CS490D: Introduction to Data Mining
Prof. Chris Clifton

March 8, 2004

Midterm Review

Midterm Wednesday, March 10, in class. Open book/notes.

Seminar Thursday: Support Vector Machines

- Massive Data Mining via Support Vector Machines
- Hwanjo Yu, University of Illinois
  - Thursday, March 11, 2004
  - 10:30-11:30
  - CS 111
- Support Vector Machines for:
  - classifying from large datasets
  - single-class classification
  - discriminant feature combination discovery

Course Outline

www.cs.purdue.edu/~clifton/cs490d

1. Introduction: What is data mining?
   – What makes it a new and unique discipline?
   – Relationship between Data Warehousing, On-line Analytical Processing, and Data Mining
2. Data mining tasks - Clustering, Classification, Rule learning, etc.
3. Data mining process: Data preparation/cleansing, task identification
   – Introduction to WEKA
4. Association Rule mining
5. Association rules - different algorithm types
6. Classification/Prediction
7. Classification - tree-based approaches
8. Classification - Neural Networks

   Midterm
9. Clustering basics
10. Clustering - statistical approaches
11. Clustering - Neural-net and other approaches
12. More on process - CRISP-DM
    – Preparation for final project
13. Text Mining
14. Multi-Relational Data Mining
15. Future trends

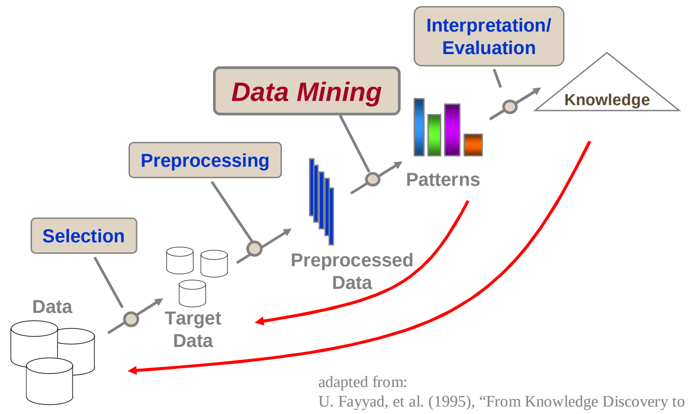
    Final

Text: Jiawei Han and Micheline Kamber, *Data Mining: Concepts and Techniques*. Morgan Kaufmann Publishers, August 2000.

Data Mining: Classification Schemes

- General functionality
  – Descriptive data mining
  – Predictive data mining
- Different views, different classifications
  – Kinds of data to be mined
  – Kinds of knowledge to be discovered
  – Kinds of techniques utilized
  – Kinds of applications adapted

Knowledge Discovery in Databases: Process



adapted from:
U. Fayyad, et al. (1995), "From Knowledge Discovery to Data Mining: An Overview," Advances in Knowledge Discovery and Data Mining, U. Fayyad et al. (Eds.), AAAI/MIT Press

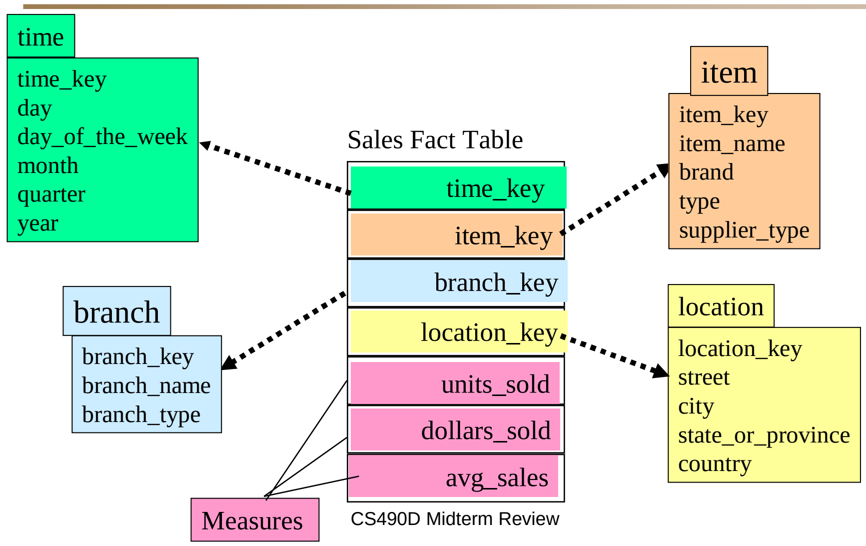
What Can Data Mining Do?

