Data, Classification, Model Selection

CS 584 Data Mining (Fall 2016)

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Slides are adapted from the available book slides developed by Tan, Steinbach and Kumar

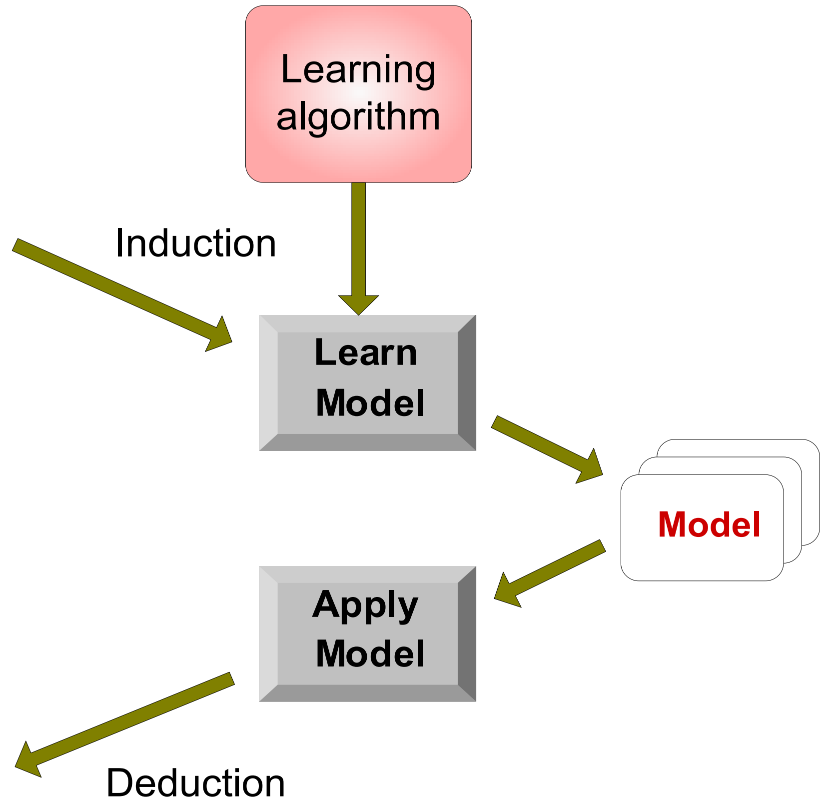
Lesson Plan

- Classification
  - Nearest Neighbor
- Definitions/Terms
  - Data
- Text-Data: Similarity Function
- Problems
  - Curse of Dimensonality
- Model Selection
  - Metrics/Plan

Illustrating Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set



Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set

Classification: Definition

- Given a collection of records (*training set*)
  - Each record contains a set of *attributes*, one of the attributes is the *class*.
- Find a *model* for class attribute as a function of the values of other attributes.
- Goal: <u>previously unseen</u> records should be assigned a class as accurately as possible.
  - A *test set* is used to determine the accuracy of the model. Usually, the given data set is divided into training and test sets, with training set used to build the model and test set used to validate it.

Instance-Based Classifiers

Set of Stored Cases

Atr1	……...	AtrN	Class
			A
			B
			B
			C
			A
			C
			B

- Store the training records
- Use training records to predict the class label of unseen cases

Unseen Case

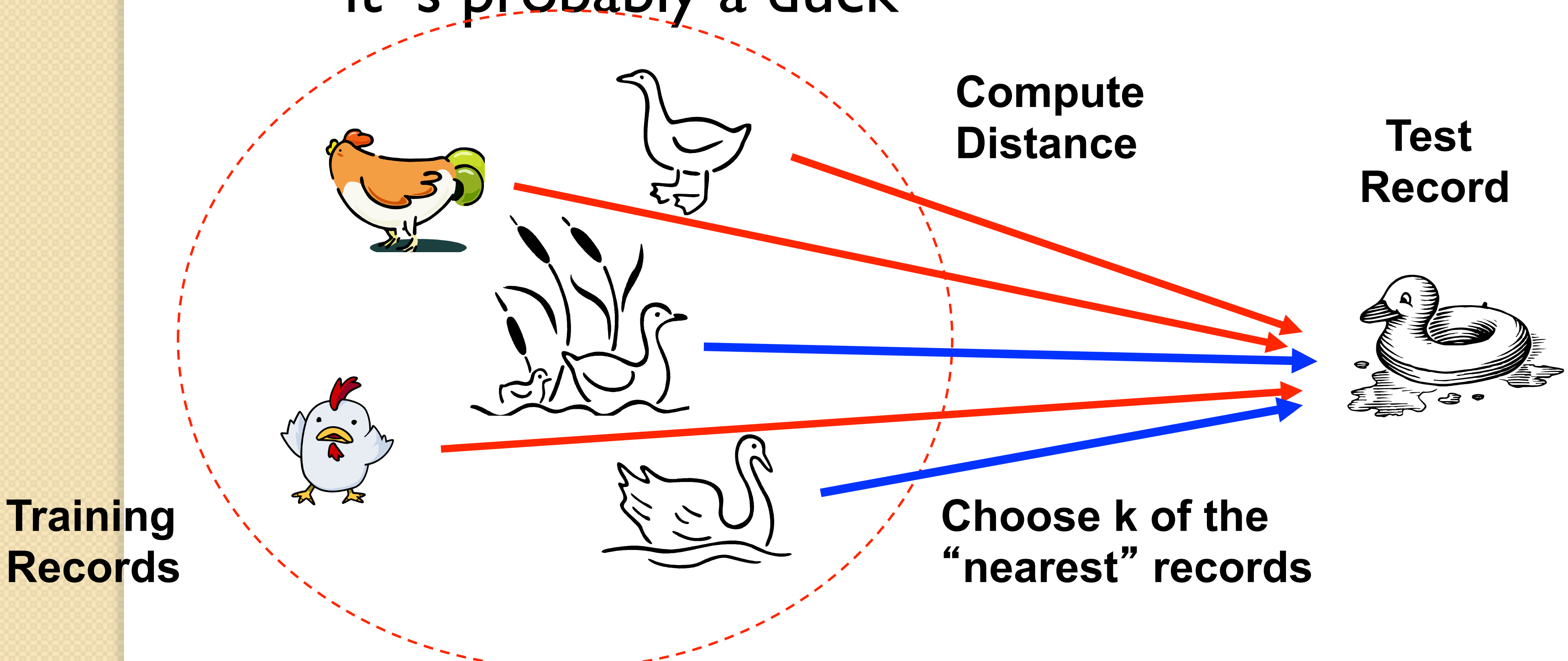
Atr1	……...	AtrN

Instance Based Classifiers

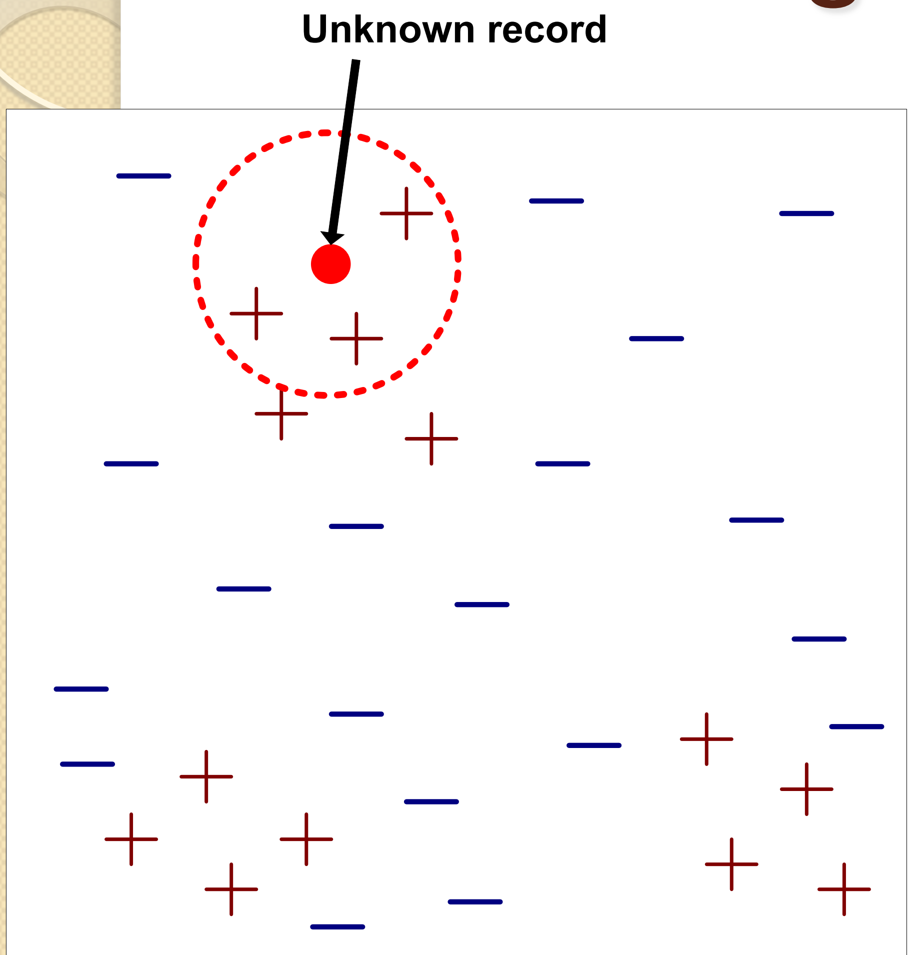
- Examples:
  - Rote-learner
    - Memorizes entire training data and performs classification only if attributes of record match one of the training examples exactly
  - Nearest neighbor
    - Uses k "closest" points (nearest neighbors) for performing classification

Nearest Neighbor Classifiers

- Basic idea:
  - If it walks like a duck, quacks like a duck, then it' s probably a duck

