Data Mining

Lecture 3
Preprocessing Methods

http://www.informatik.uni-hamburg.de/WTM/

Data Preprocessing

- Data Preprocessing: An Overview
  - Data Quality
  - Major Tasks in Data Preprocessing
- Data Cleaning
- Data Integration
- Data Reduction
- Data Transformation
- Data Discretization

Data Quality: why preprocess the Data?

Measures for data quality: A multidimensional view

- Accuracy: correct or wrong, accurate or not
- Completeness: not recorded, unavailable, …
- Consistency: some modified but some not, dangling, …
- Timeliness: timely update?
- Believability: how trustable are the data are?
- Interpretability: how easily the data can be understood?

Why We should Clean Dirty Data

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 reduction***
  - Dimensionality reduction
  - Data compression
- ***Data transformation*** and ***data discretization***
  - Normalization
  - Concept hierarchy generation

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Data Cleaning

- Data in the real world is "dirty" or incorrect, e.g., instrument faulty, human or computer error, transmission error
- ***Incomplete***: lacking attribute values, lacking certain attributes of interest, or only aggregate data available
  - e.g., *Occupation*=" " (missing data)
- ***Noisy***: containing noise, errors, or outliers
  - e.g., *Salary*="−10" (an error)
- ***Inconsistent***: containing discrepancies in codes or names, e.g.,
  - *Age*="42", *Birthday*="03/07/2012"
  - Was rating "1, 2, 3", now rating "A, B, C"
  - discrepancy between duplicate records
- ***Intentionally imprecise*** (e.g., *disguised missing* data)
  - Jan. 1 as everyone's birthday?

Incomplete (Missing) Data

- Data is not always available
  - E.g., many tuples have no recorded value for several attributes, such as customer income in sales data
- Missing data may be due to
  - equipment malfunction
  - inconsistent with other recorded data and thus deleted
  - data not entered due to misunderstanding
  - certain data may not be considered important at the time of entry
  - not register history or changes of the data
- Missing data may need to be inferred

How to handle missing Data?

- Ignore the tuple: usually done when class label is missing (when doing classification) — not effective when the % of missing values per attribute varies considerably
- Fill in the missing value manually: tedious + infeasible?
- Fill it in 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

Missing Data

- One possible interpretation of missing values – ***"don't care"*** values:

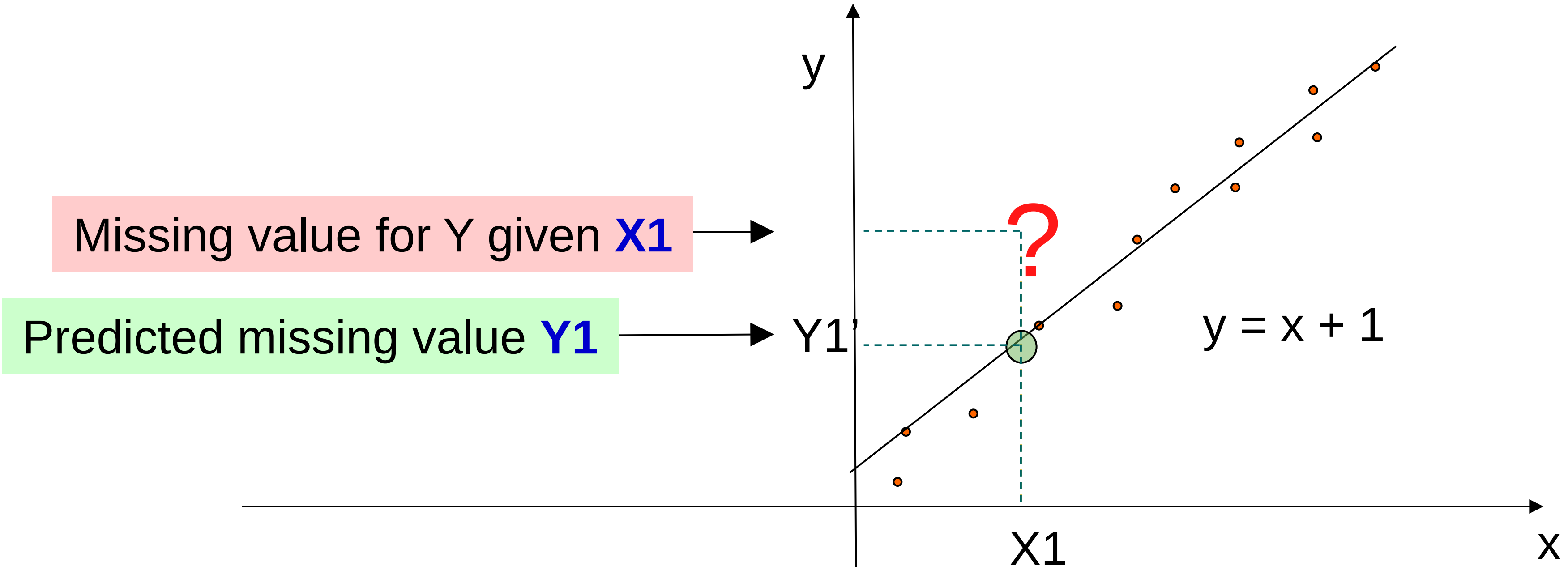
```
X = {1,?,3}
```

→ for the second feature the domain is `[0,1,2,3,4]`:

```
X1 = {1,0,3}, X2 = {1,1,3}, X3 = {1,2,3},
  X4 = {1,3,3}, X5 = {1,4,3}
```

- *Data miner* can generate model of ***correlation between features***.
  - Different techniques possible: regression, Bayesian formalism, clustering, or decision tree induction.

Missing Data Replacement with Regression Analysis



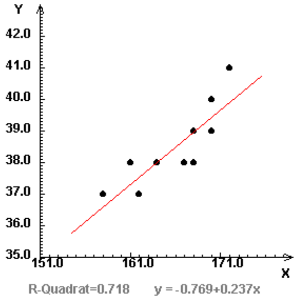
- In general, replacement of missing values using a simple, artificial schema of data preparation is *speculative and often misleading*.
- It is best to generate multiple solutions of data mining ***with and without features*** that have missing values, and then make comparison, analysis and interpretation.

Noisy Data

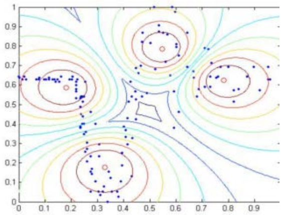
- Noise: random error or variance in a measured variable
- Incorrect attribute values may be due to
  - technology limitation
  - faulty data collection instruments
  - data entry problems
  - data transmission problems
  - inconsistency in naming convention
- Other data problems which require data cleaning
  - duplicate records
  - incomplete data
  - inconsistent data

How to handle noisy Data?

- Binning
  - first sort data and partition into (equal-frequency) bins
  - then one can smooth by bin means, smooth by bin median, smooth by bin boundaries, etc.
- Regression
  - smooth by fitting the data into regression functions



- Clustering
  - detect and remove outliers



- Combined computer and human inspection
  - detect suspicious values and check by human (e.g., deal with possible outliers)

Data Quality: why preprocess the Data?

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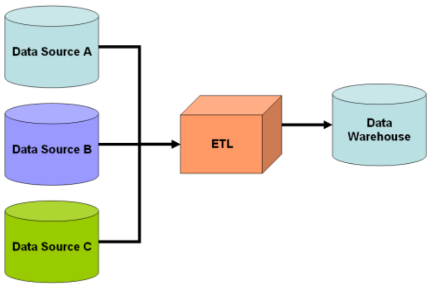
Data Integration



- Data integration:
  - Combines data from multiple sources into a coherent store
- Schema integration: e.g., A.cust-id ≡ B.cust-#
  - Integrate metadata from different sources
- Entity identification problem:
  - Identify real world entities from multiple data sources, e.g., Bill Clinton = William Clinton
- Detecting and resolving data value conflicts
  - For the same real world entity, attribute values from different sources are different
  - Possible reasons: different representations, different scales, e.g., metric vs. British units

Handling Redundancy in Data Integration

- Redundant data occur often when integrating multiple databases
  - ***Object identification***: The same attribute or object may have different names in different databases
  - ***Derivable data:*** One attribute may be a "derived" attribute in another table, e.g., annual revenue
- Redundant attributes may be possible to detect by ***correlation analysis***
- Careful integration of the data from multiple sources may reduce/avoid redundancies and inconsistencies and improve mining speed and quality

Correlation Analysis (Nominal Data)

- ***X^2 (chi-square) test***

$$\chi^2 = \sum \frac{(Observed - Expected)^2}{Expected}$$

- The cells that contribute the most to the X^2 value are those whose actual count is very different from the expected count
- Correlation does not imply causality
  - # of hospitals and # of car-thefts in a city are correlated
  - Both are causally linked to the third variable: population

Chi-Square Calculation: an Example

- Questionnaire among N=1500 participants:

	Play chess	Not play chess	Sum (row)
Like science fiction	250	250	500
Not like science fiction	50	950	1000
Sum (column)	300	1200	1500

- Expected results e_{ij} from the null hypothesis stating that "preferred reading" and "game favour" are uncorrelated):

	Play chess	Not play chess	Sum (row)
Like science fiction	100	400	500
Not like science fiction	200	800	1000
Sum (column)	300	1200	1500

$$e_{ij} = sum(col\ \ i) \cdot sum(row\ \ j) / N$$

Chi-Square Calculation: an Example

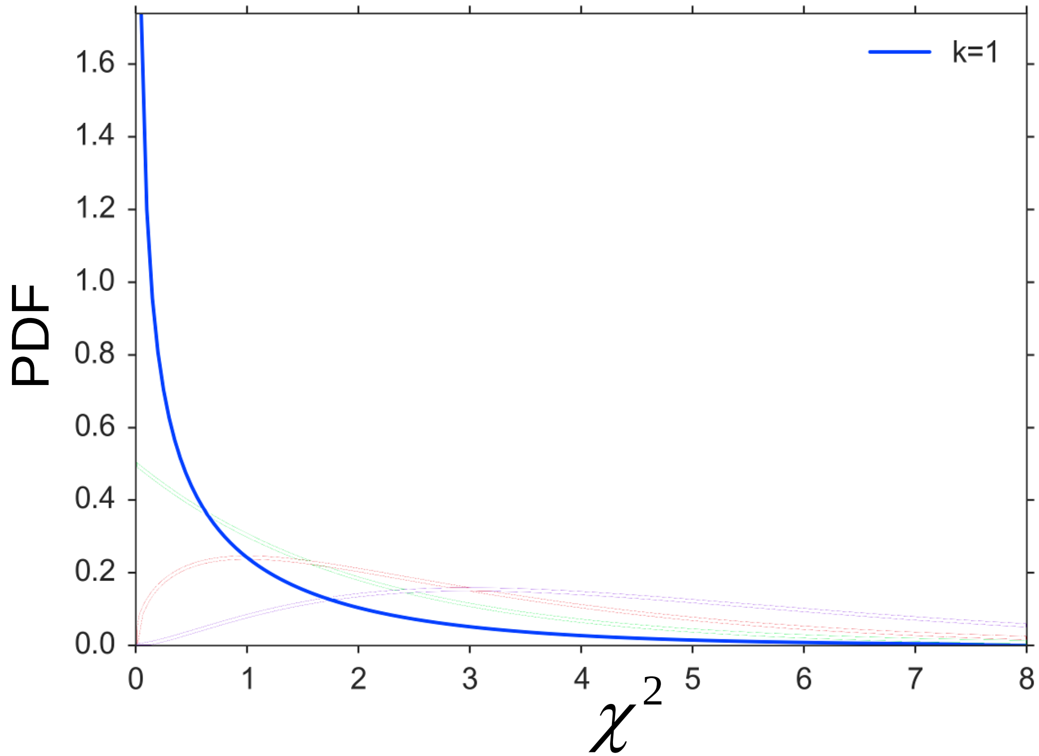
- X^2 (chi-square) calculation:

$$\chi^2 = \frac{(250-100)^2}{100} + \frac{(50-200)^2}{200} + \frac{(250-400)^2}{400} + \frac{(950-800)^2}{800} = \underline{421.9}$$

- What does it show?

Chi-square Test

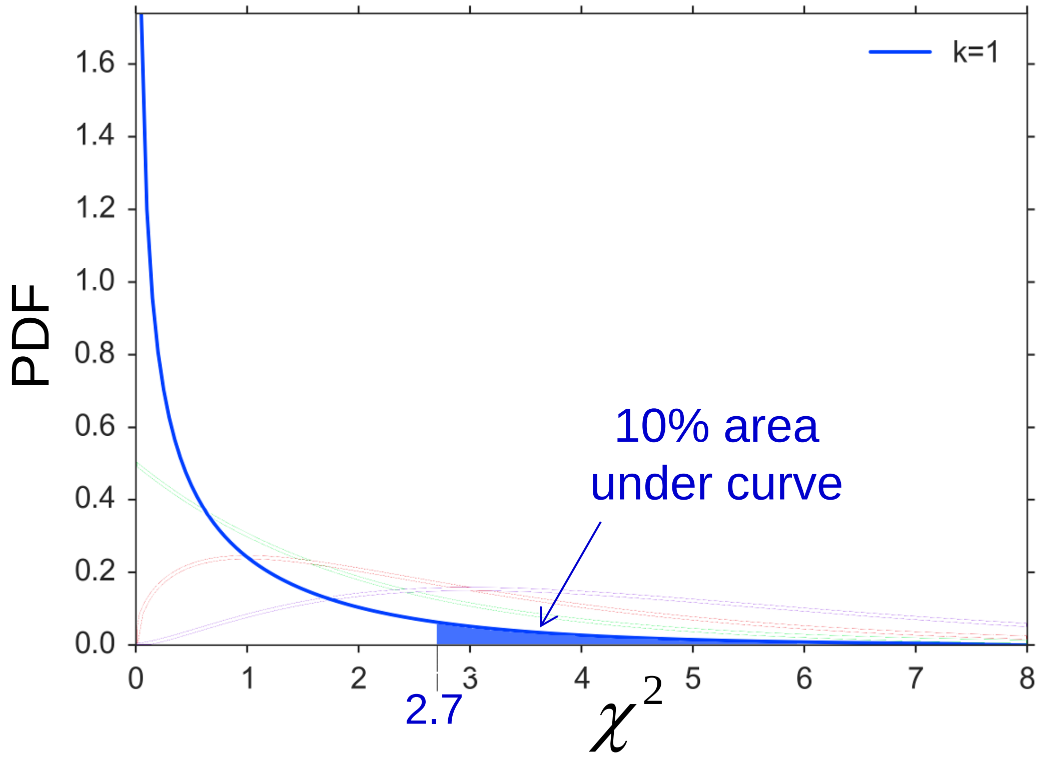
- Small deviations are more expected than large deviations:



- Random variable Y has a normal distribution
  $\rightarrow Y^2$ has a chi-square distribution (with 1 degree of freedom)

