COMP5121 Data Mining and Data Warehousing Applications

Week 8: Course Review for Mid-term Exam

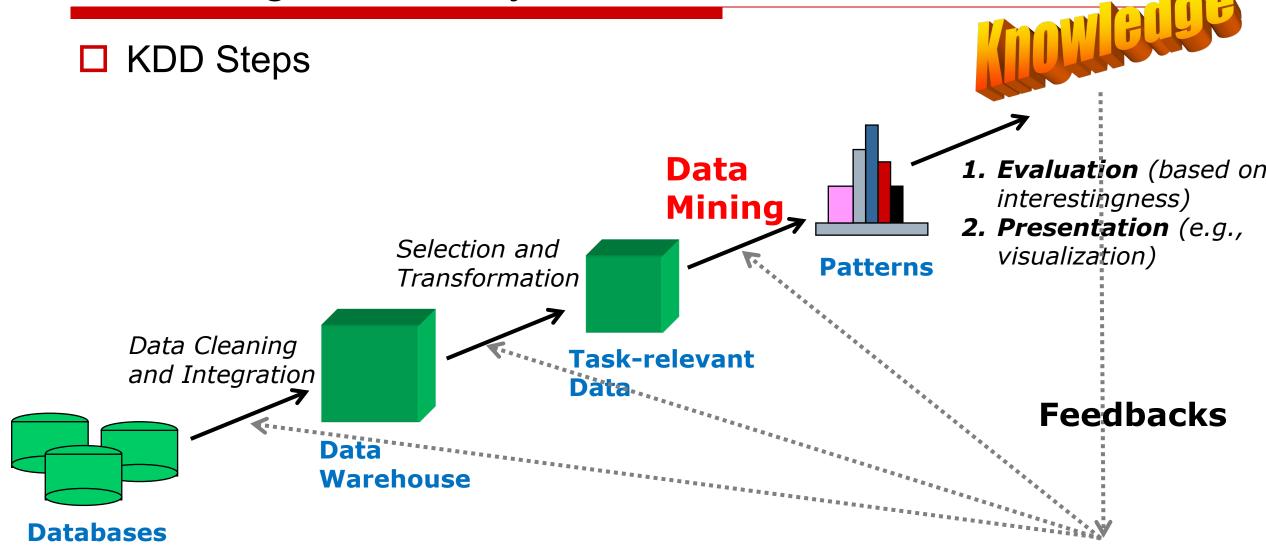
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The KDD process

KNOWLEDGE DISCOVERY FROM DATA

Knowledge discovery in databases



Data Objects

- ☐ Databases/Datasets are made up of data objects.
- ☐ A data object represents an entity.
 - ☐ Sales DB: customers, store items, sales
 - ☐ Medical DB: patients, treatments
 - □University DB: students, professors, courses
- □ Database rows → data objects, described by attributes
 - Also called as *samples*, *examples*, *instances*, *data points*, *tuples*
- ☐ Database columns → attributes
 - Also called as data field, characteristic, dimension, feature, variable

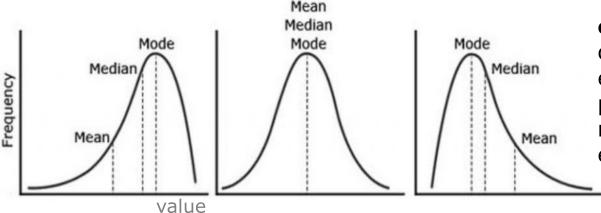
Classify Attribute Types

- ☐ To describe a **qualitative** feature of an object that does not provide actual size or quantity **nominal**, **binary**, **ordinal**
 - Values are typically words representing categories.
 - Integers are used to embed categories as codes.
 - □ 0 for small drink size, 1 for medium, and 2 for large.
- ☐ To provide quantitative measurements of an object numeric
 - Interval-scaled: No true zero.
 - Radio-scaled: True zero, enabling meaningful ratios.

Basic Statistical Descriptions of Data (I)

- Motivation: To better understand the data, identify properties of the data, and highlight what values shall be treated as *noise*
 - Central tendency: to measure the middle or center of the data
 - Mean: The average of the data (sensitive to extremes/outliers)
 - Median: The middle value when data is ordered (a more robust measure when data is skewed)
 - Mode: The most frequently occurring value

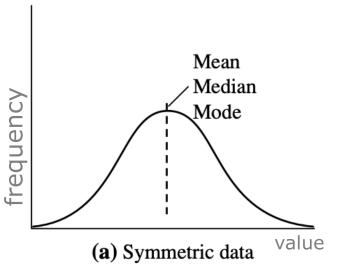
example: a strong middle class and fewer low-income households, e.g., Sweden, Finland, Denmark.

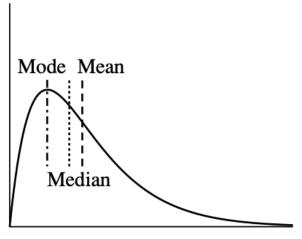


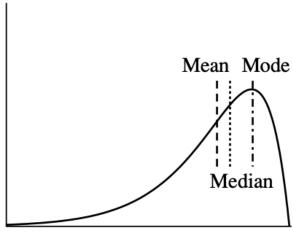
example: a small group of extremely high-income earners and a large population of low- to middle-income workers, e.g., New York, HK

Symmetric vs. Skewed Data

□ Compare the central tendency (i.e., median, mean and mode) of symmetric, positively-skewed and negatively-skewed data







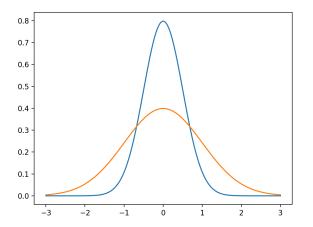
(b) Positively skewed data

*the long tail is on the **positive** side (higher values)

