# Machine Learning: Symbolische Ansätze



#### **Data Pre-Processing**

- Data Mining
  - Motivation
  - Data Mining Process Models
- Pre-Processing
  - Supervised vs.Unsupervised

- Feature Subset Selection
  - Filter and Wrapper Approaches
- Discretization
  - Bottom-Up (Chi-Merge) and Top-Down (Entropy-Split)
- Sampling
  - Windowing
- Data Cleaning
  - Outlier Detection and Noise Filtering

V2.0 | WS 10/11 | J. Fürnkranz

## **Data Mining - Motivation**



"Computers have promised us a fountain of wisdom but delivered a flood of data."

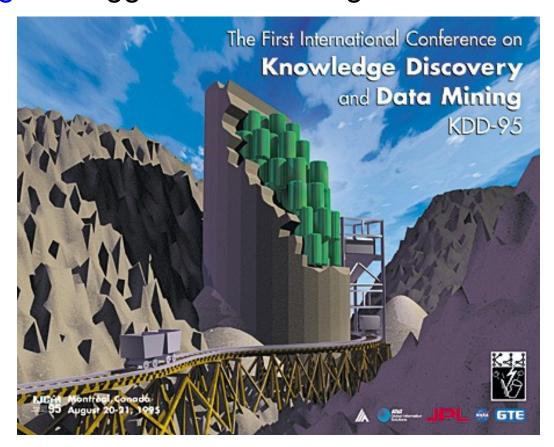
"It has been estimated that the amount of information in the world doubles every 20 months."

(Frawley, Piatetsky-Shapiro, Matheus, 1992)

## **Knowledge Discovery in Databases (KDD)**



Mining for nuggets of knowledge in mountains of Data.



#### **Definition**



# Data Mining is the non-trivial process of identifying

- valid
- novel
- potentially useful
- ultimately understandable
   patterns in data.
   (Fayyad et al. 1996)

#### It employs techniques from

- machine learning
- statistics
- databases

#### Or maybe:

Data Mining is torturing your database until it confesses.
 (Mannila (?))



# **Knowledge Discovery in Databases: Key Steps**



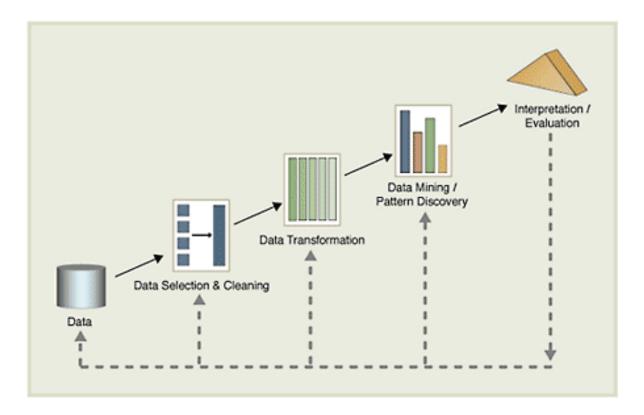
#### Key steps in the Knowledge Discovery cycle:

- 1. Data Cleaning: remove noise and inconsistent data
- 2. Data Integration: combine multiple data sources
- Data Selection: select the part of the data that are relevant for the problem
- 4. Data Transformation: transform the data into a suitable format (e.g., a single table, by summary or aggregation operations)
- Data Mining: apply machine learning and machine discovery techniques
- 6. Pattern Evaluation: evaluate whether the found patterns meet the requirements (e.g., interestingness)
- Knowledge Presentation: present the mined knowledge to the user (e.g., visualization)

# **Data Mining is a Process!**



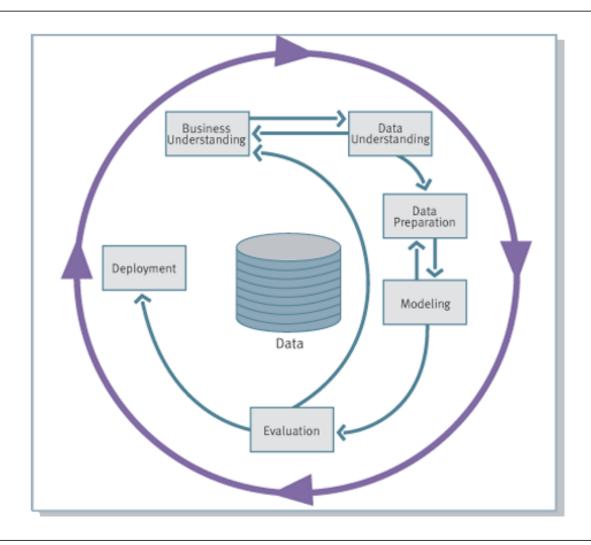
The steps are not followed linearly, but in an iterative process.