Chi-square Test

- Some percentage of expected deviations is over a threshold



- E.g.: 10% of all χ^2 values are larger than critical value 2.7
- Values can be looked up in a chi-square distribution table

Chi-square Distribution Table

probability level

α	0.5	**0.1**	**0.05**	0.02	0.01	0.001
	0.455	**2.706**	**3.841**	5.412	6.635	10.827

- α=0.1: 90% of values are below critical value 2.706
- α=0.05: 95% of values are below critical value 3.841

  …

- α: significance level

- Earlier, we have found a value of 421.9

→ Our data are extremely unlikely given the null hypothesis

Chi-Square Calculation: an Example

- X^2 (chi-square) calculation:

$$\chi^2 = \frac{(250-100)^2}{100} + \frac{(50-200)^2}{200} + \frac{(250-400)^2}{400} + \frac{(950-800)^2}{800} = \underline{421.9}$$

- It shows that "preferred reading" and "game favour" are correlated in the group (since X^2 larger than 10.827, from X^2 table – a statistical measure for significance of 2x2 table)
- What if all numbers were 10x smaller (N=150 participants)?

$$\rightarrow \quad \chi^2 = \ldots = 42.19$$

- What if all numbers were 50x smaller (N=30 participants)?

$$\chi^2 = \frac{(5-2)^2}{2} + \frac{(1-4)^2}{4} + \frac{(5-8)^2}{8} + \frac{(19-16)^2}{16} = 8.4375$$

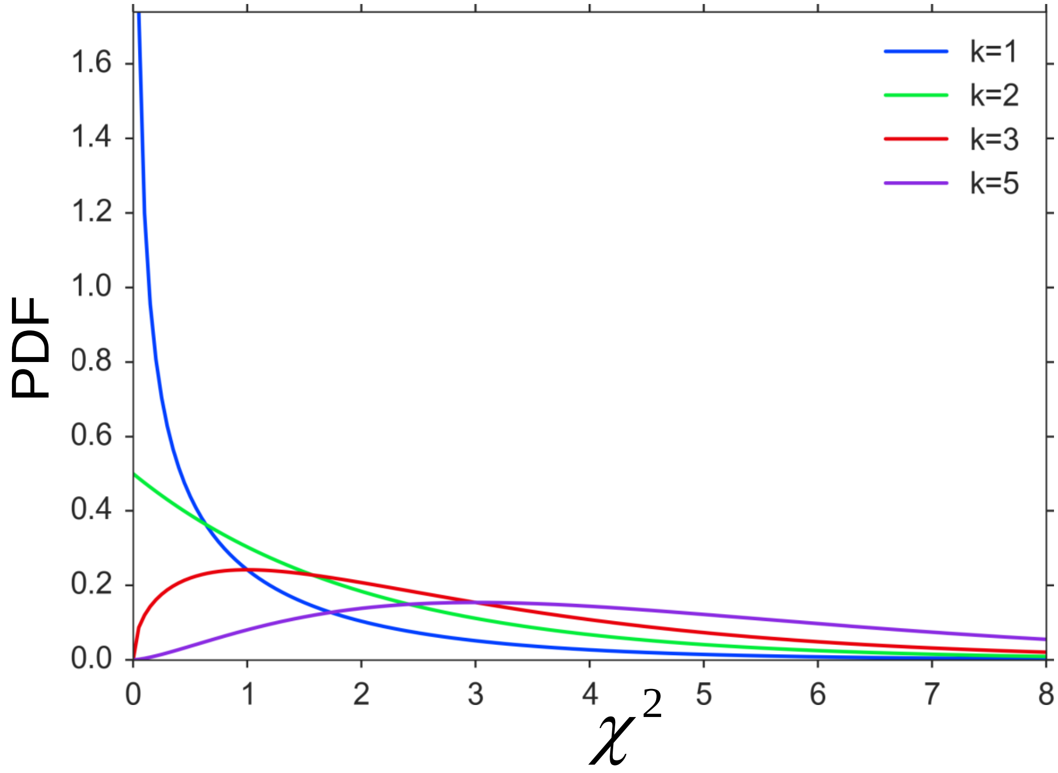
Chi-Square Calculation: Degrees of Freedom

		Category 1 Levels				Sum (row)
		L1	L2	...	LJ	
Category 2 Levels	L1					
	...					
	LI					
Sum (col.)						N

- If the two categories have several levels (J levels for category 1 and I levels for category 2), then there are more degrees of freedom in which the entries can differ
- I *x* J ***contingency table***
- Number of degrees of freedom: (I-1) *x* (J-1)

Chi-Square Calculation: Degrees of Freedom

- More degrees of freedom make larger deviations probable:



- Sum of k independ. random variables Y_i with normal distrib. $\rightarrow \Sigma_i Y_i^2$ has a χ^2 distribution with k degrees of freedom

Chi-square Distribution Table

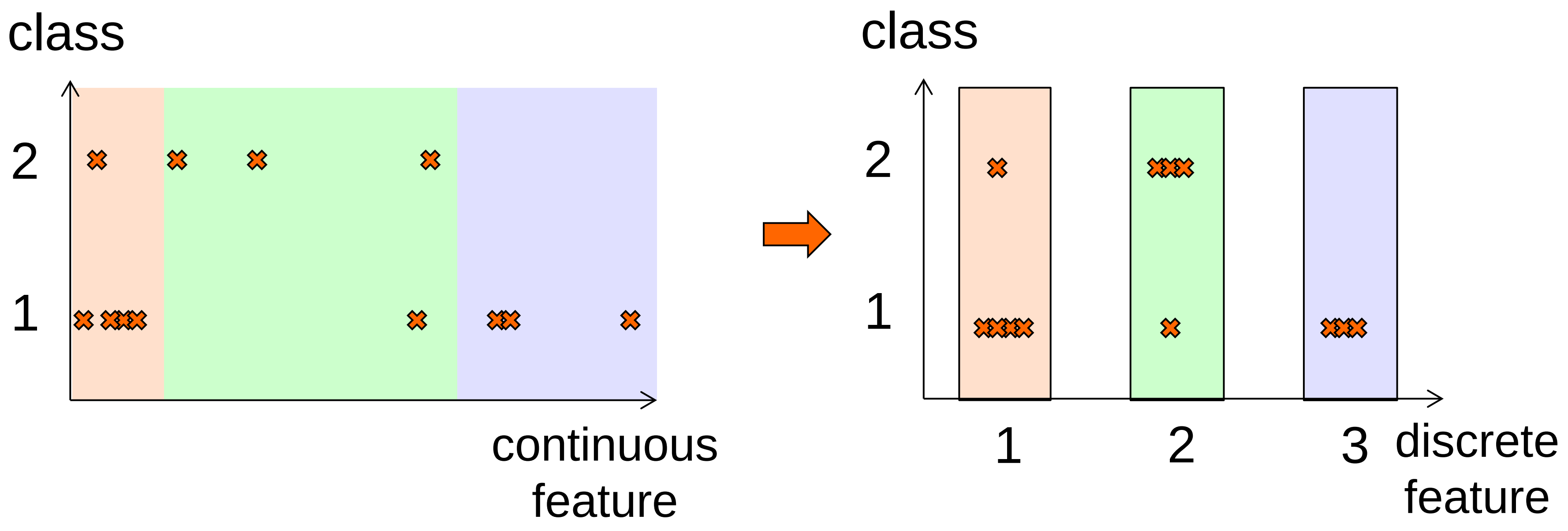
probability level

DF	0.5	0.1	**0.05**	0.02	0.01	0.001
1	0.455	2.706	**3.841**	5.412	6.635	10.827
2	1.386	4.605	**5.991**	7.824	9.210	13.815
3	2.366	6.251	**7.815**	9.837	11.345	16.268
4	3.357	7.779	**9.488**	11.668	13.277	18.465
5	4.351	9.236	**11.070**	13.388	15.086	20.517

- Degrees of freedom

Values Reduction

Data often have continuous features



Many classification algorithms require data with discrete attributes

Values Reduction – ChiMerge Technique

1. ***Sort*** the data for the given feature in ascending order
2. ***Define initial intervals*** so that every value of the feature is in a separate interval
3. ***Repeat***:

   3.1 Compute X^2 tests for each pair of adjacent intervals

   3.2 Merge two adjacent intervals with the lowest X^2 value, if calculated X^2 is less than threshold

   Until no X^2 test of any two adjacent intervals is less than threshold value

Values Reduction – Contingency Table

- A ChiMerge requires computation of X^2 test for the contingency table 2 x 2 of categorical data:

	Class 1	Class 2	Σ
Interval-1	A_{11}	A_{12}	R_1
Interval-2	A_{21}	A_{22}	R_2
Σ	C_1	C_2	N

X^2 test is:

$$\chi^2 = \sum_{i=1}^{2} \sum_{j=1}^{k} \frac{\left(A_{ij} - E_{ij}\right)^2}{E_{ij}}$$

where:

k = number of classes,

A_{ij} = number of instances in the i-th interval, j-th class,

E_{ij} = ***expected frequency*** of A_{ij}, which is computed as $(R_i \cdot C_j) / N$,

R_i = number of instances in the i-th interval = $\sum A_{ij}$, j = 1,…k,

C_j = number of instances in the j-th class = $\sum A_{ij}$, i = 1,2,

N = total number of instances = $\sum R_i$, i = 1,2.

Values Reduction – ChiMerge Technique Example

Data Set

Sample:	F	K
1	1	1
2	3	2
3	7	1
4	8	1
5	9	1
6	11	2
7	23	2
8	37	1
9	39	2
10	45	1
11	46	1
12	59	1

Initial interval points

0
2
5
7.5
8.5
.
.
.

Values Reduction – ChiMerge Technique Example

- X^2 was minimum for intervals: [7.5,8.5] and [8.5,10]

Sample:	F	K
1	1	1
2	3	2
3	7	1
4	8	1
5	9	1
6	11	2
7	23	2
8	37	1
9	39	2
10	45	1
11	46	1
12	59	1

	Class 1	Class 2	Σ
Interval [7.5,8.5]	A_{11}=1	A_{12}=0	R_1=1
Interval [8.5,10]	A_{21}=1	A_{22}=0	R_2=1
Σ	C_1=2	C_2=0	N=2

Based on the table's values, we can calculate expected values:

E11 = 1*2/2 = 1, E12 = 1*0/2 = 0,
E21 = 1*2/2 = 1, & E22 = 1*0/2 = 0

and corresponding X^2 test:

$$X^2 = (1-1)^2/1 + (0-0)^2/0 + (1-1)^2/1 + (0-0)^2/0 = \mathbf{0}$$

For d=1 degree of freedom: X^2 **= 0 < 2.706** $\longrightarrow$ **merge !**
(α=0.1)

Values Reduction – ChiMerge Technique Example

- … one of the following iterations:

Sample:	F	K
1	1	1
2	3	2
3	7	1
4	8	1
5	9	1
6	11	2
7	23	2
8	37	1
9	39	2
10	45	1
11	46	1
12	59	1

	Class 1	Class 2	Σ
Interval [**0.0**,**7.5**]	$A_{11}=2$	$A_{12}=1$	$R_1=3$
Interval [**7.5**,**10**]	$A_{21}=2$	$A_{22}=0$	$R_2=2$
Σ	$C_1=4$	$C_2=1$	$N=5$

E11 = 3*4/5 = 2.4, E12 = 3*1/5 = 0.6,
E21 = 2*4/5 = 1.6, E22 = 2*1/5 = 0.4

$$X^2 = (2-2.4)^2/2.4 + (1-0.6)^2/0.6 + (2-1.6)^2/1.6 + (0-0.4)^2/0.4 = \mathbf{0.834}$$

For d=1 degree of freedom: X^2 **= 0.834 < 2.706** (α=0.1) $\longrightarrow$ **merge !**

Values Reduction – ChiMerge Technique Example

- … One of the additional iterations:

Sample:	F	K
1	1	1
2	3	2
3	7	1
4	8	1
5	9	1
6	11	2
7	23	2
8	37	1
9	39	2
10	45	1
11	46	1
12	59	1

	Class 1	Class 2	Σ
Interval [**0.0,10**]	$A_{11}=4$	$A_{12}=1$	$R_1=5$
Interval [**10 ,42**]	$A_{21}=1$	$A_{22}=3$	$R_2=4$
Σ	$C_1=5$	$C_2=4$	N=9

E11 = 2.78, E12 = 2.22,
E21 = 2.22, E22 = 1.78

$X^2 =$ 2.72 **>** 2.706 → **NO merge !**

Final discretization: [0, 10], [10, 42], and [42, 60]

Interval representatives: 5 (low) 26 (medium) 51 (high)

Values Reduction – ChiMerge Technique Example

Original set

Sample:	F	K
1	1	1
2	3	2
3	7	1
4	8	1
5	9	1
6	11	2
7	23	2
8	37	1
9	39	2
10	45	1
11	46	1
12	59	1

Final data set with reduced set of values F:

Sample:	F	K
1	5	1
2	5	2
3	5	1
4	5	1
5	5	1
6	26	2
7	26	2
8	26	1
9	26	2
10	51	1
11	51	1
12	51	1

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Feature Reduction

- Which features to select, and how?

TRS_DT	TRS_TYP_CD	REF_DT	REF_NUM	CO_CD	GDS_CD	QTY	UT_CD	UT_PRIC
21/05/93	00001	04/05/93	25119	10002J	001M	10	CTN	22.000
21/05/93	00001	05/05/93	25124	10002J	032J	200	DOZ	1.370
21/05/93	00001	05/05/93	25124	10002J	033Q	500	DOZ	1.000
21/05/93	00001	13/05/93	25217	10002J	024K	5	CTN	21.000
21/05/93	00001	13/05/93	25216	10026H	006C	20	CTN	69.000
21/05/93	00001	13/05/93	25216	10026H	008Q	10	CTN	114.000
21/05/93	00001	14/05/93	25232	10026H	006C	10	CTN	69.000
21/05/93	00001	14/05/93	25235	10027E	003A	5	CTN	24.000
21/05/93	00001	14/05/93	25235	10027E	001M	5	CTN	24.000
21/05/93	00001	22/04/93	24974	10035E	009F	50	CTN	118.000
21/05/93	00001	27/04/93	25033	10035E	015A	375	GRS	72.000
21/05/93	00001	20/05/93	25313	10041Q	010F	10	CTN	26.000
21/05/93	00001	12/05/93	25197	10054R	002E	25	CTN	24.000

Features Reduction

Two standard approaches:

- ***Feature selection***: A process that chooses an optimal subset of features according to an objective function:
  - feature ranking algorithms,
  - minimum subset algorithms.

