

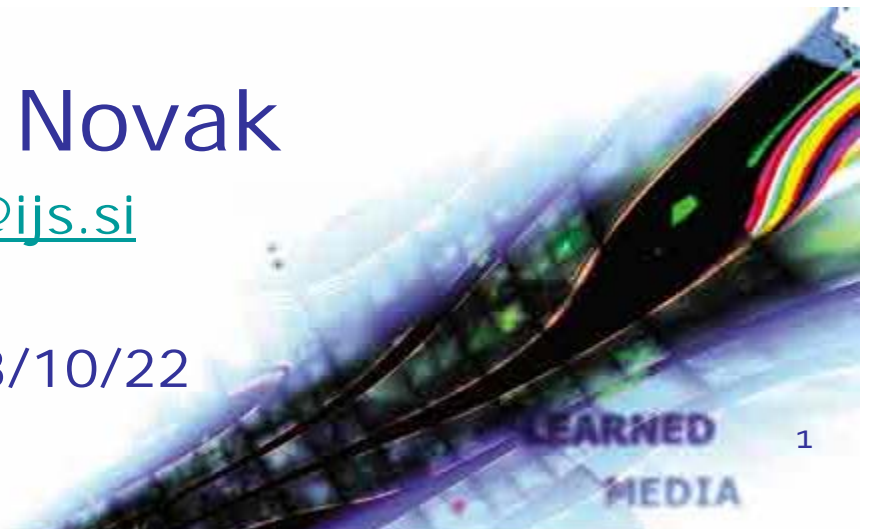
Data Mining and Knowledge Discovery

Knowledge Discovery and Knowledge Management in e-Science

Petra Kralj Novak

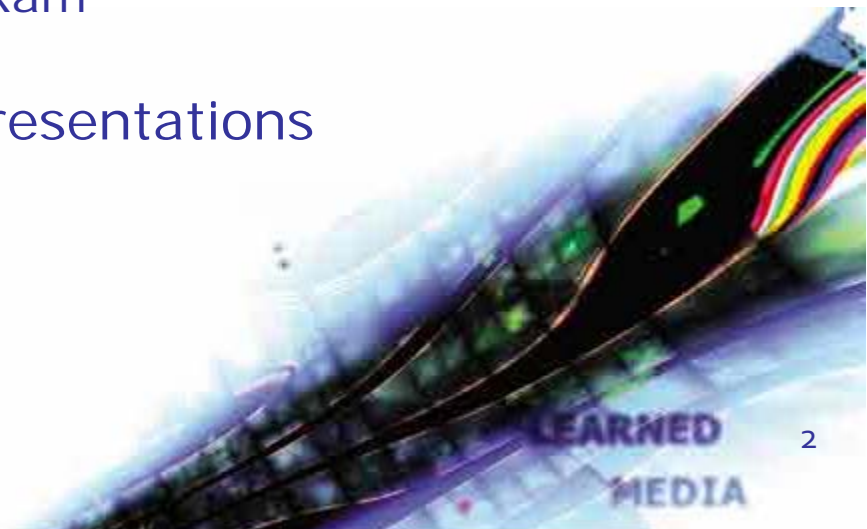
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Practice, 2008/10/22



Practice plan

- 2008/10/22: Predictive data mining
 - Decision trees
 - Naïve Bayes classifier
 - Evaluating classifiers (separate test set, cross validation, confusion matrix, classification accuracy)
 - Predictive data mining in Weka
- 2008/11/12: Numeric prediction and descriptive data mining
 - Regression models
 - Association rules
 - Regression models and evaluation in Weka
 - Descriptive data mining in Weka
 - Discussion about seminars and exam
- 2008/12/1: Written exam
- 2008/12/8: Seminar proposals presentations



