### **Chapter 12**

# Discovering New Knowledge – Data Mining

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### **Chapter Objectives**

- Introduce the student to the concept of Data Mining (DM), also known as Knowledge Discovery in Databases (KDD).
  - How it is different from knowledge elicitation from experts
  - How it is different from extracting existing knowledge from databases.
- The objectives of data mining
  - Explanation of past events (descriptive DM)
  - Prediction of future events (predictive DM)
- (continued)

### **Chapter Objectives (cont.)**

- Introduce the student to the different classes of statistical methods available for DM
  - Classical statistics (e.g., regression, curve fitting, ...)
  - Induction of symbolic rules
  - Neural networks (a.k.a. "connectionist" models)
- Introduce the student to the details of some of the methods described in the chapter.

### **Historical Perspective**

- DM, a.k.a. KDD, arose at the intersection of three independently evolved research directions:
  - Classical statistics and statistical pattern recognition
  - Machine learning (from symbolic AI)
  - Neural networks

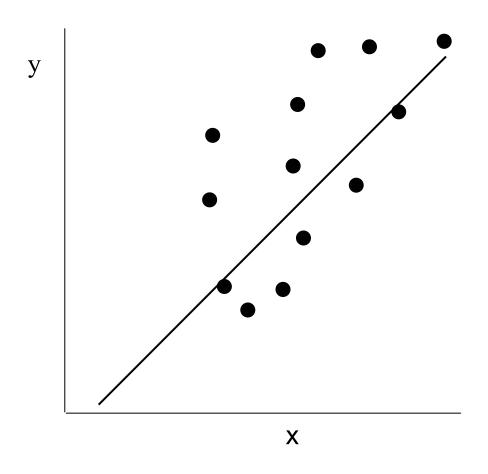
### **Objectives of Data Mining**

- Descriptive DM seeks patterns in past actions or activities to affect these actions or activities
  - eg, seek patterns indicative of fraud in past records
- Predictive DM looks at past history to predict future behavior
  - Classification classifies a new instance into one of a set of discrete predefined categories
  - Clustering groups items in the data set into different categories
  - Affinity or association finds items closely associated in the data set

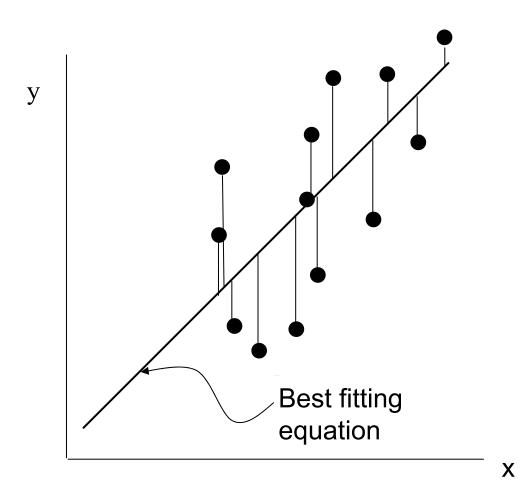
# Classical statistics & statistical pattern recognition

- Provide a detailed description of the most important statistical methods for data mining
  - Curve fitting with least squares method
  - Multi-variate correlation
  - K-Means clustering
  - Market Basket analysis
  - Discriminant analysis
  - Logistic regression

# Figure 12.14 – 2-D input data plotted on a graph



# Figure 12.15 – data and deviations



### **Induction of symbolic rules**

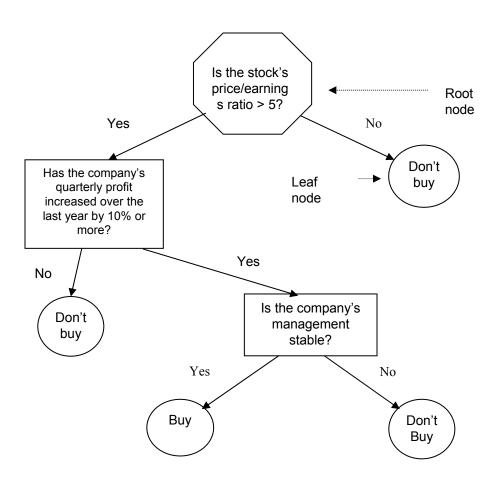
- Present a detailed description of the symbolic approach to data mining - rule induction by learning decision trees
- Present the main algorithm for rule induction
  - C5.0 and its ancestors, ID3 and CLS (from machine learning)
  - CART (Classification And Regression Trees) and CHAID, very similar algorithms for rule induction (independently developed in statistics)
- Present several example applications of rule induction