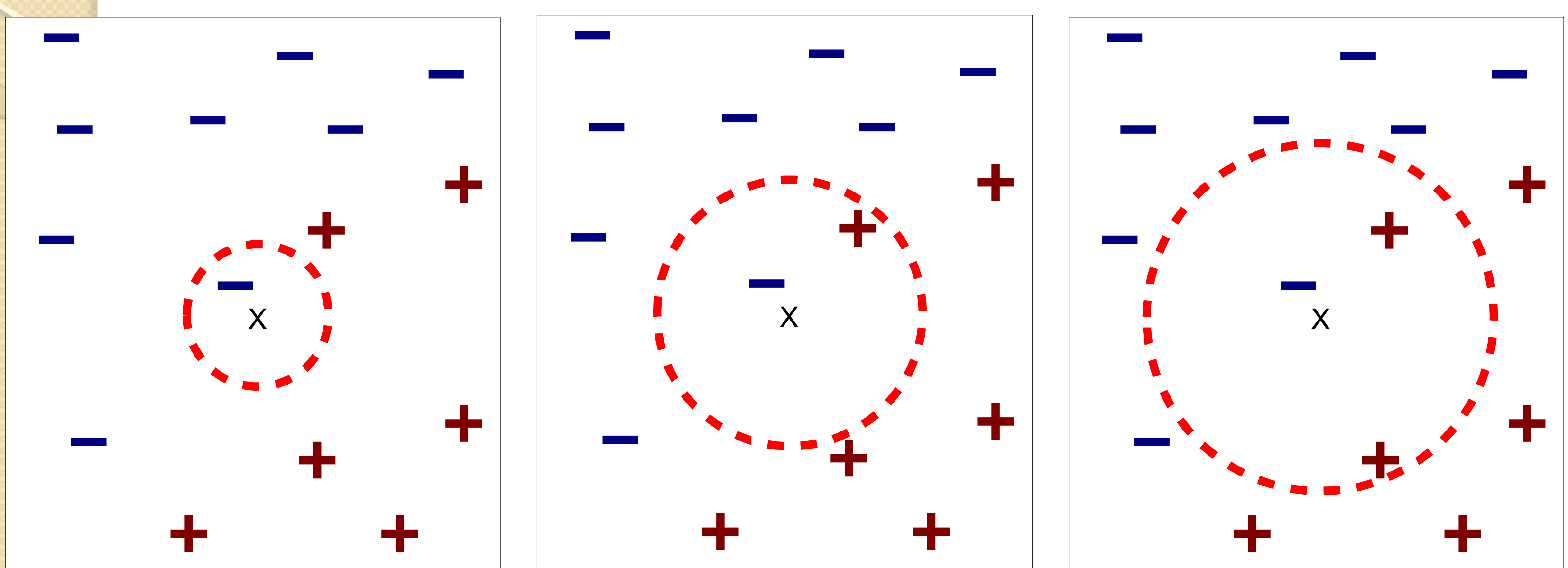


Nearest-Neighbor Classifiers



- Requires three things
  - The set of stored records
  - Distance Metric (Sim) to compute distance (Sim) between records
  - The value of *k*, the number of nearest neighbors to retrieve
- To classify an unknown record:
  - Compute distance to other training records
  - Identify *k* nearest neighbors
  - Use class labels of nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

Definition of Nearest Neighbor

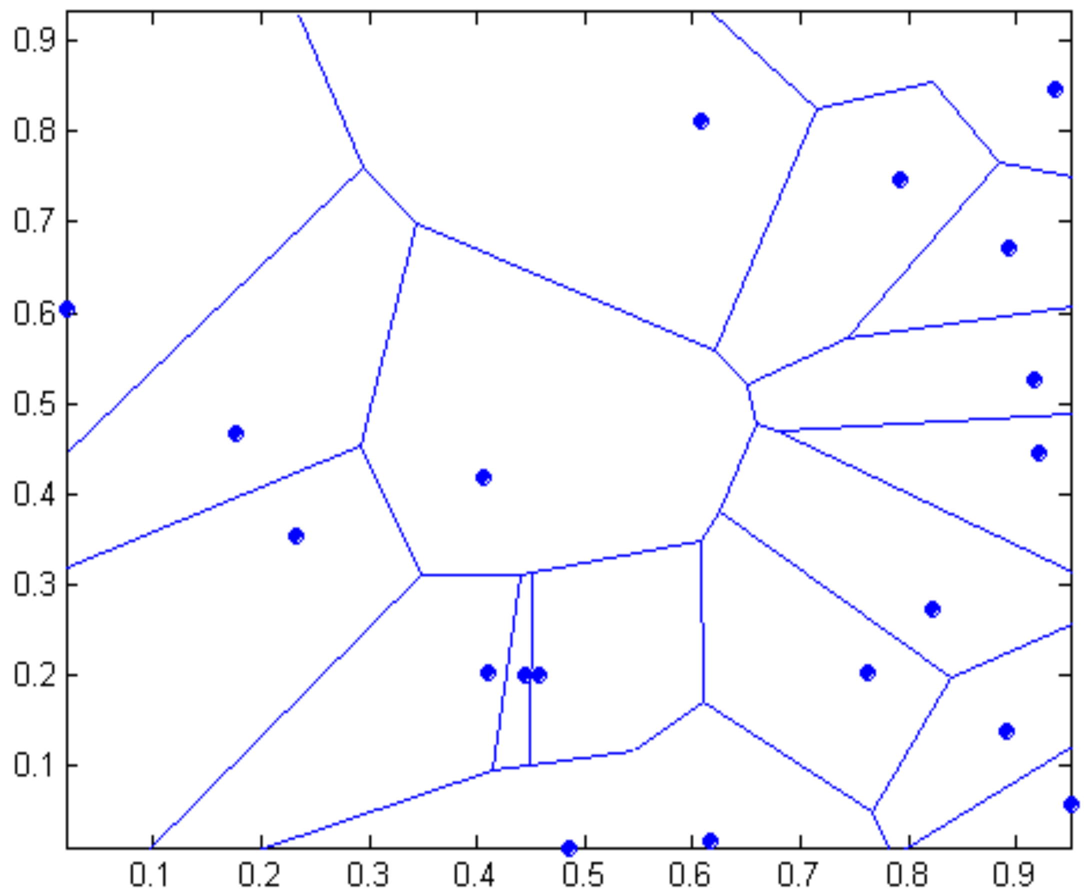


(a) 1-nearest neighbor　　(b) 2-nearest neighbor　　(c) 3-nearest neighbor

K-nearest neighbors of a record x are data points that have the k smallest distance to x

1 nearest-neighbor

Voronoi Diagram



Nearest Neighbor Classification

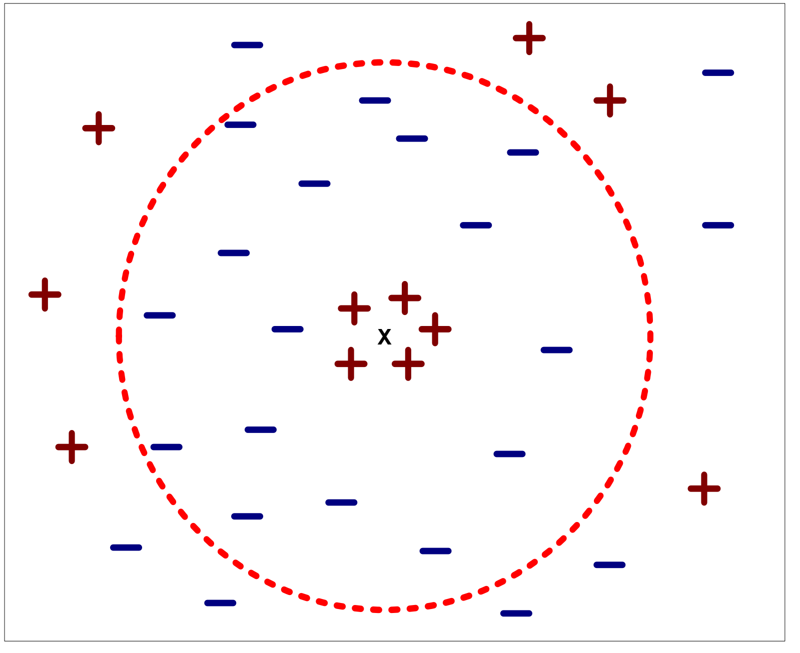
- Compute distance between two points:
  - Euclidean distance

$$d(p,q) = \sqrt{\sum_i (p_i - q_i)^2}$$

- Determine the class from nearest neighbor list
  - take the majority vote of class labels among the k-nearest neighbors
  - Weigh the vote according to distance
    - weight factor, $w = 1/d^2$

Nearest Neighbor Classification…

- Choosing the value of k:
  - If k is too small, sensitive to noise points
  - If k is too large, neighborhood may include points from other classes



Nearest neighbor Classification…

- k-NN classifiers are lazy learners
  - It does not build models explicitly
  - Unlike eager learners such as decision tree induction.
  - Classifying unknown records are relatively expensive

What is Data ?

Tid	**Refund**	**Marital Status**	**Taxable Income**	**Cheat**
1	Yes	Single	125K	**No**
2	No	Married	100K	**No**
3	No	Single	70K	**No**
4	Yes	Married	120K	**No**
5	No	Divorced	95K	**Yes**
6	No	Married	60K	**No**
7	Yes	Divorced	220K	**No**
8	No	Single	85K	**Yes**
9	No	Married	75K	**No**
10	No	Single	90K	**Yes**

What is Data?