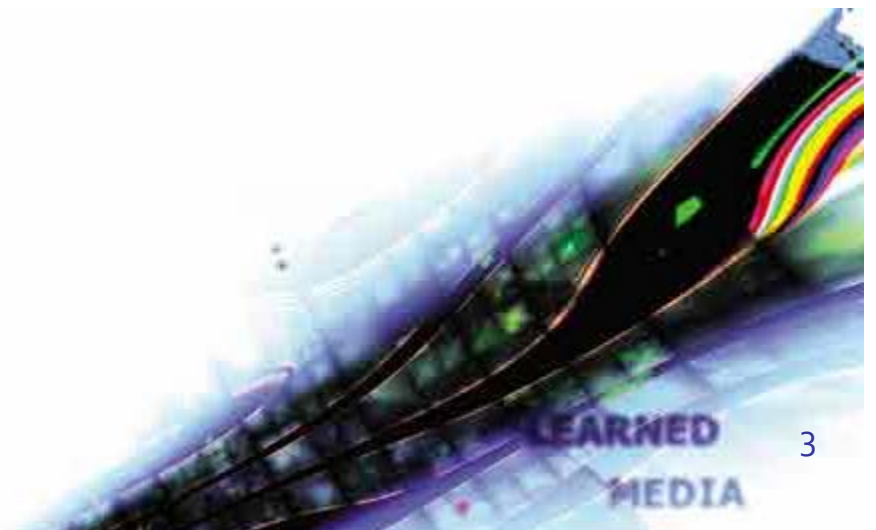
Decision tree induction

Given

- Attribute-value data with nominal target variable

Induce

- A decision tree and estimate its performance on new data



Decision tree induction (ID3)

Given:

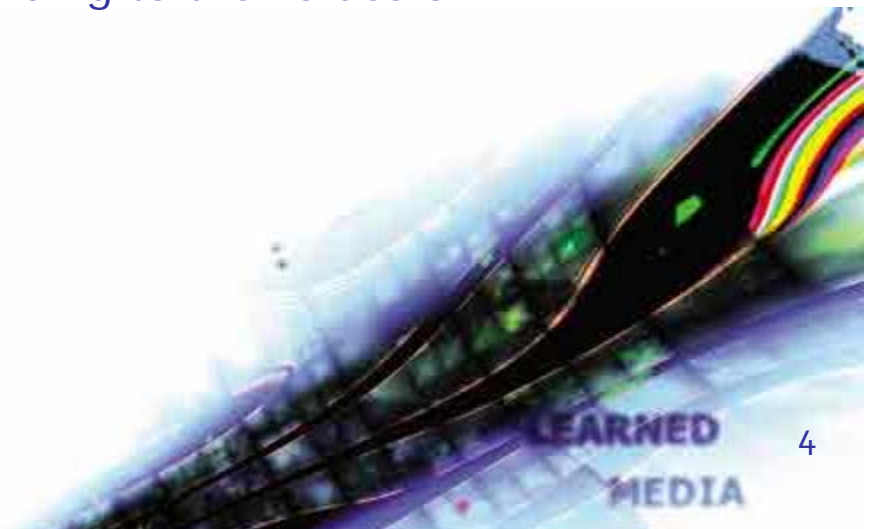
Attribute-value data with nominal target variable

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 $\text{Gain}(S, A)$
6. The attribute A with the highest information gain becomes the root
7. Divide the set S into subsets S_i according to the values of A
8. Repeat steps 1-7 on each S_i

Test the model on the test set T



Attribute-value data

(nominal)
target
variable

attributes

examples

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
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
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

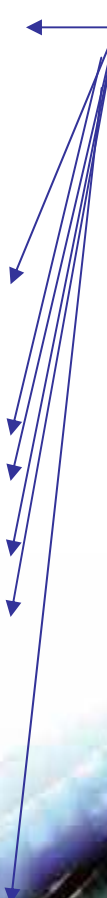
classes
=
values of
the
(nominal)
target
variable



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
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
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

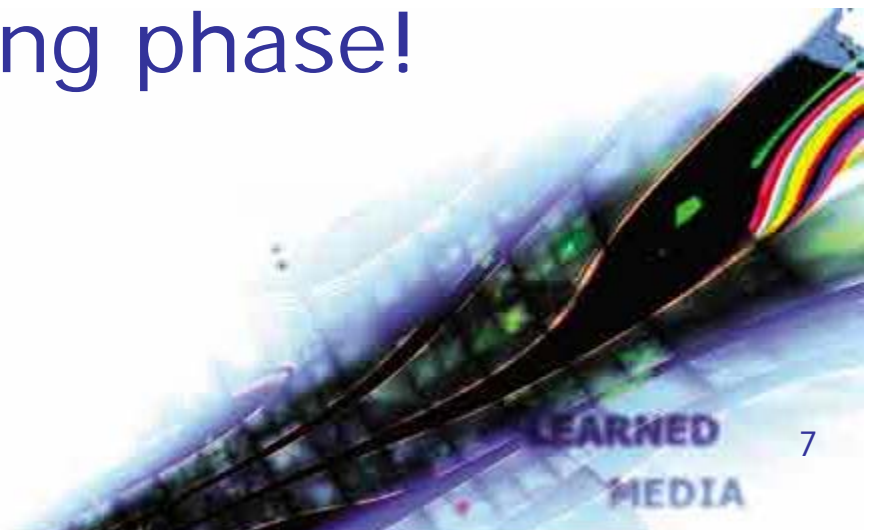
Put 30% of examples in a separate test set