(c) Negatively skewed data

Basic Statistical Descriptions of Data (II)

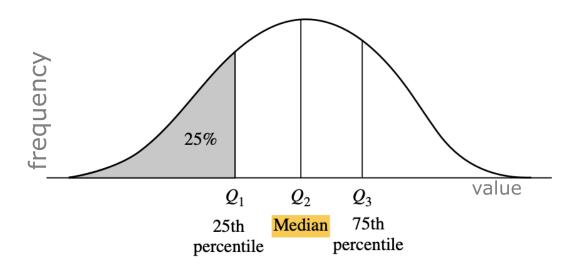
- Motivation: To better understand the data, identify properties of the data, and highlight what values shall be treated as *noise*
 - Data dispersion: how are the data spread out?
 - □ Range: difference between max and min values
 - ☐ Interquartile Range (IQR): Measures spread around the **median**
 - □ Variance / Standard Deviation: Indicate deviation from the mean



Measures of Data Dispersion

30, 36, 47, 50, 52, 52, 56, 60, 63, 70, 70, 110.

□ q-Quantiles: q - 1 data points where the data distribution is split into q equal-size consecutive sets, e.g., 2-quantile (i.e., median), 4-quantiles (called quartile), 100-quantiles (called percentiles)



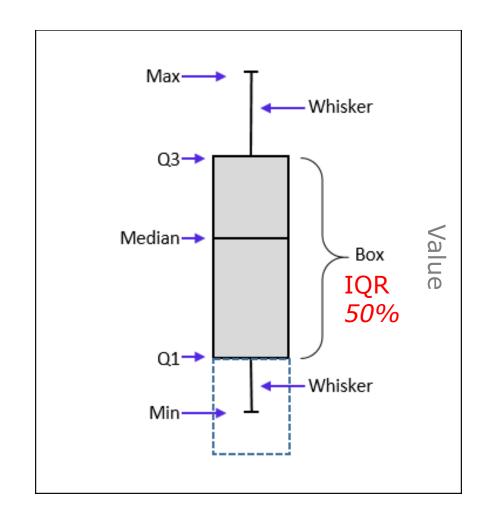
Interquartile Range (IQR)

- to identify the spread of the central portion of a dataset
- calculated as the difference between:
 - Upper quartile, Q3
 - Lower quartile, Q1
 - IQR = Q3 Q1 = 63 47 = 16

A plot of the data distribution for some attribute *X*. The quantiles plotted are quartiles. The three quartiles divide the distribution into four equal-size consecutive subsets. The second quartile corresponds to the median.

Graphic Displays: Boxplot

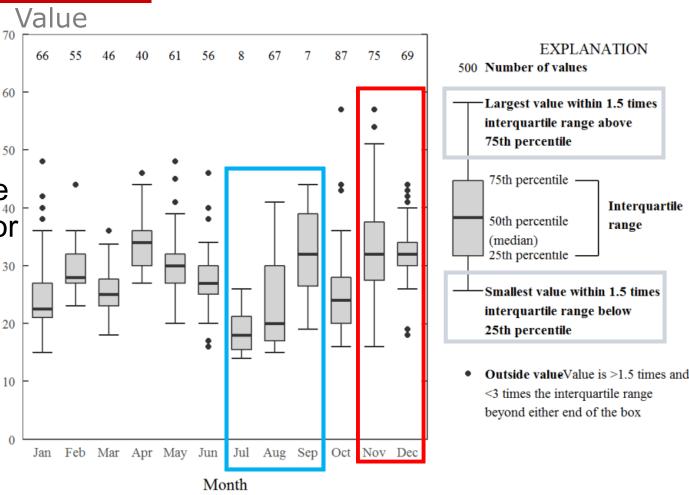
- □ Quartiles (i.e., 4-quantiles)
 - Five-number summary: min, Q1, median (Q2), Q3, max
 - Boxplot: data is represented by a box
 - □ IQR: the two ends of the box are at Q1 and Q3, i.e., the height of the box is IQR
 - Median: marked by a line within the box
 - □ Whiskers: two lines outside the box extended to min and max



Graphic Displays: Boxplot's Application

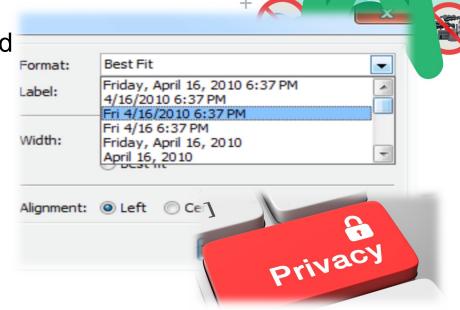
Outliers

- data points beyond a specified threshold
 - Usually, outside values are $1.5 \times IQR$ higher than Q3 or lower than Q1
- Plotted individually
 - □ The whiskers shall stop at the most extreme low/high observations within 1.5 × IQR of the quartile.
 - ☐ Then, outliers show up.



Why Preprocess the Data? Data Quality!

- □ Data quality depends on the intended use of data.
- Multidimensional views of data quality:
 - Accuracy: data must correctly reflect the real-world scenario without errors or noise.
 - Completeness: all required data fields should be present and valid.
 - Consistency: data should follow the same rules and format across all records.
 - **Timeliness**: data should be up-to-date.
 - Believability: data should be credible and from trusted sources.
 - Interpretability: data should be clear and understandable.



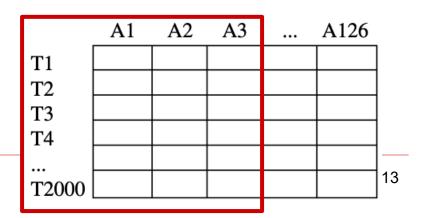
What is your date of birth?



