UNIVERSITAT DE BARCELONA

Week 5

Course. Introduction to Machine Learning

Theory 5. Visualization

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Introduction to Machine Learning

Unsupervised Learning			Supervised Learning					Decision Learning Theory
Cluster Analysis	Factor Analysis	Visualization	Non Linear Decision				Linear Decision	Basic concepts of Decision Learning Theory
K-Means , EM	PCA, ICA	SOM, MDS	Lazy Learning (K-NN, IBL, CBR)	Overfitting, model selection and feature selection	Kernel Learning	Ensemble Learning (NN, Trees, Adaboost)	Perceptron, SVM	Bias/Variance, VC dimension, Practical advice of how to use learning algorithms

Contents

Introduction to Visualization

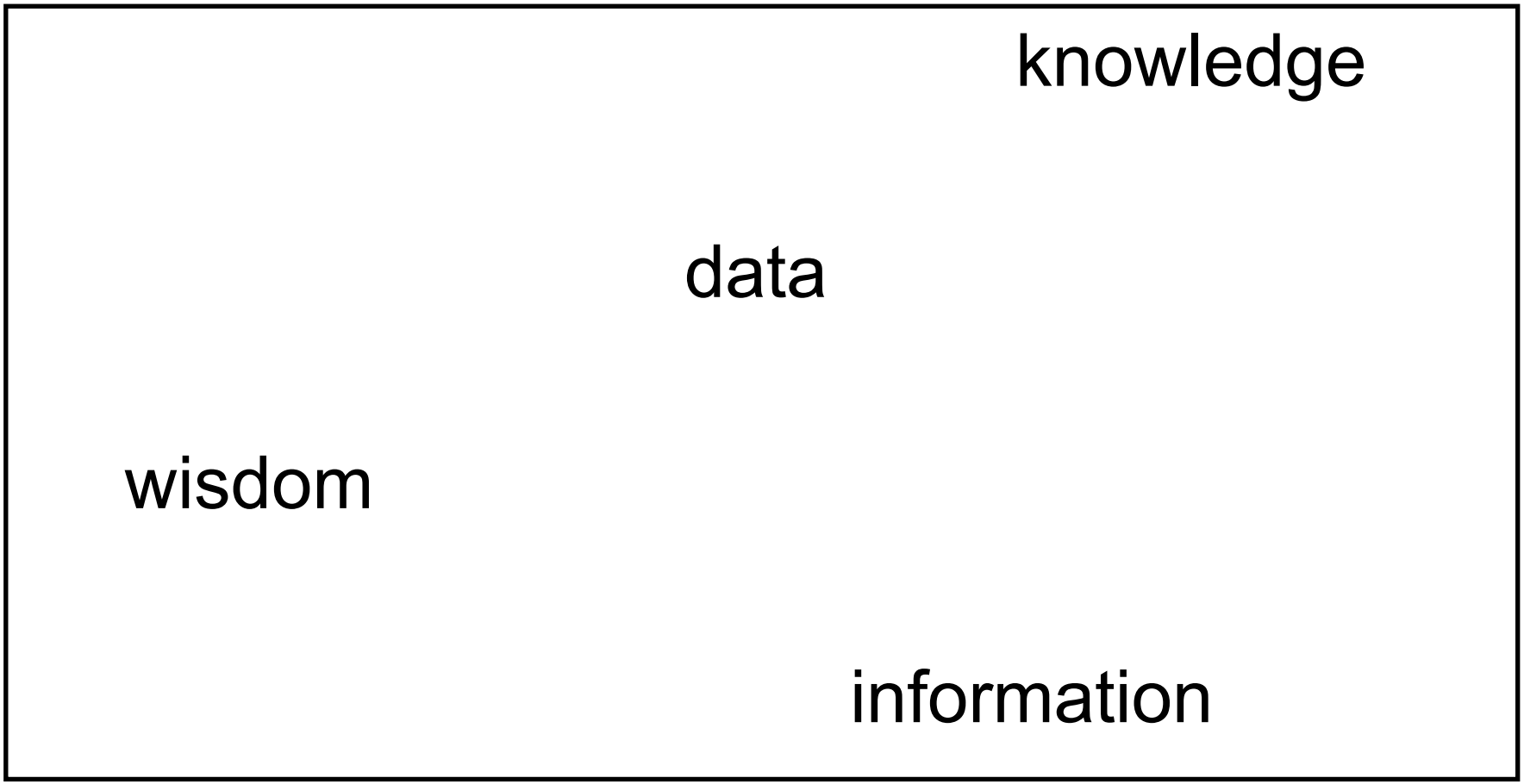
Introduction to visualization

- **Objective**: Visualizing low-dimensional views of high-dimensional data

- This lecture is mainly devoted to:
  - Self-Organizing Maps
  - Multi-Dimensional Scaling