# Table 12.1 – decision tables (if ordered, then decision lists)

| Name         | Outlook | Temperature | Humidity | Class         |
|--------------|---------|-------------|----------|---------------|
| Data sample1 | Sunny   | Mild        | Dry      | Enjoyable     |
| Data sample2 | Cloudy  | Cold        | Humid    | Not Enjoyable |
| Data sample3 | Rainy   | Mild        | Humid    | Not Enjoyable |
| Data sample4 | Sunny   | Hot         | Humid    | Not Enjoyable |

Note: DS = Data Sample

# Figure 12.1 – decision trees (a.k.a. classification trees)

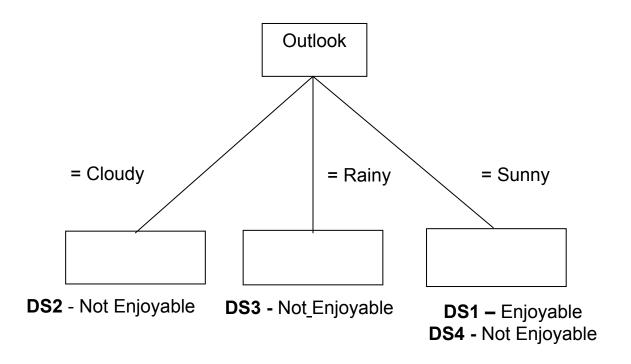


#### **Induction trees**

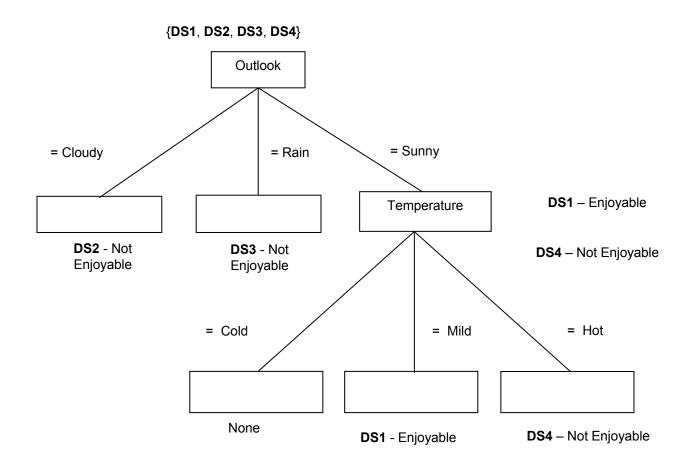
- An induction tree is a decision tree holding the data samples (of the training set)
- Built progressively by gradually segregating the data samples

# Figure 12.2 – simple induction tree (step 1)

{DS1, DS2, DS3, DS4}



# Figure 12.3 – simple induction tree (step 2)



#### Writing the induced tree as rules

- Rule 1. If the Outlook is cloudy, then the Weather is not enjoyable.
- Rule 2. If the Outlook is rainy, then the Weather is not enjoyable.
- Rule 3. If the Outlook is sunny and Temperature
  is mild, then the Weather is enjoyable.
- Rule 4. If the Outlook is sunny and Temperature
  is cold, then the Weather is not enjoyable.