- Cluster
- Classify
  - Categorical, Regression
- Summarize
  - Summary statistics, Summary rules
- Link Analysis / Model Dependencies
  - Association rules
- Sequence analysis
  - Time-series analysis, Sequential associations
- Detect Deviations

What is Data Warehouse?

- Defined in many different ways, but not rigorously.
  - A decision support database that is maintained separately from the organization's operational database
  - Support information processing by providing a solid platform of consolidated, historical data for analysis.
- "A data warehouse is a subject-oriented, integrated, time-variant, and nonvolatile collection of data in support of management's decision-making process."—W. H. Inmon
- Data warehousing:
  - The process of constructing and using data warehouses

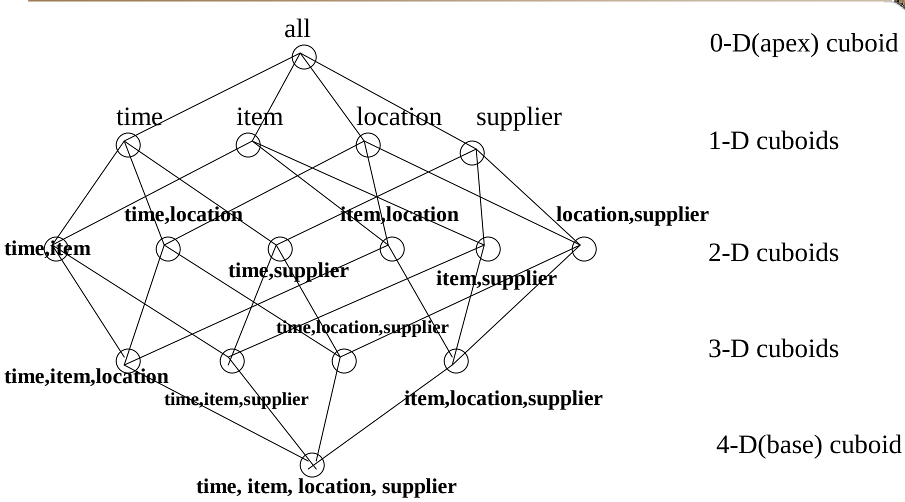
Example of Star Schema



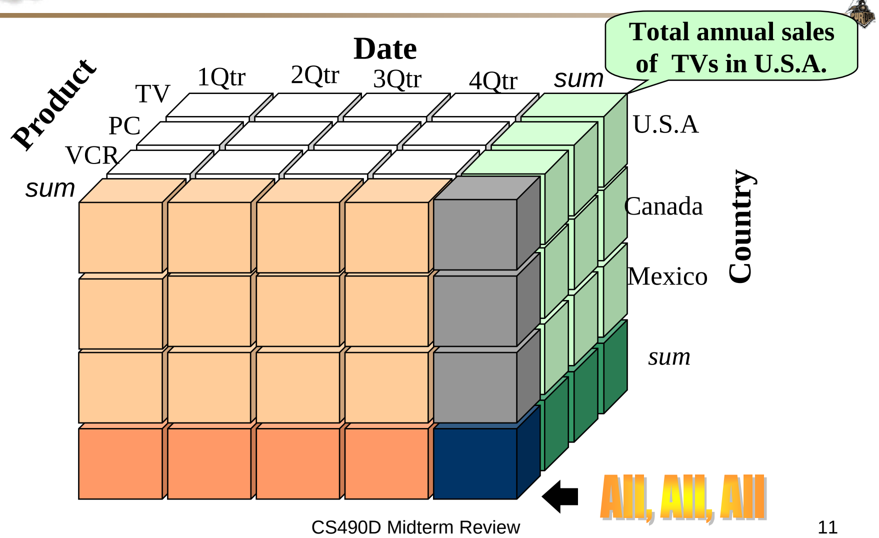
From Tables and Spreadsheets to Data Cubes

- A data warehouse is based on a multidimensional data model which views data in the form of a data cube
- A data cube, such as sales, allows data to be modeled and viewed in multiple dimensions
  - Dimension tables, such as item (item_name, brand, type), or time(day, week, month, quarter, year)
  - Fact table contains measures (such as dollars_sold) and keys to each of the related dimension tables
- In data warehousing literature, an n-D base cube is called a base cuboid. The top most 0-D cuboid, which holds the highest-level of summarization, is called the apex cuboid. The lattice of cuboids forms a data cube.