Major Tasks of Data Preprocessing

messy

- □ Data Cleaning
 - To fill in missing data, smooth noisy data, identify or remove outliers, and resolve inconsistencies
- □ Data Integration (e.g., Bill Gates, William Gates, B. Gates, ...)
 - To merge multiple databases into a coherent data store
- □ Data **Reduction** (efficiency of mining process)
 - To obtain a reduced representation of the data with similar results
- Data Transformation
 - To normalize data for similarity-based mining (e.g., age vs salary)



data cube

DATA WAREHOUSE AND OLAP

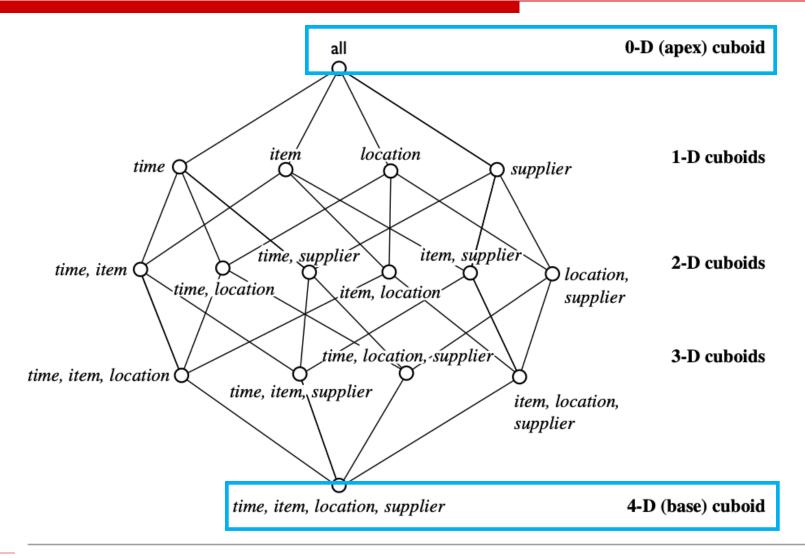
Why a Separate Data Warehouse?

- ☐ High performance for both systems:
- DBMS tuned for OLTP: access methods, indexing, hashing, concurrency control, recovery
- Warehouse tuned for OLAP: complex OLAP queries, consolidation, multi-dimensional view
 - ☐ Different data and functions:
 - Data warehouses are structured for analysis, with standardized schemas and consolidated information from diverse sources.
 - Data warehouses support complex analytics on historical data.
 Operational databases handle frequent transactions and updates.
 - □ Some systems perform OLAP directly on DBs, but performance and scalability may be limited.

From Tables and Spreadsheets to Data Cubes

- ☐ A data warehouse is based on a multi-dimensional data mode, which *views data* in the form of a data cube, defined by:
 - **Dimension tables**: to describe a dimension, e.g., item (item_name, brand, type), or time (day, week, month, quarter, year)
 - Fact table: to store numeric measures (e.g., dollars_sold) and keys linking to dimension tables analyze relationships between dimensions
- \square Data cube is typically n-dimensional.
 - The n-dimensional base cube is called a base cuboid.
 - The topmost 0-dimensional cuboid, which provides the highest-level summarization, is called the apex cuboid.
 - All levels of cuboids form the entire data cube.

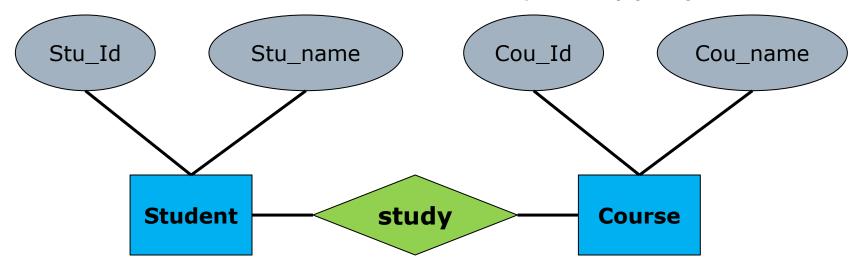
Example: Structure of Data Cube



Lattice of cuboids, making up a 4-D data cube for *time*, *item*, *location*, and *supplier*. Each cuboid represents a different degree of summarization.

Schemas for Multi-dimensional Data Models

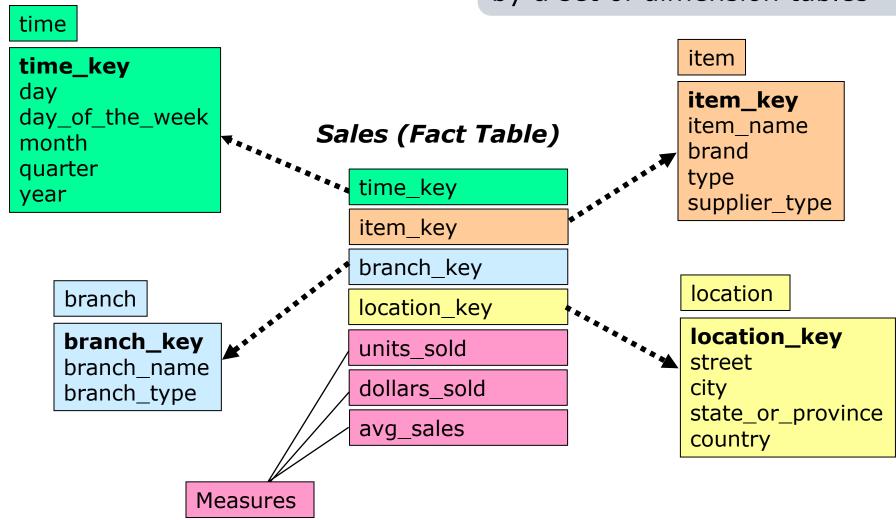
- ☐ Entity-Relationship (ER) model and the schema
 - a set of entities and their relationships appropriate for OLTP