## Learning decision trees for classification into multiple classes

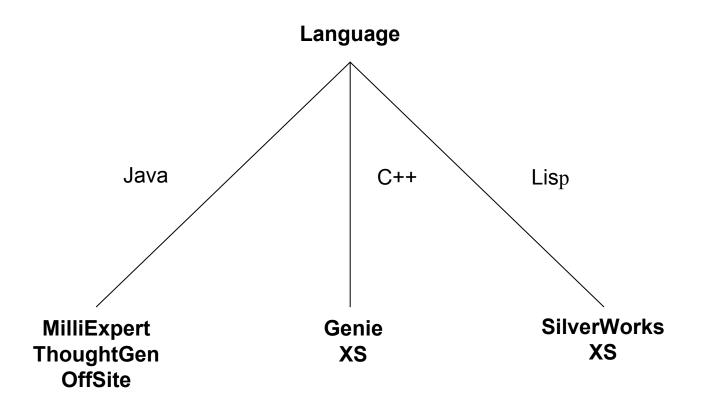
- In the previous example, we were learning a function to predict a boolean (enjoyable = true/false) output.
- The same approach can be generalized to learn a function that predicts a class (when there are multiple predefined classes/categories).
- For example, suppose we are attempting to select a KBS shell for some application:
  - with the following as our options:
    - ThoughtGen, Offsite, Genie, SilverWorks, XS, MilliExpert
  - using the following attributes and range of values:
    - Development language: { java, C++, lisp }
    - Reasoning method: { forward, backward }
    - External interfaces: { dBase, spreadsheetXL, ASCII file, devices }
    - Cost: any positive number
    - Memory: any positive number

#### **Table 12.2 -**

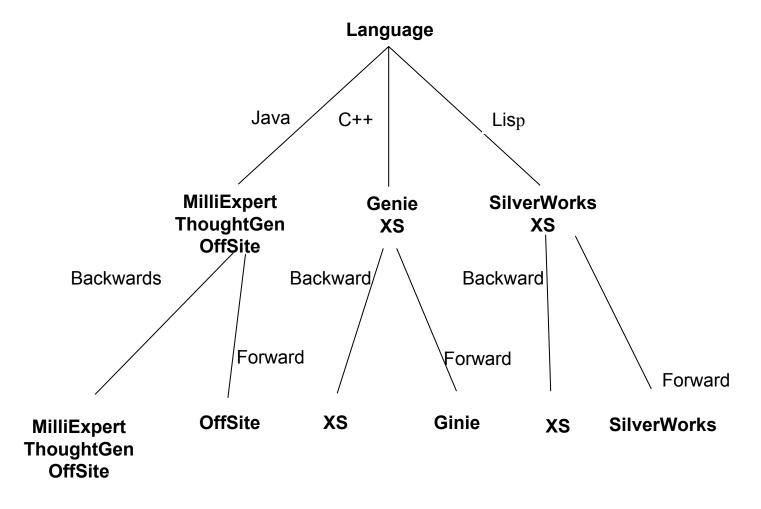
### collection of data samples (training set) described as vectors of attributes (feature vectors)

| Language | Reasoning method | Interface<br>Method | Cost  | Memory | Classification |
|----------|------------------|---------------------|-------|--------|----------------|
| Java     | Backward         | SpreadsheetXL       | 250   | 128MB  | MilliExpert    |
| Java     | Backward         | ASCII               | 250   | 128MB  | MilliExpert    |
| Java     | Backward         | dBase               | 195   | 256MB  | ThoughtGen     |
| Java     | *                | Devices             | 985   | 512MB  | OffSite        |
| C++      | Forward          | *                   | 6500  | 640MB  | Genie          |
| LISP     | Forward          | *                   | 15000 | 5GB    | Silverworks    |
| C++      | Backward         | *                   | 395   | 256MB  | XS             |
| LISP     | Backward         | *                   | 395   | 256MB  | XS             |

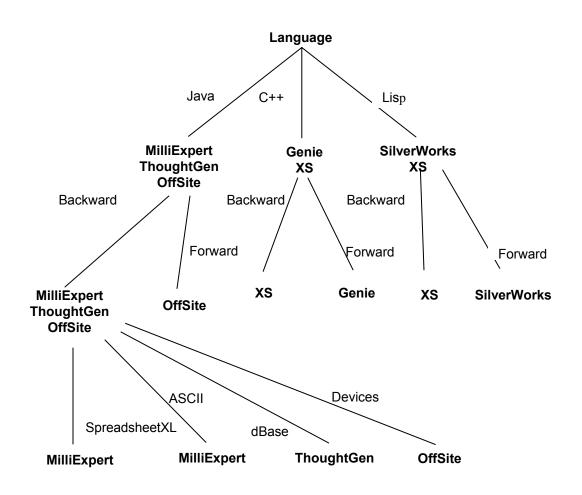
### **Figure 12.4 –** decision tree resulting from selection of the language attribute