Cube: A Lattice of Cuboids



A Sample Data Cube



Warehouse Summary

- Data warehouse
- A multi-dimensional model of a data warehouse
  - Star schema, snowflake schema, fact constellations
  - A data cube consists of dimensions & measures
- OLAP operations: drilling, rolling, slicing, dicing and pivoting
- OLAP servers: ROLAP, MOLAP, HOLAP
- Efficient computation of data cubes
  - Partial vs. full vs. no materialization
  - Multiway array aggregation
  - Bitmap index and join index implementations
- Further development of data cube technology
  - Discovery-drive and multi-feature cubes
  - From OLAP to OLAM (on-line analytical mining)

Data Preprocessing

- Data in the real world is dirty
  - incomplete: lacking attribute values, lacking certain attributes of interest, or containing only aggregate data
    - e.g., occupation=“”
  - noisy: containing errors or outliers
    - e.g., Salary=“-10”
  - inconsistent: containing discrepancies in codes or names
    - e.g., Age=“42” Birthday=“03/07/1997”
    - e.g., Was rating “1,2,3”, now rating “A, B, C”
    - e.g., discrepancy between duplicate records

Multi-Dimensional Measure of Data Quality

- A well-accepted multidimensional view:
  - Accuracy
  - Completeness
  - Consistency
  - Timeliness
  - Believability
  - Value added
  - Interpretability
  - Accessibility
- Broad categories:
  - intrinsic, contextual, representational, and accessibility.

Major Tasks in Data Preprocessing

- Data cleaning
  - Fill in missing values, smooth noisy data, identify or remove outliers, and resolve inconsistencies
- Data integration
  - Integration of multiple databases, data cubes, or files
- Data transformation
  - Normalization and aggregation
- Data reduction
  - Obtains reduced representation in volume but produces the same or similar analytical results
- Data discretization
  - Part of data reduction but with particular importance, especially for numerical data

How to Handle Missing Data?

- Ignore the tuple: usually done when class label is missing (assuming the tasks in classification—not effective when the percentage of missing values per attribute varies considerably.
- Fill in the missing value manually: tedious + infeasible?
- Fill in it automatically with
  - a global constant : e.g., “unknown”, a new class?!
  - the attribute mean
  - the attribute mean for all samples belonging to the same class: smarter
  - the most probable value: inference-based such as Bayesian formula or decision tree

How to Handle Noisy Data?

- Binning method:
  - first sort data and partition into (equi-depth) bins
  - then one can smooth by bin means, smooth by bin median, smooth by bin boundaries, etc.
- Clustering
  - detect and remove outliers
- Combined computer and human inspection
  - detect suspicious values and check by human (e.g., deal with possible outliers)
- Regression
  - smooth by fitting the data into regression functions

Data Transformation

- Smoothing: remove noise from data
- Aggregation: summarization, data cube construction
- Generalization: concept hierarchy climbing
- Normalization: scaled to fall within a small, specified range
  - min-max normalization
  - z-score normalization
  - normalization by decimal scaling
- Attribute/feature construction
  - New attributes constructed from the given ones

Data Reduction Strategies

- A data warehouse may store terabytes of data
  - Complex data analysis/mining may take a very long time to run on the complete data set
- Data reduction
  - Obtain a reduced representation of the data set that is much smaller in volume but yet produce the same (or almost the same) analytical results
- Data reduction strategies
  - Data cube aggregation
  - Dimensionality reduction — remove unimportant attributes
  - Data Compression
  - Numerosity reduction — fit data into models
  - Discretization and concept hierarchy generation

Principal Component Analysis

- Given N data vectors from k-dimensions, find c ≤ k orthogonal vectors that can be best used to represent data
  - The original data set is reduced to one consisting of N data vectors on c principal components (reduced dimensions)
- Each data vector is a linear combination of the c principal component vectors
- Works for numeric data only
- Used when the number of dimensions is large

Discretization

- Three types of attributes:
  - Nominal — values from an unordered set
  - Ordinal — values from an ordered set
  - Continuous — real numbers
- Discretization:
  - divide the range of a continuous attribute into intervals
  - Some classification algorithms only accept categorical attributes.
  - Reduce data size by discretization
  - Prepare for further analysis