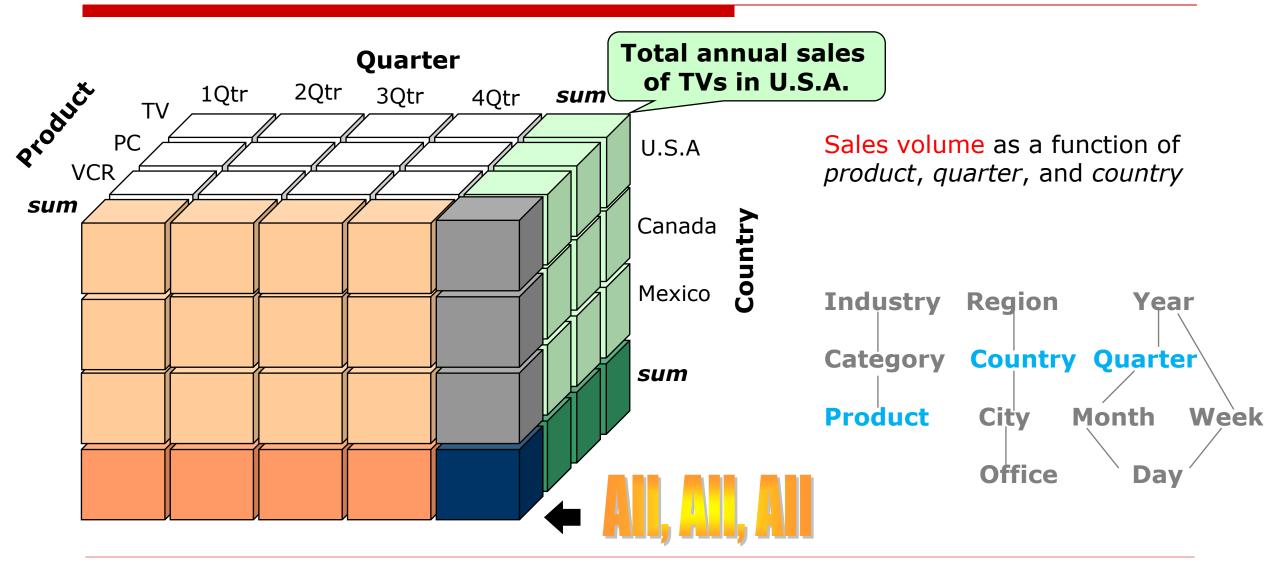
- ☐ A multi-dimensional model for data warehouses: focus on dimensions and measures, in the form of:
 - star schema, snowflake schema, fact constellation schema

(1) Star Schema

A fact table in the center, surrounded by a set of dimension tables



A Sample Data Cube



Typical OLAP Operations

- □ Roll up (drill-up): summarize data by climbing up hierarchy or by dimension reduction techniques
- ☐ Drill down (roll-down): reverse of roll-up
 - from higher-level summary to lower-level summary or detailed data, or introducing new dimensions
- ☐ Slice and dice: project and select
- ☐ Pivot (rotate): reorient the cube, visualization, 3D to series of 2D planes
- Other operations:
 - Drill-across: involving (across) more than one fact table
 - Drill-through: through the bottom level of the cube to its back-end relational tables (using SQL)

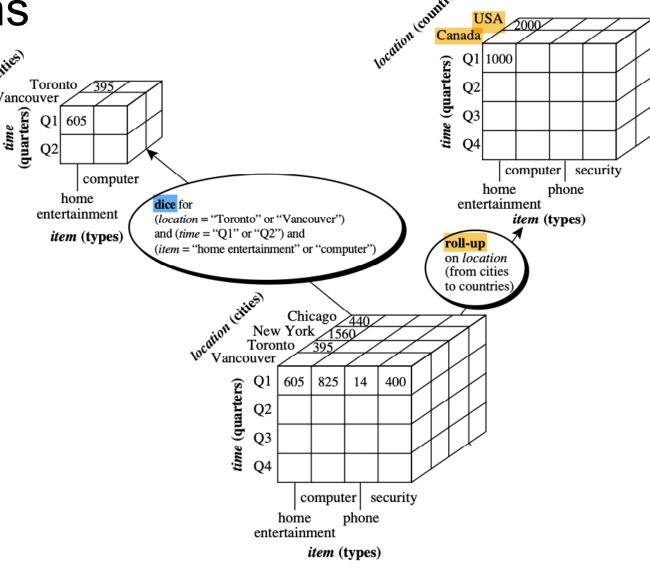
Typical OLAP Operations

☐ Roll up (drill-up)

summarize data by climbing up hierarchy for a dimension or by dimension reduction