### **Figure 12.5** – decision tree resulting from addition of the reasoning method attribute



# Figure 12.6 – final decision tree

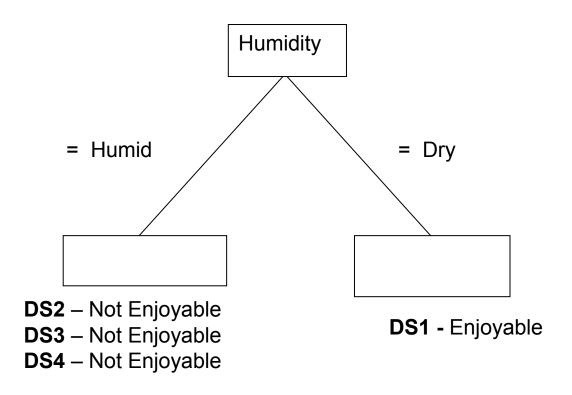


### Order of choosing attributes

 Note that the decision tree that is built depends greatly on which attributes you choose first

### **Figure 12.7**

{DS1, DS2, DS3, DS4}



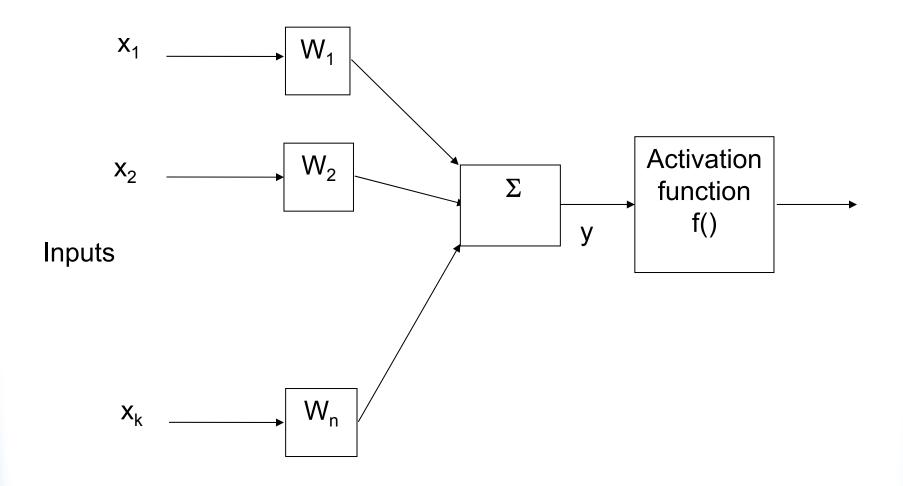
# Order of choosing attributes (cont)

- One sensible objective is to seek the minimal tree, ie, the smallest tree required to classify all training set samples correctly
  - Occam's Razor principle: the simplest explanation is the best
- What order should you choose attributes in, so as to obtain the minimal tree?
  - Often too complex to be feasible
  - Heuristics used
  - Information gain, computed using information theoretic quantities, is the best way in practice

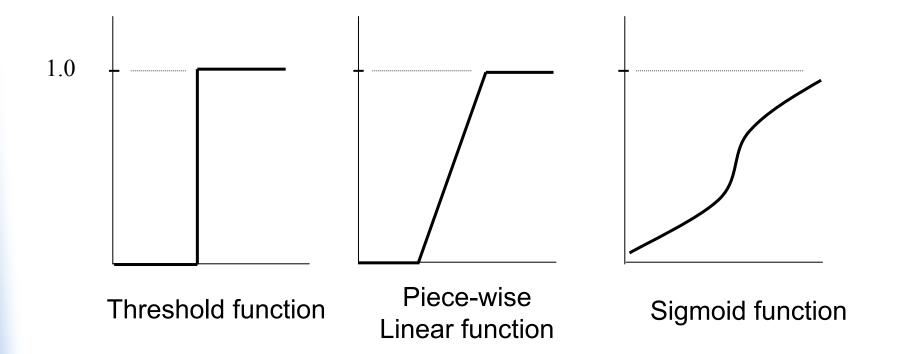
#### **Artificial Neural Networks**

- Provide a detailed description of the connectionist approach to data mining - neural networks
- Present the basic neural network architecture the multi-layer feed forward neural network
- Present the main supervised learning algorithm backpropagation
- Present the main unsupervised neural network architecture - the Kohonen network