- Information that can be easily processed.
- Collection of data objects and their attributes
- An attribute is a property or characteristic of an object
  - Examples: eye color of a person, temperature, etc.
  - Attribute is also known as variable, field, characteristic, or feature
- A collection of attributes describe an object
  - Object is also known as record, point, case, sample, entity, or instance

Attributes

Objects

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Types of Attributes

- There are different types of attributes
  - Nominal
    - Examples: ID numbers, eye color, zip codes
  - Ordinal
    - Examples: rankings (e.g., taste of potato chips on a scale from 1-10), grades, height in {tall, medium, short}
  - Interval
    - Examples: calendar dates, temperatures in Celsius or Fahrenheit.
  - Ratio
    - Examples: temperature in Kelvin, length, time, counts

Properties of Attribute Values

- The type of an attribute depends on which of the following properties it possesses:
  - Distinctness: $=$ $\neq$
  - Order: $<$ $>$
  - Addition: $+$ $-$
  - Multiplication: $*$ $/$

Nominal attribute: distinctness
Ordinal attribute: ?
Interval attribute: ?
Ratio attribute: all 4 properties

Attribute Type	Description	Examples	Operations
Nominal	The values of a nominal attribute are just different names, i.e., nominal attributes provide only enough information to distinguish one object from another. (=, ≠)	zip codes, employee ID numbers, eye color, sex: {*male, female*}	mode, entropy, contingency correlation, χ^2 test
Ordinal	The values of an ordinal attribute provide enough information to order objects. (<, >)	hardness of minerals, {*good, better, best*}, grades, street numbers	median, percentiles, rank correlation, run tests, sign tests
Interval	For interval attributes, the differences between values are meaningful, i.e., a unit of measurement exists. (+, -)	calendar dates, temperature in Celsius or Fahrenheit	mean, standard deviation, Pearson's correlation, *t* and *F* tests
Ratio	For ratio variables, both differences and ratios are meaningful. (*, /)	temperature in Kelvin, monetary quantities, counts, age, mass, length, electrical current	geometric mean, harmonic mean, percent variation

Attribute Level	Transformation	Comments
Nominal	Any permutation of values	If all employee ID numbers were reassigned, would it make any difference?
Ordinal	An order preserving change of values, i.e., *new_value = f(old_value)* where *f* is a monotonic function.	An attribute encompassing the notion of good, better best can be represented equally well by the values {1, 2, 3} or by { 0.5, 1, 10}.
Interval	*new_value =a * old_value + b* where a and b are constants	Thus, the Fahrenheit and Celsius temperature scales differ in terms of where their zero value is and the size of a unit (degree).
Ratio	*new_value = a * old_value*	Length can be measured in meters or feet.

Discrete and Continuous Attributes

- Discrete Attribute
  - Has only a finite or countably infinite set of values
  - Examples: zip codes, counts, or the set of words in a collection of documents
  - Often represented as integer variables.
  - Note: binary attributes are a special case of discrete attributes

- Continuous Attribute
  - Has real numbers as attribute values
  - Examples: temperature, height, or weight.
  - Practically, real values can only be measured and represented using a finite number of digits.
  - Continuous attributes are typically represented as floating-point variables.

Record Data

- Data that consists of a collection of records, each of which consists of a fixed set of attributes

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
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Data Matrix

- If data objects have the same fixed set of numeric attributes, then the data objects can be thought of as points in a multi-dimensional space, where each dimension represents a distinct attribute
- Such data set can be represented by an m by n matrix, where there are m rows, one for each object, and n columns, one for each attribute

Projection of x Load	Projection of y load	Distance	Load	Thickness
10.23	5.27	15.22	2.7	1.2
12.65	6.25	16.22	2.2	1.1

How would you represent

- Document Data

Document Data

- Each document becomes a `term' vector,
  - each term is a component (attribute) of the vector,
  - the value of each component is the number of times the corresponding term occurs in the document.

	team	coach	pla y	ball	score	game	wi n	lost	timeout	season
Document 1	3	0	5	0	2	6	0	2	0	2
Document 2	0	7	0	2	1	0	0	3	0	0
Document 3	0	1	0	0	1	2	2	0	3	0

Transaction Data

- A special type of record data, where
  - each record (transaction) involves a set of items.
  - For example, consider a grocery store. The set of products purchased by a customer during one shopping trip constitute a transaction, while the individual products that were purchased are the items.

TID	*Items*
1	**Bread, Coke, Milk**
2	**Beer, Bread**
3	**Beer, Coke, Diaper, Milk**
4	**Beer, Bread, Diaper, Milk**
5	**Coke, Diaper, Milk**

Graph Data

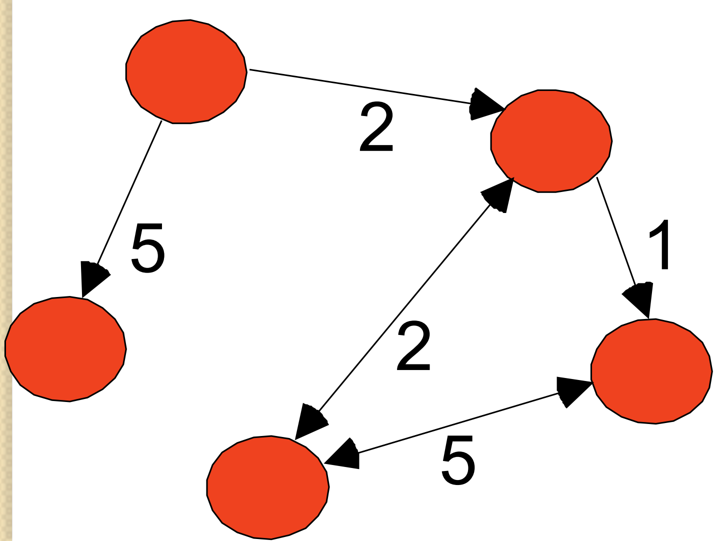
- Examples: Generic graph and HTML Links

Data Mining

Graph Partitioning

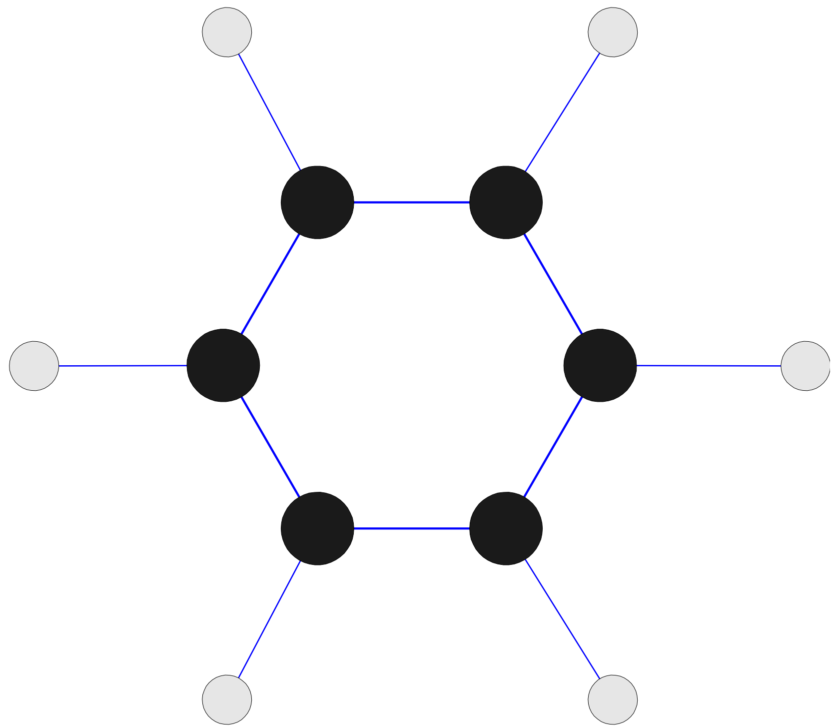
Parallel Solution of Sparse Linear System of Equations

<a href="papers/papers.html#ffff">
N-Body Computation and Dense Linear System Solvers



Chemical Data

- Benzene Molecule: C_6H_6



Ordered Data

- Sequences of transactions

Items/Events

(A B) (D) (C E)
(B D) (C) (E)
(C D) (B) (A E)

An element of the sequence

Ordered Data

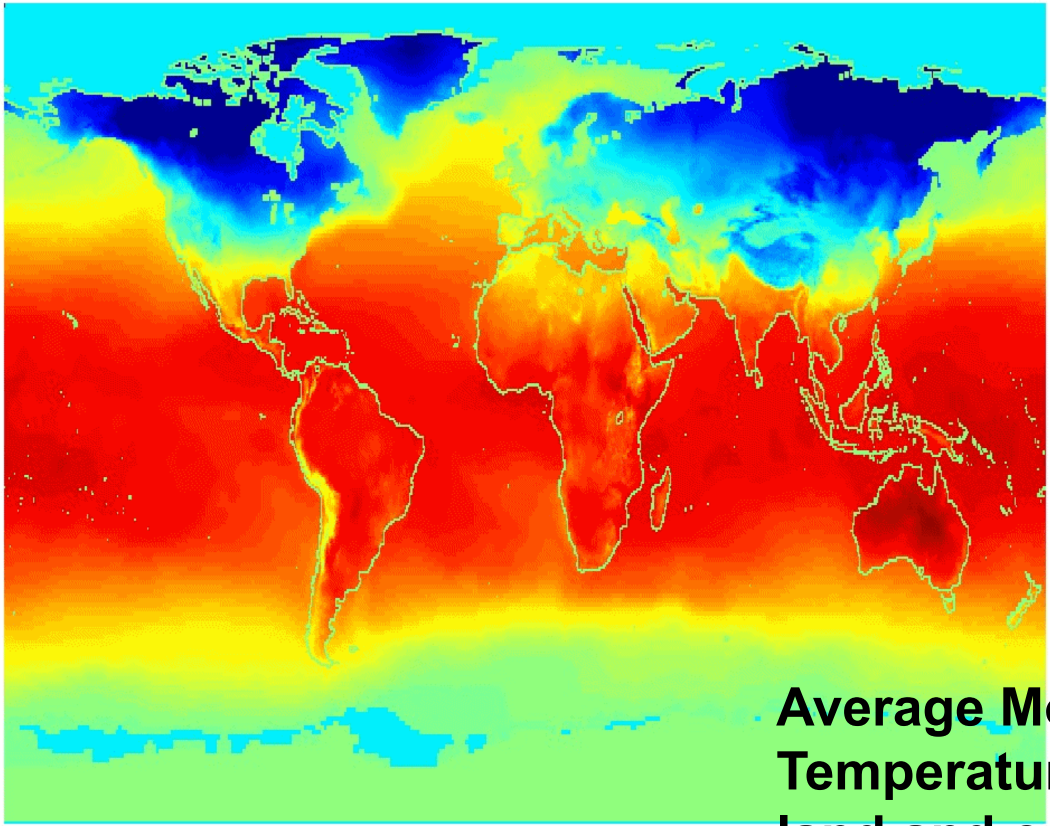
- Genomic sequence data

```
GGTTCCGCCTTCAGCCCCGCGCC
CGCAGGGCCCGCCCCGCGCCGTC
GAGAAGGGCCCGCCTGGCGGGCG
GGGGGAGGCGGGGCCGCCCGAGC
CCAACCGAGTCCGACCAGGTGCC
CCCTCTGCTCGGCCTAGACCTGA
GCTCATTAGGCGGCAGCGGACAG
GCCAAGTAGAACACGCGAAGCGC
TGGGCTGCCTGCTGCGACCAGGG
```

Ordered Data

- Spatio-Temporal Data

Jan



Average Monthly Temperature of land and ocean

What is Similarity?