Test set

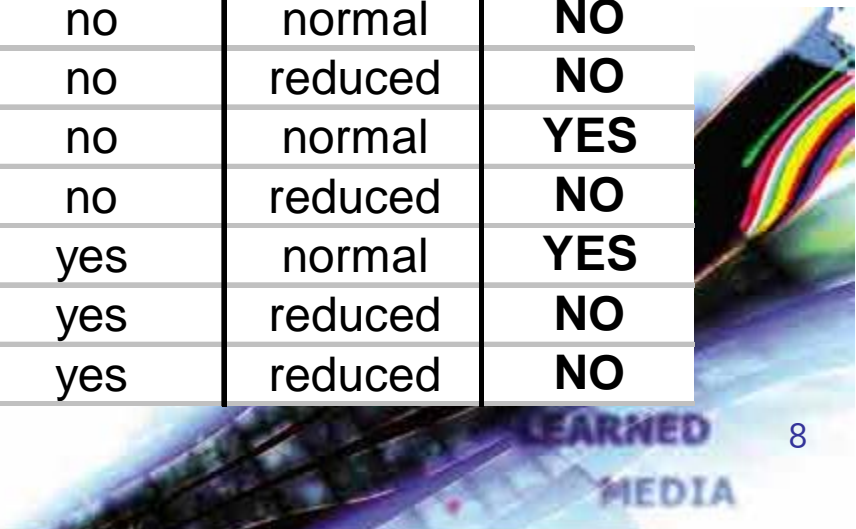
Person	Age	Prescription	Astigmatic	Tear_Rate	Lenses
P3	young	hypermetrope	no	normal	YES
P9	pre-presbyopic	myope	no	normal	YES
P12	pre-presbyopic	hypermetrope	no	reduced	NO
P13	pre-presbyopic	myope	yes	normal	YES
P15	pre-presbyopic	hypermetrope	yes	normal	NO
P16	pre-presbyopic	hypermetrope	yes	reduced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