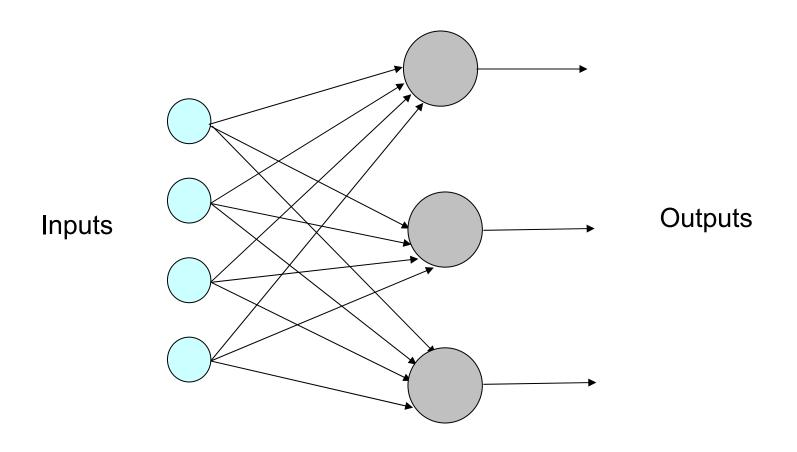
# Figure 12.8 – simple model of a neuron



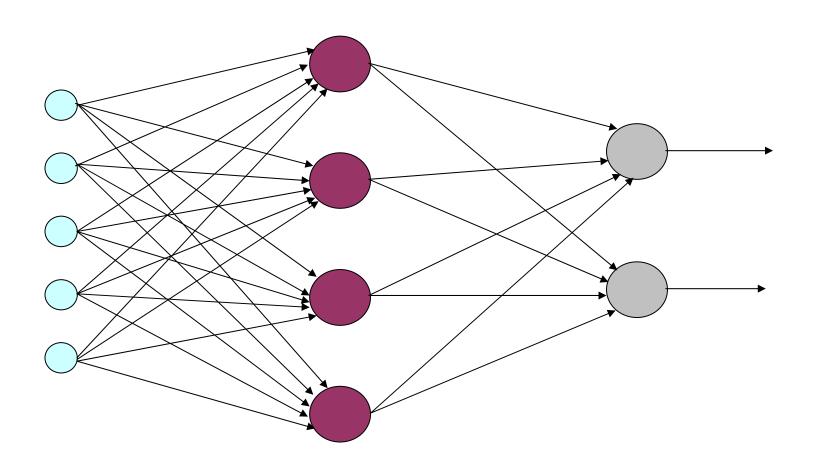
## Figure 12.9 – three common activation functions



### Figure 12.10 – simple singlelayer neural network



## Figure 12.11 – two-layer neural network



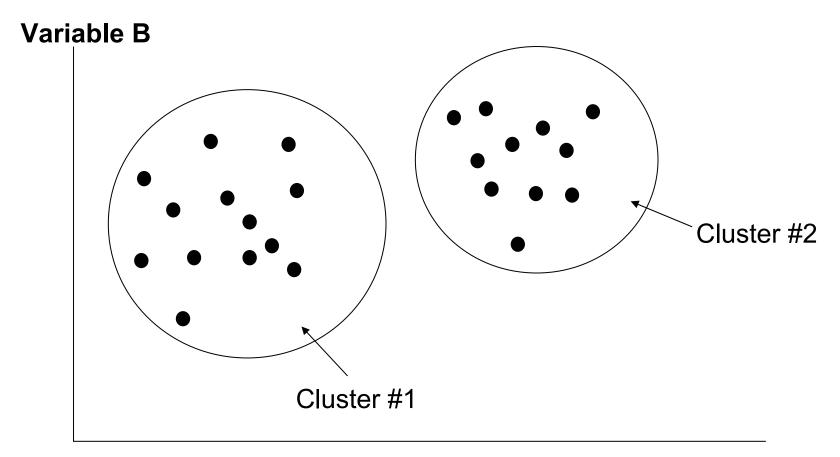
# Supervised Learning: Back Propagation

- An iterative learning algorithm with three phases:
  - 1. Presentation of the examples (input patterns with outputs) and feed forward execution of the network
  - 2. Calculation of the associated errors when the output of the previous step is compared with the expected output and back propagation of this error
  - 3. Adjustment of the weights