The quality or state of being similar; likeness; resemblance; as, a similarity of features. **Webster's Dictionary**

Similarity is hard to define, but…
“*We know it when we see it*”

The real meaning of similarity is a philosophical question.

We will take a more pragmatic approach.

Similarity and Dissimilarity

- Similarity
  - Numerical measure of how alike two data objects are.
  - Is higher when objects are more alike.
  - Often falls in the range [0,1]
- Dissimilarity
  - Numerical measure of how different are two data objects
  - Lower when objects are more alike
  - Minimum dissimilarity is often 0
  - Upper limit varies
- Proximity refers to a similarity or dissimilarity

Similarity/Dissimilarity for Simple Attributes

p and *q* are the attribute values for two data objects.

Attribute Type	Dissimilarity	Similarity
Nominal	$d = \begin{cases} 0 & \text{if } p = q \\ 1 & \text{if } p \neq q \end{cases}$	$s = \begin{cases} 1 & \text{if } p = q \\ 0 & \text{if } p \neq q \end{cases}$
Ordinal	$d = \frac{\lvert p-q \rvert}{n-1}$ (values mapped to integers 0 to $n-1$, where n is the number of values)	$s = 1 - \frac{\lvert p-q \rvert}{n-1}$
Interval or Ratio	$d = \lvert p - q \rvert$	$s = -d$, $s = \frac{1}{1+d}$ or $s = 1 - \frac{d - min\_d}{max\_d - min\_d}$

Table 5.1. Similarity and dissimilarity for simple attributes

Defining Distance Measures

Definition: Let O_1 and O_2 be two objects from the universe of possible objects. The distance (dissimilarity) is denoted by $D(O_1,O_2)$

What properties should a distance measure have?

- $D(A,B) = D(B,A)$ *Symmetry*
- $D(A,A) = 0$ *Constancy of Self-Similarity*
- $D(A,B) = 0$ IIf $A= B$ *Positivity*
- $D(A,B) \leq D(A,C) + D(B,C)$ *Triangular Inequality*

When the last one holds, we call the measure a metric

Euclidean Distance

- Euclidean Distance

$$dist = \sqrt{\sum_{k=1}^{n} (p_k - q_k)^2}$$

Where *n* is the number of dimensions (attributes) and p_k and q_k are, respectively, the kth attributes (components) or data objects *p* and *q*.

- Standardization is necessary, if scales differ.

Minkowski Distance

- Minkowski Distance is a generalization of Euclidean Distance

$$dist = \left(\sum_{k=1}^{n} | p_k - q_k |^r \right)^{\frac{1}{r}}$$

Where r is a parameter, n is the number of dimensions (attributes) and p_k and q_k are, respectively, the kth attributes (components) or data objects p and q.

Minkowski Distance: Examples

- $r = 1$. City block (Manhattan, taxicab, L1 norm) distance.
  - A common example of this is the Hamming distance, which is just the number of bits that are different between two binary vectors
- $r = 2$. Euclidean distance
- $r \to \infty$. "supremum" (Lmax norm, L_∞ norm) distance.
  - This is the maximum difference between any component of the vectors
- Do not confuse r with n, i.e., all these distances are defined for all numbers of dimensions.

Euclidean vs. City block geometry

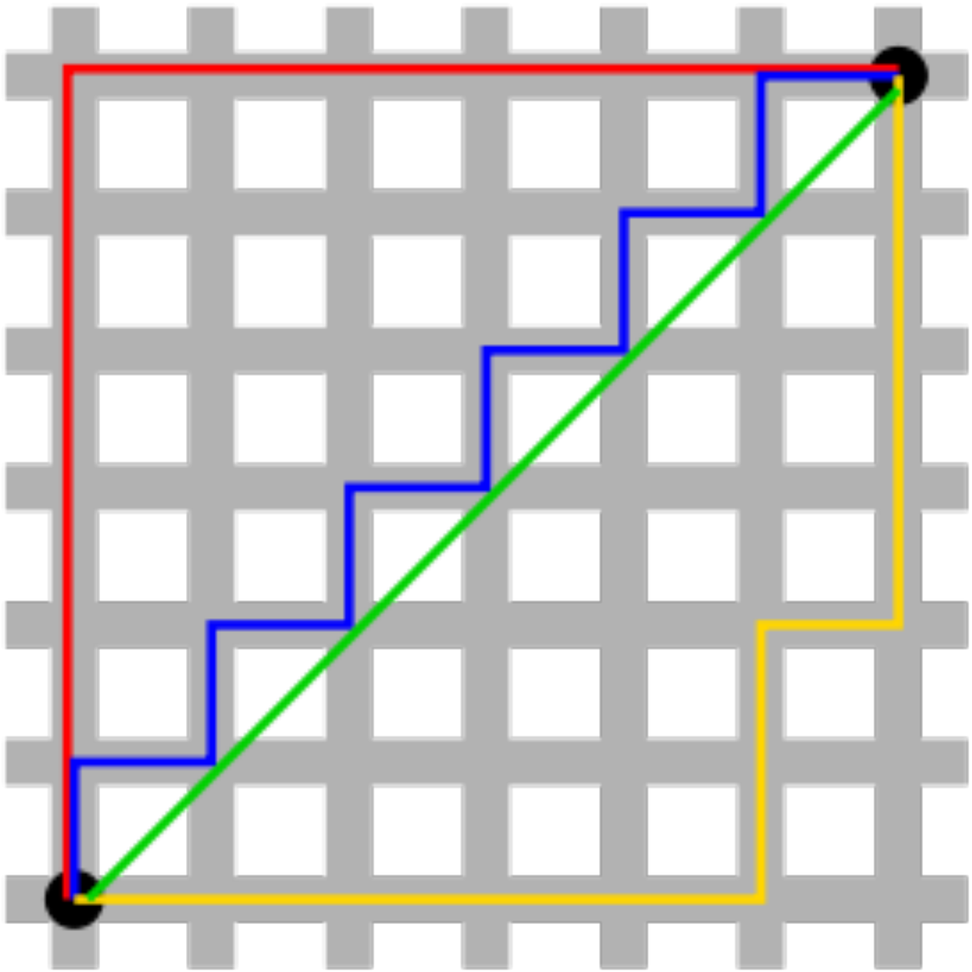
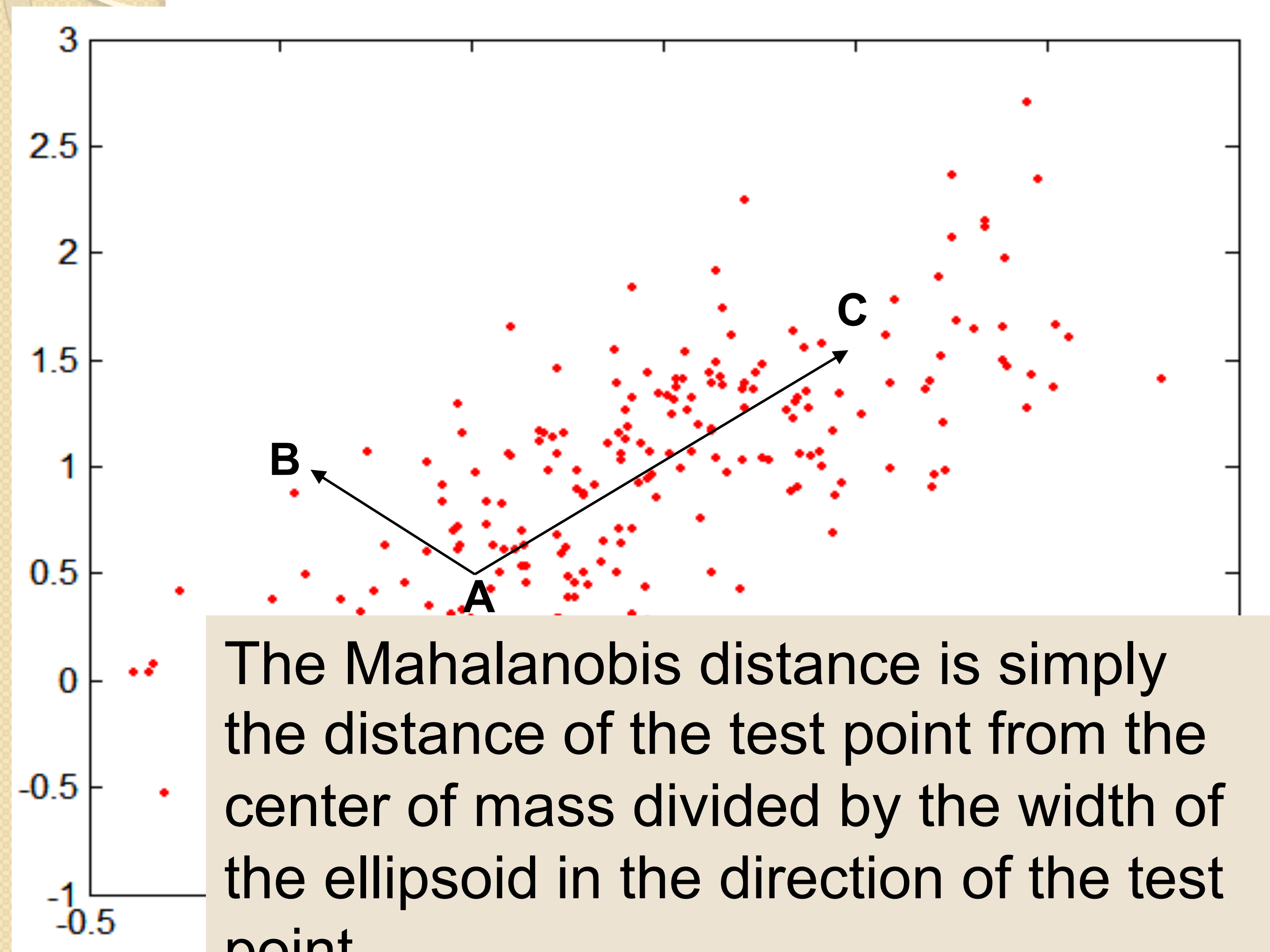


