Data Mining und Maschinelles Lernen

TECHNISCHE UNIVERSITÄT DARMSTADT

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 | J. Fürnkranz

Knowledge Discovery in Databases: Key Steps

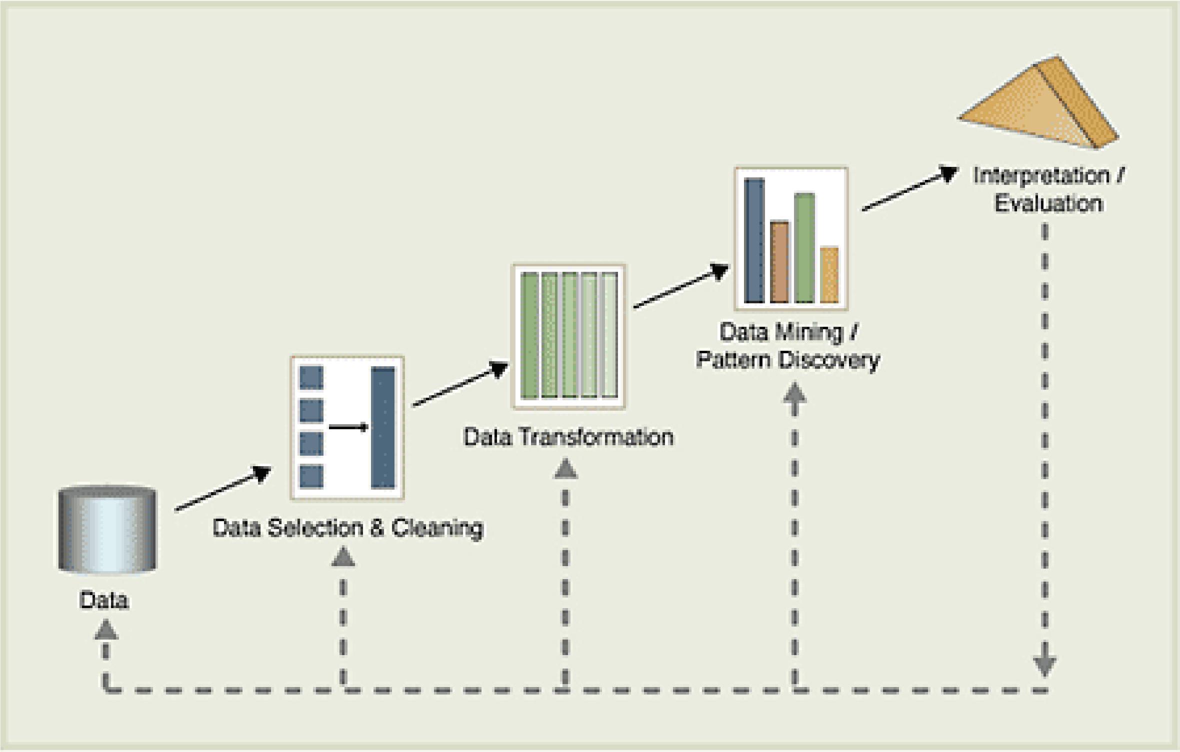
TECHNISCHE UNIVERSITÄT DARMSTADT

Key steps in the Knowledge Discovery cycle:

1. Data Cleaning: remove noise and inconsistent data
2. Data Integration: combine multiple data sources
3. 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)
5. Data Mining: apply machine learning and machine discovery techniques
6. Pattern Evaluation: evaluate whether the found patterns meet the requirements (e.g., interestingness)
7. Knowledge Presentation: present the mined knowledge to the user (e.g., visualization)

