## **COMP90051 Statistical Machine Learning**

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## COMP90049 Revision

## **Covered Knowledge**

- un/supervised learning
- probability theory; entropy
- association rule mining
- k-means clustering
- naive Bayes
- instance-based learning (IB1)

- feature selection (mutual information)
- decision stump/tree induction (0R, 1R, ID5)
- basic sampling (hold-out, cross-validation)
- evaluation (precision/recall/F, ROC)
- Seen: SVMs, bit of Bayes nets

## **Entropy**

The entropy of a discrete random event x with possible states 1, ..n
 is:

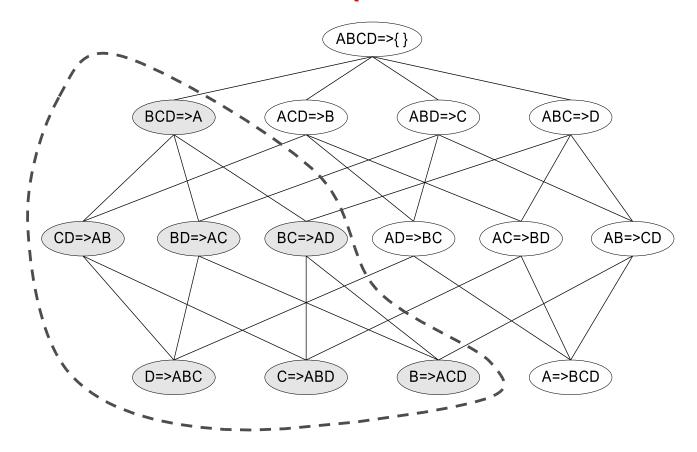
$$H(x) = -\sum_{i=1}^{n} P(i) \log_2 P(i)$$

where  $0 \log_2 0 =^{def} 0$ 

#### **Association Rules: Definitions**

- An association rule is an implication  $A \to B$ , where A and B are disjoint itemsets
  - $\star A =$ antecedent
  - $\star B = consequent$
- N.B. in association mining parlance:
  - $\star$  item = attribute-value pair (I = set of items)
  - ★ itemset = set of attribute-value pairs
  - $\star$  k-itemset = set of k attribute-value pairs
  - $\star$  transaction = exemplar (T = set of transactions)

## APriori Algorithm (Rule Generation)



## k-means Clustering

- Given k, the k-means algorithm is implemented in four steps:
  - 1. Select k points at random to act as seed clusters
  - Compute seed points as the centroids of the clusters of the current partition (the centroid is the centre, i.e., mean point, of the cluster)
  - 3. Assign each instance to the cluster with the nearest centroid
  - 4. Go back to 2, stop when no reassignments
- Exclusive, deterministic, partitioning, batch clustering method

## Naive Bayes (NB) Classifiers

• Classify instance 
$$D = \langle x_1, x_2, ..., x_n \rangle$$
 as class  $c_j \in C$  
$$c = \underset{c_j \in C}{\operatorname{arg max}} P(c_j | x_1, x_2, ..., x_n)$$
 
$$= \underset{c_j \in C}{\operatorname{arg max}} \frac{P(x_1, x_2, ..., x_n | c_j) P(c_j)}{P(x_1, x_2, ..., x_n)}$$
 
$$= \underset{c_j \in C}{\operatorname{arg max}} P(x_1, x_2, ..., x_n | c_j) P(c_j)$$
 
$$= \underset{c_j \in C}{\operatorname{arg max}} P(c_j) \prod_{i=1}^n P(x_i | c_j)$$

Model trained using frequencies

## **Nearest Neighbour Classification**

- Combining training—test instance scores to form an overall categorisation function:
- Method 1: index all training documents, and query the training document set with each test document; classify the test document according to the class of the top-ranked training document [1-NN]
- **Method 2:** index all training documents, and query the training document set with each test document; classify the test document according to the **majority class** within the *k* top-ranked training documents **[k-NN]**

## Similarity/Distance Metrics

• Cosine similarity:

$$sim(x,y) = \frac{\vec{x} \cdot \vec{y}}{|\vec{x}||\vec{y}|} = \frac{\sum_{i} x_{i} y_{i}}{\sqrt{\sum_{i} x_{i}^{2}} \sqrt{\sum_{i} y_{i}^{2}}}$$

Relative entropy:

$$D(x || y) = \sum_{i} x_i (\log_2 x_i - \log_2 y_i)$$

or alternatively **skew divergence**:

$$s_{\alpha}(x,y) = D(x \mid\mid \alpha y + (1 - \alpha)x)$$

### **Feature Selection**

• Mutual information:

$$MI(T;C) = \sum_{t \in \{0,1\}} \sum_{c} P(t,c) \log_2 \frac{P(t,c)}{P(t)P(c)}$$