Data Preparation Summary

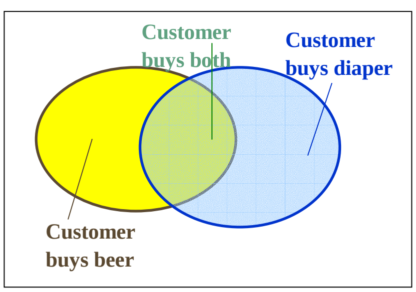
- Data preparation is a big issue for both warehousing and mining
- Data preparation includes
  - Data cleaning and data integration
  - Data reduction and feature selection
  - Discretization
- A lot a methods have been developed but still an active area of research

Association Rule Mining

- Finding frequent patterns, associations, correlations, or causal structures among sets of items or objects in transaction databases, relational databases, and other information repositories.
  - Frequent pattern: pattern (set of items, sequence, etc.) that occurs frequently in a database [AIS93]
- Motivation: finding regularities in data
  - What products were often purchased together? — Beer and diapers?!
  - What are the subsequent purchases after buying a PC?
  - What kinds of DNA are sensitive to this new drug?
  - Can we automatically classify web documents?

Basic Concepts: Association Rules

Transaction-id	Items bought
10	A, B, C
20	A, C
30	A, D
40	B, E, F



- Itemset $X=\{x_1, \ldots, x_k\}$
- Find all the rules $X \rightarrow Y$ with min confidence and support
  - support, *s*, probability that a transaction contains $X \cup Y$
  - confidence, *c*, conditional probability that a transaction having X also contains *Y*.

Let min_support = 50%, min_conf = 50%:

$A \rightarrow C$ (50%, 66.7%)

$C \rightarrow A$ (50%, 100%)

The Apriori Algorithm—An Example

Database TDB

Tid	Items
10	A, C, D
20	B, C, E
30	A, B, C, E
40	B, E

1^{st} scan

C_1

Itemset	sup
{A}	2
{B}	3
{C}	3
{D}	1
{E}	3

L_1

Itemset	sup
{A}	2
{B}	3
{C}	3
{E}	3

C_2

Itemset
{A, B}
{A, C}
{A, E}
{B, C}
{B, E}
{C, E}

2^{nd} scan

C_2

Itemset	sup
{A, B}	1
{A, C}	2
{A, E}	1
{B, C}	2
{B, E}	3
{C, E}	2

L_2

Itemset	sup
{A, C}	2
{B, C}	2
{B, E}	3
{C, E}	2

C_3

Itemset
{B, C, E}

3^{rd} scan

L_3

Itemset	sup
{B, C, E}	2

FP-Tree Algorithm

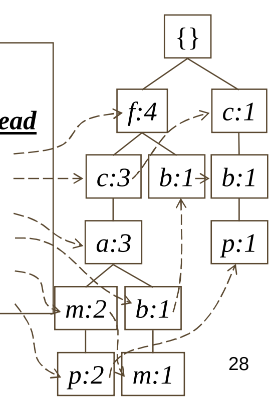
TID	***Items bought***	***(ordered) frequent items***
100	***{f, a, c, d, g, i, m, p}***	***{f, c, a, m, p}***
200	***{a, b, c, f, l, m, o}***	***{f, c, a, b, m}***
300	***{b, f, h, j, o, w}***	***{f, b}***
400	***{b, c, k, s, p}***	***{c, b, p}***
500	***{a, f, c, e, l, p, m, n}***	***{f, c, a, m, p}***

min_support = 3

1. Scan DB once, find frequent 1-itemset (single item pattern)
2. Sort frequent items in frequency descending order, f-list
3. Scan DB again, construct FP-tree