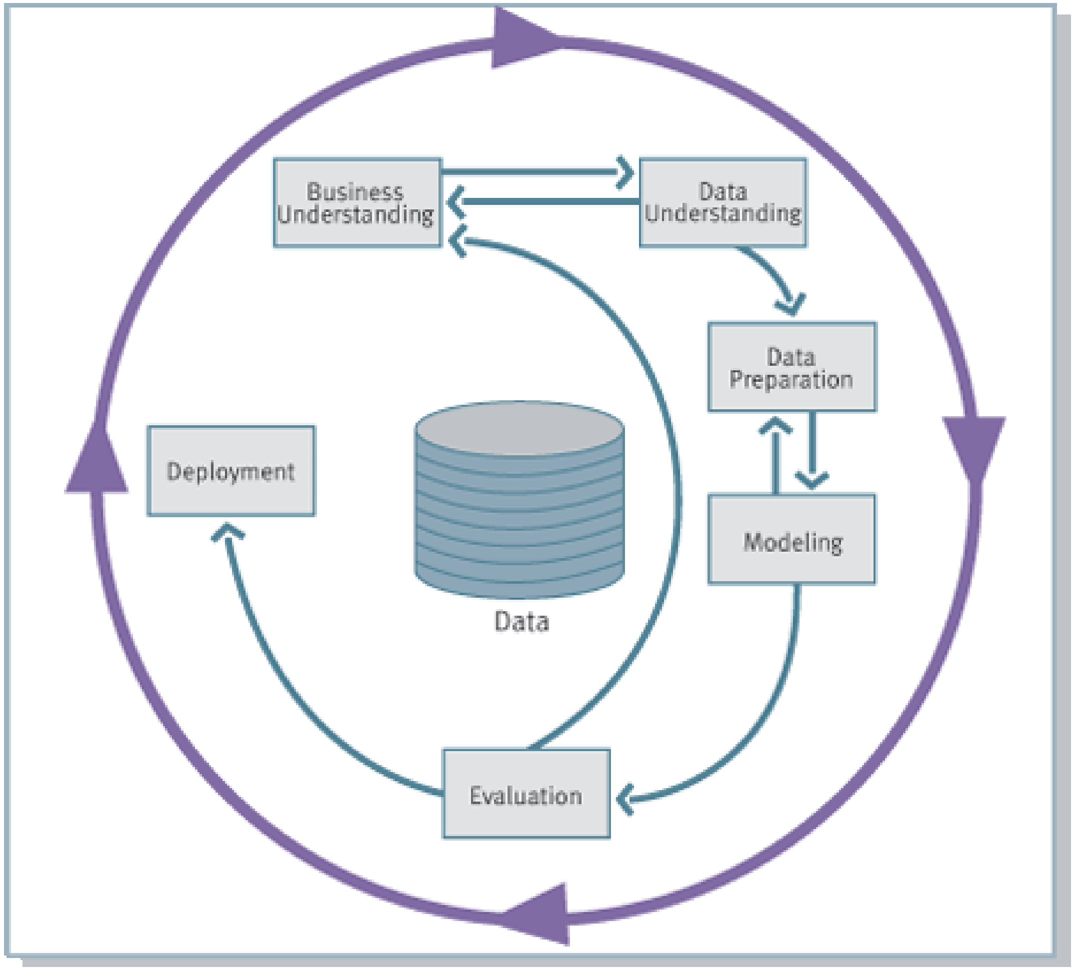
Data Mining is a Process !

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

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 pre-processing 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).