Source: http://alg.ncsa.uiuc.edu/tools/docs/d2k/manual/dataMining.html, after Fayyad, Piatetsky-Shapiro, Smyth, 1996 V2.0 | J. Fürnkranz

#### **Another Process Model**





#### **Pre-Processing**



- Databases are typically not made to support analysis with a data mining algorithm
  - pre-processing of data is necessary
- Pre-processing techniques:
  - Feature Engineering:

find the right features/attribute set

- Feature Subset Selection: select appropriate feature subsets
- Feature Transformation: bring attributes into a suitable form (e.g., discretization)
- Feature Construction: construct derived features
- Data Cleaning:
  - remove inconsistencies from the data
- Sampling:
  - select appropriate subsets of the data



# Unsupervised vs. Supervised Pre-processing



- Unsupervised
  - do not use information about the learning task
    - only prior information (from knowledge about the data)
    - and information about the distribution of the training data
- Supervised
  - use information about the learning task
    - e.g.: look at relation of an attribute to class attribute

#### WARNING:

- pre-processing may only use information from training data!
  - compute pre-processing model from training data
  - apply the model to training and test data
  - otherwise information from test data may be captured in the preprocessing step → biased evaluation
- in particular: apply pre-processing to every fold in cross-validation



#### **Feature Subset Selection**



- Databases are typically not collected with data mining in mind
- Many features may be
  - irrelevant
  - uninteresting
  - redundant
- Removing them can
  - increase efficiency
  - improve accuracy
  - prevent overfitting
- Feature Subsect Selection techniques try to determine appropriate features automatically



## **Unsupervised FSS**



- Using domain knowledge
  - some features may be known to be irrelevant, uninteresting or redundant
- Random Sampling
  - select a random sample of the feature
  - may be appropriate in the case of many weakly relevant features and/or in connection with ensemble methods

### **Supervised FSS**



#### Filter approaches:

- compute some measure for estimating the ability to discriminate between classes
- typically measure feature weight and select the best n features
- problems
  - redundant features (correlated features will all have similar weights)
  - dependent features (some features may only be important in combination (e.g., XOR/parity problems).

#### Wrapper approaches

- search through the space of all possible feature subsets
- each search subset is tried with the learning algorithm

## **Supervised FSS: Filters**



- Feature Weighting
  - a good attribute should discriminate between classes
  - use a measure of discrimination for determining the importance of attributes
    - decision tree splitting criteria (entropy/information gain, gini-index, ...)
    - attribute weighting criteria (Relief, ...), etc.
- Advantage
  - very fast
- Disadvantage
  - quality of each attribute is measured in isolation
  - some attributes may only be useful in combination with others

- foreach attribute A
  - W[A] = feature weight according to some measure of discrimination
- select the n features with highest W[A]

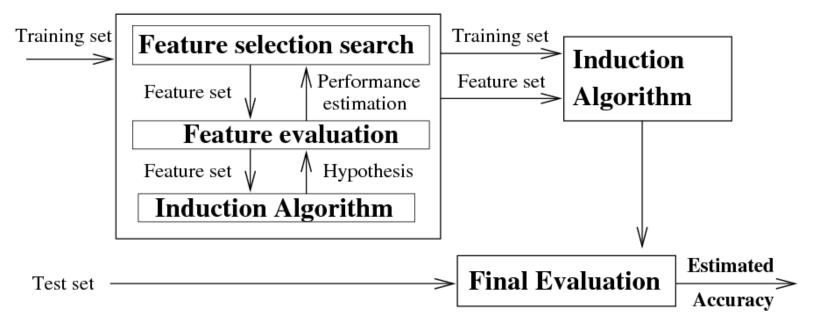


# **FSS: Wrapper Approach**

(John, Kohavi, Pfleger, ICML-94)



- Wrapper Approach:
  - try a feature subset with the learner
  - improve it by modifying the feature sets based on the result
  - repeat



The induction algorithm itself is used as a "black box" by the subset selection algorithm.