Figure taken from Wikipedia

Mahalanobis Distance



The Mahalanobis distance is simply the distance of the test point from the center of mass divided by the width of the ellipsoid in the direction of the test point.

Covariance Matrix:

$$\Sigma = \begin{bmatrix} 0.3 & 0.2 \\ 0.2 & 0.3 \end{bmatrix}$$

A: (0.5, 0.5)

B: (0, 1)

C: (1.5, 1.5)

Mahal(A,B) = 5

Mahal(A,C) = 4

Mahalanobis Distance!

$$\text{mahalanobis}(p,q) = (p-q)\sum^{-1}(p-q)^T$$

Σ is the covariance matrix of the input data *X*

$$\Sigma_{j,k} = \frac{1}{n-1}\sum_{i=1}^{n}(X_{ij}-\overline{X}_j)(X_{ik}-\overline{X}_k)$$

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{x}_i$$

2×2 covariance matrix:

$$E\left[(\boldsymbol{x}-\mu)(\boldsymbol{x}-\mu)^T\right] =$$

$$E\left[\begin{pmatrix} x_1-\mu_1 \\ x_2-\mu_2 \end{pmatrix}(x_1-\mu_1, x_2-\mu_2)\right] =$$

$$E\begin{bmatrix} (x_1-\mu_1)^2 & (x_1-\mu_1)(x_2-\mu_2) \\ (x_1-\mu_1)(x_2-\mu_2) & (x_2-\mu_2)^2 \end{bmatrix} =$$

$$\frac{1}{N-1}\sum_{i=1}^{N}\begin{bmatrix} (x_1^i-\mu_1)^2 & (x_1^i-\mu_1)(x_2^i-\mu_2) \\ (x_1^i-\mu_1)(x_2^i-\mu_2) & (x_2^i-\mu_2)^2 \end{bmatrix}$$

$$\frac{1}{N-1}\sum_{i=1}^{N}\begin{bmatrix}\left(x_1^i-\mu_1\right)^2 & \left(x_1^i-\mu_1\right)\left(x_2^i-\mu_2\right)\\ \left(x_1^i-\mu_1\right)\left(x_2^i-\mu_2\right) & \left(x_2^i-\mu_2\right)^2\end{bmatrix}=$$

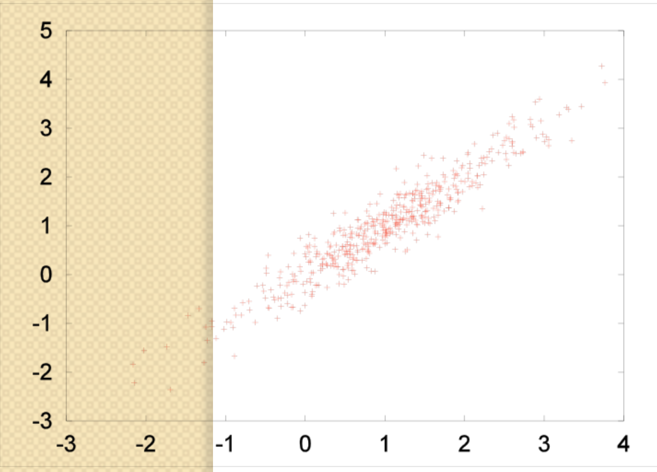
variance

covariance

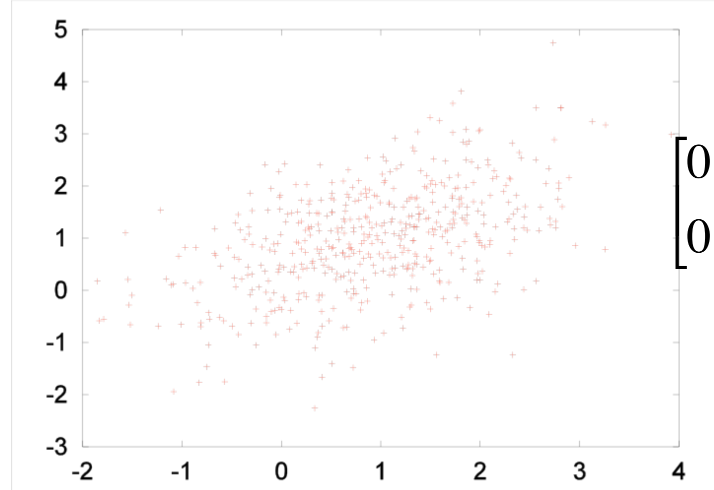
$$\begin{bmatrix}\frac{1}{N-1}\sum_{i=1}^{N}\left(x_1^i-\mu_1\right)^2 & \frac{1}{N-1}\sum_{i=1}^{N}\left[\left(x_1^i-\mu_1\right)\left(x_2^i-\mu_2\right)\right]\\ \frac{1}{N-1}\sum_{i=1}^{N}\left[\left(x_1^i-\mu_1\right)\left(x_2^i-\mu_2\right)\right] & \frac{1}{N-1}\sum_{i=1}^{N}\left(x_2^i-\mu_2\right)^2\end{bmatrix}$$

covariance

variance

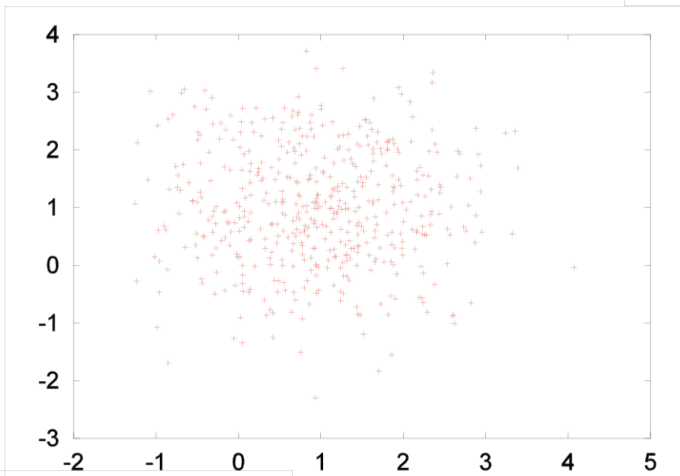


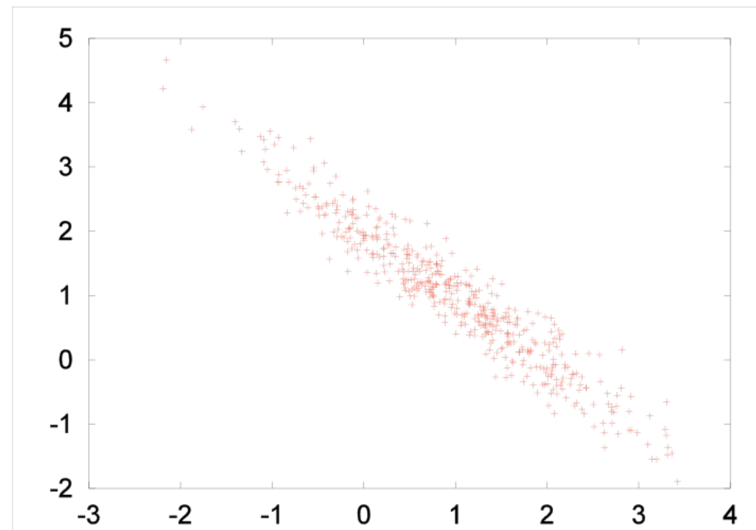
$$\begin{bmatrix} 0.94 & 0.93 \\ 0.93 & 1.03 \end{bmatrix}$$

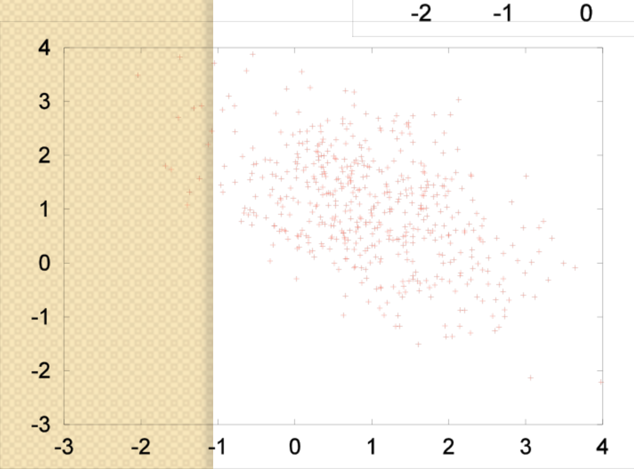


$$\begin{bmatrix} 0.97 & 0.49 \\ 0.49 & 1.04 \end{bmatrix}$$

$$\begin{bmatrix} 0.93 & 0.01 \\ 0.01 & 1.05 \end{bmatrix}$$







$$\begin{bmatrix} 0.99 & -0.5 \\ -0.5 & 1.06 \end{bmatrix}$$

$$\begin{bmatrix} 1.04 & -1.05 \\ -1.05 & 1.15 \end{bmatrix}$$

Common Properties of a Similarity

- Similarities, also have some well known properties.