- ***Feature extraction***: refers to the mapping of the original high-dimensional data onto a lower-dimensional space.
  - Descriptive setting: minimizes the information loss
  - Predictive setting: maximizes the class discrimination

Feature selection – Example for Optimal Features' Subset

F_1	F_2	F_3	F_4	F_5	C
0	0	1	0	1	0
0	1	0	0	1	1
1	0	1	0	1	1
1	1	0	0	1	1
0	0	1	1	0	0
0	1	0	1	0	1
1	0	1	1	0	1
1	1	0	1	0	1

- Data set (whole set)
  - Five Boolean features
  - $C = F_1 \vee F_2$
  - $F_3 = \neg F_2$, $F_5 = \neg F_4$
  - Optimal subset:

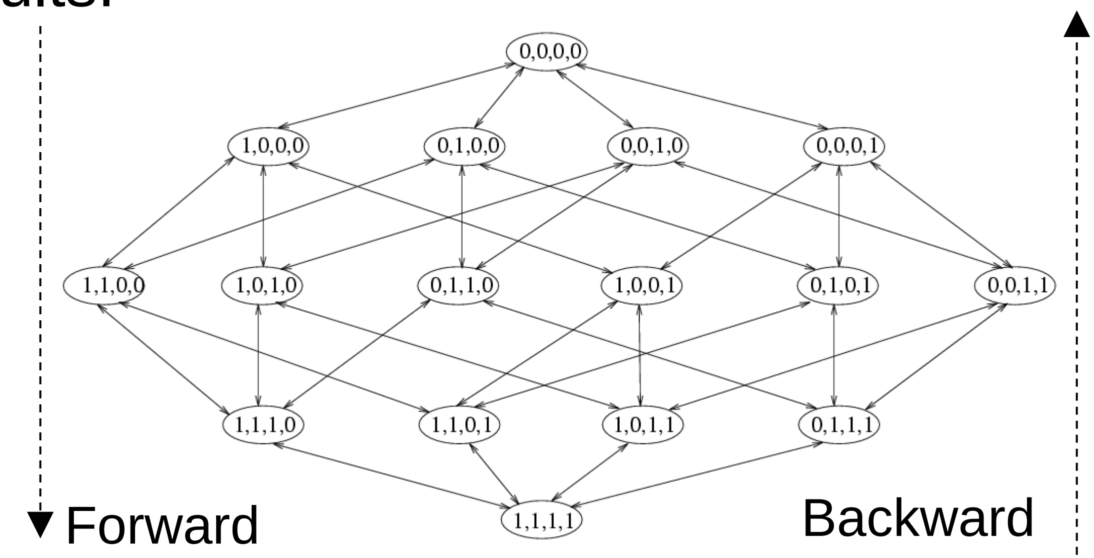
    $\{F_1, F_2\}$ or $\{F_1, F_3\}$

- Combinatorial nature of searching for an optimal subset

Feature Selection – Complexity

- **Feature selection** in general can be viewed as a search problem.

- For practical methods, an optimal search is not feasible, and simplifications are made to produce acceptable and timely reasonable results:
  - heuristic criteria
  - bottom-up approach
  - top-down approach



Methods of Feature Selection

- Univariate methods
  - Considers one variable (feature) at a time.
- Filter methods
  - Separating feature selection from classifier learning
  - Relying on general characteristics of data (information, distance, dependence, consistency)
  - No bias toward any learning algorithm, fast
- Wrapper methods
  - Relying on a predetermined classification algorithm.
  - Using predictive accuracy as goodness measure
  - High accuracy, computationally expensive
- Embedded methods
  - Combine Filter and Wrapper approaches

Features Selection: Univariate Methods

Comparison of means and variances:

- Samples of two classes (A and B) can be examined:

$$\mathrm{SE}(A-B)=\sqrt{\frac{\mathrm{var}(A)}{n_1}+\frac{\mathrm{var}(B)}{n_2}}$$

- TEST:

$$\frac{\left|\mathrm{mean}(A)-\ \mathrm{mean}(B)\right|}{\mathrm{SE}(A-B)}>\textit{threshold-value}$$

where n_1 and n_2 are the corresponding number of samples for classes A and B.

Features Selection: Univariate Methods

- Comparison of *means* and *variances* – **Example**:

X	Y	C
0.3	0.7	A
0.2	0.9	B
0.6	0.6	A
0.5	0.5	A
0.7	0.7	B
0.4	0.9	B

Threshold value is 0.5

$X_A = \{0.3, 0.6, 0.5\},$ $X_B = \{0.2, 0.7, 0.4\},$

$Y_A = \{0.7, 0.6, 0.5\},$ $Y_B = \{0.9, 0.7, 0.9\}$

Features Selection: Univariate Methods

- Comparison of *means* and *variances* – **Example**:

$$SE(X_A - X_B) = \sqrt{\frac{\mathrm{var}(X_A)}{n_1} + \frac{\mathrm{var}(X_B)}{n_2}} = \sqrt{\frac{0.0233}{3} + \frac{0.6333}{3}} = 0.4678$$

$$SE(Y_A - Y_B) = \sqrt{\frac{\mathrm{var}(Y_A)}{n_1} + \frac{\mathrm{var}(Y_B)}{n_2}} = \sqrt{\frac{0.01}{3} + \frac{0.0133}{3}} = 0.0875$$

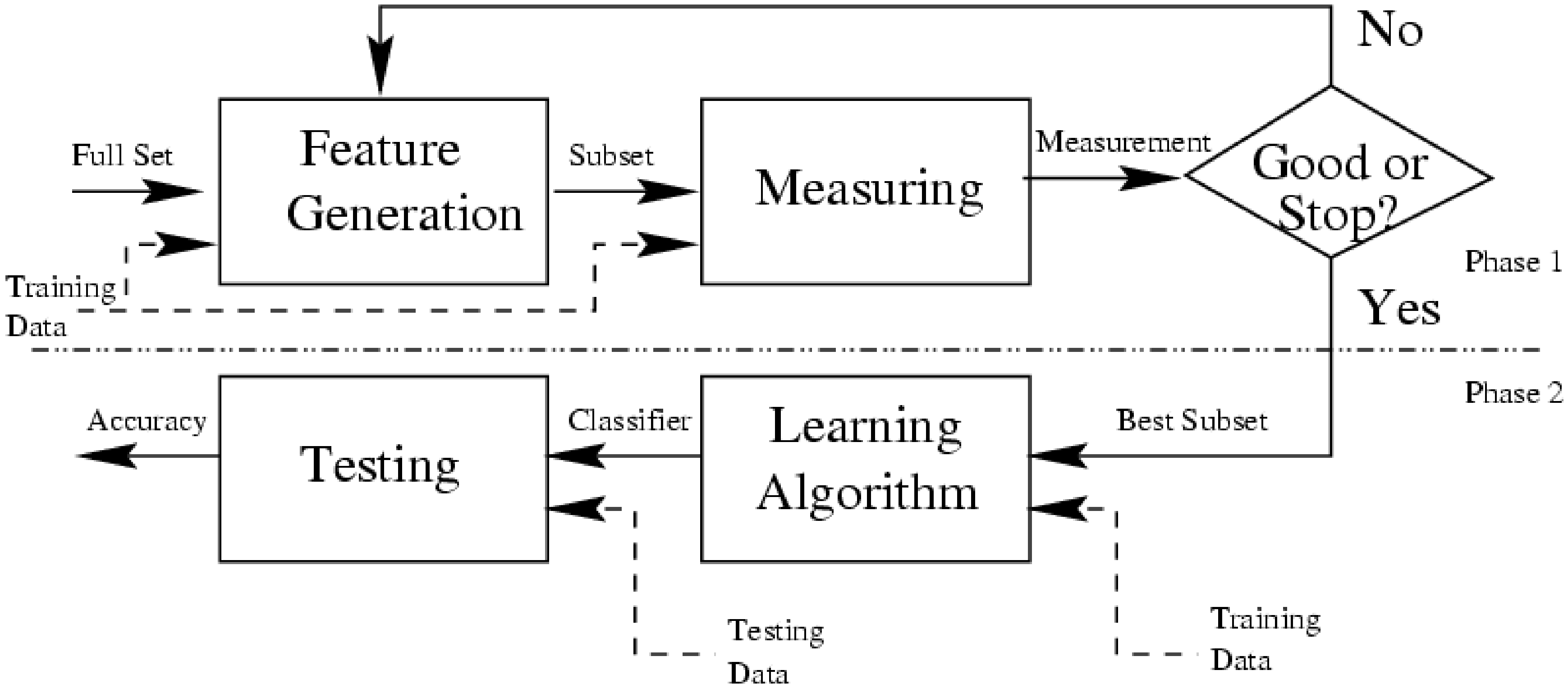
Tests:

X: $$\frac{|\mathrm{mean}(A) - \mathrm{mean}(B)|}{SE(A-B)} = \frac{|0.4667 - 0.4333|}{0.4678} < 0.5$$

Y: $$\frac{|\mathrm{mean}(A) - \mathrm{mean}(B)|}{SE(A-B)} = \frac{|0.6 - 0.8333|}{0.0875} > 0.5$$

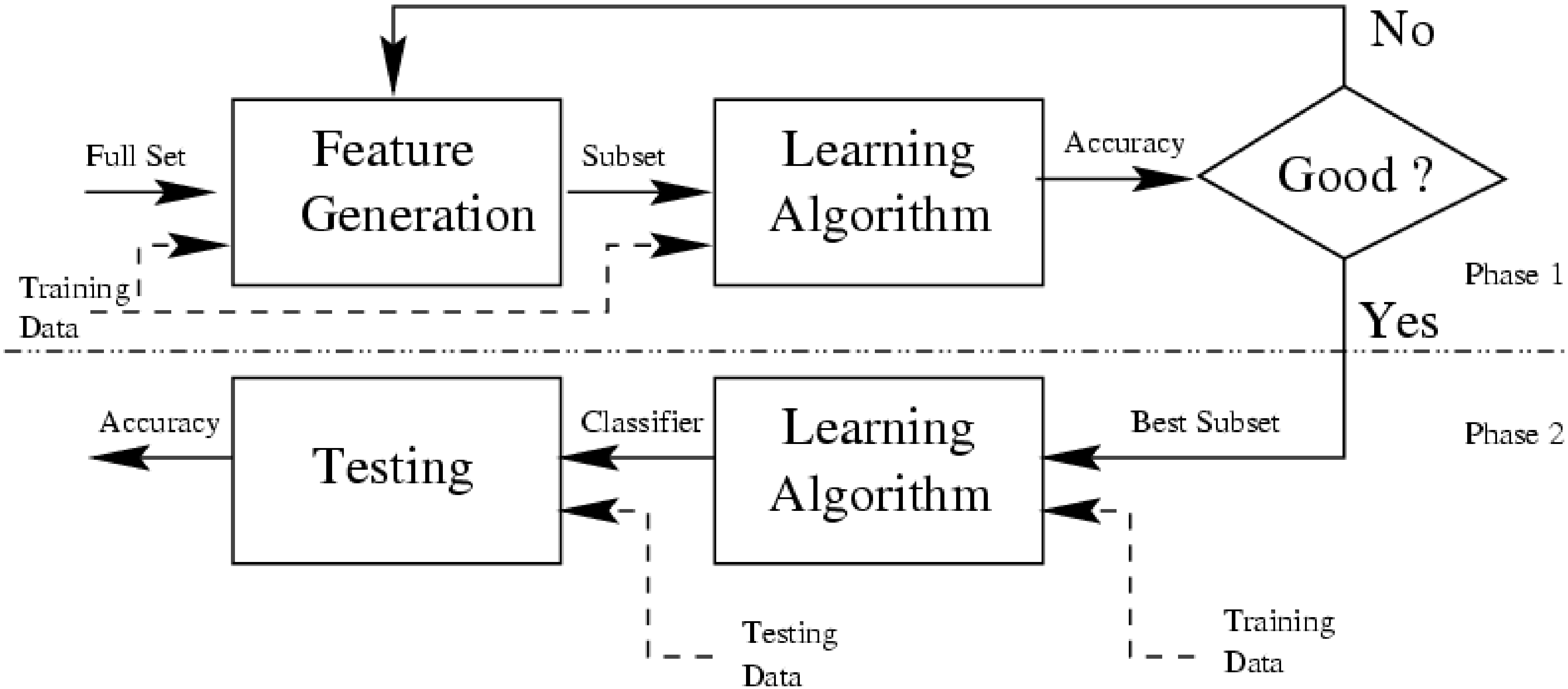
X is a candidate feature for reduction because its mean values are close, and therefore the final test is below threshold value.

Filter Model



- Example filter algorithm for feature selection:
  - ***Relief*** (Kira & Rendell 1992)

Wrapper Model



- Example wrapper algorithm for Feature Selection:
  - ***SVM***

Data Reduction: Dimensionality Reduction

- ***Curse of dimensionality***
  - When dimensionality increases, data becomes increasingly sparse
  - Density and distance between points, which is critical to clustering, outlier analysis, becomes less meaningful
  - The possible combinations of subspaces will grow exponentially

- ***Dimensionality reduction***
  - Avoid the curse of dimensionality
  - Help eliminate irrelevant features and reduce noise
  - Reduce time and space required in data mining
  - Allow easier visualization

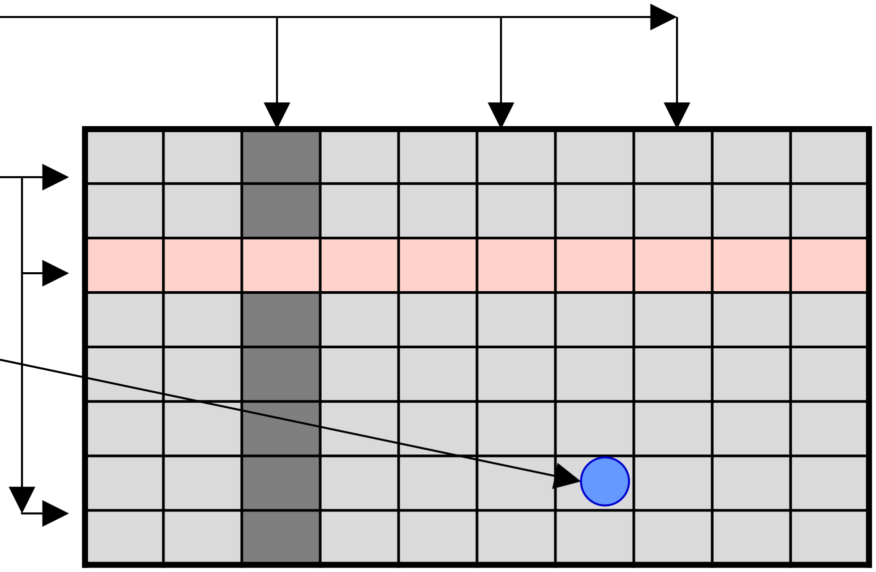
Data Reduction Strategies

- Why data reduction? — A database/data warehouse may store terabytes of data. Complex data analysis may take a very long time to run on the complete data set.
- Obtain a reduced representation of the data set that is much smaller in volume but yet produces the (almost) same analytical results
- Data reduction strategies
  - ***Dimensionality reduction***, e.g., remove unimportant attributes
    - Feature subset selection, feature creation
    - Wavelet transforms
    - Principal Components Analysis (PCA)
  - ***Numerosity*** reduction (some simply call it: Data Reduction)
    - Regression and Log-Linear Models
    - Histograms, clustering, sampling
    - Data cube aggregation
  - ***Data compression***