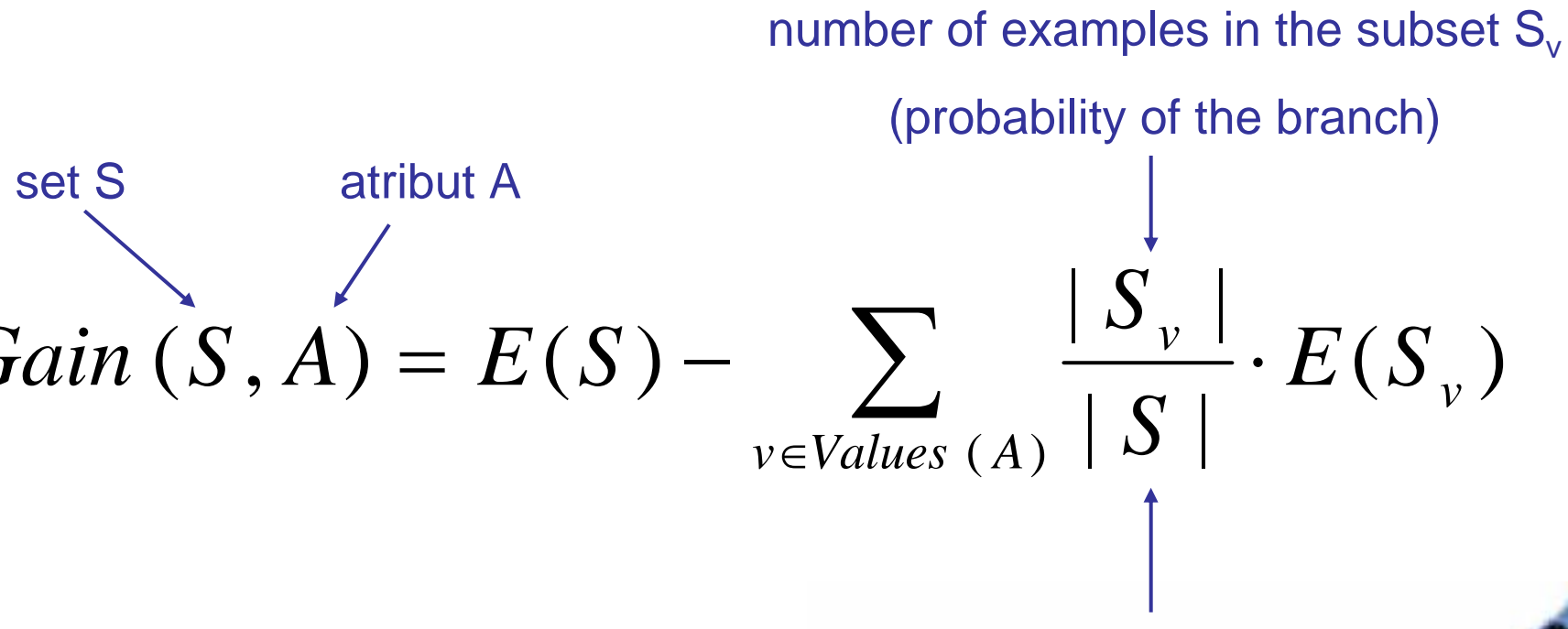
Information gain

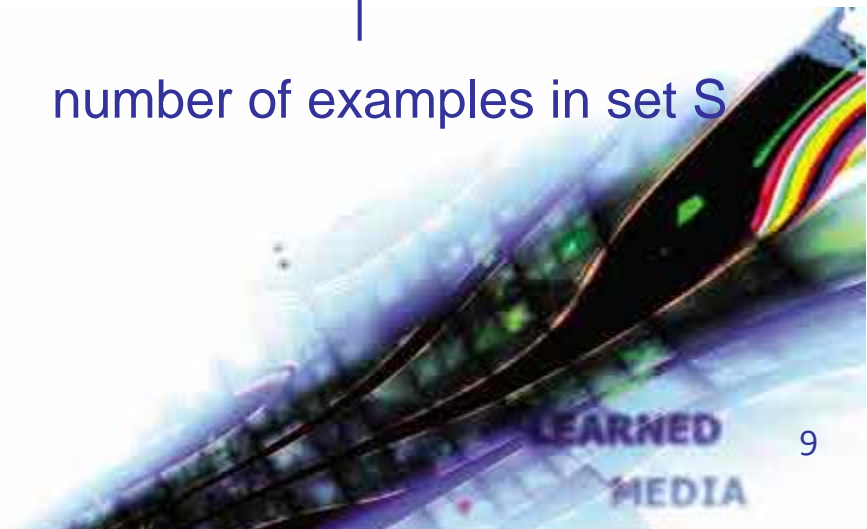
number of examples in the subset S_v
(probability of the branch)

set S atribut 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





Entropy

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

- Calculate the following entropies:

$$E(0,1) =$$

$$E(1/2, 1/2) =$$

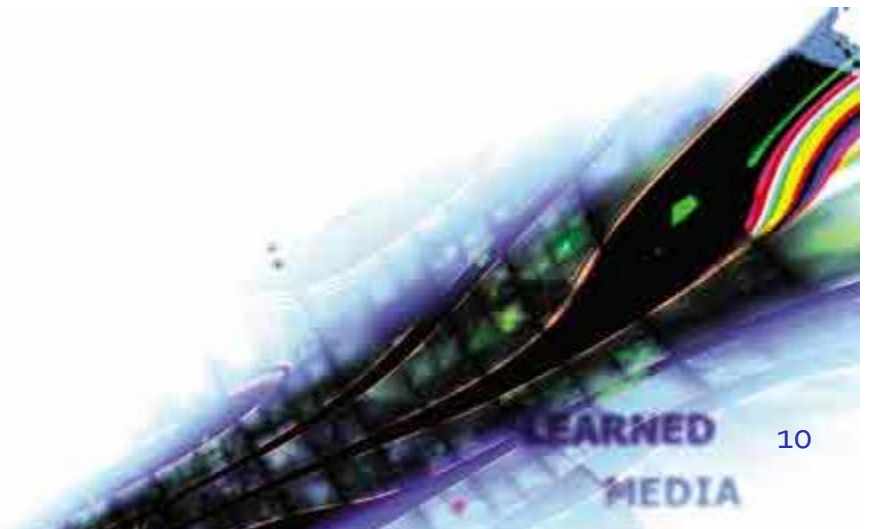
$$E(1/4, 3/4) =$$

$$E(1/7, 6/7) =$$

$$E(6/7, 1/7) =$$

$$E(0.1, 0.9) =$$

$$E(0.001, 0.999) =$$



Entropy

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

- Calculate the following entropies:

$$E(0,1) = 0$$

$$E(1/2, 1/2) = 1$$

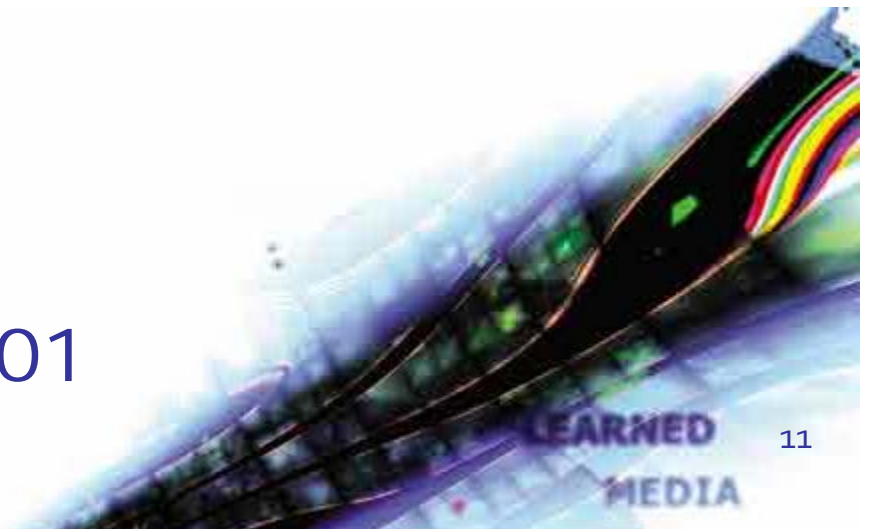
$$E(1/4, 3/4) = 0.81$$

$$E(1/7, 6/7) = 0.59$$

$$E(6/7, 1/7) = 0.59$$

$$E(0.1, 0.9) = 0.47$$

$$E(0.001, 0.999) = 0.01$$



Entropy

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$$E(0,1) = 0$$

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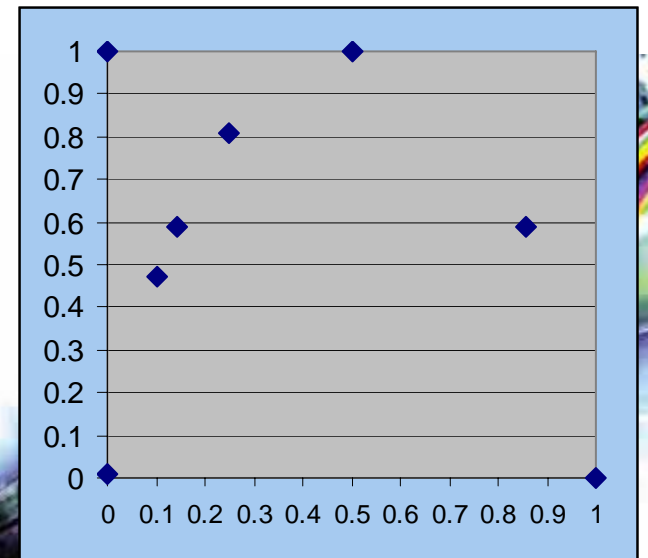
$$E(1/4, 3/4) = 0.81$$

$$E(1/7, 6/7) = 0.59$$

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Entropy

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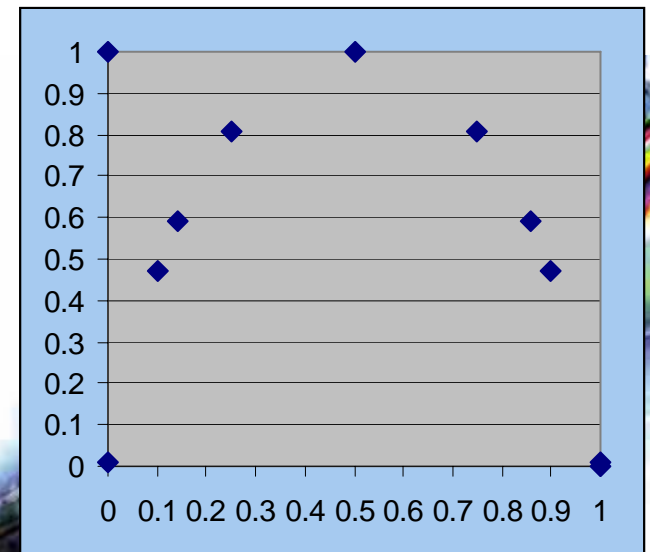
$$E(1/4, 3/4) = 0.81$$