Header Table

Item	*frequency*	*head*
f	*4*	
c	*4*	
a	*3*	
b	*3*	
m	*3*	
p	*3*	



F-list=f-c-a-b-m-p

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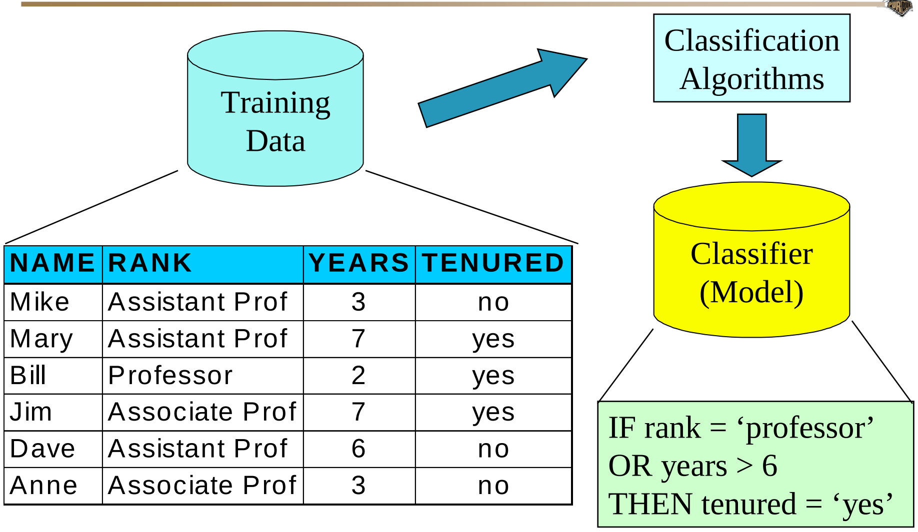
Constrained Frequent Pattern Mining: A Mining Query Optimization Problem

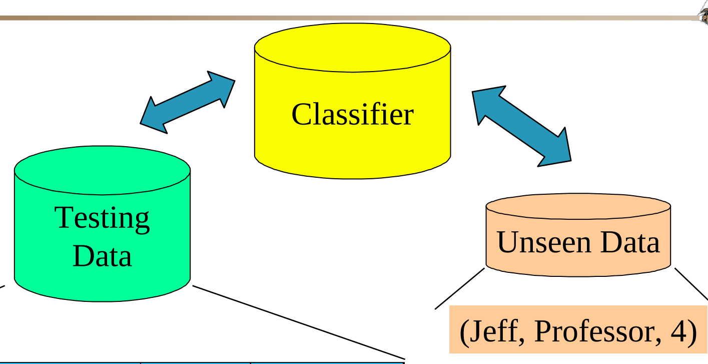
- Given a frequent pattern mining query with a set of constraints C, the algorithm should be
  - sound: it only finds frequent sets that satisfy the given constraints *C*
  - complete: all frequent sets satisfying the given constraints *C* are found
- A naïve solution
  - First find all frequent sets, and then test them for constraint satisfaction
- More efficient approaches:
  - Analyze the properties of constraints comprehensively
  - Push them as deeply as possible inside the frequent pattern computation.

Classification: Model Construction

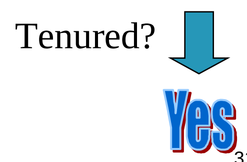


NAME	RANK	YEARS	TENURED
Mike	Assistant Prof	3	no
Mary	Assistant Prof	7	yes
Bill	Professor	2	yes
Jim	Associate Prof	7	yes
Dave	Assistant Prof	6	no
Anne	Associate Prof	3	no

Classification: Use the Model in Prediction



NAME	RANK	YEARS	TENURED
Tom	Assistant Prof	2	no
Merlisa	Associate Prof	7	no
George	Professor	5	yes
Joseph	Assistant Prof	7	yes



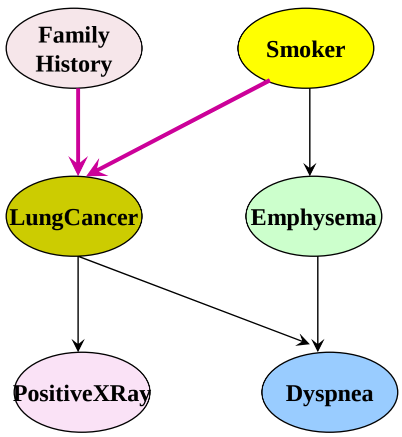
Naïve Bayes Classifier

- A simplified assumption: attributes are conditionally independent:

$$P(X|C_i) = \prod_{k=1}^{n} P(x_k|C_i)$$

- The product of occurrence of say 2 elements x_1 and x_2, given the current class is C, is the product of the probabilities of each element taken separately, given the same class $P([y_1,y_2],C) = P(y_1,C) * P(y_2,C)$
- No dependence relation between attributes
- Greatly reduces the computation cost, only count the class distribution.
- Once the probability $P(X|C_i)$ is known, assign X to the class with maximum $P(X|C_i)*P(C_i)$