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

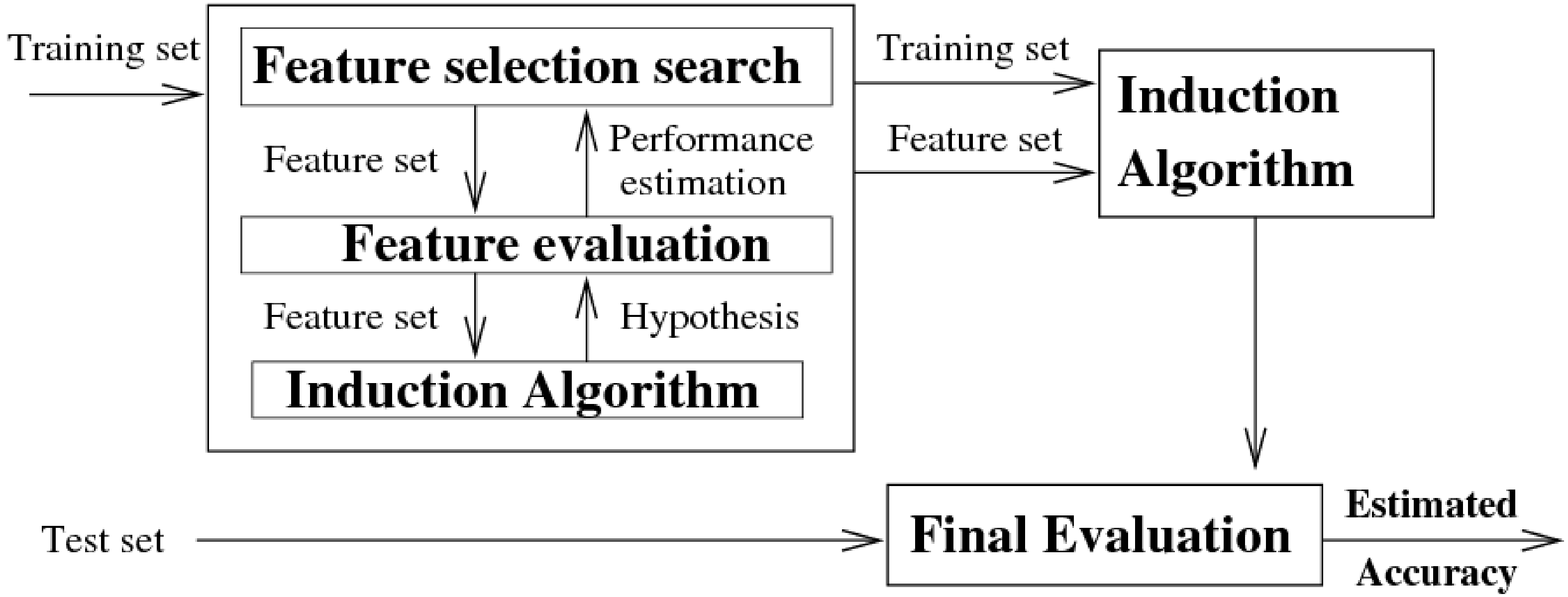
- foreach attribute A
  - $W[A]$ = feature weight according to some measure of discrimination
- select the n features with highest $W[A]$

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

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.

FSS: Wrapper Approach

- Forward selection:

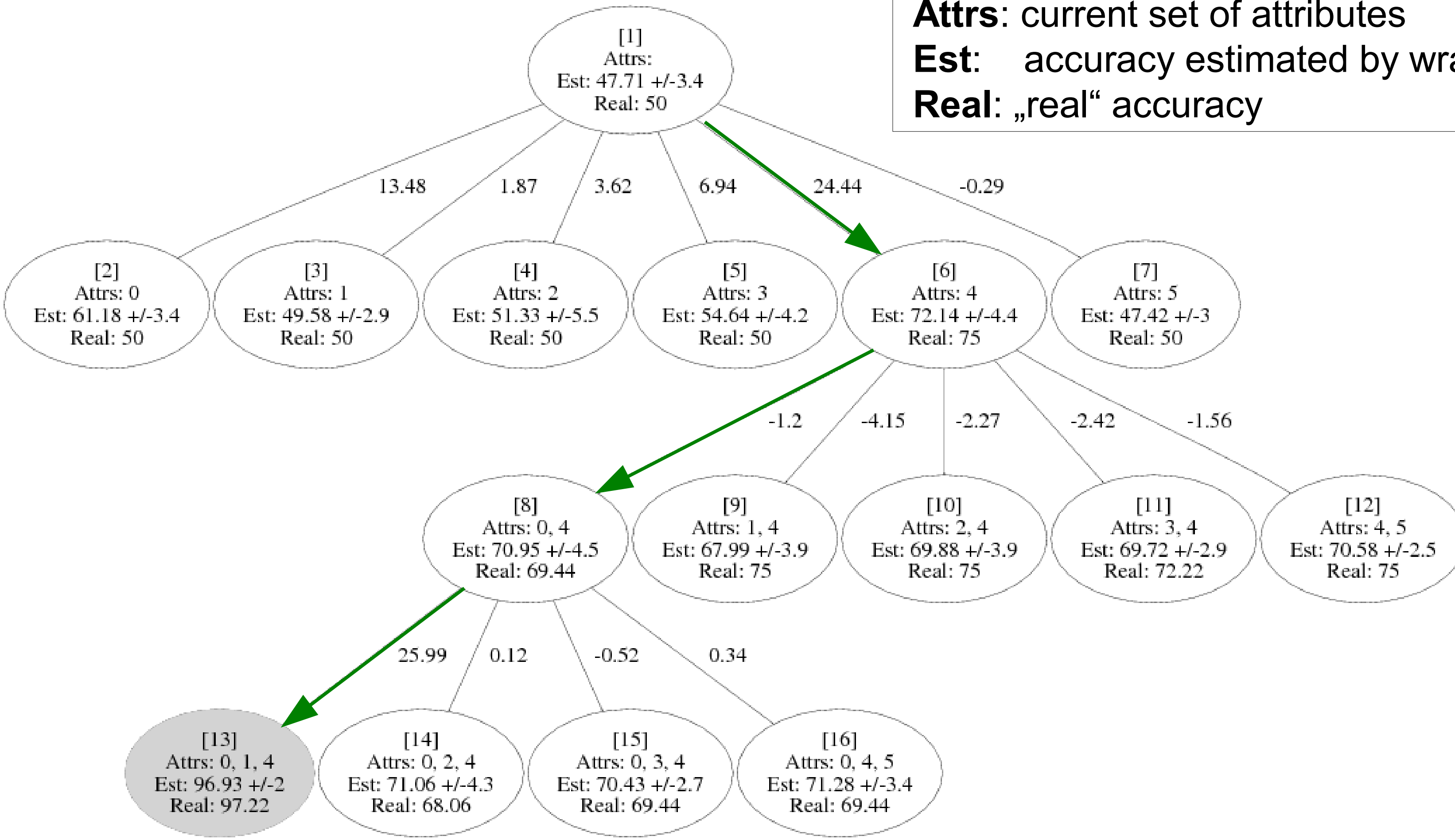
1. start with empty feature set F
2. for each attribute A
   - Estimate Accuracy of Learning algorithm on $F \cup \{A\}$
3. $F = F \cup$ {attribute with highest estimated accuracy}
4. goto 2. until n features have been found

- Backward elimination:
  - start with full feature set F
  - try to remove attributes

- Bi-directional search is also possible

Example: Forward Search for Best 3 Features

Attrs: current set of attributes
Est: accuracy estimated by wrapper
Real: „real“ accuracy



Stopping Criteria for Wrapper algorithms

- Select the best n attributes
  - Like pseudo-code on the previous slide
- Add an attribute if it increases accuracy
  - Might be too greedy
  - e.g., in the previous example, the search would have stopped after adding the first attribute
- Add an attribute until the last k added attributes did not increase attribute
  - e.g., for $k = 2$, the last example would have found the final 3-value set
- Add an attribute if it does not significantly decrease accuracy
  - Significance test can be performed with → sign test or → t-test