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$$E(6/7, 1/7) = 0.59$$

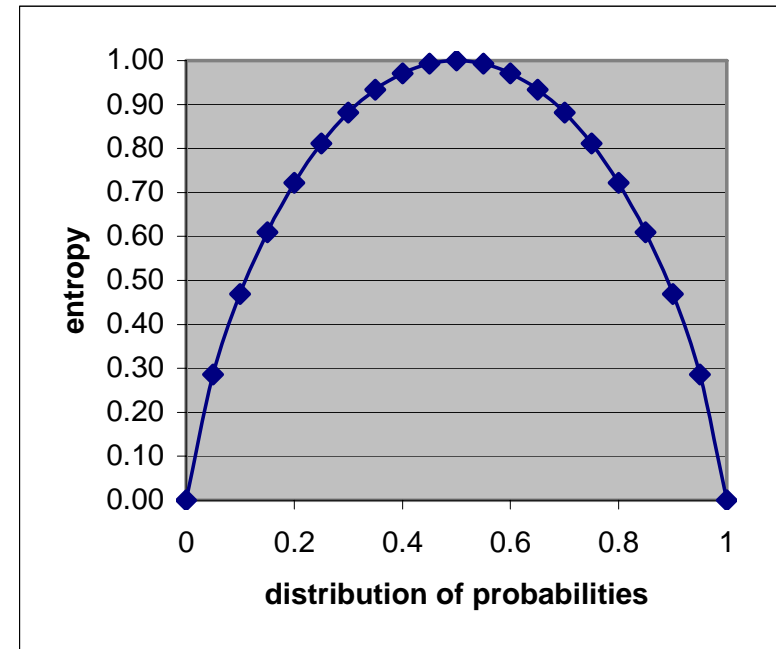
$$E(0.1, 0.9) = 0.47$$

$$E(0.001, 0.999) = 0.01$$



Entropy and information gain

probability of class 1	probability of class 2	entropy $E(p_1, p_2) = -p_1 \cdot \log_2(p_1) - p_2 \cdot \log_2(p_2)$
p_1	$p_2 = 1 - p_1$	
0	1	0.00
0.05	0.95	0.29
0.10	0.90	0.47
0.15	0.85	0.61
0.20	0.80	0.72
0.25	0.75	0.81
0.30	0.70	0.88
0.35	0.65	0.93
0.40	0.60	0.97
0.45	0.55	0.99
0.50	0.50	1.00
0.55	0.45	0.99
0.60	0.40	0.97
0.65	0.35	0.93
0.70	0.30	0.88
0.75	0.25	0.81
0.80	0.20	0.72
0.85	0.15	0.61
0.90	0.10	0.47
0.95	0.05	0.29
1	0	0.00



number of examples in the subset
probability of the "branch"