Dimensions Reduction of Large Data Sets

Main dimensions:

- ***columns*** (features),
- ***rows*** (cases or samples),
- ***values*** of the features for the given sample



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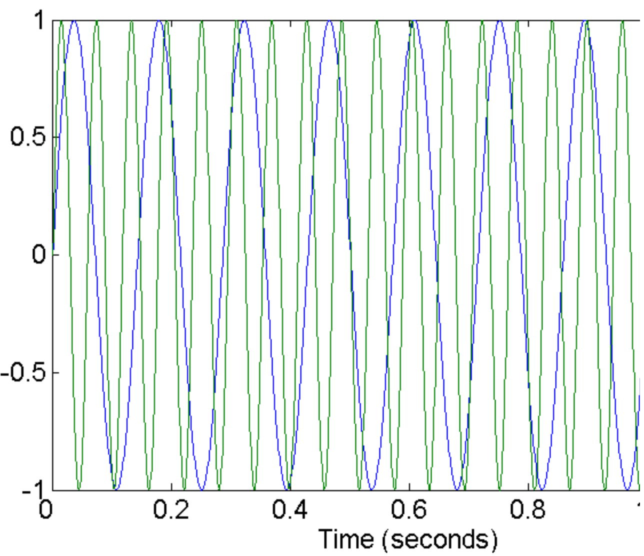
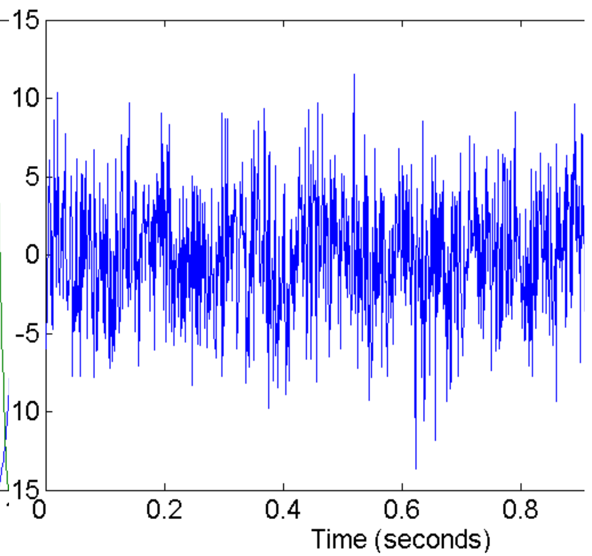
  - Major Tasks in Data Preprocessing
- Data Cleaning
- Data Integration
- Data Reduction
- Data Transformation
- Data Discretization

Mapping Data to a New Space

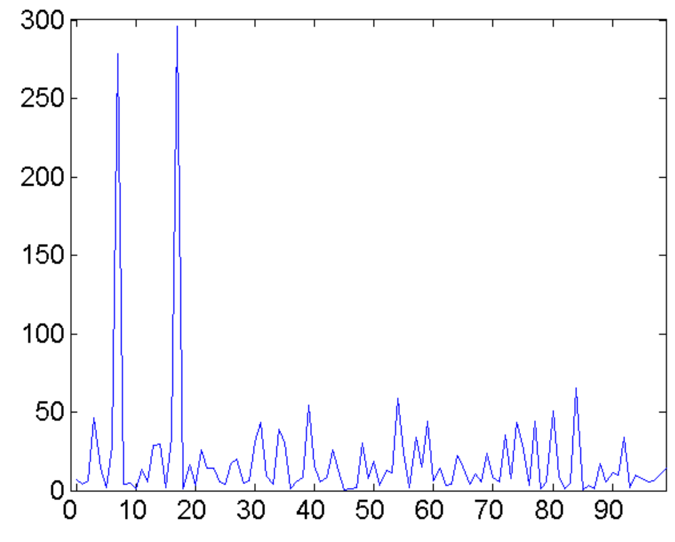
- Fourier transform: mapping from time to frequency domain
- Wavelet transform



Two Sine Waves



Two Sine Waves + Noise



Frequencies

Data Transformation

- A function that maps the entire set of values of a given attribute to a new set of replacement values so that each old value can be identified with one of the new values
- Methods
  - Smoothing: Remove noise from data
  - Attribute/feature construction
    - New attributes constructed from the given ones
  - Aggregation: Summarization
  - Normalization: Scaled to fall within a smaller, specified range
    - min-max normalization
    - z-score normalization
    - normalization by decimal scaling
  - Discretization: Concept hierarchy climbing

Normalization

- ***Min-max normalization***: to [new_min$_A$, new_max$_A$]

$$v' = \frac{v - min_A}{max_A - min_A}(new\_max_A - new\_min_A) + new\_min_A$$

  - Ex. Let income range \$12,000 to \$98,000. Normalize to [0.0, 1.0]. Then \$73,600 is mapped to $\frac{73,600-12,000}{98,000-12,000}(1.0-0)+0 = 0.716$

- ***Z-score normalization*** (μ: mean, σ: standard deviation):

$$v' = \frac{v - \mu_A}{\sigma_A}$$

  - Ex. Let μ = 54,000, σ = 16,000. Then $\frac{73,600-54,000}{16,000} = 1.225$

- ***Normalization by decimal scaling***

$$v' = \frac{v}{10^j}$$ where *j* is the smallest integer such that Max(|v'|) < 1

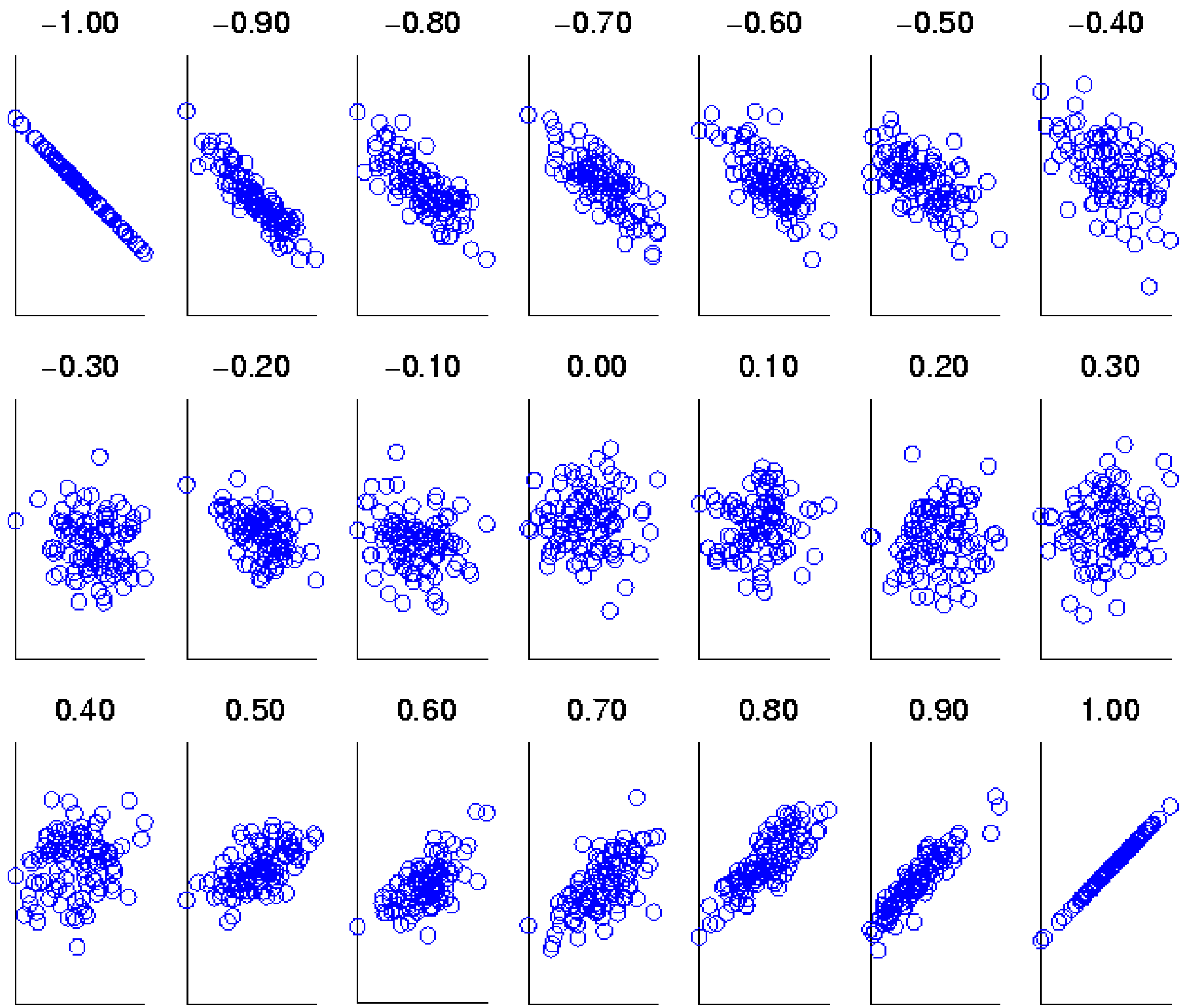
Correlation Analysis (Numeric Data)

- Correlation coefficient (also called ***Pearson's product moment coefficient***)

$$r_{A,B} = \frac{\sum_{i=1}^{N}(a_i - \overline{A})(b_i - \overline{B})}{N\sigma_A \sigma_B}$$

  - N = number of tuples
  - $\overline{A}$ and $\overline{B}$ = means of attributes A and B
  - σ_A and σ_B = standard deviations of A and B
- $r_{A,B} > 0$: A and B are positively correlated
  - A's values increase as B's. Larger $r_{A,B} \rightarrow$ stronger correlation.
- $r_{A,B} = 0$: independent
- $r_{AB} < 0$: negatively correlated

Visually Evaluating Correlation



Scatter plots

Correlation coefficients range from –1 to 1.

Covariance (Numeric Data)

- Covariance:

$$Cov(A,B) = E((A-\bar{A})(B-\bar{B})) = \frac{\sum_{i=1}^{n}(a_i-\bar{A})(b_i-\bar{B})}{n}$$

Related to correlation coefficient: $r_{A,B} = \frac{Cov(A,B)}{\sigma_A \sigma_B}$

  - n = number of tuples
  - $\overline{A}$ and $\overline{B}$ = mean or ***expected values*** of A and B
  - σ_A and σ_B = standard deviation of A and B.
- ***Positive covariance***: If $Cov_{A,B} > 0$, then A and B both tend to be larger than their expected values.
- ***Negative covariance***: If $Cov_{A,B} < 0$ then if A is larger than its expected value, B is likely to be smaller than its expected value.
- ***Independence***: $Cov_{A,B} = 0$

Co-Variance: an Example

$$Cov(A,B) = E((A-\bar{A})(B-\bar{B})) = \frac{\sum_{i=1}^{n}(a_i-\bar{A})(b_i-\bar{B})}{n}$$

- It can be simplified in computation as

$$Cov(A,B) = E(A \cdot B) - \bar{A}\bar{B}$$

- Suppose two stocks A and B have the following values in one week: (2, 5), (3, 8), (5, 10), (4, 11), (6, 14).
- **Question**: If the stocks are affected by the same industry trends, will their prices rise or fall together?
  - $E(A)$ = (2 + 3 + 5 + 4 + 6)/ 5 = 20/5 = 4
  - $E(B)$ = (5 + 8 + 10 + 11 + 14) /5 = 48/5 = 9.6
  - $Cov(A,B)$ = (2·5 + 3·8 + 5·10 + 4·11 + 6·14)/5 − 4·9.6 = 4
- Thus, A and B rise together since $Cov(A, B) > 0$.

Principal Component Analysis (Steps)

- Given *N* data vectors from *n*-dimensions, find *m* << *n* orthogonal vectors (***principal components***) to represent the data
  - Subtract mean from the input data, each attribute has mean zero
  - Compute *m* orthonormal (unit) vectors, i.e., *principal components*
  - Each input data (vector) is a linear combination of the *m* principal component vectors
  - The principal components are sorted in order of decreasing "***significance***" (1st component: data has maximum variance)
  - Since the components are sorted, the size of the data can be reduced by eliminating the *insignificant components*, i.e., those with low variance
  - Thus, using only the most significant principal components, it is possible to reconstruct a good approximation of the original data.
- Works for numeric data; reduction of higher dimensions to lower

Principal Components Analysis Algorithm

1. Compute the $n \times n$ ***covariance matrix*** S

$$S_{ij} = \frac{1}{N-1} \cdot \sum_{d=1}^{N} \left(x_i^d - \overline{x}_i \right)^T \cdot \left(x_j^d - \overline{x}_j \right) \quad \text{where} \quad \overline{x} = \frac{1}{N-1} \cdot \sum_{d=1}^{N} x^d$$

2. Calculate the ***eigenvalues*** of the covariance matrix S for the given data and sort the eigenvalues of S:
   $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n \geq 0.$

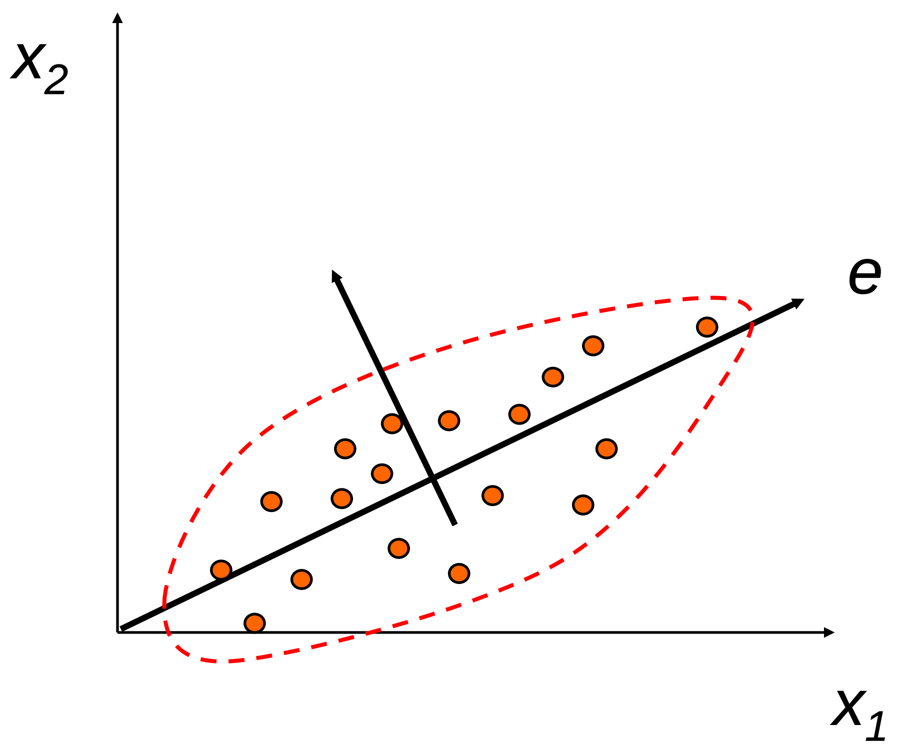
   The eigenvalues are the variances of the data in the directions of ``their´´ eigenvectors.