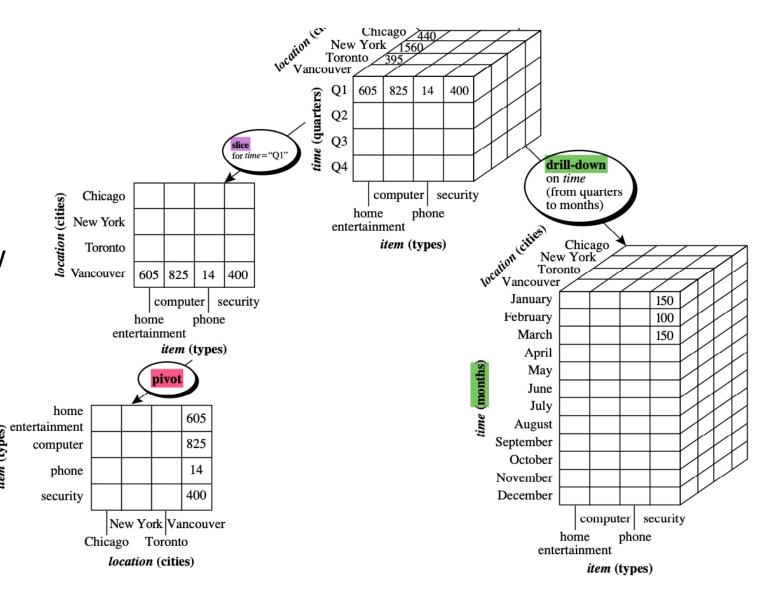
□ Dice

define a subcube by performing a selection on two or more dimensions

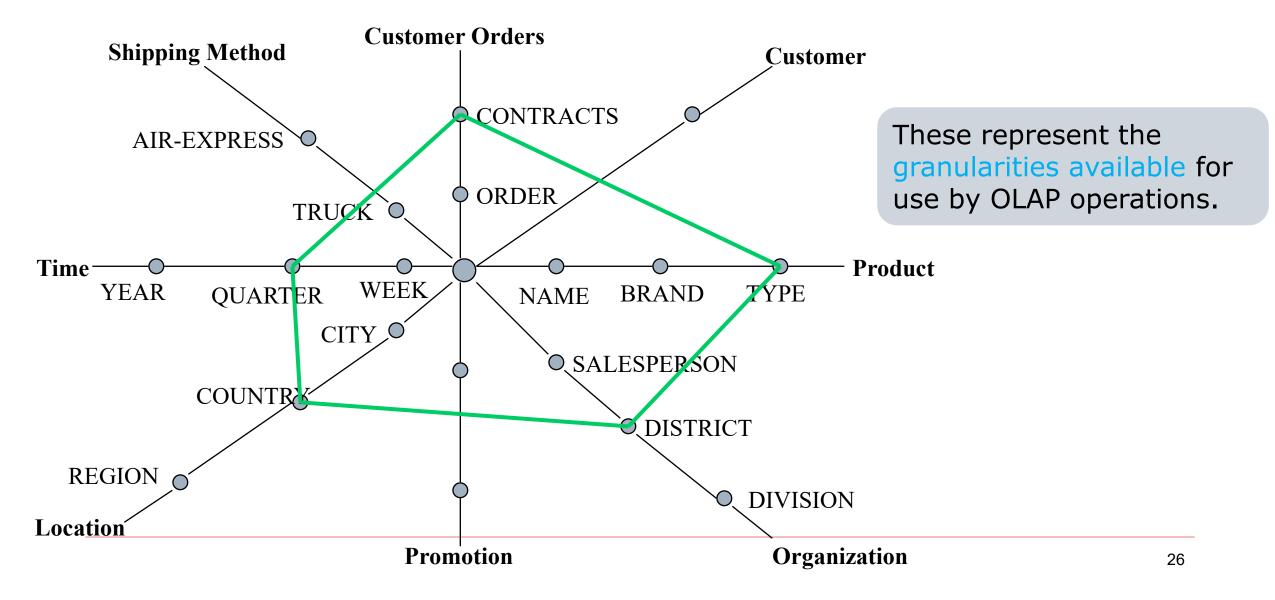


Typical OLAP Operations

- ☐ Roll-down (drill-down): reverse of roll-up
 - from higher-level summary to lower-level summary or detailed data, or introducing new dimensions
- ☐ Slice: define a subcube by performing a selection on one dimension
- ☐ Pivot (rotate): reorient the cube, visualization, 3D to series of 2D planes



A Star-Net Query Model



Efficient Data Cube Computation

- ☐ Data cube can be viewed as a lattice of cuboids
 - The bottom-most cuboid is the **base** cuboid the most specific
 - The top-most cuboid (apex) contains only one cell the most generalized (all)

Drilling down: start from apex cuboid and explore downward

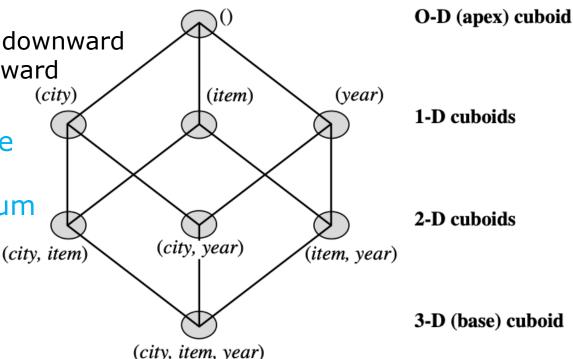
Rolling up: start at the base cuboid and explore upward

 O-D op: i.e., no group-by SQL, like "compute the sum of total sales"

1-D op: one group-by, e.g., "compute the sum of sales, group-by city"

• ...

 The cube operator is the n-dimensional generalization of the group-by operator.



Apriori algorithm, support, confidence, ...

FREQUENT ITEMSETS & ASSOCIATION RULE MINING

Basic Concepts: Frequent Itemsets

- ☐ **Itemset**: A set of one or more items
 - **k-itemset**: $X = \{x_1, \dots, x_k\}$ with k items
- ☐ Support of an itemset
 - Absolute Support (Count): the number of transactions containing the given itemset *X*
 - Relative Support: the fraction of transactions containing *X* (i.e., the probability that a transaction contains *X*)

□ Frequent Itemset: An itemset X is frequent if the support of X is no less than σ – a minsup threshold.