## **Constructing Decision Trees: ID3**

 Basic method: construct decision trees in recursive divide-andconquer fashion

FUNCTION ID3 (Root)

IF all instances at root have same class

THEN stop

ELSE Select a new attribute to use in partitioning root node instances

Create a branch for each attribute value and partition up root node instances according to each value

Call ID3(LEAF $_i$ ) for each leaf node LEAF $_i$ 

Note: we may not end up with pure leaves

## **Split Criteria**

• The **information gain** for attribute  $R_A$  (with values  $x_1,...x_m$ ) at a given root node R is:

$$IG(R_A|R) = H(R) - \sum_{i=1}^{m} P(x_i)H(x_i)$$

• The corresponding gain ratio is:

$$GR(R_A|R) = \frac{IG(R_A|R)}{H(R_A)}$$

$$= \frac{H(R) - \sum_{i=1}^{m} P(x_i)H(x_i)}{-\sum_{i=1}^{m} P(x_i)\log_2 P(x_i)}$$

#### **Evaluation**

• Classification accuracy: is the proportion of

$$ACC = \frac{TP + TN}{TP + FP + FN + TN}$$

Error rate:

$$ER = \frac{FP + FN}{TP + FP + FN + TN}$$

• Error rate reduction:

$$ERR = \frac{ER_0 - ER}{ER_0}$$

#### • Precision:

$$Precision = \frac{TP}{TP + FP}$$

• Recall:

$$Recall = \frac{TP}{TP + FN}$$

F-score:

F-score = 
$$(1 + \beta^2) \frac{PR}{R + \beta^2 P}$$

## Sampling

- Holdout = train a classifier over a fixed training dataset, and evaluate it over a fixed held-out test dataset
- Random Subsampling = perform holdout over multiple iterations, randomly selecting the training and test data (maintaining a fixed size for each dataset) on each iteration
- Cross Validation = partition data into N folds, and use N-1 as training data and 1 as test  $\times N$  iterations
- **Stratified Cross Validation** = partition the data so as to maintain the overall class distribution within individual partitions

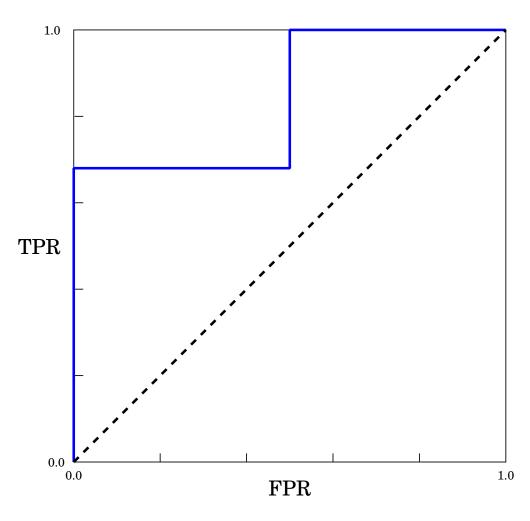
#### **ROC Curves**

- 1. Sort the test instances in ascending order of "rating"  $t_1, t_2, ..., t_k$
- 2. Initialise  $TP_{k+1} = FP_{k+1} = 0$ , and set  $FN_{k+1}$  and  $TN_{k+1}$  to the number of positive and negative instances in the dataset, resp.
- 3. For each i = k, ..., 2, 1
  - i. update  $TP_i$ ,  $FP_i$ ,  $FN_i$  and  $TN_i$  assuming positive classification of instance i, based on the actual class of  $t_i$  and  $TP_{i+1}$ ,  $FP_{i+1}$ ,  $FN_{i+1}$  and  $TN_{i+1}$
  - ii. calculate TPR and FPR at  $t_i$
- 4. Plot the TPR and FPR values for each  $t_i$

## **Generating ROC Curves: Example**

Class	_	+	_	+	+	
Score	0.85	0.85	0.87	0.93	0.95	
i	1	2	3	4	5	6
TP	3	3	2	2	1	0
FP	2	1	1	0	0	0
FN	0	0	1	1	2	3
TN	0	1	1	2	2	2
TPR	$\frac{3}{3}$	$\frac{3}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{1}{3}$	0
FPR	$\frac{3}{3}$ $\frac{2}{2}$ $\frac{2}{2}$	$\frac{3}{3}$ $\frac{1}{2}$	$\frac{\frac{2}{3}}{\frac{1}{2}}$	Ö	Ö	0

## **Generating ROC Curves: Example**



# What other topics in ML have you seen?