3. The ***eigenvectors*** $e_1, e_2, \ldots, e_n$ correspond to ``their´´ eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$,

   The eigenvectors are called the ***principal axes***.

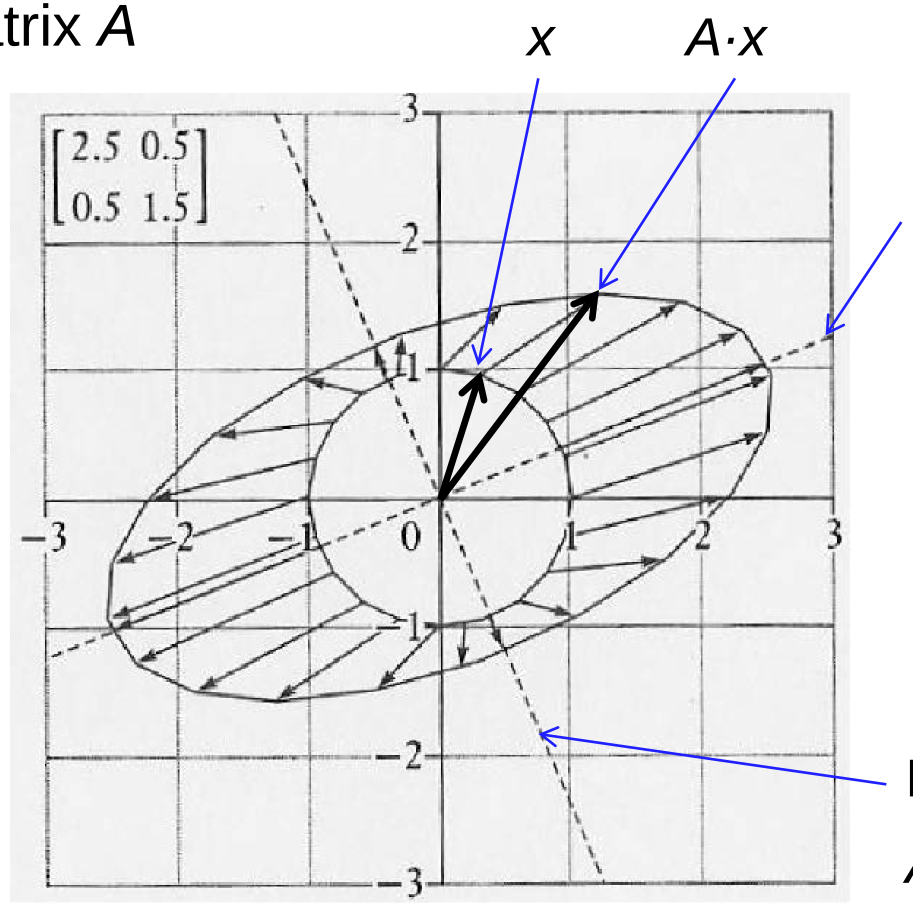
Principal Component Analysis (PCA)

- Find a projection that captures the largest amount of variation in data
- The original data are projected onto a much smaller space, resulting in dimensionality reduction. We find the eigenvectors of the covariance matrix, and these eigenvectors define the new space



Multiply a Vector with an n×n Matrix: A·x

- Symmetric matrix *A*



Eigenvector(s),

$A \cdot e_1 = \lambda_1 \cdot e_1$

large eigenvalue λ_1

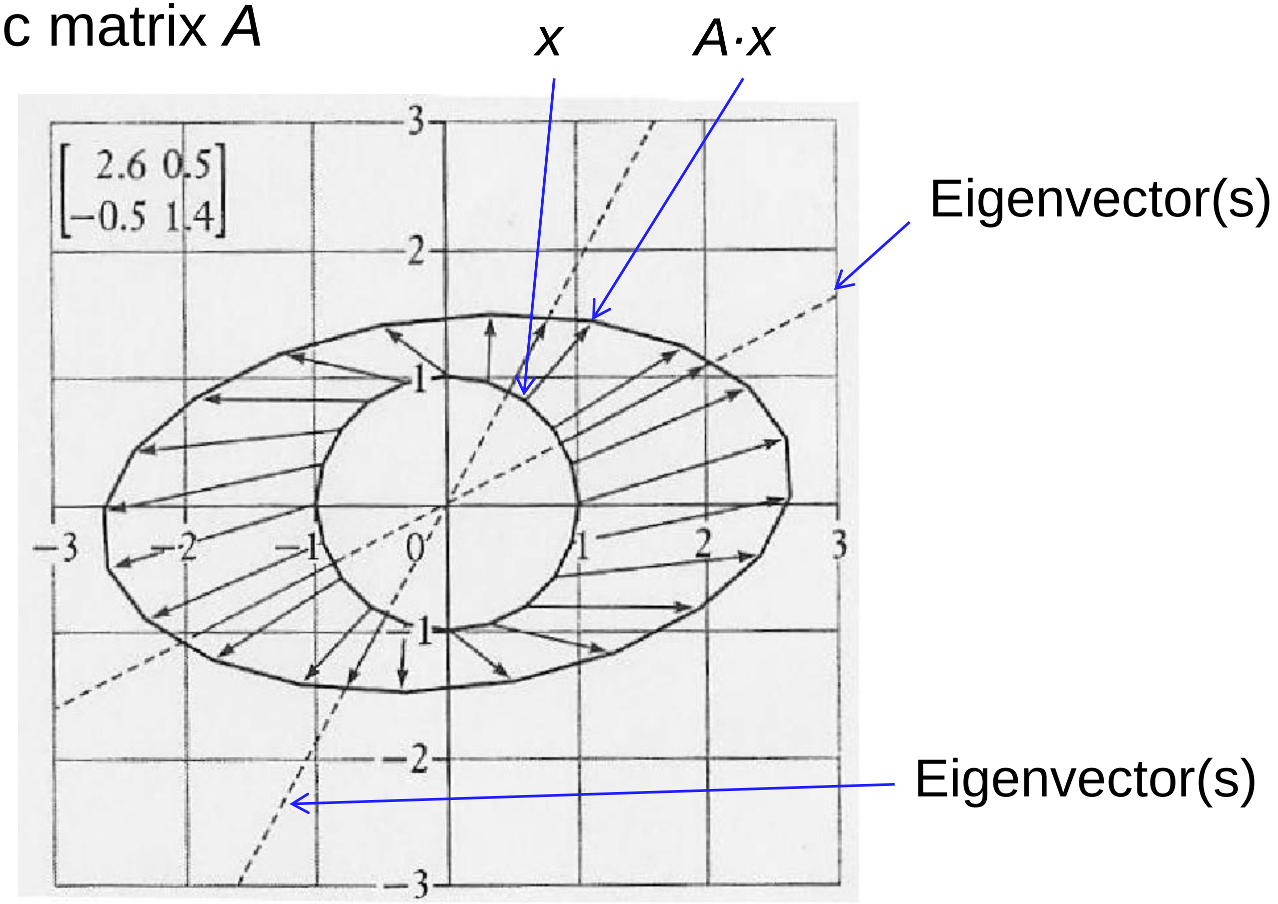
Eigenvector(s)