  - $s(p, q) = 1$ (or maximum similarity) only if $p = q$.

  - $s(p, q) = s(q, p)$ for all p and q. (Symmetry)

- where $s(p, q)$ is the similarity between points (data objects), p and q.

Similarity Between Binary Vectors

- Common situation is that objects, *p* and *q*, have only binary attributes
- Compute similarities using the following quantities

  M_{01} = the number of attributes where p was 0 and q was 1
  M_{10} = the number of attributes where p was 1 and q was 0
  M_{00} = the number of attributes where p was 0 and q was 0
  M_{11} = the number of attributes where p was 1 and q was 1
- Simple Matching and Jaccard Coefficients

  SMC = number of matches / number of attributes
  $= (M_{11} + M_{00}) / (M_{01} + M_{10} + M_{11} + M_{00})$

  J = number of 11 matches / number of not-both-zero attributes values
  $= (M_{11}) / (M_{01} + M_{10} + M_{11})$

SMC versus Jaccard: Example

p = 1 0 0 0 0 0 0 0 0 0
q = 0 0 0 0 0 0 1 0 0 1

$M_{01} = 2$ (the number of attributes where p was 0 and q was 1)
$M_{10} = 1$ (the number of attributes where p was 1 and q was 0)
$M_{00} = 7$ (the number of attributes where p was 0 and q was 0)
$M_{11} = 0$ (the number of attributes where p was 1 and q was 1)

$SMC = (M_{11} + M_{00})/(M_{01} + M_{10} + M_{11} + M_{00}) = (0+7) / (2+1+0+7) = 0.7$

$J = (M_{11}) / (M_{01} + M_{10} + M_{11}) = 0 / (2 + 1 + 0) = 0$

Cosine Similarity

- If d_1 and d_2 are two document vectors, then

  $$\cos(d_1, d_2) = (d_1 \bullet d_2) / ||d_1||\ ||d_2||,$$

  where $\bullet$ indicates vector dot product and $|| d ||$ is the length of vector d.

- Example:

  $$d_1 = \mathbf{3\ 2\ 0\ 5\ 0\ 0\ 0\ 2\ 0\ 0}$$
  $$d_2 = \mathbf{1\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 2}$$

  $d_1 \bullet d_2 = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$

  $||d_1|| = (3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{0.5} = (42)^{0.5} = 6.481$

  $||d_2|| = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{0.5} = (6)^{0.5} = 2.245$

  $$\cos(d_1, d_2) = .3150$$

Correlation

Correlation measures the linear relationship between objects

$$corr(x, y) = \frac{\text{Covariance}(x, y)}{\text{standard\_dev(x)*standard\_dev(y)}}$$

$$= \frac{S_{xy}}{S_x S_y}$$

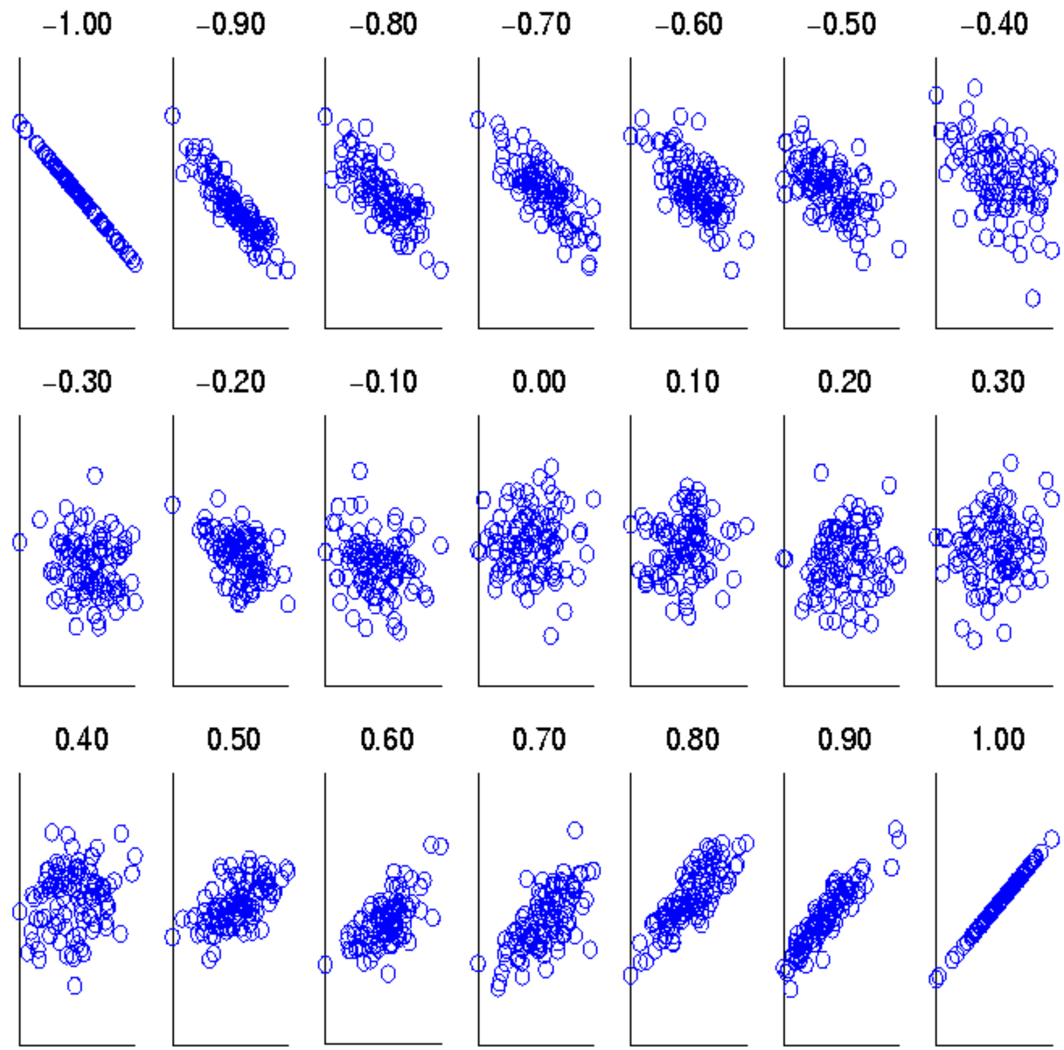
Correlation (cont.)

$$\text{covariance(x,y)}=\frac{1}{n-1}\sum_{k=1}^{n}(x_k-\overline{x})(y_k-\overline{y})$$

$$\text{standard\_dev(x)}=\mathrm{S_x}=\sqrt{\frac{1}{n-1}\sum_{k=1}^{n}(x_k-\overline{x})^2}$$

$$\text{standard\_dev(y)}=\mathrm{S_y}=\sqrt{\frac{1}{n-1}\sum_{k=1}^{n}(y_k-\overline{y})^2}$$

Visually Evaluating Correlation



General Approach for Combining Similarities

- Sometimes attributes are of many different types, but an overall similarity is needed.

1. For the k^{th} attribute, compute a similarity, s_k, in the range $[0, 1]$.
2. Define an indicator variable, δ_k, for the k_{th} attribute as follows:

$$\delta_k = \begin{cases} 0 & \text{if the } k^{th} \text{ attribute is a binary asymmetric attribute and both objects have} \\ & \text{a value of 0, or if one of the objects has a missing values for the } k^{th} \text{ attribute} \\ 1 & \text{otherwise} \end{cases}$$

3. Compute the overall similarity between the two objects using the following formula:

$$similarity(p, q) = \frac{\sum_{k=1}^{n} \delta_k s_k}{\sum_{k=1}^{n} \delta_k}$$

Using Weights to Combine Similarities

- May not want to treat all attributes the same.
  - Use weights wk which are between 0 and 1 and sum to 1.

$$similarity(p,q) = \frac{\sum_{k=1}^{n} w_k \delta_k s_k}{\sum_{k=1}^{n} \delta_k}$$