The Apriori Algorithm: Framework

- ☐ Outline of **Apriori**: level-wise, candidate generation and test
- ➤ Initially, scan DB once to get frequent 1-itemset
- > Repeat
 - Generate length-(k + 1) candidate itemsets based on frequent k-itemsets
 - Test the candidates against DB to find frequent (k + 1)-itemsets
 - Set k := k + 1
- Until no frequent or candidate set can be generated
- > Return all the frequent itemsets derived

From Frequent Itemsets to Association Rules

- □ Association Rules written as X → Y [support, confidence]
 - Both X and Y are non-empty itemsets, and $X \cap Y = \emptyset$.
 - It describes an 'if-then' relationship between two sets of items.
 - Support: The percentage of transactions containing both X and Y $\sup(X \to Y) = P(X \cup Y)$
 - \square $P(X \cup Y)$: the percentage of transactions that contains every item in X and Y, i.e., how frequently both X and Y appear together in the dataset
 - Confidence: The conditional probability that a transaction having X also contains Y, that is,

$$conf(X \to Y) = P(Y|X) = sup(X \to Y)/sup(X)$$

Final Step: Rule Generation via Frequent Itemsets

- □ Support (*min-sup*): used to mine the frequent itemsets
- ☐ Confidence (*min-conf*): used by the rule generation step to qualify the strength of the derived association rules
 - \blacksquare For each frequent itemset F, generate F's all non-empty subsets
 - For every non-empty subset s, generate a rule:

$$R: S \to (F - S)$$

If the rule R satisfies the minimum confidence, i.e.,

$$conf(s \to F - s) = \frac{sup(F)}{sup(s)} \ge min_conf$$

then *R* is a strong association rule and should be output.

Limitation of the **Support-Confidence** Framework

 \square Strong rules are not necessarily interesting: " $A \rightarrow B$ " [s, c]



■ Example: Suppose a school may have the following statistics on # students related to playing basketball and/or eating cereal:

	Play basketball	Not play basketball	sum
Eat cereal	400	350	750
Not eat cereal	200	50	250
sum	600	400	1000 (TOTAL)

Association rule mining may generate a rule:



play-basketball → eat-cereal [40%, 66.7%]

- But this strong association rule is misleading → The overall % of students eating cereal is 75% > 66.7%.
- A more telling rule:

Interestingness Measure: Lift

Measure of dependent / correlated events:

$$lift(B,C) = \frac{P(B \cup C)}{P(B)P(C)} = \frac{\sup(B \to C)}{\sup(B)\sup(C)} = \frac{\operatorname{conf}(B \to C)}{\sup(C)}$$

Tell how B and C are correlated

 \square lift(B, C) = 1: B and C are independent

 \square lift(B, C) > 1: positively correlated

 \square lift(B, C) < 1: negatively correlated

	В	Not B	sum
С	400	350	750
Not C	200	50	250
sum	600	400	1000

lift is more telling than s & c

Example:
$$lift(B,C) = \frac{400/1000}{600/1000 \times 750/1000} = 0.89 \quad lift(B,\neg C) = \frac{200/1000}{600/1000 \times 250/1000} = 1.33$$

- \square Thus, B and C are negatively correlated since lift(B,C) < 1.
- B and $\neg C$ are positively correlated since $lift(B, \neg C) > 1$.

Interestingness Measure: χ^2

- \square To test correlated events: $\chi^2 = \frac{\sum (Observed Expected)^2}{Expected}$
- $\chi^2 = 0$: independent
- $\chi^2 > 0$: correlated, either positive or negative \rightarrow needs additional test

	В	Not B	sum
С	400 (450)	750	
Not C	200 (150)	50 (100)	250
sum	600	100	1000

$$\chi^2 = \frac{(400 - 450)^2}{450} + \frac{(350 - 300)^2}{300} + \frac{(200 - 150)^2}{150} + \frac{(50 - 100)^2}{100} = 55.56$$

Expected value

Observed value

- ☐ Thus, *B* and *C* are negatively correlated since the expected value is 450 but the observed is only 400.
- \square χ^2 is also more telling than the support-confidence framework

Lift and χ^2 : Are They Always Good Measures?

□ Null transactions: Transactions that contain **neither** *B* **nor** *C*

Examine the dataset:

- BC (100, 0.1%) is much rarer than $B \neg C$ (1000) and $\neg BC$ (1000)
- There are many $\neg B \neg C$ (100000, 98%).
- Unlikely B & C will happen together!

	В	¬B	Σ_{row}
С	100	1000	1100
¬С	1000	100000	101000
$\Sigma_{\text{col.}}$	1100	101000	102100

null transactions

- ☐ However, B and C seem to be strongly positively correlated based on:
 - \Box *lift*(*B*, *C*) = 8.44 \gg 1
 - $\Box \chi^2(B,C) = 670$ and Observed (100) >> Expected (11.85)
- ☐ Too many null transactions may "spoil the soup"!

Contingency table with expected values added

	В	¬В	Σ_{row}
С	100 (11.85)	1000	1100
¬C	1000 (988.15)	100000	101000
$\Sigma_{\text{col.}}$	1100	101000	102100

Interestingness Measures: Null-Invariant

- □ Null invariance: value does not change with # null-transactions
 - \blacksquare χ^2 and lift are NOT null-invariant with the range of $[0, \infty]$.
- Null-invariant Measures:
 - All Confidence: the minimum confidence of the two association rules related to A and B, namely, "A → B" and "B → A"

$$all_conf(A,B) = \frac{sup(A \cup B)}{max\{sup(A), sup(B)\}} = min\{P(A|B), P(B|A)\} \qquad max_conf(A,B) = max\{P(A|B), P(B|A)\}$$

- Max Confidence: the maximum confidence of the two rules
- Kulczynski (Kulc): an average of two confidence values
- **Cosine**: a harmonized *lift* measure (unaffected by # total transactions)

$$Kulc(A, B) = \frac{1}{2}(P(A|B) + P(B|A)) - \frac{cosine(A, B)}{\sqrt{P(A) \times P(B)}} = \frac{sup(A \cup B)}{\sqrt{sup(A) \times sup(B)}} - \frac{sup(A \cup B)}{\sqrt{sup(A) \times sup(B)}} = \frac{\sqrt{P(A|B) \times P(B|A)}}{\sqrt{sup(A) \times sup(B)}}$$