$A \cdot e_2 = \lambda_2 \cdot e_2$

small eigenvalue λ_2

Multiply a Vector with an n×n Matrix: A·x

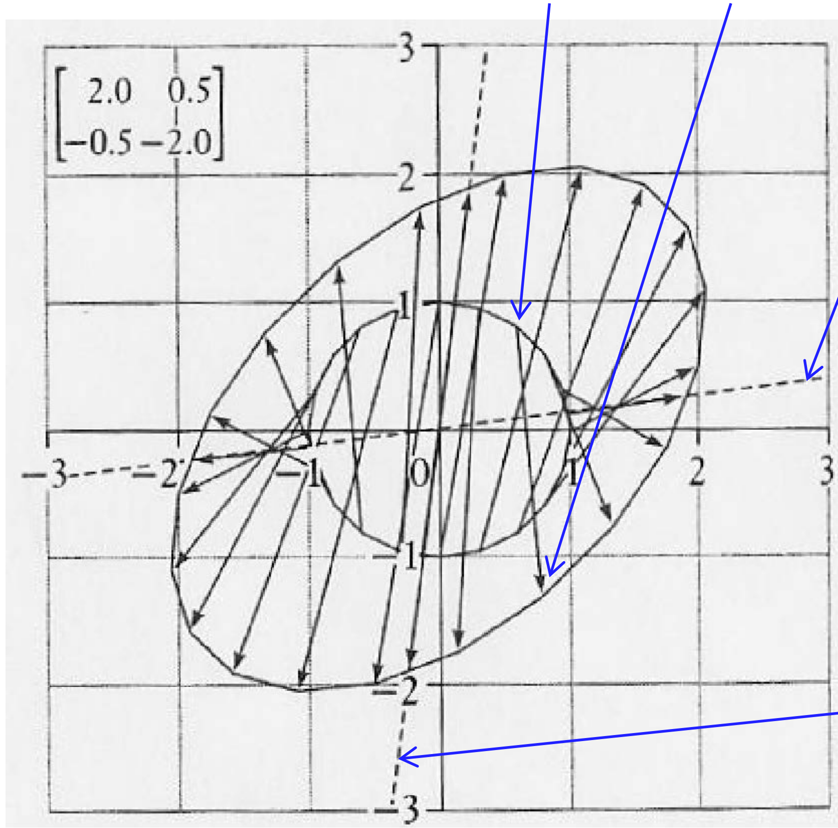
- Non-symmetric matrix *A*



Multiply a Vector with an n×n Matrix: A·x

- Arbitrary matrix *A*

x *A·x*

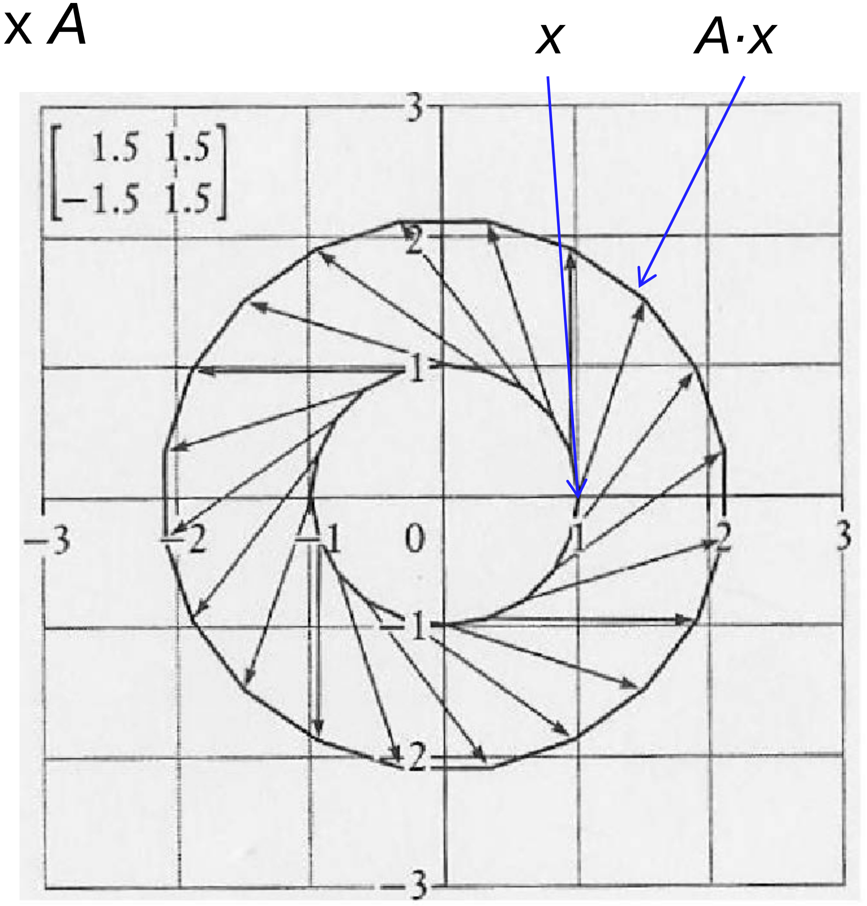


Eigenvector(s), eigenvalue $\lambda_1 > 0$

Eigenvector(s), eigenvalue $\lambda_2 < 0$

Multiply a Vector with an n×n Matrix: A·x

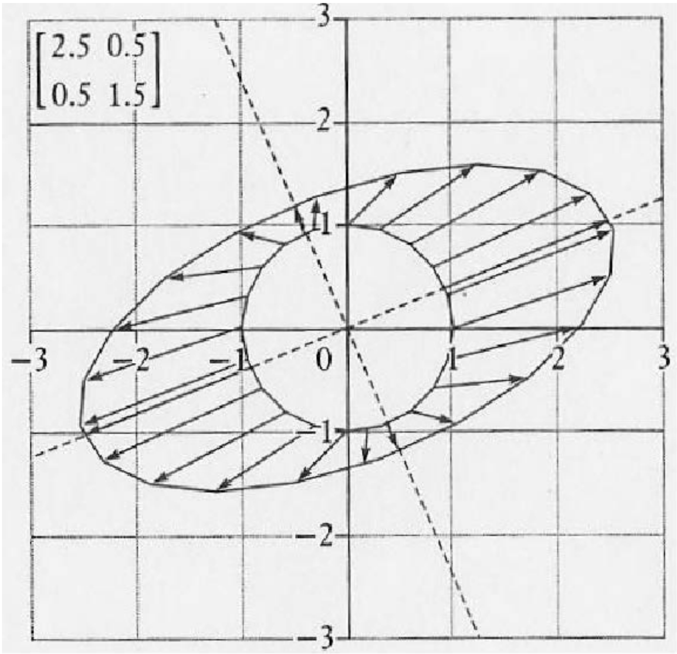
- Rotation matrix *A*



No eigenvectors

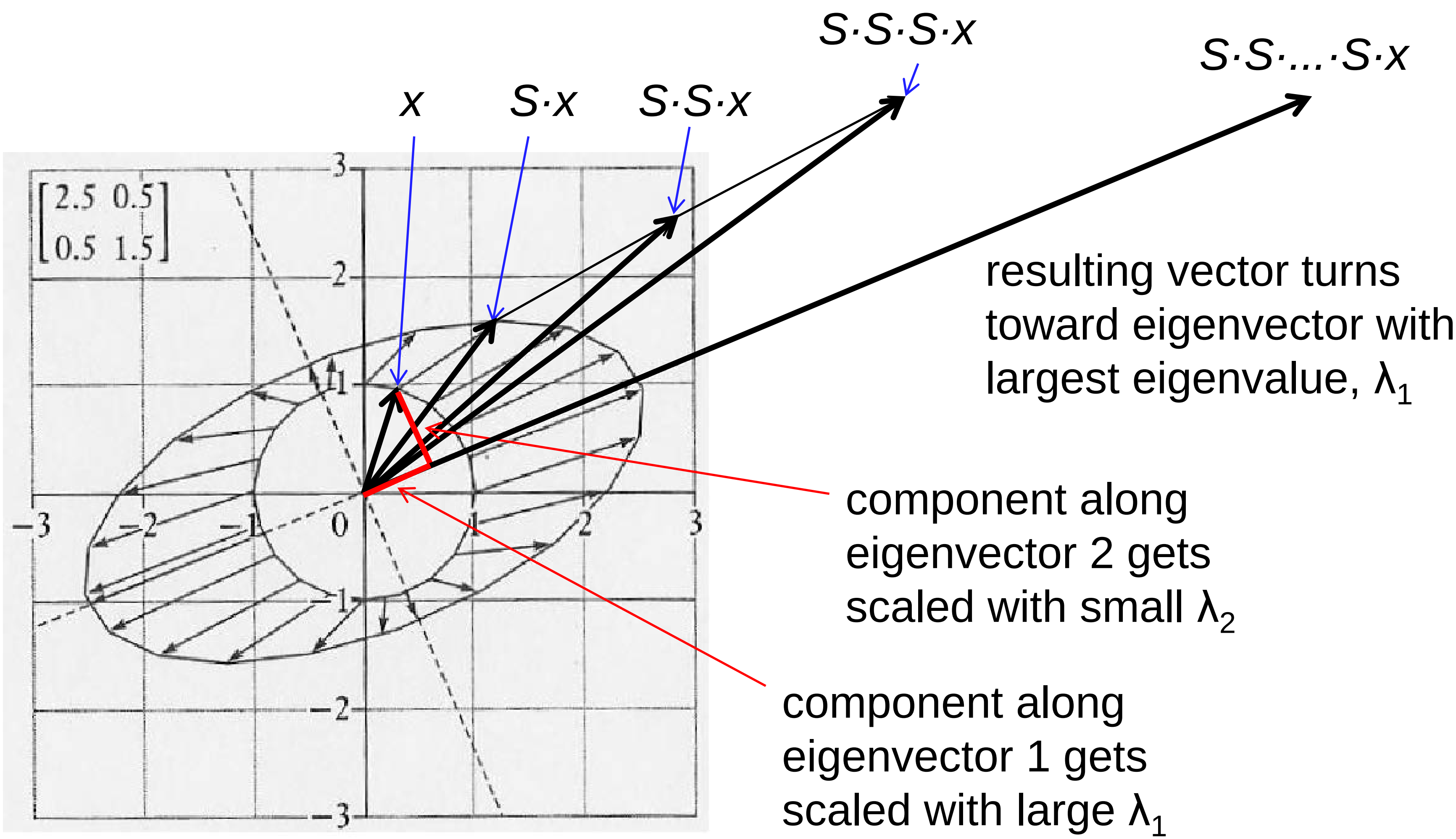
Multiply a Vector with a Covariance Matrix

- The covariance matrix *S* is a symmetric matrix
  - It always has eigenvectors
  - Eigenvectors are orthogonal to each other, if their eigenvalues differ
- Its eigenvalues are ≥ 0
  - *S* is positive (semi-) definite
- Eigenvalues are variances of the data in the directions of the corresponding eigenvectors

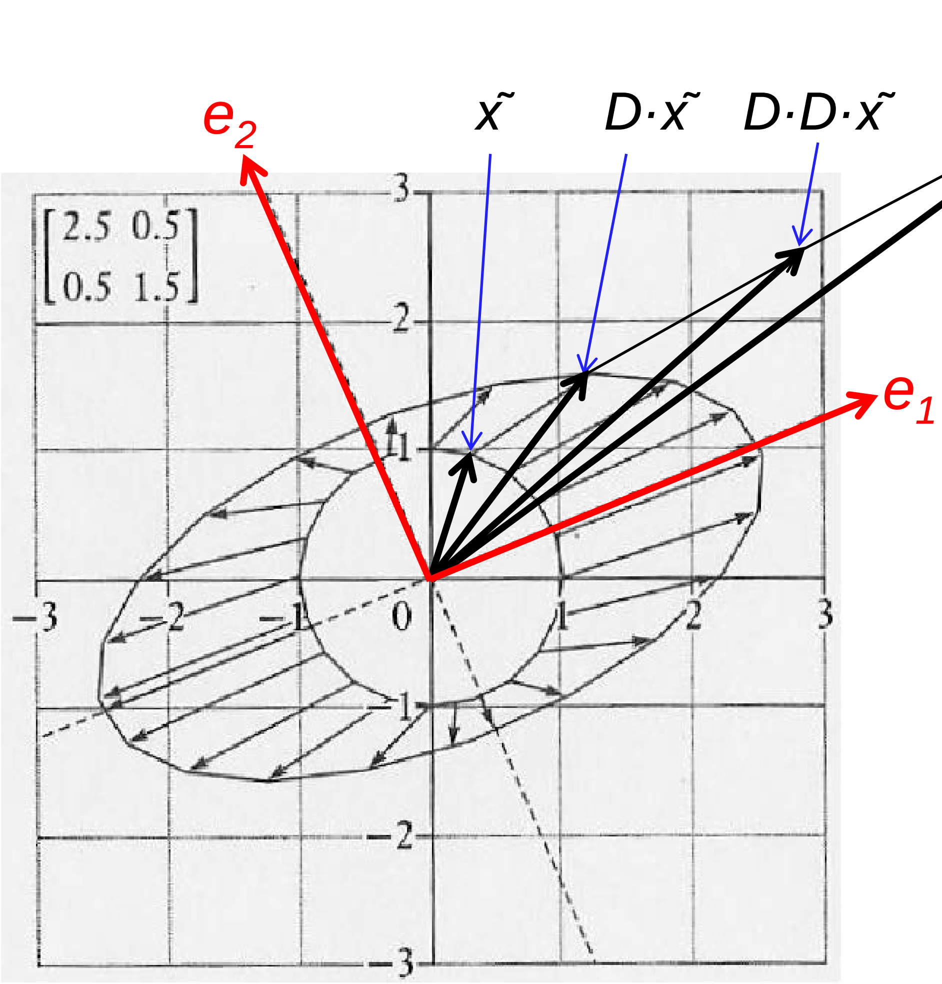


- Multiplying by *S* does not rotate any vector by more than 90°

Repeatedly Multiply with the Covariance Matrix



Repeatedly Multiply with the Covariance Matrix



New coordinate system:

Axes defined by the eigenvectors e_i

Here: $x \rightarrow \tilde{x}$

Here, covariance matrix expressed as a diagonal matrix D

The diagonal elements of D are the eigenvalues λ_i

Easy to see: individual dimensions/components *i* of $\tilde{x}$ are multiplied by λ_i

Obtain Largest Eigenvalue and Eigenvector

Iterative method

- Choose an initial random vector x
- Repeat
  - $x \leftarrow S \cdot x$
  - Normalize x to length 1
- Until converged. Then ***normalized eigenvector*** $e_1 = x$

Compute corresponding ***eigenvalue*** as the norm:

$$\lambda_1 = |S \cdot e_1|$$

- Other linear algebra methods, e.g. SVD, compute ***all*** eigenvectors and corresponding eigenvalues.

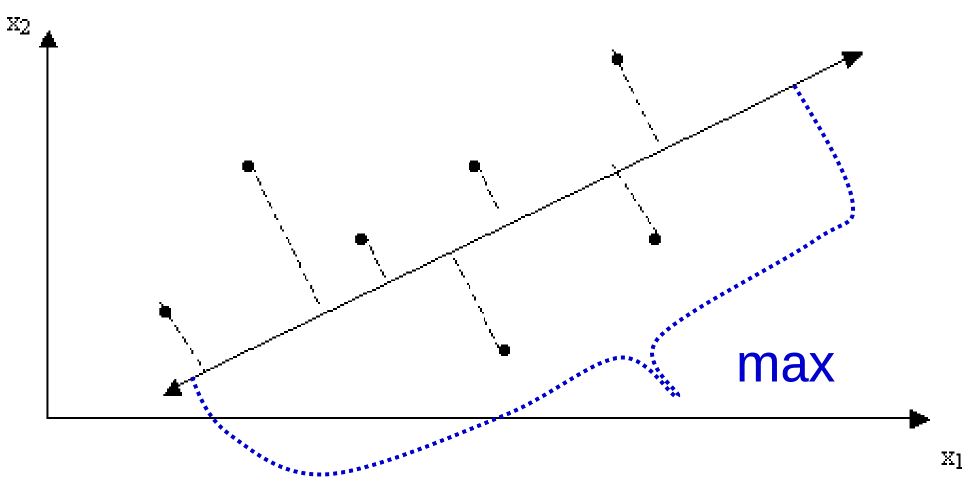
Principal Components Analysis

- The data can be expressed in the new coordinate system

$$x = \bar{x} + \sum_{j=1}^{m} w_j \cdot e_j$$

- w_j are the data coordinates along the eigenvector axes
- $m < n$: data are only approximately reconstructed

The first principal component is an axis in the direction of maximum variance.



Principal Components Analysis

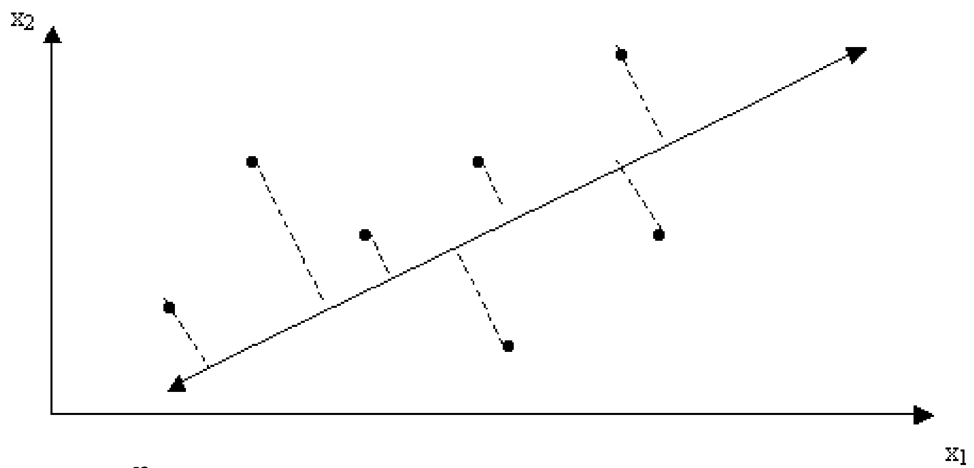
- The criterion for features selection is based on the ratio *R* of the sum of the *m* largest eigenvalues ($m \le n$) of *S* to the trace of *S* (for example R>90%):

$$R = \frac{\sum_{i=1}^{m} \lambda_i}{\sum_{i=1}^{n} \lambda_i}$$

sum over all explained variances

Trace of *S*

= sum over all variances



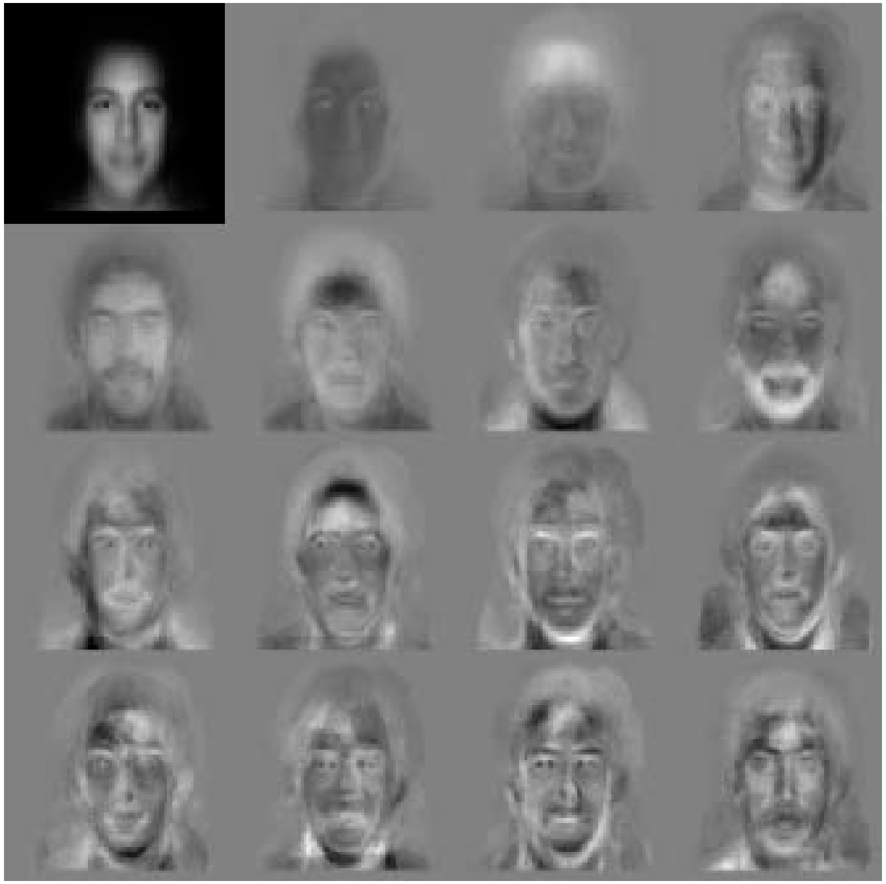
- Benefit:
  - non-explained variance $\sum_{i=m+1}^{n} \lambda_i$ may be small, even if *m* << *n*.