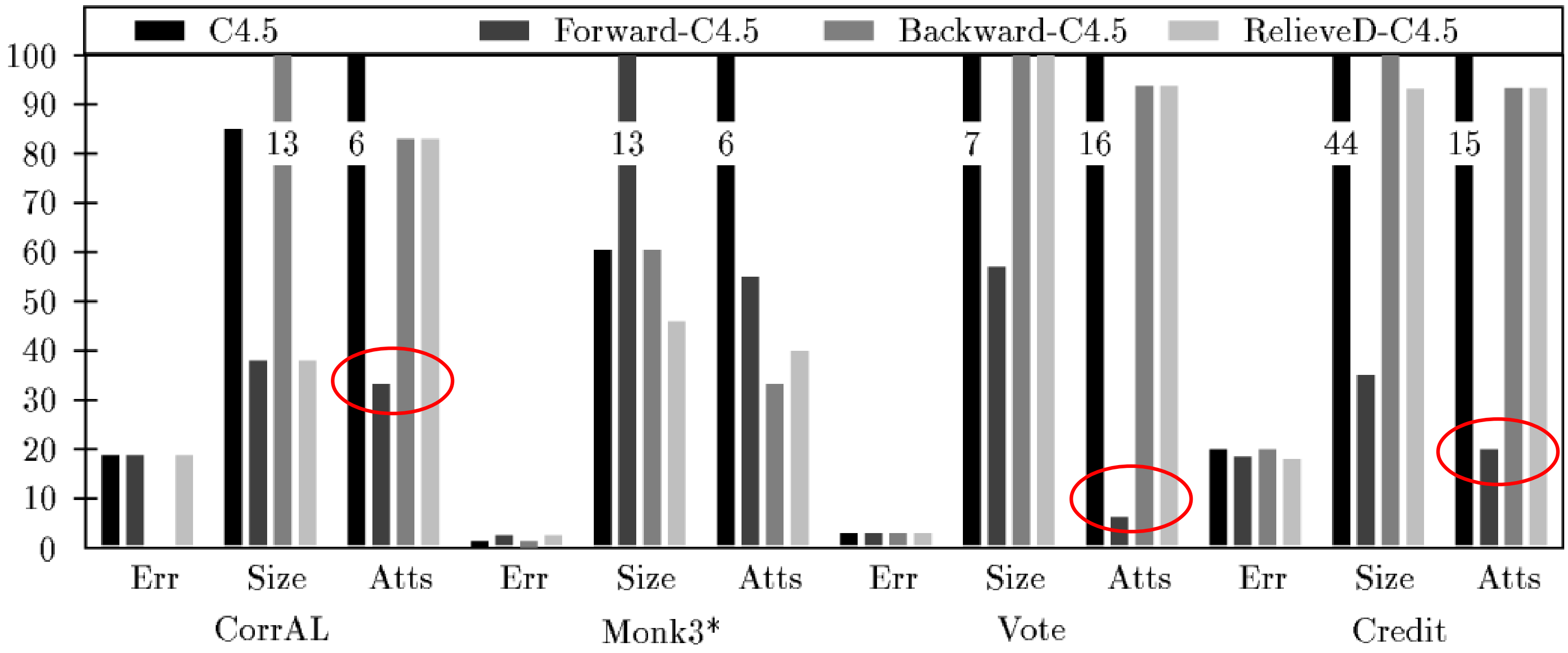
Wrapper Approaches - Discussion

- 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 sub-intervals

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) → (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 χ^2 value for each pair of adjacent intervals

$$\chi^2 = \sum_{i=1}^{2} \sum_{j=1}^{c} \frac{(A_{ij} - E_{ij})^2}{E_{ij}} \quad \text{where} \quad E_{ij} = N_i \frac{C_j}{N_1 + N_2}$$

$$C_j = A_{1j} + A_{2j}$$

$$N_i = \sum_{j=1}^{c} A_{ij}$$

A_{ij} = number of examples in i-th interval that are of class j

E_{ij} = expected number of examples in i-th interval that are of class j

= examples in i-th interval N_i $\times$ fraction of examples of class j in both intervals

  - merge those with lowest χ^2 value
- stop
  - when the χ^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