Decision tree: ID3 algorithm driven by entropy and information gain

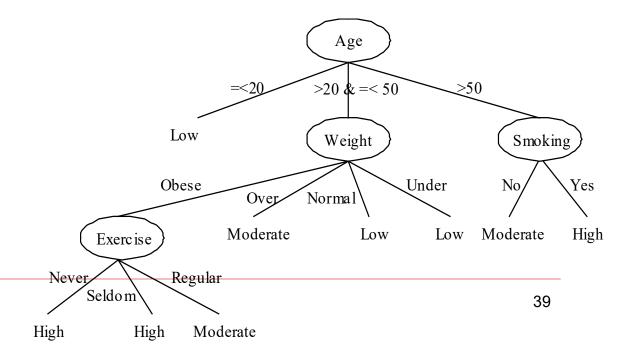
CLASSIFICATION

Decision Tree Structure

- ☐ A flow-chart-like structure used for classification
 - Internal node: a test on an attribute (e.g., age, exercise, weight, smoking)
 - **Branch**: an outcome of the test
 - Leaf nodes: class labels (e.g., high-, moderate-, and low-risk)

How it works:

An object is classified by traversing the tree from its root to a leaf.



Entropy

- ☐ A measure of randomness, uncertainty, and disorder in a system with probability distributions of outcome.
- ☐ Entropy is formulated as a *function* that measures disorder.
 - "The higher the entropy, the greater the disorder."
 - For classification, it tells how diverse the classes are in a set.
- \square Let D be a set of examples from m classes.

$$Info(D) = -\sum_{i=1}^{m} p_i \cdot \log_2(p_i)$$

- Input: Distribution of outcomes
- Output: A value indicating how disordered the outcomes are
- p_i : The proportion of examples observed in D that belong to i-th class within [0,1].

Example: Tossing Coins in Casino

☐ Casino A with real coins (50/50 chances):

$$Info(Coin Toss) = -p(head) \log_2 p(head) - p(tail) \log_2 p(tail)$$

$$= -\frac{1}{2}\log_2\left(\frac{1}{2}\right) - \frac{1}{2}\log_2\left(\frac{1}{2}\right) = 1$$



HEAD



TAIL

☐ Casino B with fake coins (75/25 chances):

$$Info(Coin \, Toss) = -p(head) \log_2 p(head) - p(tail) \log_2 p(tail)$$

$$= -\frac{3}{4}\log_2\left(\frac{3}{4}\right) - \frac{1}{4}\log_2\left(\frac{1}{4}\right) = 0.811$$

Entropy is a measure of randomness and disorder. Higher entropy means higher uncertainty.

Information Gain and Iterative Dichotomiser (ID3)

- ☐ Classification Goal: To split the dataset in a way that reduces entropy the most.
- □ Information Gain: To measure the reduction in entropy after splitting the dataset on an attribute A

$$Gain(D, A) = Info(D) - Info_A(D)$$

- Weighted entropy after split: $Info_A(D) = \sum_{j=1}^n p(D_j|A)Info(D_j)$
 - \square D_i : subsets of D created by splitting on A

ID3 Algorithm: Repeatedly selects the attribute with the highest information gain at each step to build the decision tree.

ID3 Example (Decision: buy computer or not)

- □ Class P: buys_computer = 'yes' → 9
- \square Class N: buys_computer = 'no' \rightarrow 5

•	Info(D) =	$\sum -p_i \times \log_2 p_i$
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- Info_A(D) = $\sum [p(D_j|A) \times Info(D_j)]$
- $Gain(D, A) = Info(D) Info_A(D)$

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
3140	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
3140	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
3140	medium	no	excellent	yes
3140	high	yes	fair	yes
>40	medium	no	excellent	no

$$Info(D) = I(9,5) = -\frac{9}{14}\log_2(\frac{9}{14}) - \frac{5}{14}\log_2(\frac{5}{14}) = 0.940$$

age	p _i	n _i	I(p _i , n _i)
<=30	2	3	0.971
3140	4	0	0
>40	3	2	0.971

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

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

Hence,

$$Gain(age) = Info(D) - Info_{age}(D) = 0.246$$

Similarly,
$$Gain(income) = 0.029$$

 $Gain(student) = 0.151$
 $Gain(credit_rating) = 0.048$

Bayesian Theorem

- \square P(H|E): Posterior probability, the probability of H holds given E
 - E: Evidences (e.g., a data tuple) with attribute description
 - \blacksquare H: Hypothesis to be verified (e.g., a class label that E belongs to)

$$P(H|E) = \frac{P(E|H) P(H)}{P(E)}$$

- \square P(H): prior probability, i.e., the initial probability of hypothesis H before observing evidence E
- \square P(E): marginal probability, i.e., the total probability of observing evidence E under all possible hypotheses
- \square P(E|H): likelihood, i.e., the probability of observing evidence E given that the hypothesis H = true

Bayesian Classification

- \square A data tuple: $X = (A_1 = x_1, A_2 = x_2, A_3 = x_3, ..., A_n = x_n)$
- \square To classify X, we need to estimate $P(C_i \mid X)$
 - lacksquare C_i represents the **hypothesis** that X belongs to C_i .
 - We say X belongs to C_i iff: $P(C_i|X) > P(C_j|X)$, $for \ all \ j \neq i$
- \square How to estimate $P(C_i \mid X)$ for classifying X?
 - **Bayesian theorem**: $P(C_i|X) = \frac{P(X|C_i)P(C_i)}{P(X)}$
 - The problem becomes \rightarrow estimating $P(X|C_i)$ and $P(C_i)$

Bayesian Classification

□ Estimate the priori probability of the i-th class C_i from the training set D: $P(C_i) = \frac{|C_i|}{|D|}$

Independence Assumption: For $P(X \mid C_i)$, we assume that the effect of each attribute A_i is independent to others:

$$P(X = (A_1 = x_1, A_2 = x_2, ..., A_n = x_n) | C_i)$$

$$= P(A_1 = x_1 | C_i) \times P(A_2 = x_2 | C_i) \times \cdots$$

$$\times P(A_n = x_n | C_i)$$

where $P(A_i = x_i | C_i)$ can also be estimated from the training set D.