Principle Components Example: Eigenfaces

Eigenfaces are the (first few) principle components of a face image database.

reconstructed face

eigenfaces



Sampling

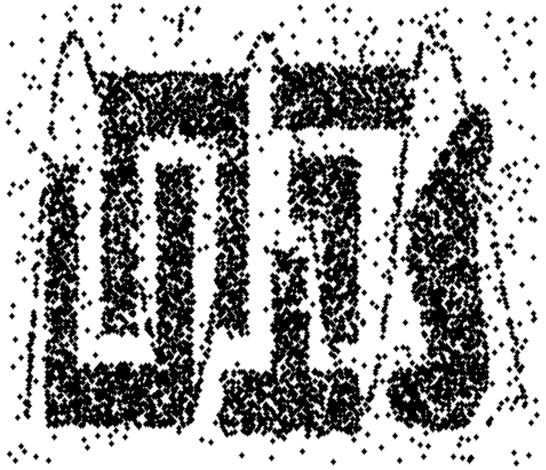
- Sampling: obtaining a small sample *s* to represent the whole data set *N*
- Allow a mining algorithm to run in complexity that is potentially sub-linear to the size of the data
- Key principle: Choose a ***representative*** subset of the data
  - Simple random sampling may have very poor performance in the presence of skewed data
  - Develop adaptive sampling methods, e.g., stratified sampling

Cases Reduction: Sampling …

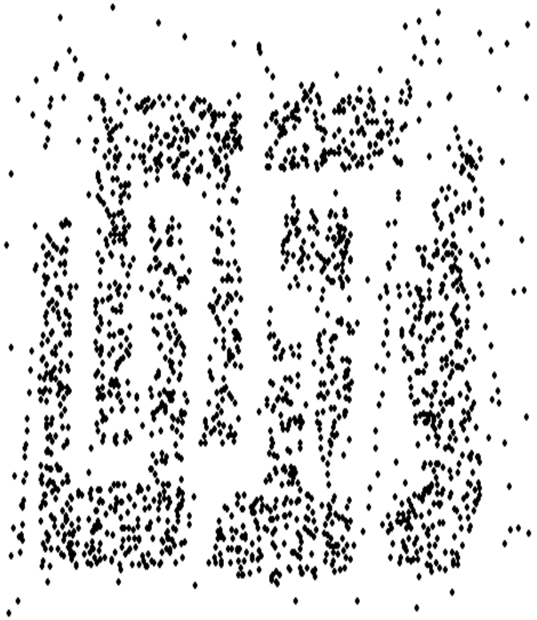
Key principle for effective sampling:

- Using a sample will work almost as well as using the entire data sets, if the sample is ***representative***.
- A sample is representative if it has approximately the same property (of interest) as the original set of data.

Cases Reduction: Sample Size



8000 points

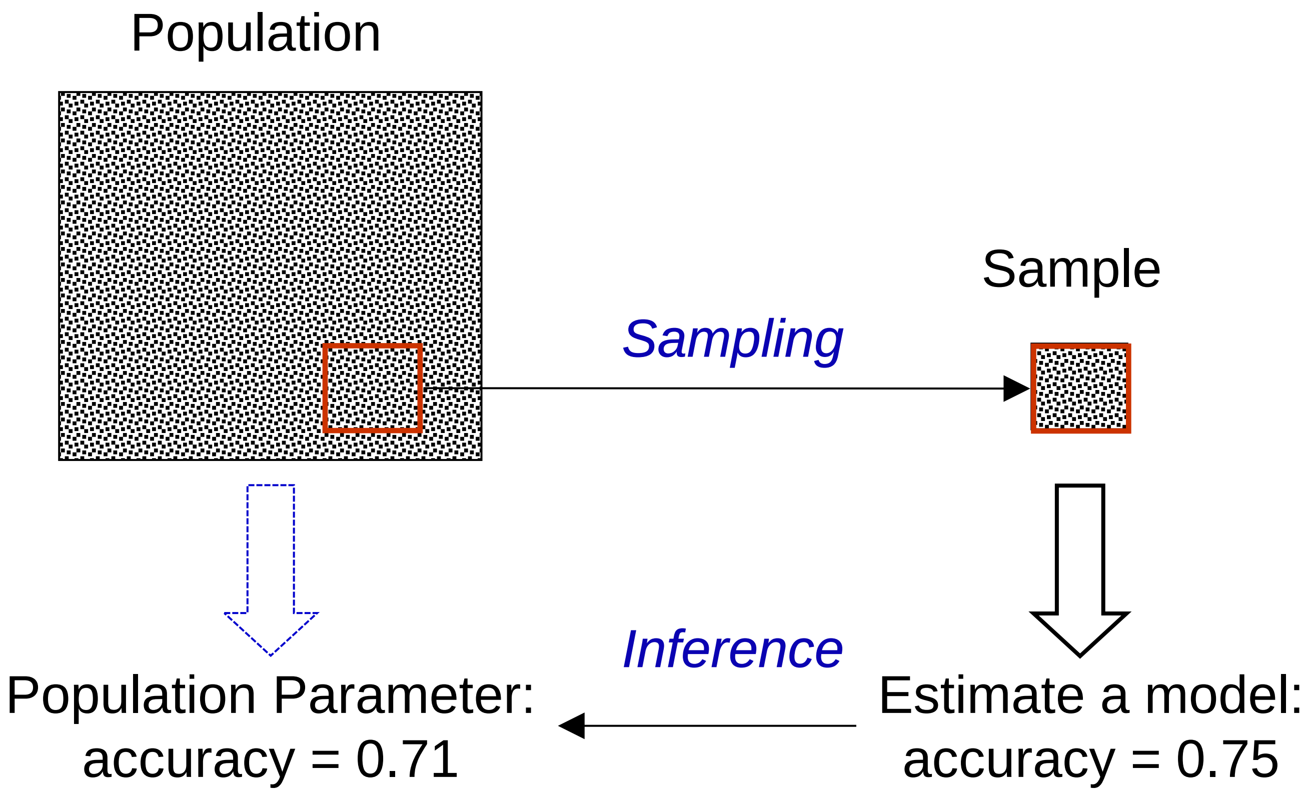


2000 Points

500 Points

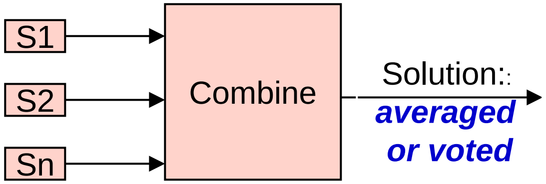
Cases Reduction: Accuracy Parameter Estimation

- ***Challenging task***: Infer the value of a population parameter based on a sample model.

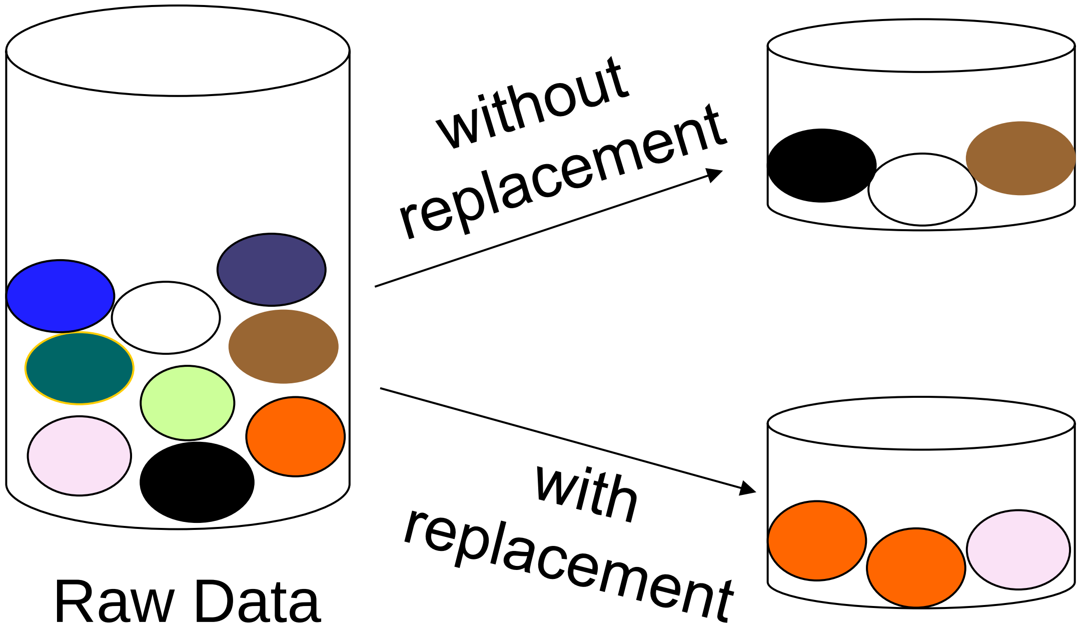


General-purpose Sampling Methods

- ***Systematic sampling*:**
  - For example 50% of a data set (every second sample)
  - Simplest.
  - Built in most of Data Mining tools
  - Problem: regularities in data set!
- ***Random sampling***
  - Random sampling without replacement,
  - Random sampling with replacement.
  - Average sampling: Combined solution from several subsets (randomly selected)
    - Stratified sampling



Sampling With or Without Replacement



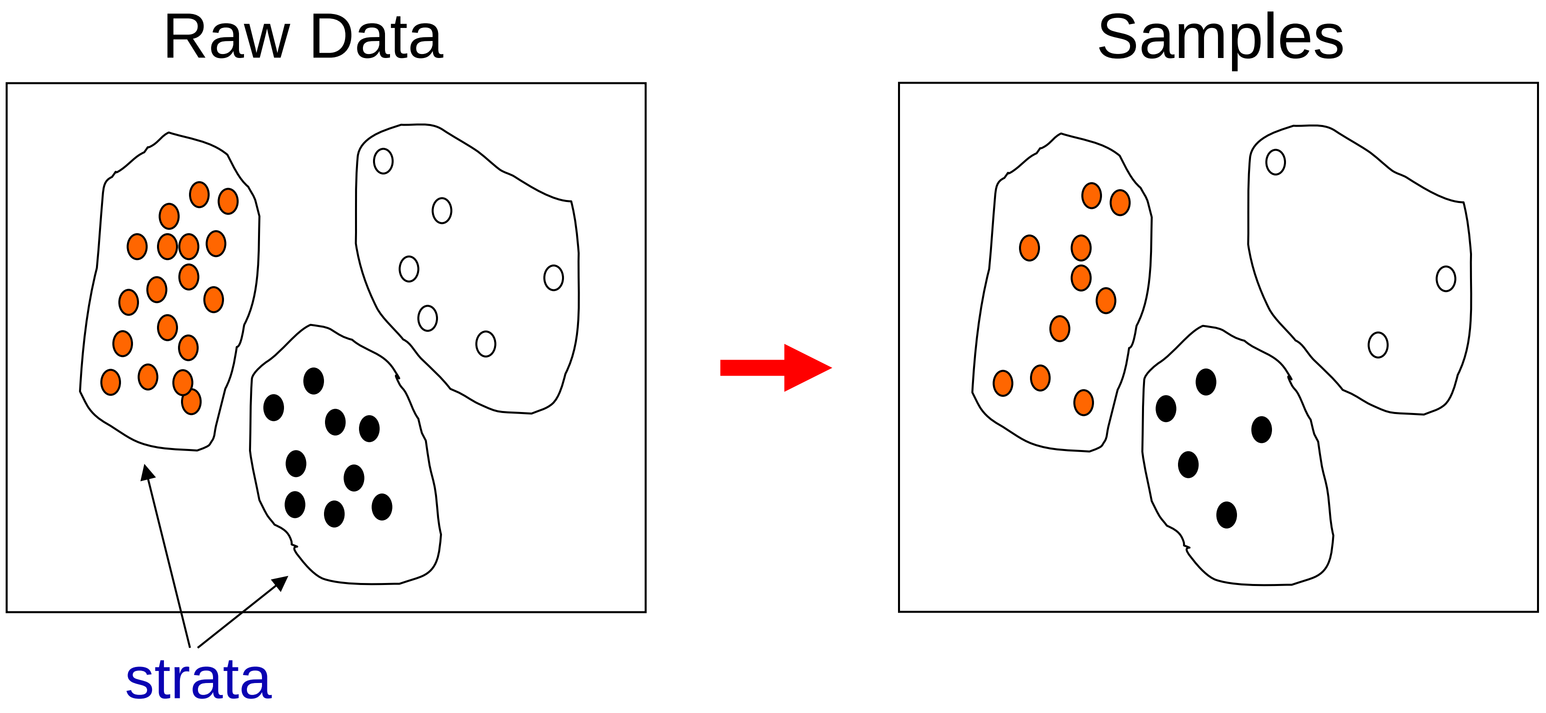
Raw Data (population)

Once an object is selected, it is removed from the population

A selected object is not removed from the population

Stratified Sampling

- Partition the data set into strata (non-overlapping)
- Draw samples from each partition proportionally to its percentage in the data



Data Preprocessing

- Data Preprocessing: An Overview
  - Data Quality
  - Major Tasks in Data Preprocessing
- Data Cleaning
- Data Integration
- Data Reduction
- Data Transformation
- Data Discretization

Data Discretization Methods

- Reduce number of values for given continuous attribute by dividing into intervals
  - ***Binning***: equal width binning and replacing bin by mean
    - Top-down split, unsupervised, no class information used
  - ***Histogram analysis***
    - Top-down split, unsupervised, no class information used
  - ***Clustering analysis*** (unsupervised, top-down split or bottom-up merge)
  - ***Decision-tree analysis*** (supervised, top-down split)
  - ***Correlation*** (e.g., χ^2) ***analysis*** (unsupervised, bottom-up merge)

Simple Discretization: Binning

- ***Equal-width*** (distance) partitioning
  - Divides the range into *N* intervals of equal size: uniform grid
  - If *A* and *B* are the lowest and highest values of the attribute, the width of intervals will be: $W = (B - A)/N$.
  - Simple, but outliers may dominate presentation
  - Skewed data is not handled well
- ***Equal-depth*** (frequency) partitioning
  - Divides the range into *N* intervals, each containing approximately same number of samples
  - Good data scaling

Binning Methods for Data Smoothing

Sorted data for price (in dollars): 4, 8, 9, 15, 21, 21, 24, 25, 26, 28, 29, 34

Partition into equal-frequency (*equi-depth*) bins:

- Bin 1: 4, 8, 9, 15
- Bin 2: 21, 21, 24, 25
- Bin 3: 26, 28, 29, 34

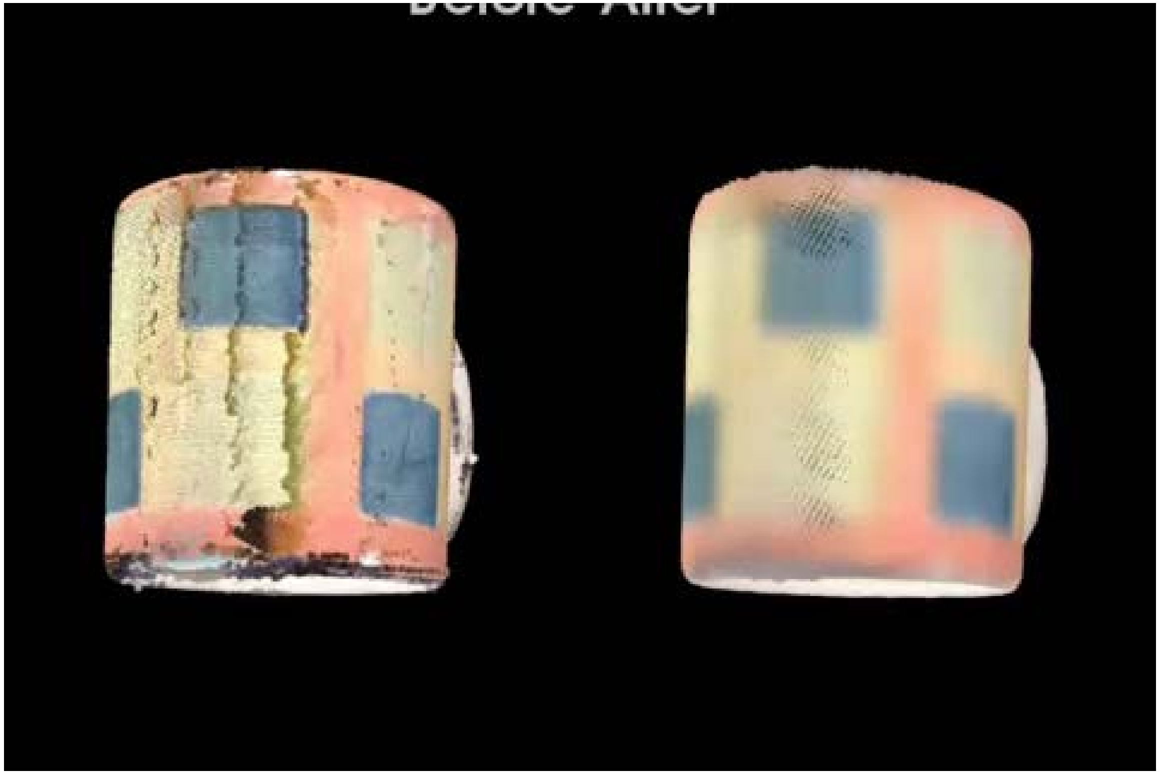
Smoothing by ***bin means***:

- Bin 1: 9, 9, 9, 9
- Bin 2: 23, 23, 23, 23
- Bin 3: 29, 29, 29, 29

Smoothing by ***bin boundaries***:

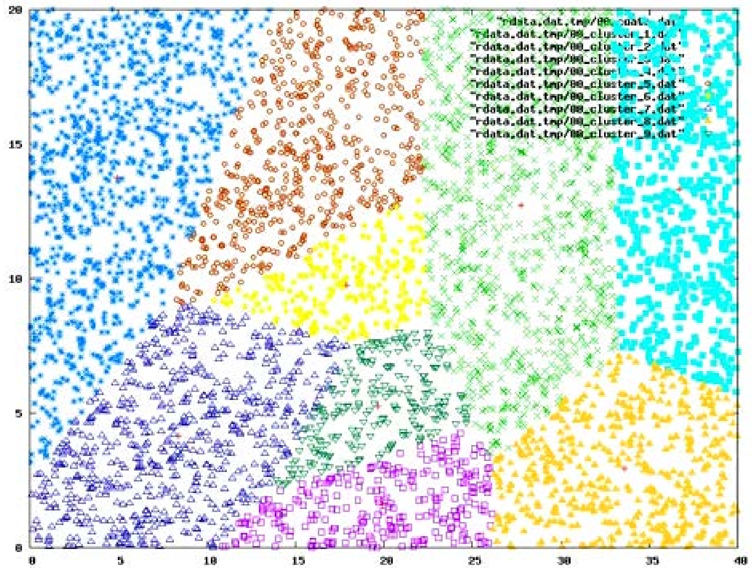
- Bin 1: 4, 4, 4, 15
- Bin 2: 21, 21, 21, 25
- Bin 3: 26, 26, 26, 34

Example: Data Resampling and Smoothing in Point Cloud Application



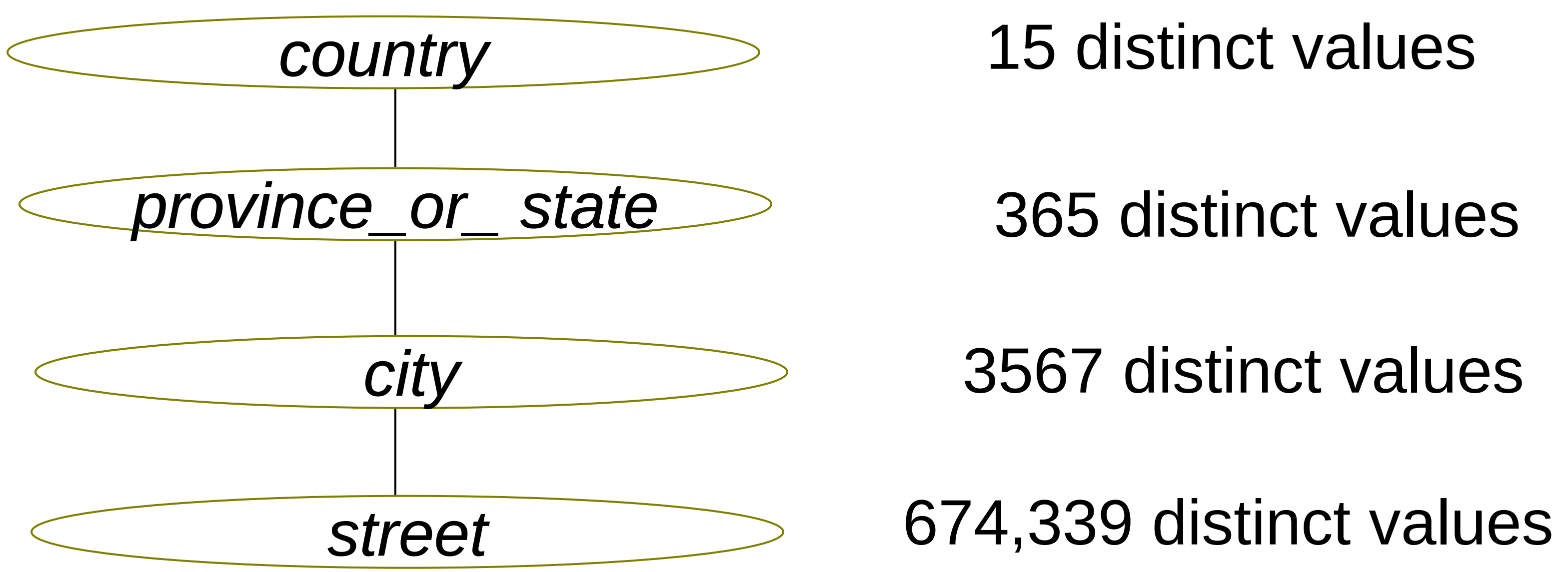
Clustering

- Partition data set into clusters based on similarity, and store cluster representation (e.g., centroid and diameter) only
- Can have hierarchical clustering and be stored in multi-dimensional index tree structures
- There are many choices of clustering definitions and clustering algorithms



Automatic Concept Hierarchy Generation

- Some hierarchies can be automatically generated based on the analysis of the number of distinct values per attribute in the data set
  - The attribute with the most distinct values is placed at the lowest level of the hierarchy
  - Exceptions, e.g., weekday, month, quarter, year



Time-dependent Data

- The ***time series*** of values can be expressed as a list:

  X = $\{t(1), t(2), t(3), \ldots, t(n)\}$,

  where $t(n)$ is the most recent value.

- For many problems based on time series the goal is to:
  - ***forecast*** $t(n+1)$ from previous n values of the feature (or more general forecast $t(n+j)$), where these values are directly related to the predicted value, or
  - ***find patterns*** in time series.

- The most important step in preprocessing of row time-dependent data is specification of a window or a time lag

Time-dependent Data

- Example: time series consisting of eleven measurements:

X = {t(0), t(1), t(2), t(3), t(4), t(5), t(6), t(7), t(8), t(9), t(10)}

- window size: w=5
- next value: **j=1**

Sample	WINDOW					Next Value
	M1	M2	M3	M4	M5	
1	t(0)	t(1)	t(2)	t(3)	t(4)	t(5)
2	t(1)	t(2)	t(3)	t(4)	t(5)	t(6)
3	t(2)	t(3)	t(4)	t(5)	t(6)	t(7)
4	t(3)	t(4)	t(5)	t(6)	t(7)	t(8)
5	t(4)	t(5)	t(6)	t(7)	t(8)	t(9)
6	t(5)	t(6)	t(7)	t(8)	t(9)	t(10)

Time-dependent Data

- Example: time series consisting of eleven measurements:

X = {t(0), t(1), t(2), t(3), t(4), t(5), t(6), t(7), t(8), t(9), t(10)}

- window size: w=5
- next value: **j=3**

Sample	W	I	N	D	O W	Next Value
	M1	M2	M3	M4	M5	
1	t(0)	t(1)	t(2)	t(3)	t(4)	t(7)
2	t(1)	t(2)	t(3)	t(4)	t(5)	t(8)
3	t(2)	t(3)	t(4)	t(5)	t(6)	t(9)
4	t(3)	t(4)	t(5)	t(6)	t(7)	t(10)

Time-dependent Data

Time-dependent ***2D*** data

Time	a	b
1	5	117
2	8	113
3	4	116
4	9	118
5	10	119
6	12	120

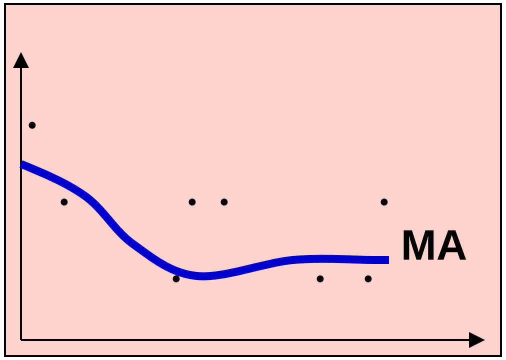
Samples prepared for ***window*** w = 3

Sample	a (n-2)	a (n-1)	a(n)	b (n-2)	b (n-1)	b(n)
1	5	8	4	117	113	116
2	8	4	9	113	116	118
3	4	9	10	116	118	119
4	9	10	12	118	119	120

Time-dependent Data

- One way of ***summarizing*** features in the data set is to average them, producing "***moving averages***" (MA):

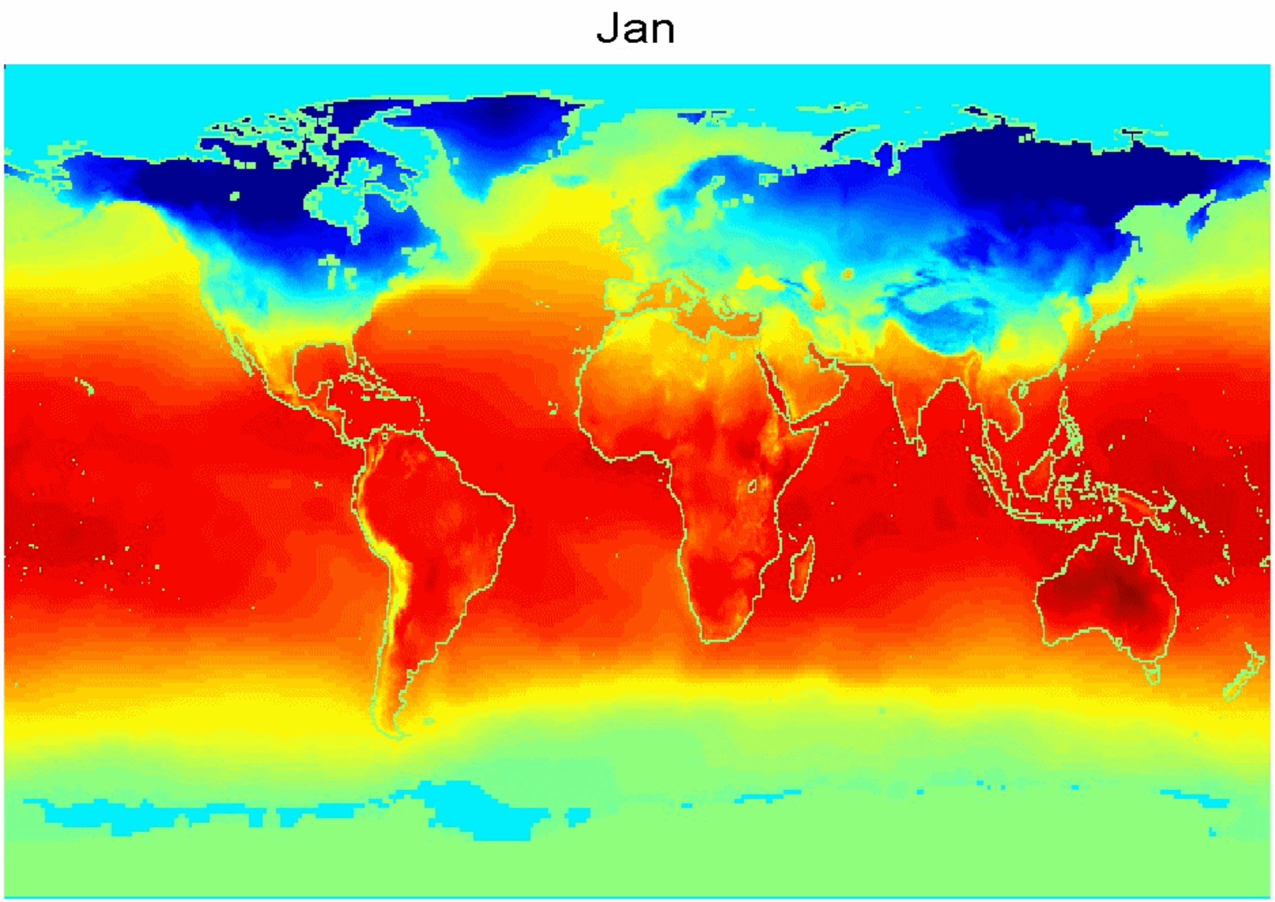
$$\mathrm{MA}(i,m) = \frac{1}{m} \cdot \sum_{j=i-m+1}^{i} t(j)$$



- The objective is to ***smooth*** neighboring time points by a moving average to reduce the random variation and noise components:

$$\mathrm{MA}(i,m) = t(i) = \mathrm{mean}(i) + error$$

Spatial-Temporal Data



Average monthly temperature

New disciplines: Temporal, Spatial, and Streaming Data Mining

Noise example in real world from the WTM lab

www.informatik.uni-hamburg.de/WTM or
www.knowledge-technology.info

Summary

- ***Data quality***: accuracy, completeness, consistency, timeliness, believability, interpretability
- ***Data cleaning***: e.g. missing/noisy values, outliers
- ***Data integration*** from multiple sources:
  - Entity identification problem; Remove redundancies; Detect inconsistencies
  - Chi-square for correlation analysis
- ***Data reduction***
  - Dimensionality reduction, e.g. by comparison of means and variances; Numerosity reduction; Data compression
- ***Data transformation***
  - Normalization
  - PCA
- ***Data discretization***
  - Binning, Clustering, Concept hierarchy generation

HiWi Position at WTM Available

- 20 - 40 hours (one-off, approx. €400-€500)
- Immediate availability
- Task: Organize the Publications on the WTM Web Page