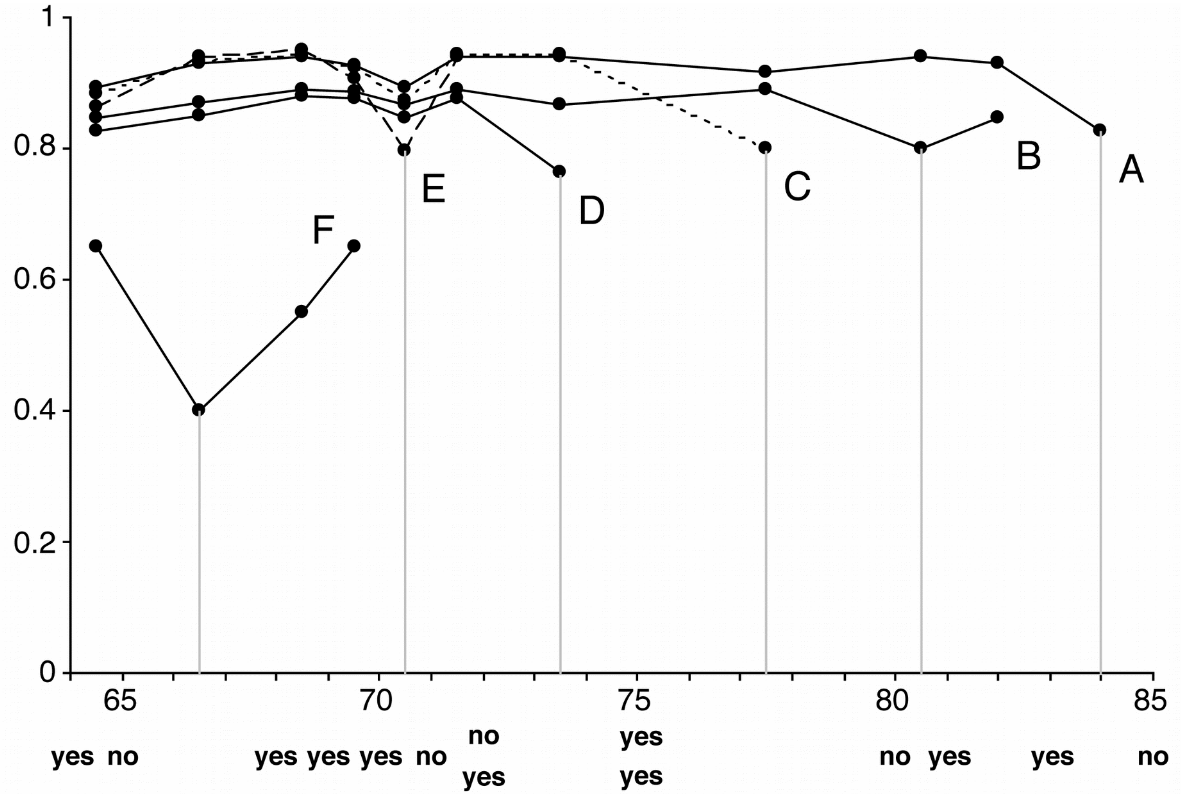
- initialization:
  - initialize intervals with a single interval covering all examples S
  - sort all examples according to the attribute value
  - initialize the set of possible split points
    - simple: all values
- interval splitting:
  - select split point with the minimum weighted entropy

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

  - recursively apply Entropy-Split to $S_{A<T_{max}}$ and $S_{A\geq T_{max}}$
- 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



Example

- Possible Split points:

  64.5, 66.5, 68.5, 69.5, 70.5, 71.5, 73.5, 77.5, 80.5, 82.0, 84.0
- Compute Information gain for every split point
  - As in decision tree induction for numeric attributes
- Select the point with the highest information gain
  - In this case 84.0 (→ point A in graph in previous slide)
- Repeat in both successor nodes until a full decision tree is grown
  - In the example only the left branch contains examples

Note:

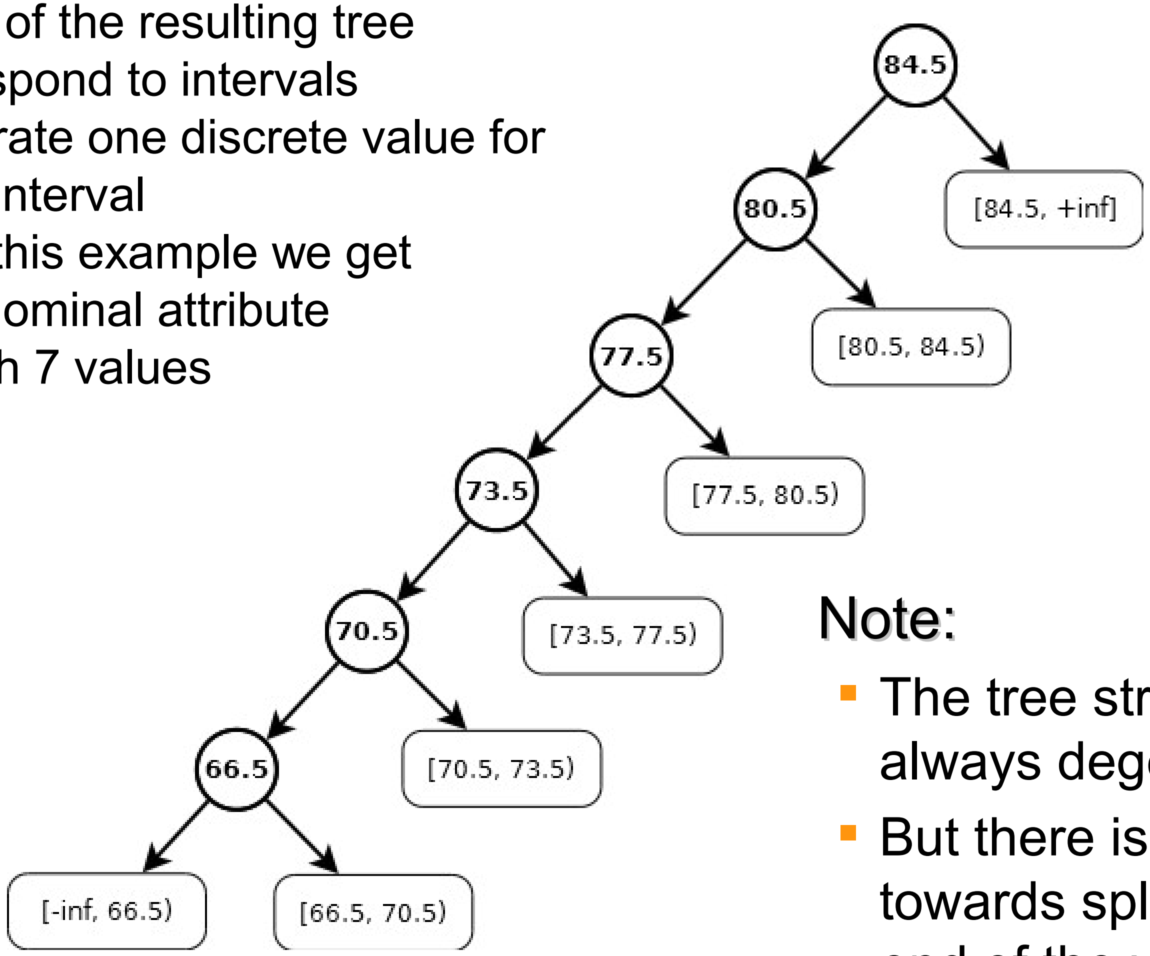
- One can proof that a split point can only lie on a change between classes, i.e., we would only have to consider split points

  64.5, 66.5, 70.5, 71.5, 73.5, 77.5, 80.5, 84.0

  (we cannot split the yes/no examples at 72.0, so we have to split left and right of it)

Resulting Tree

- Leafs of the resulting tree correspond to intervals
- Generate one discrete value for each interval
  - In this example we get a nominal attribute with 7 values



Note:

- The tree structure does not always degenerate to a list
- But there is a selection bias towards split points near the end of the value ranges

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 multi-dimensional 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