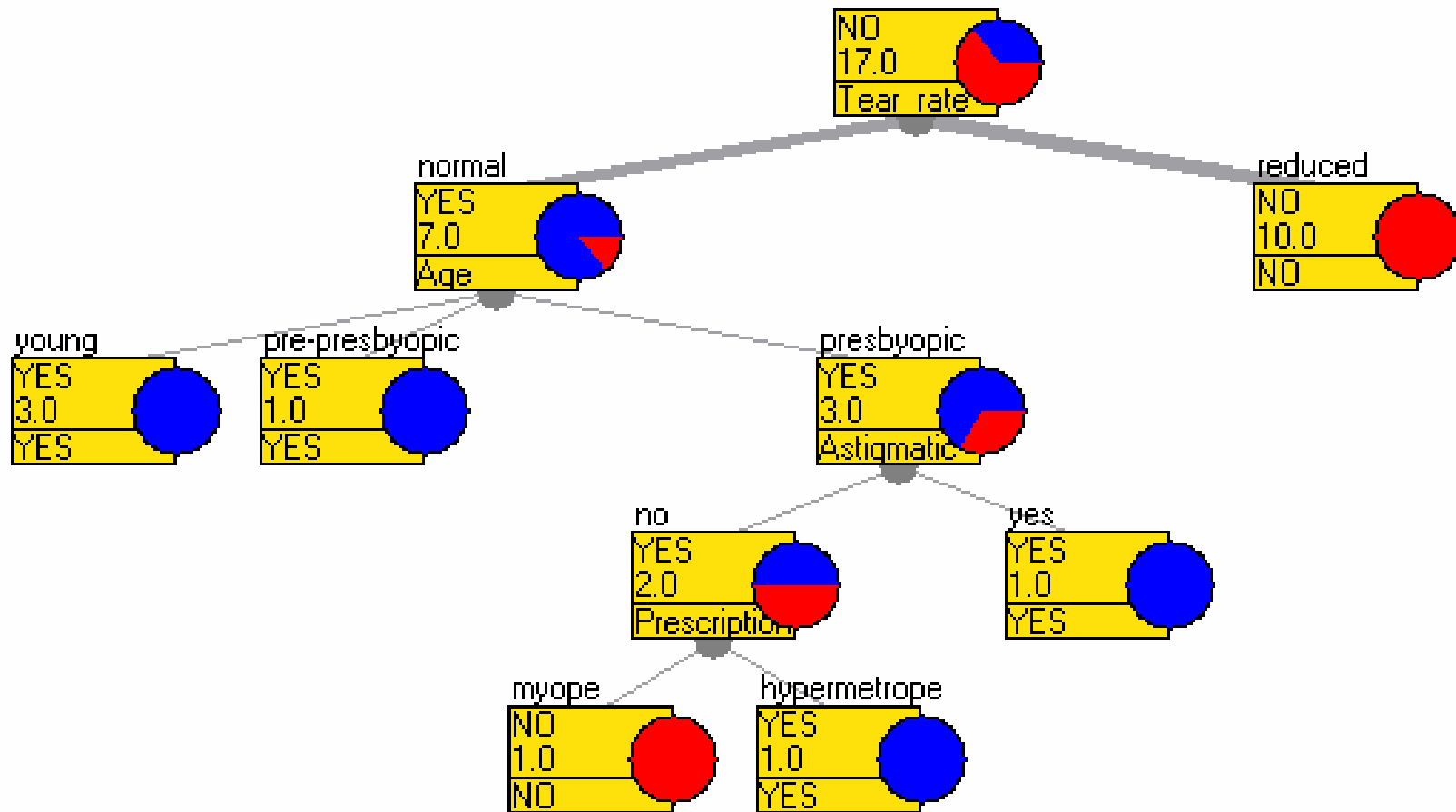
attribut A

$$Gain(S, A) = E(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} E(S_v)$$

set S

number of examples in set S

Decision tree



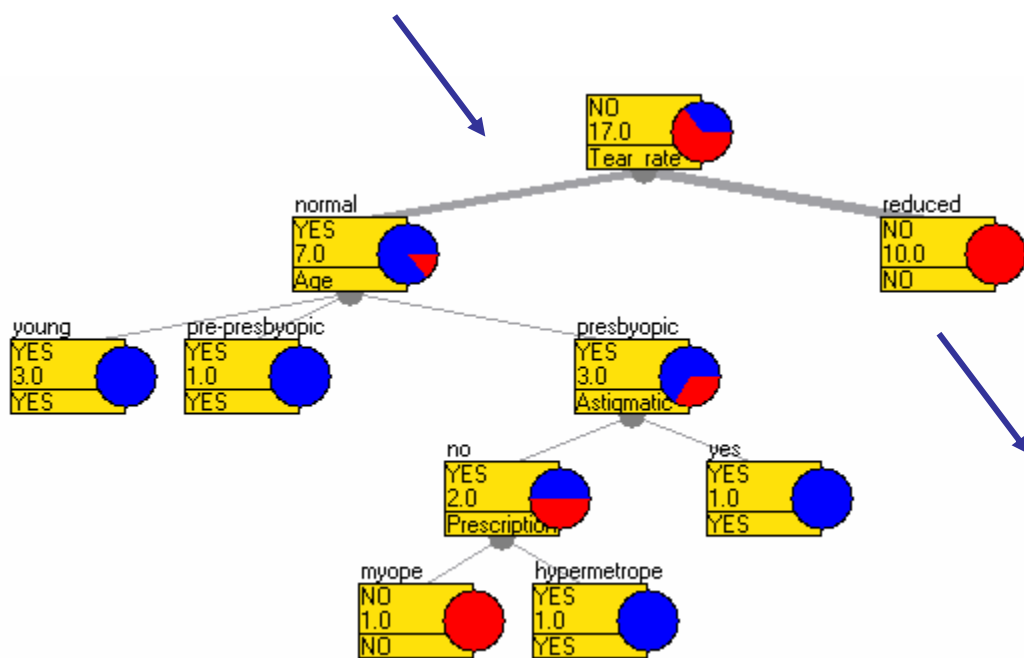
Confusion matrix

		predicted	
		Predicted positive	Predicted negative
actual	Actual positive	TP	FN
	Actual negative	FP	TN

- Confusion matrix is a matrix showing actual and predicted classifications
- Classification measures can be calculated from it, like classification accuracy
 - = $\#(\text{correctly classified examples}) / \#(\text{all examples})$
 - = $(TP + TN) / (TP + TN + FP + FN)$

Evaluating decision tree accuracy

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



$$Ca = (3+2) / (3+2+2+0) = 0,71\%$$

	Predicted positive	Predicted negative
Actual positive	TP=3	FN=0
Actual negative	FP=2	TN=2