Example

Bayesian: $P(C_i|X) = \frac{P(X|C_i)P(C_i)}{P(X)}$

- ☐ Given a training set, predict if a person *X* will buy a computer
 - X: {age = youth, income = medium, student = yes, credit_rating = fair}
 - Yes or No? $P(buy_computer|X)$

Priori Probability in training Data:

- $P(buy_computer = yes) = 9/14 = 0.643$
- $P(buy_computer = no) = 5/14 = 0.357$

	buys_computer	
age	yes	no
youth	2	3
middle_aged	4	0
senior	3	2

	buys_computer	
income	yes	no
low medium high	3 4 2	1 2 2

To calculate $P(X \mid buy_computer = yes)$:

- $P(age = youth \mid yes) = 2/9 = 0.222$
- $P(income = medium \mid yes) = 4/9 = 0.444$
- $P(student = yes \mid yes) = 6/9 = 0.667$
- $P(credit_rating = fair \mid yes) = 6/9 = 0.667$
- $\rightarrow P(X \mid buy_computer = yes) = 0.044$
- \rightarrow Similarly, $P(X \mid buy_computer = no) = 0.019$

	buys_computer	
student	yes	no
yes no	6 3	1 4

	buys_computer	
credit_ratting	yes	no
fair excellent	6 3	2 3



Through Bayesian:

- $P(X \mid yes) \times P(buy_computer = yes) = 0.028$
- $P(X \mid no) \times P(buy_computer = no) = 0.007$

Conclusion: X will buy a computer.

Evaluation Measures

- ☐ To assess how "accurate" your classifier is at predicting the class label of tuples compared to actual labels
 - True Positives TP: positive tuples that were correctly labeled
 □ Positive tuples: tuples of the main class of interest
 - True Negatives TN: negative tuples that were correctly labeled
 - False Positives FP: negative tuples that were incorrectly labeled as positive (e.g., people who do not buy computers but are labeled as buys_computer = yes)
 Predicted class
 - False Negatives FN: positive tuples that were mislabeled as negative (e.g., people who really buy computers but are labeled as buys_computer = no)

Actual class

	yes	no	Total		
yes	TP	FN	P		
no	FP	TN	N		
Total	P'	N'	$^{48}P + N$		

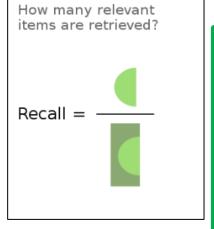
Evaluation Measures

Actual class

Predicted clas	S
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	yes	no	Total
yes	TP	FN	P
по	FP	TN	N
Total	P'	N'	P+1

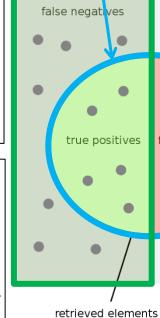
Measure	Formula
accuracy, recognition rate	$\frac{TP + TN}{P + N}$
error rate, misclassification rate	$\frac{FP + FN}{P + N}$
sensitivity, true positive rate, recall	$\frac{TP}{P}$
specificity, true negative rate	$\frac{TN}{N}$
precision	$\frac{TP}{TP + FP}$
F , F_1 , F -score, harmonic mean of precision and recall	$\frac{2 \times precision \times recall}{precision + recall}$
F_{β} , where β is a non-negative real number	$\frac{(1+\beta^2) \times precision \times recall}{\beta^2 \times precision + recall}$



How many retrieved items are relevant?

Precision =

 $\beta^2 \times precision + recall$



relevant elements

true negatives

false positives

49

0

CLUSTERING

Partitioning Algorithms: Basic Concepts

Partitioning method

 Discover groupings in the data by optimizing a specific objective function and iteratively improving the quality of partitions

☐ *K*-partitioning method

- Objective: Divide a dataset D of n objects into a set of K clusters, so that an objective function is optimized (e.g., minimizing the sum of distances within clusters)
- Typical objective function: Sum of Squared Errors (SSE)

$$SSE(C) = \sum_{k=1}^{K} \sum_{x_{i \in C_k}} ||x_i - c_k||^2$$

where c_k is the centroid or medoid of cluster C_k

The *K*-Means Clustering Algorithm

- ☐ Idea: each cluster is represented by the centroid, which is the mean position of all data points in the cluster
 - It may not correspond to an actual data point in the dataset!
- ☐ Given *K*, the number of clusters, the *K*-Means clustering algorithm is outlined as follows:

Initialization: Select *K* data points as initial centroids **Repeat**

- Form K clusters by assigning each point to its closest centroid
- Re-compute the centroids (i.e., mean point) of each cluster
 Until centroids no longer change or convergence criterion is met

Discussion on *K*-Means Clustering (I)

Limitations

- Need to specify *K* in advance
 - \square There are ways to automatically determine the 'best' K.
 - □ In practice, one often runs a range of values and selected the 'best'.
- Only for objects in a continuous data space: K-modes for nominal data
- K-means clustering often terminates at a local optimum.
 - Poor initialization can lead to suboptimal clusters.
- Sensitive to noisy data and outliers (extreme values)

Measuring Clustering Quality

- □ **Evaluation**: Evaluating the goodness of clustering results
 - No universally recognized 'best' measure in practice!
- □ Three categorization of measures
 - Internal: Unsupervised, criteria derived from data itself
 - □ How well the clusters are separated and how compact the clusters are
 - **External**: Supervised, employ criteria not inherent to the dataset
 - ☐ Compare a clustering against prior or expert-specified knowledge (i.e., the ground truth) using certain clustering quality measures
 - Relative: Directly compare different clustering, usually those obtained by varying parameters for the same algorithm

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THANK YOU!