Bayesian Belief Network



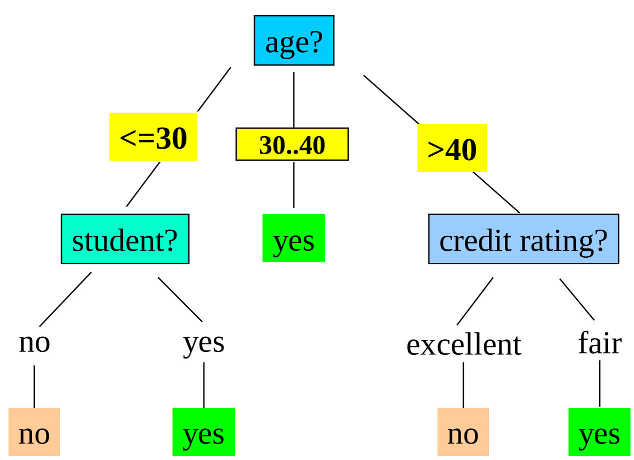
	(FH, S)	(FH, ~S)	(~FH, S)	(~FH, ~S)
LC	**0.8**	**0.5**	**0.7**	**0.1**
~LC	**0.2**	**0.5**	**0.3**	**0.9**

The conditional probability table for the variable LungCancer: Shows the conditional probability for each possible combination of its parents

$$P(z1,\ldots,zn) = \prod_{i=1}^{n} P(z_i \mid Parents(Z_i))$$

Bayesian Belief Networks

Decision Tree



Algorithm for Decision Tree Induction

- Basic algorithm (a greedy algorithm)
  - Tree is constructed in a top-down recursive divide-and-conquer manner
  - At start, all the training examples are at the root
  - Attributes are categorical (if continuous-valued, they are discretized in advance)
  - Examples are partitioned recursively based on selected attributes
  - Test attributes are selected on the basis of a heuristic or statistical measure (e.g., information gain)
- Conditions for stopping partitioning
  - All samples for a given node belong to the same class
  - There are no remaining attributes for further partitioning – majority voting is employed for classifying the leaf
  - There are no samples left

Attribute Selection Measure: Information Gain (ID3/C4.5)

- Select the attribute with the highest information gain
- S contains s_i tuples of class C_i for i = {1, …, m}
- information measures info required to classify any arbitrary tuple

$$I(s_1,s_2,\ldots,s_m) = -\sum_{i=1}^{m} \frac{s_i}{s} \log_2 \frac{s_i}{s}$$

- entropy of attribute A with values $\{a_1,a_2,\ldots,a_v\}$

$$E(A) = \sum_{j=1}^{v} \frac{s_{1j}+\ldots+s_{mj}}{s} I(s_{1j},\ldots,s_{mj})$$

- information gained by branching on attribute A

$$Gain(A) = I(s_1,s_2,\ldots,s_m) - E(A)$$

Definition of Entropy

- Entropy $H(X) = \sum_{x \in A_X} -P(x) \log_2 P(x)$
- Example: Coin Flip
  - A_X = *{heads, tails}*
  - *P(heads) = P(tails) = ½*
  - *½* $\log_2$*(½) = ½ * - 1*
  - *H(X) = 1*
- What about a two-headed coin?
- Conditional Entropy: $H(X \mid Y) = \sum_{y \in A_Y} P(y) H(X \mid y)$

Attribute Selection by Information Gain Computation

- Class P: buys_computer = "yes"
- Class N: buys_computer = "no"
- I(p, n) = I(9, 5) =0.940
- Compute the entropy for *age*:

age	p_i	n_i	$I(p_i, n_i)$
<=30	2	3	0.971
30…40	4	0	0
>40	3	2	0.971

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

$$E(age) = \frac{5}{14} I(2,3) + \frac{4}{14} I(4,0) + \frac{5}{14} I(3,2) = 0.694$$