Figure by Kohavi & John



## **FSS: Wrapper Approach**

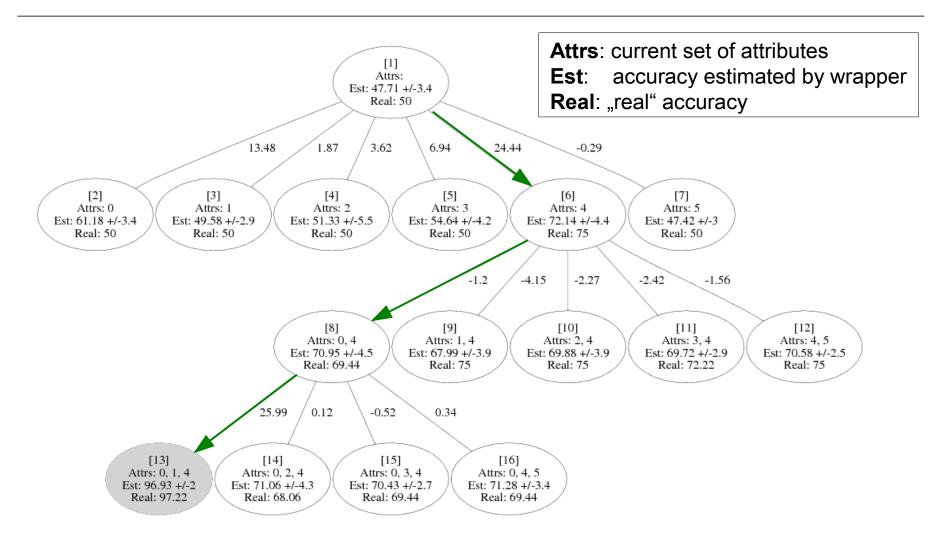


- Forward selection:
  - 1. start with empty feature set *F*
  - 2. for each attribute A
    - Estimate Accuracy of Learning algorithm on  $F \cup \{A\}$
  - 3.  $F = F \cup \{\text{attribute with highest estimated accuracy}\}\$
  - 4. goto 2. unless estimated accuracy decreases significantly
- Backward elimination:
  - start with full feature set F
  - try to remove attributes
- Bi-directional search is also possible



### **Example: Forward Search**





## **Wrapper Approaches - Discussion**



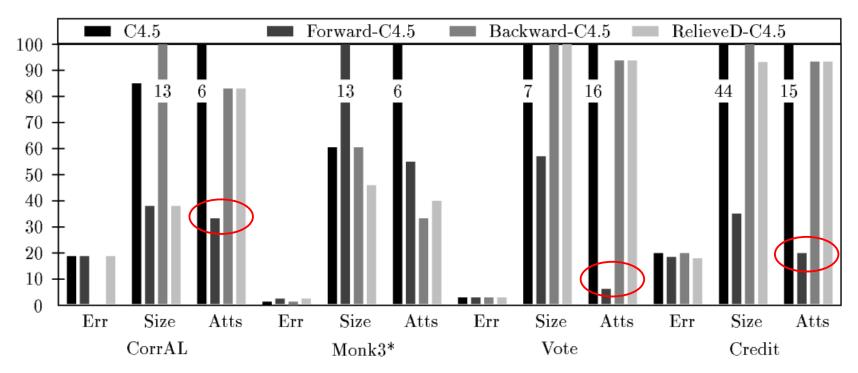
- Advantage:
  - find feature set that is tailored to learning algorithm
  - considers combinations of features, not only individual feature weights
  - can eliminate redundant features
     (picks only as many as the algorithm needs)

- Disadvantage:
  - very inefficient: many learning cycles necessary

## **Comparison Wrapper / Filter(Relief)**



Note: RelieveD is a version of Relief that uses all examples instead of a random sample



- on these datasets:
  - forward selection reduces attributes w/o error increase
- in general, it may also reduce error



#### **Feature Transformation**



#### numerization

- some algorithms can only use numeric data
- nominal → binary
  - a nominal attribute with n values is converted into n binary attributes
- binary → numeric
  - binary features may be viewed as special cases of numeric attributes with two values

#### standardization

- normalize numerical attributes to useful ranges
- sometimes logarithmic transformations are necessary

#### discretization

- some algorithms can only use categorical data
  - transform numeric attributes into (ordered) categorical values