$$distance(p,q) = \left(\sum_{k=1}^{n} w_k |p_k - q_k|^r \right)^{1/r}$$

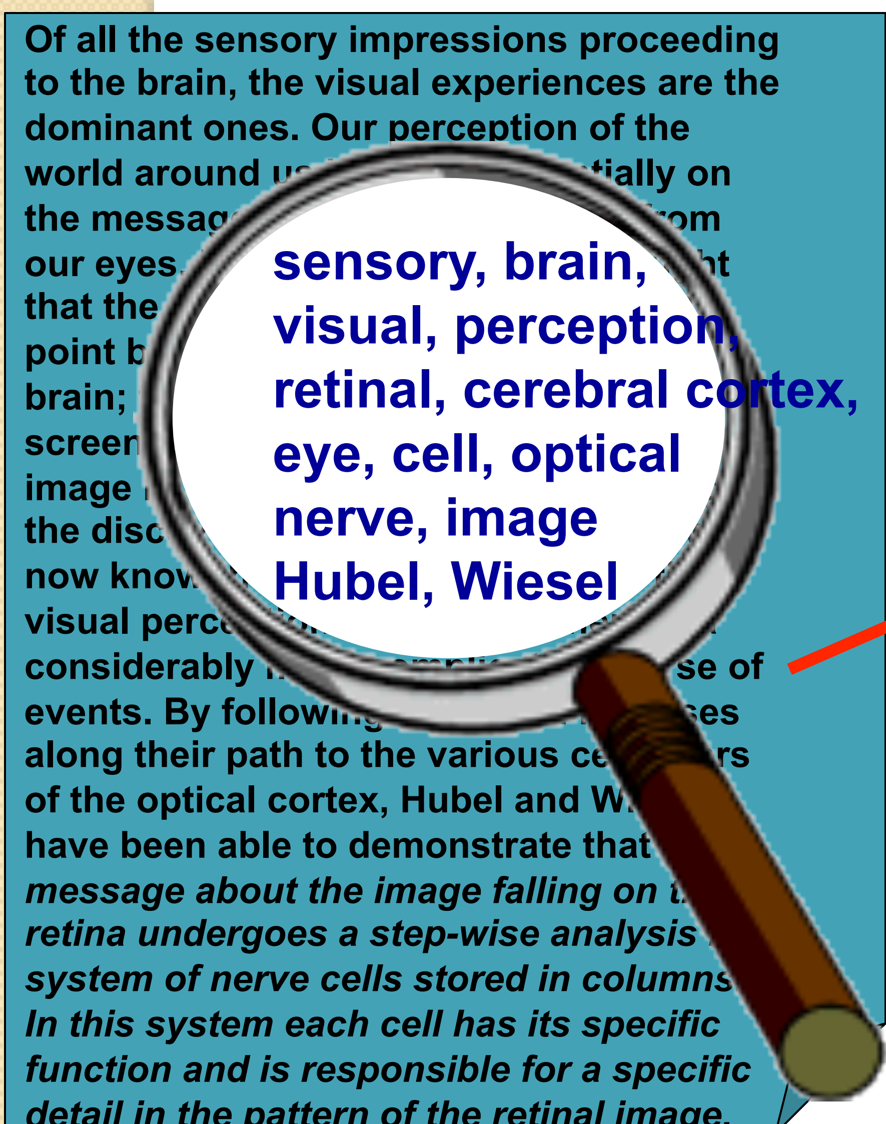
Which similarity function to use ?

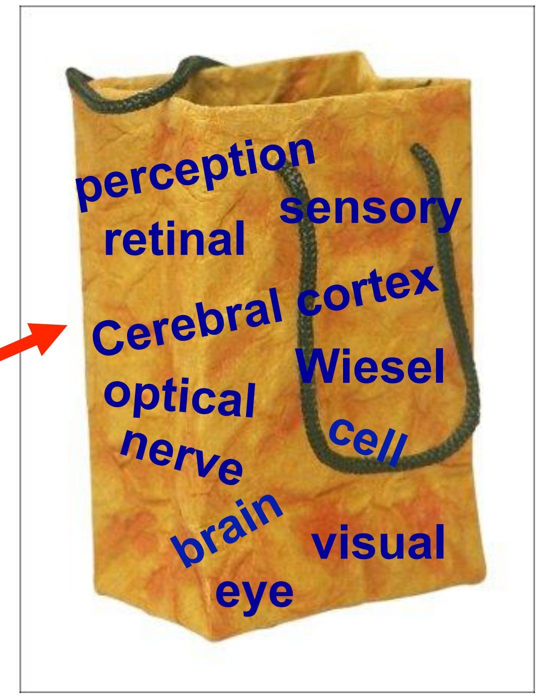
- Depends on the application.
  - Analyze the attributes.
  - See their properties, min, max, etc
  - See their dependency on other attributes
  - Do you need similarity or distance ?
  - Do you need a metric ?
  - Try several functions.
  - Combine/merge.
- Active area of research!

Curse of Dimensionality

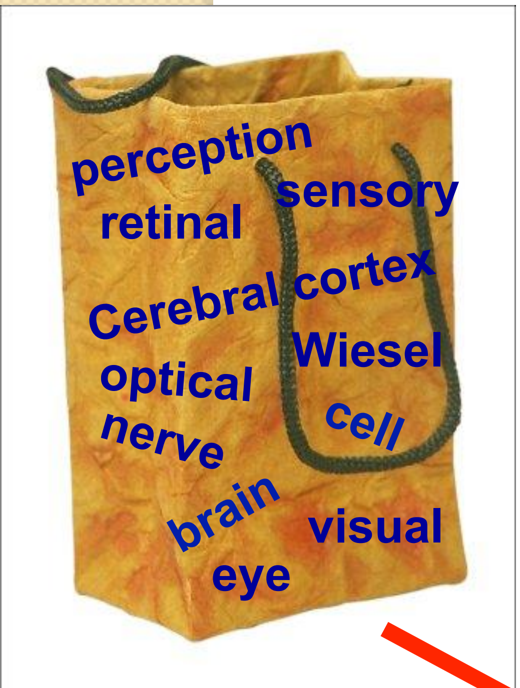
- Many problems of interest have objects with a large number of dimensions.
- An example…

Document Classification





Bag-of-words representation of a document



Of all the sensory impressions proceeding to
Of all the sensory impressions proceeding to the brain, the visual experiences are the
Of all the sensory impressions proceeding to

Of all the sensory impressions proceeding to the brain, the visual experiences are the dominant ones. Our perception of the world around us is based essentially on the messages that reach the brain from our eyes. For a long time it was thought that the retinal image was transmitted point by point to visual centers in the brain; the cerebral cortex was a movie screen, so to speak, upon which the image in the eye was projected. Through the discoveries of Hubel and Wiesel we

dictionary

w1	*w2*	....	*wq*

$$\boldsymbol{d} = \left(d_1, d_2, \cdots, d_q\right)$$

$$TF\left(w_2, \boldsymbol{d}\right)$$

Term Frequency

What's the size of the dictionary?

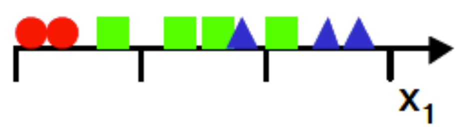
Curse of Dimensionality

- When dimensionality increases, data becomes increasingly sparse in the space that it occupies

- Also distances between objects gets skewed
  - More dimensions that contribute to the notion of distance or proximity which makes it uniform. This leads to trouble in clustering and classification settings.

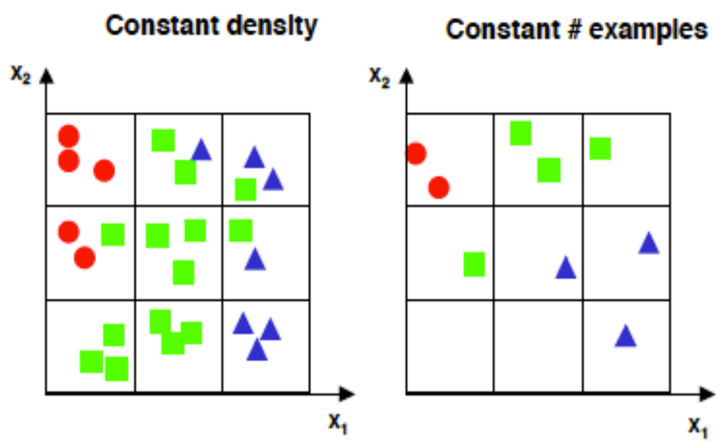
Driving the point ..

- **Consider a 3-class pattern recognition problem**
  - A simple approach would be to
    - Divide the feature space into uniform bins
    - Compute the ratio of examples for each class at each bin and,
    - For a new example, find its bin and choose the predominant class in that bin
  - In our toy problem we decide to start with one single feature and divide the real line into 3 segments

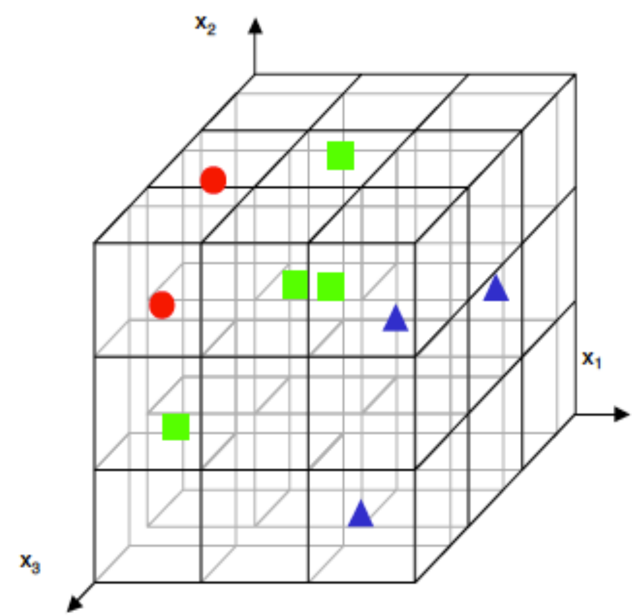


  - After we have done this, we notice that there exists too much overlap for the classes, so we decide to incorporate a second feature to try and improve the classification rate

- **We decide to preserve the granularity of each axis, which raises the number of bins from 3 (in 1D) to 3^2=9 (in 2D)**
  - At this point we are faced with a decision: do we maintain the density of examples per bin or do we keep the number of examples we used for the one-dimensional case?
    - Choosing to maintain the density increases the number of examples from 9 (in 1D) to 27 (in 2D)
    - Choosing to maintain the number of examples results in a 2D scatter plot that is very sparse