$\frac{5}{14} I(2,3)$ means "age <=30" has 5 out of 14 samples, with 2 yes'es and 3 no's. Hence

$$Gain(age) = I(p,n) - E(age) = 0.246$$

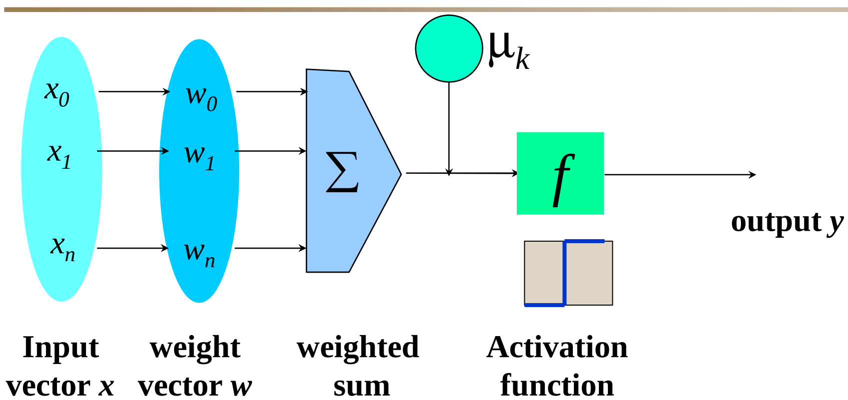
Similarly,

$$Gain(income) = 0.029$$
$$Gain(student) = 0.151$$
$$Gain(credit\_rating) = 0.048$$

Overfitting in Decision Trees

- Overfitting: An induced tree may overfit the training data
  - Too many branches, some may reflect anomalies due to noise or outliers
  - Poor accuracy for unseen samples
- Two approaches to avoid overfitting
  - Prepruning: Halt tree construction early—do not split a node if this would result in the goodness measure falling below a threshold
    - Difficult to choose an appropriate threshold
  - Postpruning: Remove branches from a "fully grown" tree—get a sequence of progressively pruned trees
    - Use a set of data different from the training data to decide which is the "best pruned tree"

Artificial Neural Networks: A Neuron

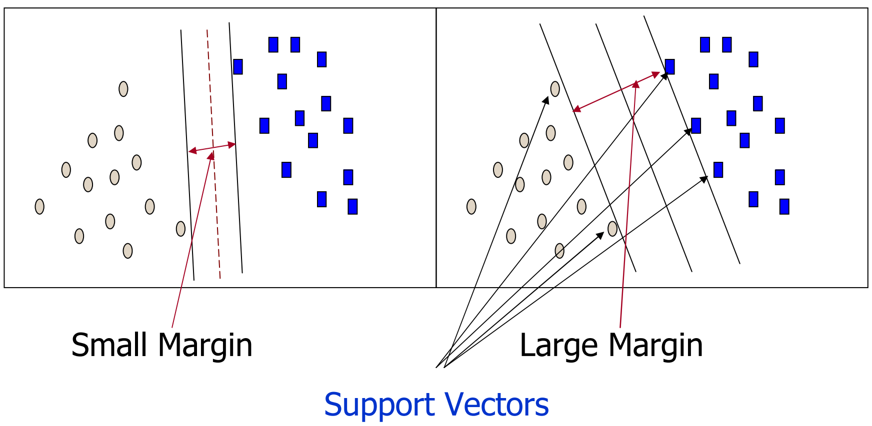


- The n-dimensional input vector x is mapped into variable y by means of the scalar product and a nonlinear function mapping

Artificial Neural Networks: Training

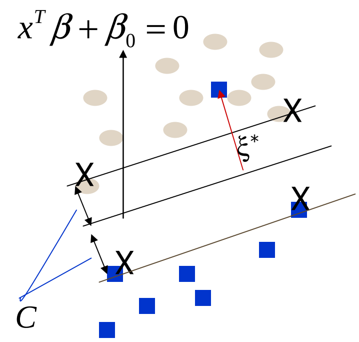
- The ultimate objective of training
  - obtain a set of weights that makes almost all the tuples in the training data classified correctly
- Steps
  - Initialize weights with random values
  - Feed the input tuples into the network one by one
  - For each unit
    - Compute the net input to the unit as a linear combination of all the inputs to the unit
    - Compute the output value using the activation function
    - Compute the error
    - Update the weights and the bias

SVM – Support Vector Machines



Non-separable case

When the data set is non-separable as shown in the right figure, we will assign weight to each support vector which will be shown in the constraint.



Non-separable Cont.