#### **Discretization**



- Supervised vs. Unsupervised:
  - Unsupervised:
    - only look at the distribution of values of the attribute
  - Supervised:
    - also consider the relation of attribute values to class values
- Merging vs. Splitting:
  - Merging (bottom-up discretization):
    - Start with a set of intervals (e.g., each point is an interval) and successively combine neighboring intervals
  - Splitting (top-down discretization):
    - Start with a single interval and successively split the interval into subintervals

## **Unsupervised Discretization**



- domain-dependent:
  - suitable discretizations are often known
  - age (0-18) → baby (0-3), child (3-6), school child (6-10), teenager (11-18)
- equal-width:
  - divide value range into a number of intervals with equal width
  - age  $(0-18) \rightarrow (0-3, 4-7, 8-11, 12-15, 16-18)$
- equal-frequency:
  - divide value range into a number of intervals so that (approximately) the same number of datapoints are in each interval
  - e.g., N = 5: each interval will contain 20% of the training data
  - good for non-uniform distributions (e.g., salary)

# Supervised Discretization: Chi-Merge (Kerber, AAAI-92)



**Basic Idea:** merge neighboring intervals if the class information is independent of the interval an example belongs to

- initialization:
  - sort examples according to feature value
  - construct one interval for each value
- interval merging:

• compute  $\chi^2$  value for each pair of adjacent intervals  $C_j = A_{1j} + A_{2j}$   $\chi^2 = \sum_{i=1}^2 \sum_{j=1}^c \frac{(A_{ij} - E_{ij})^2}{E_{ij}} \quad \text{where} \quad E_{ij} = N_i \frac{C_j}{N_1 + N_2} \qquad N_i = \sum_{j=1}^c A_{ij}$ 

 $A_{ij}$  = number of examples in *i*-th interval that are of class j  $\overline{j=1}$   $E_{ij}$  = expected number of examples in *i*-th interval that are of class j

= examples in *i*-th interval  $N_i \times$  fraction  $C_j/N$  of (all) examples of class j

- merge those with lowest x<sup>2</sup> value
- stop
- when the  $\chi^2$  values of all pairs exceed a significance threshold



# Supervised Discretization: Entropy-Split (Fayyad & Irani, IJCAI-93)



Basic Idea: grow a decision tree using a single numeric attribute and use the value ranges in the leaves as ordinal values

- initialization:
  - initialize intervals with a single interval covering all examples S
  - sort all examples according to the attribute value
  - initialize the set of possible split points
    - simple: all values
    - more efficient: only between class changes in sorted list
- interval splitting:
  - select split point with the minimum weighted entropy

$$T_{max} = arg \min_{T} \left( \frac{|S_{A < T}|}{|S|} Entropy(S_{A < T}) + \frac{|S_{A \ge T}|}{|S|} Entropy(S_{A \ge T}) \right)$$

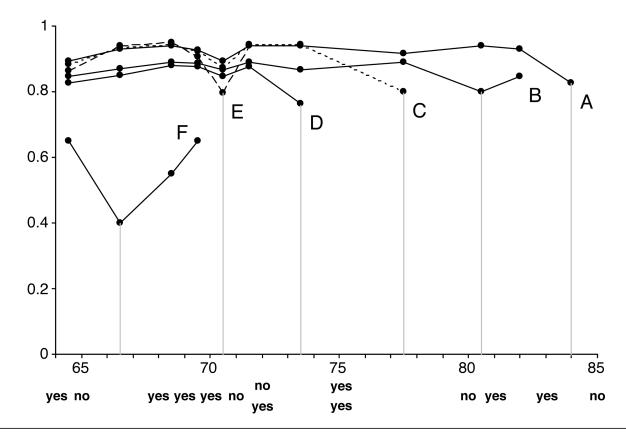
- ullet recursively apply Entropy-Split to  $S_{A < T_{max}}$  and  $S_{A \ge T_{max}}$
- stop
- when a given number of splits is achieved
- or when splitting would yield too small intervals
- or MDL-based stopping criterion (Fayyad & Irani, 1993)



# **Example**



Temperature	64	65	68	69	70	71	72	72	75	75	80	81	83	85
Play	Yes	No	Yes	Yes	Yes	No	No	Yes	Yes	Yes	No	Yes	Yes	No