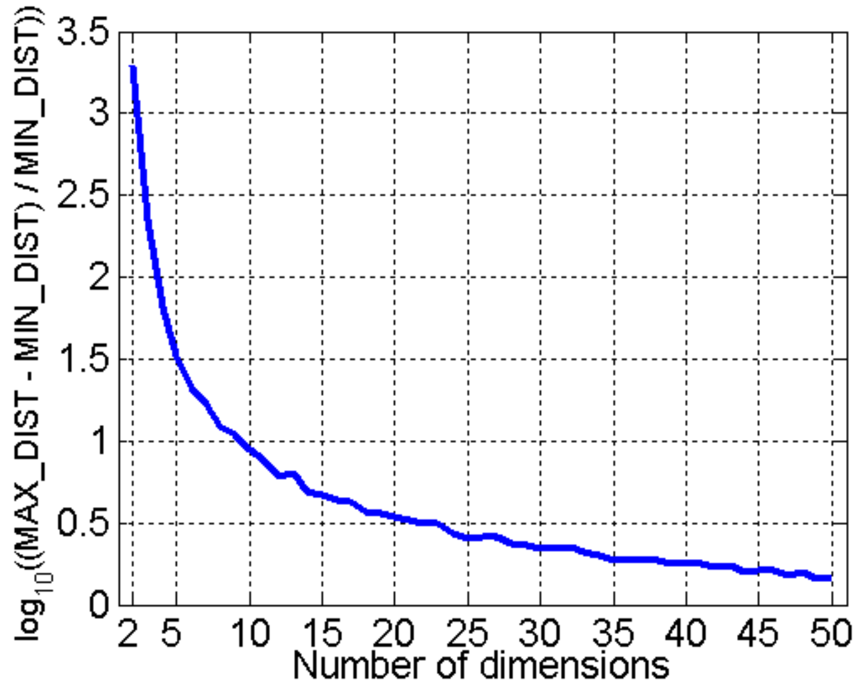


- **Moving to three features makes the problem worse:**
  - The number of bins grows to 3^3=27
  - For the same density of examples the number of needed examples becomes 81
  - For the same number of examples, well, the 3D scatter plot is almost empty



Curse of Dimensionality

- Definitions of density and distance between points, which is critical for clustering and outlier detection, become less meaningful



- **Randomly generate 500 points**
- **Compute difference between max and min distance between any pair of points**

Dimensionality Reduction

- Purpose:
  - Avoid curse of dimensionality
  - Reduce amount of time and memory required by data mining algorithms
  - Allow data to be more easily visualized
  - May help to eliminate irrelevant features or reduce noise
- Techniques
  - Principle Component Analysis
  - Singular Value Decomposition
  - Others: supervised and non-linear techniques

Nearest Neighbor Classification…

- Scaling issues
  - Attributes may have to be scaled to prevent distance measures from being dominated by one of the attributes
  - Example:
    - height of a person may vary from 1.5m to 1.8m
    - weight of a person may vary from 90lb to 300lb
    - income of a person may vary from $10K to $1M

Nearest Neighbor Classification…

- Problem with Euclidean measure:
  - High dimensional data
    - curse of dimensionality
  - Can produce counter-intuitive results

1 1 1 1 1 1 1 1 1 1 1 0	vs	1 0 0 0 0 0 0 0 0 0 0 0
0 1 1 1 1 1 1 1 1 1 1 1		0 0 0 0 0 0 0 0 0 0 0 1
d = 1.4142		d = 1.4142

- Solution: Normalize the vectors to unit length

Model Selection

Model Evaluation

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Model Comparison
  - How to compare the relative performance among competing models?

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Metrics for Performance Evaluation

- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

	PREDICTED CLASS		
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	a	b
	Class=No	c	d

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

Metrics for Performance Evaluation…

	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a (TP)	b (FN)
	Class=No	c (FP)	d (TN)

- Most widely-used metric:

$$\text{Accuracy} = \frac{a+d}{a+b+c+d} = \frac{TP+TN}{TP+TN+FP+FN}$$

Methods of Estimation

- Holdout
  - Reserve 2/3 for training and 1/3 for testing
- Random subsampling
  - Repeated holdout
- Cross validation
  - Partition data into k disjoint subsets
  - k-fold: train on k-1 partitions, test on the remaining one
  - Leave-one-out: k=n
- Stratified sampling
  - oversampling vs undersampling
- Bootstrap
  - Sampling with replacement

Limitation of Accuracy

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10

- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
  - Accuracy is misleading because model does not detect any class 1 example

Cost Matrix

	PREDICTED CLASS		
ACTUAL CLASS	C(i|j)	**Class=Yes**	**Class=No**
	Class=Yes	C(Yes|Yes)	C(No|Yes)
	Class=No	C(Yes|No)	C(No|No)

C(i|j): Cost of misclassifying class j example as class i

Computing Cost of Classification

Cost Matrix	PREDICTED CLASS		
ACTUAL CLASS	C(i|j)	+	-
	+	-1	100
	-	1	0

Model M_1	PREDICTED CLASS		
ACTUAL CLASS		+	-
	+	150	40
	-	60	250

Model M_2	PREDICTED CLASS		
ACTUAL CLASS		+	-
	+	250	45
	-	5	200

Accuracy = 80%

Cost = 3910

Accuracy = 90%

Cost = 4255

Cost vs Accuracy

Count	PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a	b
	Class=No	c	d

Cost	PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	p	q
	Class=No	q	p

Accuracy is proportional to cost if

1. C(Yes|No)=C(No|Yes) = q
2. C(Yes|Yes)=C(No|No) = p

$N = a + b + c + d$

$\text{Accuracy} = (a + d)/N$

$$\begin{aligned}\text{Cost} &= p\,(a + d) + q\,(b + c)\\ &= p\,(a + d) + q\,(N - a - d)\\ &= q\,N - (q - p)(a + d)\\ &= N\,[q - (q-p) \times \text{Accuracy}]\end{aligned}$$

Cost-Sensitive Measures

$$\text{Precision (p)} = \frac{a}{a+c}$$

$$\text{Recall (r)} = \frac{a}{a+b}$$

$$\text{F - measure (F)} = \frac{2rp}{r+p} = \frac{2a}{2a+b+c}$$

- Precision is biased towards C(Yes|Yes) & C(Yes|No)
- Recall is biased towards C(Yes|Yes) & C(No|Yes)
- F-measure is biased towards all except C(No|No)

$$\text{Weighted Accuracy} = \frac{w_1 a + w_4 d}{w_1 a + w_2 b + w_3 c + w_4 d}$$

Model Evaluation

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?

- Methods for Model Comparison
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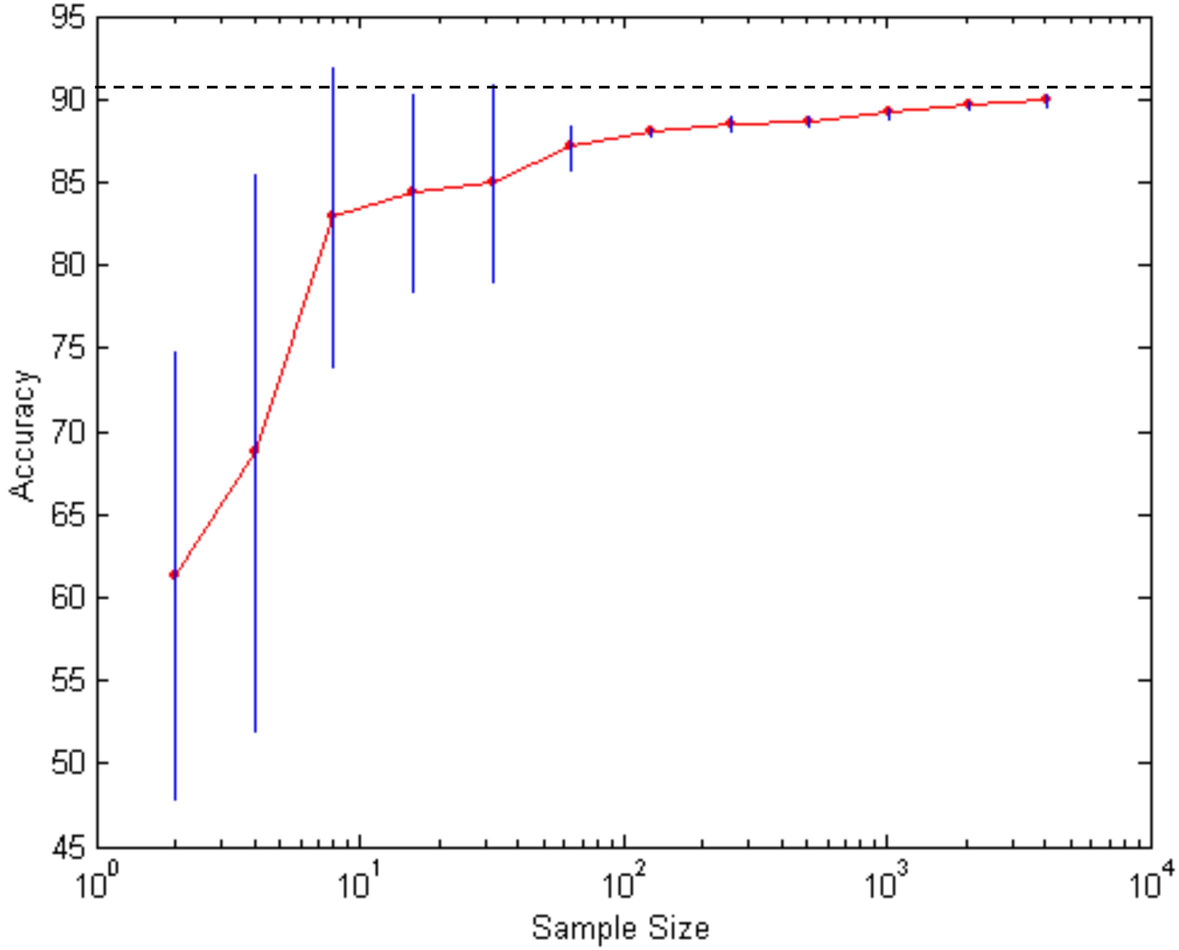
Methods for Performance Evaluation

- How to obtain a reliable estimate of performance?

- Performance of a model may depend on other factors besides the learning algorithm:
  - Class distribution
  - Cost of misclassification
  - Size of training and test sets

Learning Curve



- Learning curve shows how accuracy changes with varying sample size
- Requires a sampling schedule for creating learning curve:
  - Arithmetic sampling (Langley, et al)
  - Geometric sampling (Provost et al)

Effect of small sample size:

- Bias in the estimate
- Variance of estimate