1. Constraint changes to the following:

$y_i(x_i^T\beta + \beta_0), > C(1-\xi_i)$, Where

$$\forall i, \xi_i > 0, \sum_{i=1}^{N} \xi_i < const.$$

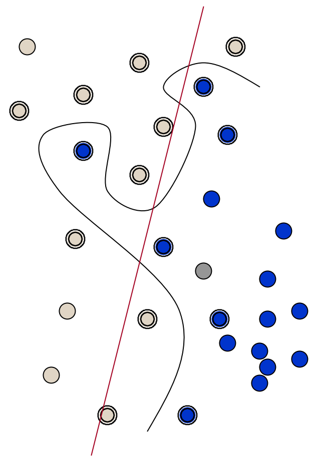
2. Thus the optimization problem changes to:

Min $\|\beta\|$ subject to $\begin{cases} y_i(x_i^T\beta+\beta_0) > 1-\xi_i, i=1,\ldots,N. \\ \forall i, \xi_i > 0, \sum_{i=1}^{N}\xi_i < const. \end{cases}$

General SVM

This classification problem clearly do not have a good optimal linear classifier.

Can we do better?
A non-linear boundary as shown will do fine.



General SVM Cont.

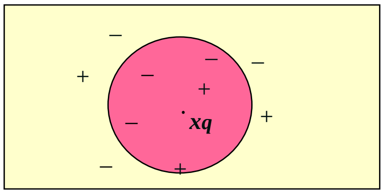
- The idea is to map the feature space into a much bigger space so that the boundary is linear in the new space.
- Generally linear boundaries in the enlarged space achieve better training-class separation, and it translates to non-linear boundaries in the original space.

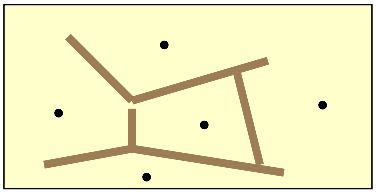
Mapping

- Mapping $\Phi : \mathbb{R}^d \mapsto H$
  - Need distances in *H*: $\Phi(x_i) \cdot \Phi(x_j)$
- Kernel Function: $K(x_i, x_j) = \Phi(x_i) \cdot \Phi(x_j)$
  - Example: $K(x_i, x_j) = e^{-\|x_i - x_j\|^2 / 2\sigma^2}$
- In this example, *H* is infinite-dimensional

The *k*-Nearest Neighbor Algorithm

- All instances correspond to points in the n-D space.
- The nearest neighbor are defined in terms of Euclidean distance.
- The target function could be discrete- or real- valued.
- For discrete-valued, the *k*-NN returns the most common value among the k training examples nearest to *xq*.
- Voronoi diagram: the decision surface induced by 1-NN for a typical set of training examples.





Case-Based Reasoning

- Also uses: lazy evaluation + analyze similar instances
- Difference: Instances are not "points in a Euclidean space"
- Example: Water faucet problem in CADET (Sycara et al'92)
- Methodology
  - Instances represented by rich symbolic descriptions (e.g., function graphs)
  - Multiple retrieved cases may be combined
  - Tight coupling between case retrieval, knowledge-based reasoning, and problem solving
- Research issues
  - Indexing based on syntactic similarity measure, and when failure, backtracking, and adapting to additional cases

Regress Analysis and Log-Linear Models in Prediction

- Linear regression: $Y = \alpha + \beta X$
  - Two parameters , α and β specify the line and are to be estimated by using the data at hand.
  - using the least squares criterion to the known values of $Y_1, Y_2, \ldots, X_1, X_2, \ldots$.
- Multiple regression: Y = b0 + b1 X1 + b2 X2.
  - Many nonlinear functions can be transformed into the above.
- Log-linear models:
  - The multi-way table of joint probabilities is approximated by a product of lower-order tables.
  - Probability: $p(a, b, c, d) = \alpha_{ab} \beta_{ac} \chi_{ad} \delta_{bcd}$

Bagging and Boosting

- General idea

Training data $\xrightarrow{\text{Classification method (CM)}}$ **Classifier C**

Altered Training data $\xrightarrow{\text{CM}}$ **Classifier C1**

Altered Training data $\xrightarrow{\text{CM}}$ **Classifier C2**

……..

Aggregation …. $\longrightarrow$ **Classifier C***

Test Taking Hints

- Open book/notes
  - Pretty much any non-electronic aid allowed
- See old copies of my exams (and solutions) at my web site
  - CS 526
  - CS 541
  - CS 603
- Time will be tight
  - Suggested "time on question" provided

Seminar Thursday: Support Vector Machines

- Massive Data Mining via Support Vector Machines
- Hwanjo Yu, University of Illinois
  - Thursday, March 11, 2004
  - 10:30-11:30
  - CS 111
- Support Vector Machines for:
  - classifying from large datasets
  - single-class classification
  - discriminant feature combination discovery