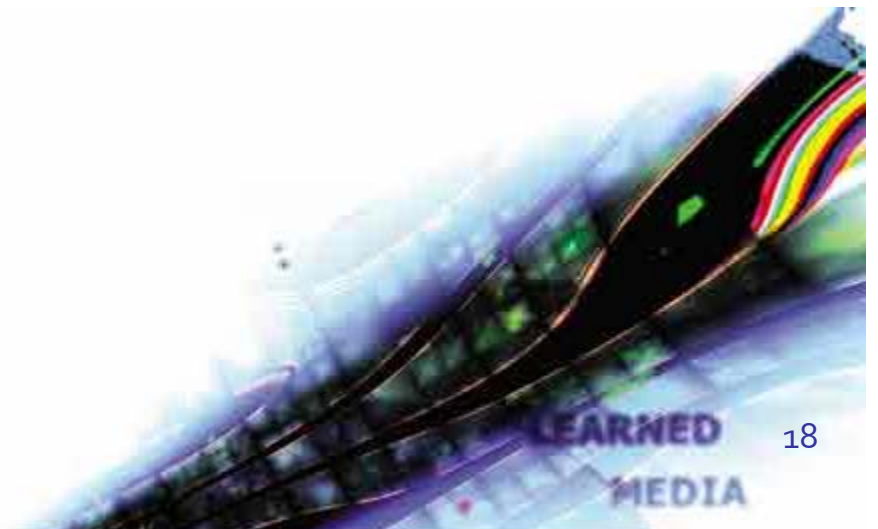
Predicting with Naïve Bayes

Given

- Attribute-value data with nominal target variable

Induce

- Build a Naïve Bayes classifier and estimate its performance on new data



Naïve Bayes classifier

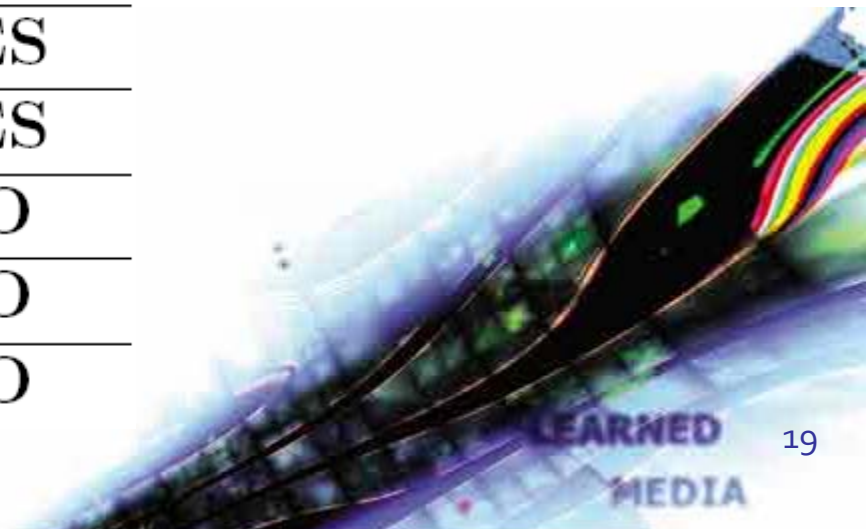
$$P(c | a_1, a_2, \dots, a_n) = P(c) \prod_i \frac{P(c | a_i)}{P(c)}$$

Assumption: conditional independence of attributes given the class.

Will the spider catch these two ants?

- Color = white, Time = night
- Color = black, Size = large, Time = day

Color	Size	Time	Caught
black	large	day	YES
white	small	night	YES
black	small	day	YES
red	large	night	NO
black	large	night	NO
white	large	night	NO



Naïve Bayes classifier -example

Color	Size	Time	Caught
black	large	day	YES
white	small	night	YES
black	small	day	YES
red	large	night	NO
black	large	night	NO
white	large	night	NO

$$v_1 = \text{“Color = white”}$$

$$v_2 = \text{“Time = night”}$$

$$c_1 = YES$$

$$c_2 = NO$$

$$p(Caught = YES) * \frac{p(Caught = YES|Color = white)}{p(Caught = YES)} * \frac{p(Caught = YES|Time = night)}{p(Caught = YES)} =$$

$$\frac{1}{2} * \frac{1}{2} * \frac{1}{4} = \frac{1}{4}$$

Discussion

- List evaluation methods for classification.
- How much is the information gain for the “attribute” Person? How would it perform on the test set?
- How do we compute entropy for a target variable that has three values? Lenses = {hard=4, soft=5, none=13}
- How would you compute the information gain for a numeric attribute?
- What would be the classification accuracy of our decision tree if we pruned it at the node *Astigmatic*?
- Compare the naïve Bayes classifier and decision trees regarding
 - the handling of missing values
 - numeric attributes
 - interpretability of the model