## **Unsupervised Learning: Kohonen Networks**

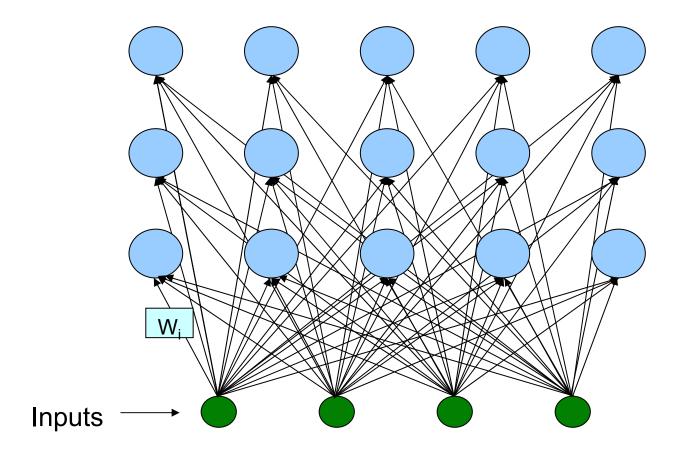
- Clustering by an iterative competitive algorithm
- Note relation to CBR

# Figure 12.12 – clusters of related data in 2-D space



Variable A

### Figure 12.13 – Kohonen selforganizing map



#### When to use what

 Provide useful guidelines for determining what technique to use for specific problems

#### **Table 12.3**

| Goal  | Input<br>Variables<br>(Predictors) | Output<br>Variables<br>(Outcomes) | Statistical<br>Technique                  | Examples<br>[SPSS, 2000]   |
|---|------------------------------------|-----------------------------------|---|--|
| Find linear<br>combination of<br>predictors that<br>best separate the<br>population | Continuous                         | Discrete                          | Discriminant<br>Analysis                  | <ul> <li>Predict instances of fraud</li> <li>Predict whether customers will remain or leave (churners or not)</li> <li>Predict which customers will respond to a new product or offer</li> <li>Predict outcomes of various medical procedures</li> </ul> |
| Predict the probability of outcome being in a particular category                   | Continuous                         | Discrete                          | Logistic and<br>Multinomial<br>Regression | <ul> <li>Predicting insurance policy renewal</li> <li>Predicting fraud</li> <li>Predicting which product a customer will buy</li> <li>Predicting that a product is likely to fail</li> </ul>   |

### **Table 12.3 (cont.)**

| Goal   | Input<br>Variables<br>(Predictors) | Output<br>Variables<br>(Outcomes) | Statistical<br>Technique           | Examples<br>[SPSS, 2000]  |
|--|------------------------------------|-----------------------------------|------------------------------------|---|
| Output is a linear combination of input variables                              | Continuous                         | Continuous                        | Linear<br>Regression               | Predict expected revenue in dollars from a new customer Predict sales revenue for a store Predict waiting time on hold for callers to an 800 number. Predict length of stay in a hospital based on patient characteristics and medical condition. |
| For experiments and repeated measures of the same sample                       | Most inputs<br>must be<br>Discrete | Continuous                        | Analysis of<br>Variance<br>(ANOVA) | Predict which<br>environmental factors are<br>likely to cause cancer  |
| To predict future events whose history has been collected at regular intervals | Continuous                         | Continuous                        | Time Series<br>Analysis            | Predict future sales data<br>from past sales records  |