# **Unsupervised Feature Construction**



- based on domain knowledge
  - Example: Body Mass Index

$$BMI = \frac{weight(kg)}{height(m)^2}$$

- automatic
  - Examples:
    - kernel functions
      - may be viewed as feature construction modules
      - → support vector machines
    - principal components analysis
      - transforms an n-dimensional space into a lower-dimensional subspace w/o losing much information
    - GLEM:
      - uses an Apriori -like algorithms to compute all conjunctive combinations of basic features that occur at least n times
      - application to constructing evaluation functions for game Othello

### **Supervised Feature Construction**



- use the class information to construct features that help to solve the classification problem
- Examples:
  - Wrapper approach
    - use rule or decision tree learning algorithm
    - observe frequently co-occurring features or feature values
    - encode them as separate features
  - Neural Network
    - nodes in hidden layers may be interpreted as constructed features

# **Scalability**



- databases are often too big for machine learning algorithms
  - ML algorithms require frequent counting operations and multidimensional access to data
  - only feasible for data that can be held in main memory
- two strategies to make DM algorithms scalable
  - design algorithms that are explicitly targetted towards minimizing the number of database operations (e.g., Apriori)
  - use sampling to work on subsets of the data

## Windowing



- Idea:
  - focus the learner on the parts of the search space that are not yet correctly covered
- Algorithm:
  - 1. Initialize the window with a random subsample of the available data
  - 2. Learn a theory from the current window
  - 3. If the learned theory correctly classifies all examples (including those outside of the window), return the theory
  - 4. Add some mis-classified examples to the window and goto 2.
- Properties:
  - may learn a good theory from a subset of the data
  - problems with noisy data



#### **Outlier Detection**



#### unsupervised Data Cleaning method

- Goal:
  - detect examples which deviate a lot from other examples
  - they are probably due to measurement errors
- 2-Sigma Rule:
  - common statistical Method for outlier detection
  - An example is classified as an outlier if
    - there exists one (numerical) attribute A
    - whose value deviates from the mean by more than two standard deviations

$$|x_A - \overline{x}_A| > 2 \cdot \sigma_A$$

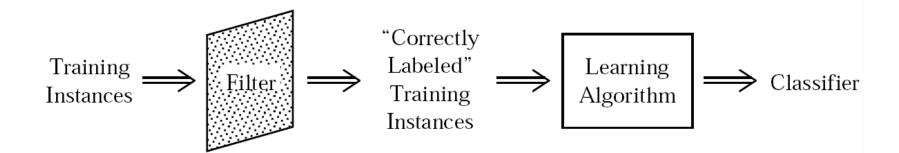


# **Identifying Mislabeled Examples**

(Friedl & Brodley, 1999)



- Identify noisy examples
  - correct them or remove them from the database
  - train the classifier on a corrected database



#### **Robust Decision Trees**

(John, KDD-95)



- supervised data cleaning method
  - 1. train a decision tree T
  - 2. remove all training examples that are misclassified by T
  - 3. learn a new tree from the remaining examples
  - 4. repeat until convergence
- thus the final tree is trained on a subset of original data
  - but may not only be simpler but also more accurate
- may be viewed as an inverse windowing

#### **Ensemble Filters**



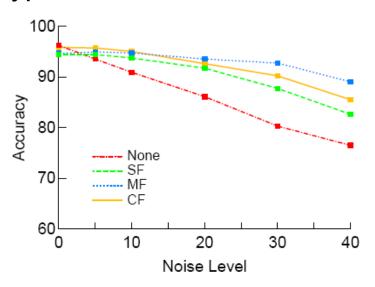
- Generalization of the previous approach to ensembles
  - filter an example if  $\geq c\%$  of the base classifiers misclassify it
- Majority Filter
  - filter if more than half of the classifiers mislabel the example
- Consensus Filter
  - special case where only unanimous misclassifications count

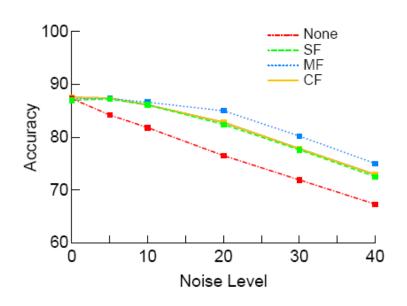
## **Experimental Comparison**

(Friedl & Brodley, 1999)



#### Typical results:





- majority performs best
- consensus is too conversative
  - not enough examples removed
- single algorithm filter (≈ robust decision trees) is too loose
  - too many examples removed