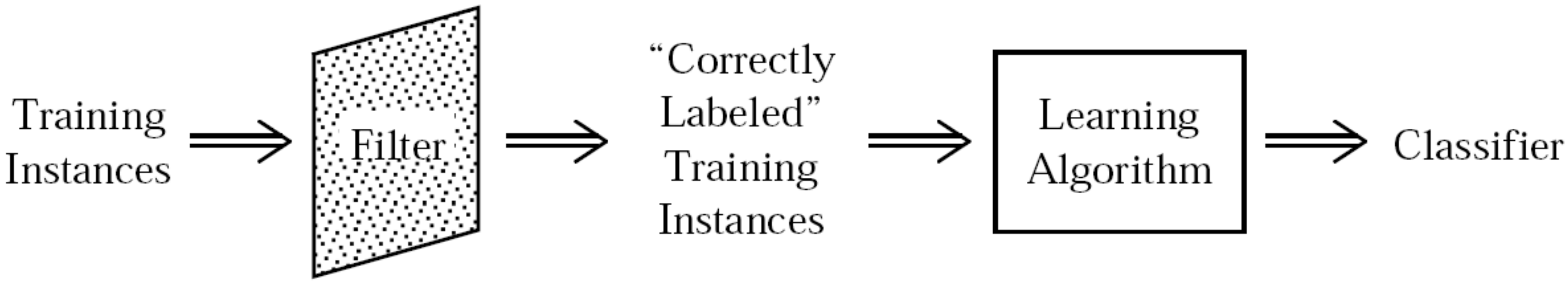
unsupervised Data Cleaning method

- 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

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

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

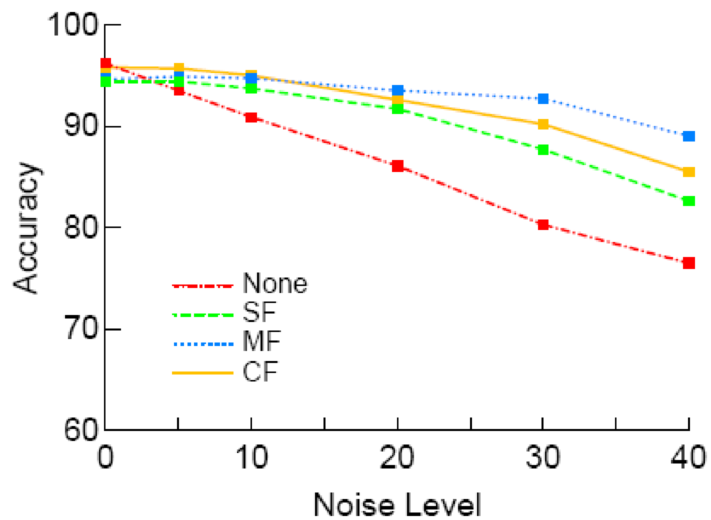
Ensemble Filters

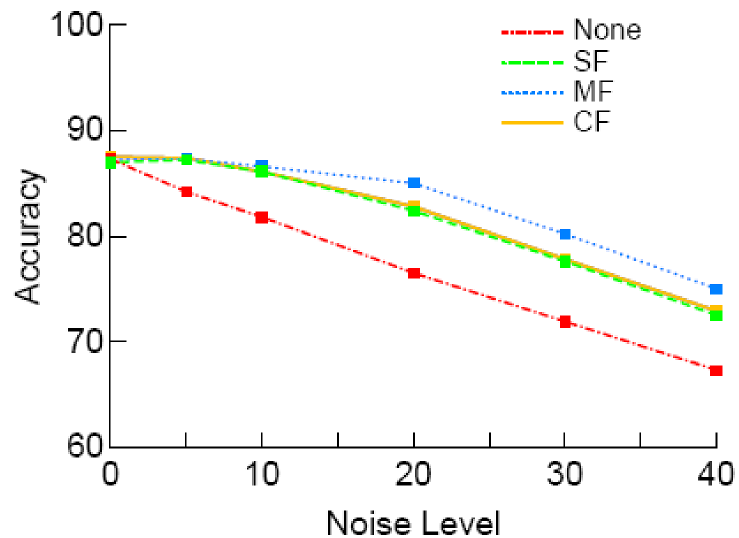
- Generalization of the previous approach to ensembles
  - filter an example if $\geq c\%$ of the base classifiers misclassify it

- 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