0.59E(6/7, 1/7) = 0.59E(0.1, 0.9) = 0.47E(0.001, 0.999) = 0.01

14



### Entropy

$$E(S) = -\sum_{c=1}^{N} p_c . \log_2 p_c$$

 Calculate the following entropies: E(0,1) = 0E(1/2, 1/2) = 1E(1/4, 3/4) = 0.81E(1/7, 6/7) = 0.590.9 0.8 0.7 E(6/7, 1/7) = 0.590.6 0.5 E(0.1, 0.9) = 0.470.4 0.3 E(0.001, 0.999) = 0.010.2

0.1

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9



### Entropy

$$E(S) = -\sum_{c=1}^{N} p_c . \log_2 p_c$$

 Calculate the following entropies: E(0,1) = 0E(1/2, 1/2) = 1E(1/4, 3/4) = 0.81E(1/7, 6/7) = 0.590.9 0.8 0.7 E(6/7, 1/7) = 0.590.6 0.5 E(0.1, 0.9) = 0.470.4 0.3 E(0.001, 0.999) = 0.010.2 0.1

0

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1



## Entropy and information gain

probability of	probability of		
class 1	class 2	entropy E(p <sub>1</sub> , p <sub>2</sub> ) =	1.00
<b>p</b> <sub>1</sub>	p <sub>2</sub> = 1-p <sub>1</sub>	-p <sub>1</sub> *log <sub>2</sub> (p <sub>1</sub> ) - p <sub>2</sub> *log <sub>2</sub> (p <sub>2</sub> )	0.90
0	1	0.00	0.80
0.05	0.95	0.29	
0.10	0.90	0.47	<b>d</b> 0.50
0.15	0.85	0.61	<b>a</b> 0.60 0.50 0.40 0.40
0.20	0.80	0.72	0.30
0.25	0.75	0.81	0.20
0.30	0.70	0.88	0.10
0.35	0.65	0.93	0.00
0.40	0.60	0.97	0 0.2 0.4 0.6 0.8 1
0.45	0.55	0.99	distribution of probabilities
0.50	0.50	1.00	
0.55	0.45	0.99	
0.60	0.40	0.97	number of examples in the subset
0.65	0.35	0.93	probability of the "branch"
0.70	0.30	0.88 a	attribut A
0.75	0.25	0.81	
0.80	0.20	0.72 Gai	$in(S, A) = E(S) - \sum_{v \in S_v} \left( \frac{TS_v}{S_v} \right) E(S_v)$
0.85	0.15	0.61	$V \in Values (A \cup S \cup S \cup S)$
0.90	0.10	0.47	
0.95	0.05	0.29	`set S
1	0	0.00	number of examples in set S
DERARTMENT OF			LEARNED 17



# Decision tree induction (ID3)

Given:

Attribute-value data with nominal target variable Divide the data into training set (S) and test set (T)

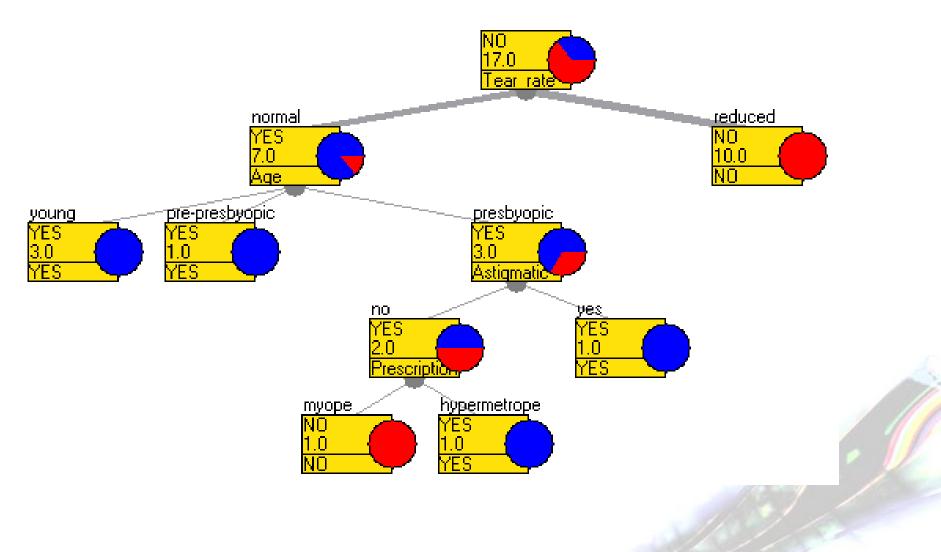
Induce a decision tree on training set S:

- 1. Compute the entropy E(S) of the set S
- 2. **IF** E(S) = 0
- 3. The current set is "clean" and therefore a leaf in our tree
- 4. **IF** E(S) > 0
- 5. Compute the information gain of each attribute Gain(S, A)
- 6. The attribute A with the highest information gain becomes the root
- 7. Divide the set S into subsets S<sub>i</sub> according to the values of A
- 8. Repeat steps 1-7 on each Si

Test the model on the test set T



### **Decision tree**





## **Confusion** matrix

predicted

20

		Predicted positive	Predicted negative
ctua	Actual positive	TP	FN
а	Actual negative	FP	TN

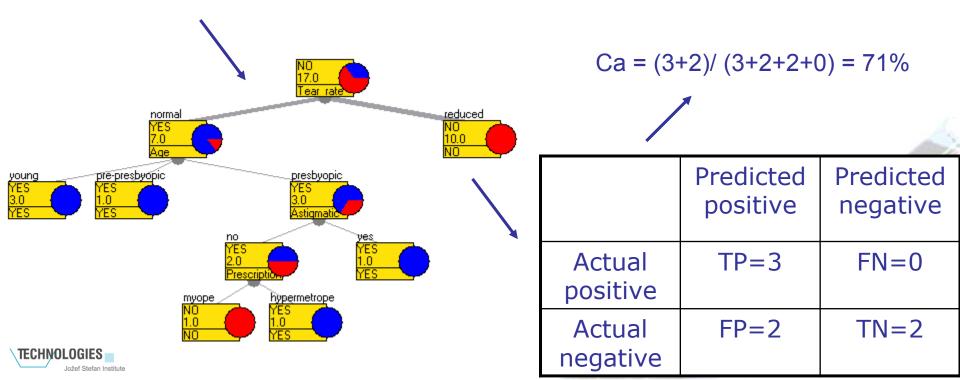
- Confusion matrix is a matrix showing actual and predicted classifications
- Classification measures can be calculated from it:
  - Classification accuracy = (TP+TN) / (TP + TN + FP + FN)
  - Precision = TP / (TP + FP)
  - Recall = TP / (TP + FN)



- ...

#### Evaluating decision tree accuracy

Person	Age	Prescription	Astigmatic	Tear_Rate	Lenses
P3	young	hypermetrope	no	normal	YES
P9	pre-presbyopic	туоре	no	normal	YES
P12	pre-presbyopic	hypermetrope	no	reduced	NO
P13	pre-presbyopic	туоре	yes	normal	YES
P15	pre-presbyopic	hypermetrope	yes	normal	NO
P16	pre-presbyopic	hypermetrope	yes	reduced	NO
P23	presbyopic	hypermetrope	yes	normal	NO



#### Predicting with Naïve Bayes

#### Given

- Attribute-value data with nominal target variable Induce
- Build a Naïve Bayes classifier and estimate its performance on new data



## Naïve Bayes classifier

$$P(c \mid a_1, a_2, \dots, a_n) = P(c) \prod_i \frac{P(c \mid a_i)}{P(c)}$$

Assumption: conditional independence of attributes given the class.

Will the spider catch these two ants?