#### **Table 12.4**

| Goal   | Input<br>(Predictor)<br>Variables  | Output<br>(Outcome)<br>Variables   | Statistical<br>Technique               | Examples<br>[SPSS, 2000]  |
|--|--|--|--|---|
| Predict outcome based on values of nearest neighbors         | Continuous,<br>Discrete, and<br>Text   | Continuous or<br>Discrete  | Memory-<br>based<br>Reasoning<br>(MBR) | Predicting medical outcomes   |
| Predict by<br>splitting data into<br>subgroups<br>(branches) | Continuous or Discrete (Different techniques used based on data characteristics) | Continuous or Discrete (Different techniques used based on data characteristics) | Decision<br>Trees                      | Predicting which customers will leave Predicting instances of fraud |
| Predict outcome in complex non-linear environments           | Continuous or<br>Discrete  | Continuous or<br>Discrete  | Neural<br>Networks                     | Predicting expected revenue Predicting credit risk                  |

#### **Table 12.5**

| Goal  | Input<br>(Predictor)<br>Variables      | Output<br>(Outcome)<br>Variables | Statistical<br>Technique                                 | Examples [SPSS, 2000]   |
|---|--|----------------------------------|--|---|
| Predict by<br>splitting data into<br>more than two<br>subgroups<br>(branches) | Continuous,<br>Discrete, or<br>Ordinal | Discrete                         | Chi-square Automatic<br>Interaction Detection<br>(CHAID) | Predict which demographic combinations of predictors yield the highest probability of a sale     Predict which factors are causing product defects in manufacturing |
| Predict by<br>splitting data into<br>more than two<br>subgroups<br>(branches) | Continuous                             | Discrete                         | C5.0   | <ul> <li>Predict which loan customers are considered a "good" risk</li> <li>Predict which factors are associated with a country's investment risk</li> </ul>        |

### **Table 12.5 (cont.)**

| Goal  | Input<br>(Predictor)<br>Variables | Output<br>(Outcome)<br>Variables | Statistical<br>Technique                                   | Examples [SPSS, 2000]   |
|---|-----------------------------------|----------------------------------|--|---|
| Predict by<br>splitting data into<br>binary subgroups<br>(branches) | Continuous                        | Continuous                       | Classification and<br>Regression Trees<br>(CART)           | Predict which factors are associated with a country's competitiveness     Discover which variables are predictors of increased customer profitability |
| Predict by splitting data into binary subgroups (branches)          | Continuous                        | Discrete                         | Quick, Unbiased,<br>Efficient, Statistical<br>Tree (QUEST) | •Predict who needs additional care after heart surgery  |

### **Table 12.6**

| Goal  | Input<br>Variables<br>(Predictor) | Output<br>Variables<br>(Outcome) | Statistical<br>Technique                           | Examples [SPSS, 2000]   |
|---|-----------------------------------|----------------------------------|--|---|
| Find large groups<br>of cases in large<br>data files that are<br>similar on a small<br>set of input<br>characteristics, | Continuous<br>or Discrete         | No<br>outcome<br>variable        | K-means<br>Cluster<br>Analysis                     | Customer segments for<br>marketing     Groups of similar insurance<br>claims  |
| To create large cluster memberships   |                                   |                                  | Kohonen<br>Neural<br>Networks                      | Cluster customers into<br>segments based on<br>demographics and buying<br>patterns  |
| Create small set<br>associations and<br>look for patterns<br>between many<br>categories                                 | Logical                           | No<br>outcome<br>variable        | Market Basket or Association Analysis with Apriori | Identify which products are likely to be purchased together     Identify which courses students are likely to take together |

# Errors and their significance in DM

- Discuss the importance of errors in data mining studies
- Define the types of errors possible in data mining studies

#### **Table 12.7**

| Heart Disease Diagnostic   | Predicted<br>No Disease | Predicted<br>Presence of Disease |
|----------------------------|-------------------------|----------------------------------|
| Actual<br>No Disease       | 118 (72%)               | 46 (28%)                         |
| Actual Presence of Disease | 43 (30.9%)              | 96 (69.1%)                       |

#### **Conclusions**

- The student should be able to use:
  - Curve-fitting algorithms.
  - Statistical methods for clustering.
  - The C5.0 algorithm to capture rules from examples.
  - Basic feedforward neural networks with supervised learning.
  - Unsupervised learning, clustering techniques and the Kohonen networks.
  - Other statistical techniques.

### **Chapter 12**

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