- Color = white, Time = night
- Color = black, Size = large, Time = dayTime Size Color Caught YES black day large YES white  $\operatorname{small}$ night YES black  $\operatorname{small}$ day night NO red large NO black large night NO white night large

## Naïve Bayes classifier -example

Color	Size	Time	Caught
black	large	day	YES
white	$\operatorname{small}$	night	YES
black	$\operatorname{small}$	day	YES
red	large	night	NO
black	large	night	NO
white	large	night	NO

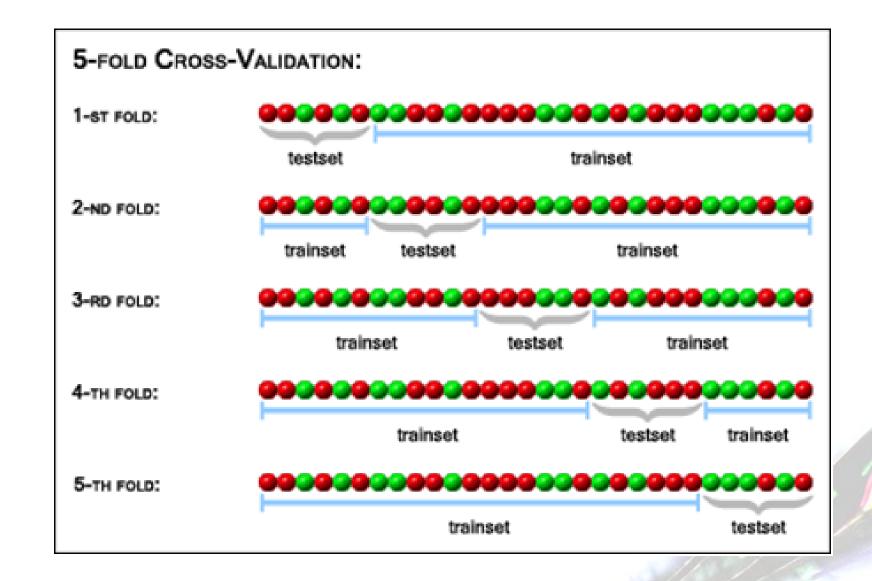
$$v_1 = "Color = white"$$
  
 $v_2 = "Time = night"$   
 $c_1 = YES$   
 $c_2 = NO$ 

$$p(c_1|v_1, v_2) = p(Caught = YES|Color = white, Time = night) = p(Caught = YES) * \frac{p(Caught = YES|Color = white)}{p(Caught = YES)} * \frac{p(Caught = YES|Time = night)}{p(Caught = YES)} = \frac{1}{2} * \frac{\frac{1}{2}}{\frac{1}{2}} * \frac{\frac{1}{4}}{\frac{1}{2}} = \frac{1}{4}$$

## K-fold cross validation

- 1. The sample set is partitioned into K subsets ("folds") of about equal size
- A single subset is retained as the validation data for testing the model (this subset is called the "testset"), and the remaining K - 1 subsets together are used as training data ("trainset").
- 3. A model is trained on the trainset and its performance (accuracy or other performance measure) is evaluated on the testset
- 4. Model training and evaluation is repeated K times, with each of the K subsets used exactly once as the testset.
- 5. The average of all the accuracy estimations obtained after each iteration is the resulting accuracy estimation.







## Discussion

- 1. How much is the information gain for the "attribute" Person? How would it perform on the test set?
- 2. How do we compute entropy for a target variable that has three values? Lenses = {hard=4, soft=5, none=13}
- 3. What would be the classification accuracy of our decision tree if we pruned it at the node *Astigmatic*?
- 4. What are the stopping criteria for building a decision tree?
- 5. Why do we prune decision trees?
- 6. How would you compute the information gain for a numeric attribute?
- 7. Compare naïve Bayes and decision trees (similarities and differences) .
- 8. Can KNN be used for classification tasks?
- 9. Compare KNN and Naïve Bayes.
- 10. Compare cross validation and testing on a separate test set.
- 11. List 3 numeric prediction methods.
- 12. What is discretization.