Keywords

Consider the following ideas

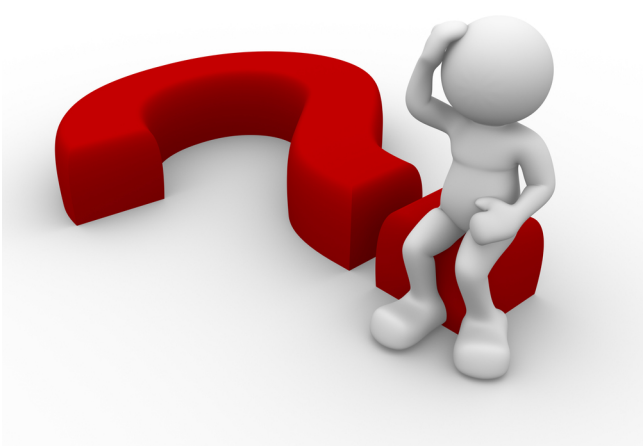


Graph comes from the book "Introduction to Data Visualization & Storytelling a Guide For the Data Scientist"

Exercise

- Now, order previous terms as logically as possible

_____ > _____ > _____ > _____



Take a moment to think about it

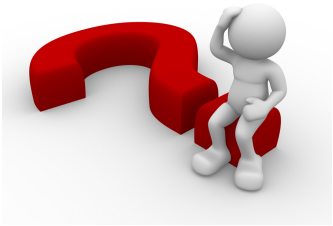
….

make a note that explain your decision

(You will have the answer in the online session)

Connect keywords

Connect each keyword with its corresponding image



data

information

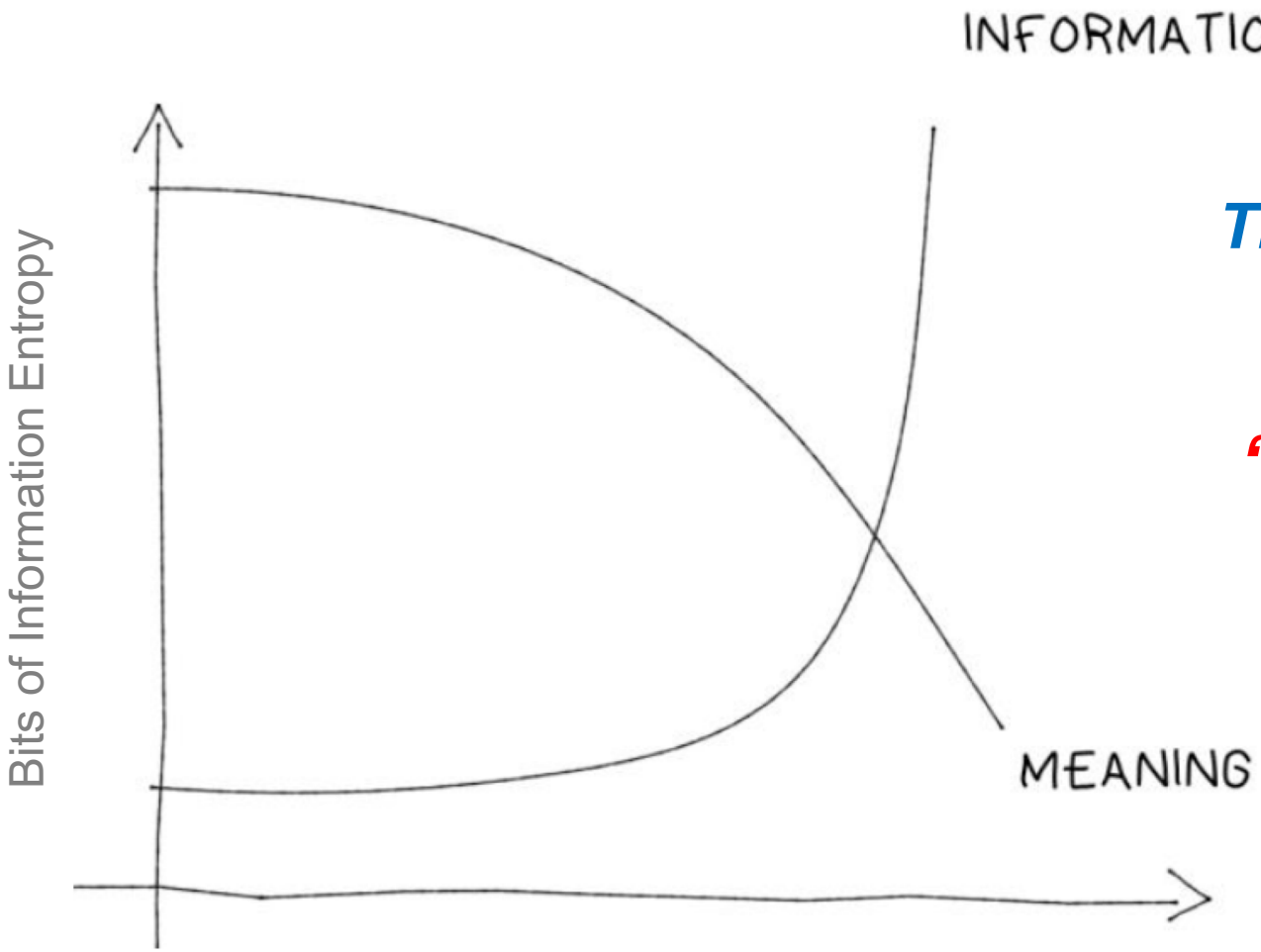
knowledge

wisdom

How is wisdom made?

*One way to arrive at wisdom is the **Synthesis** process*

Information vs Meaning



There is no peace in more

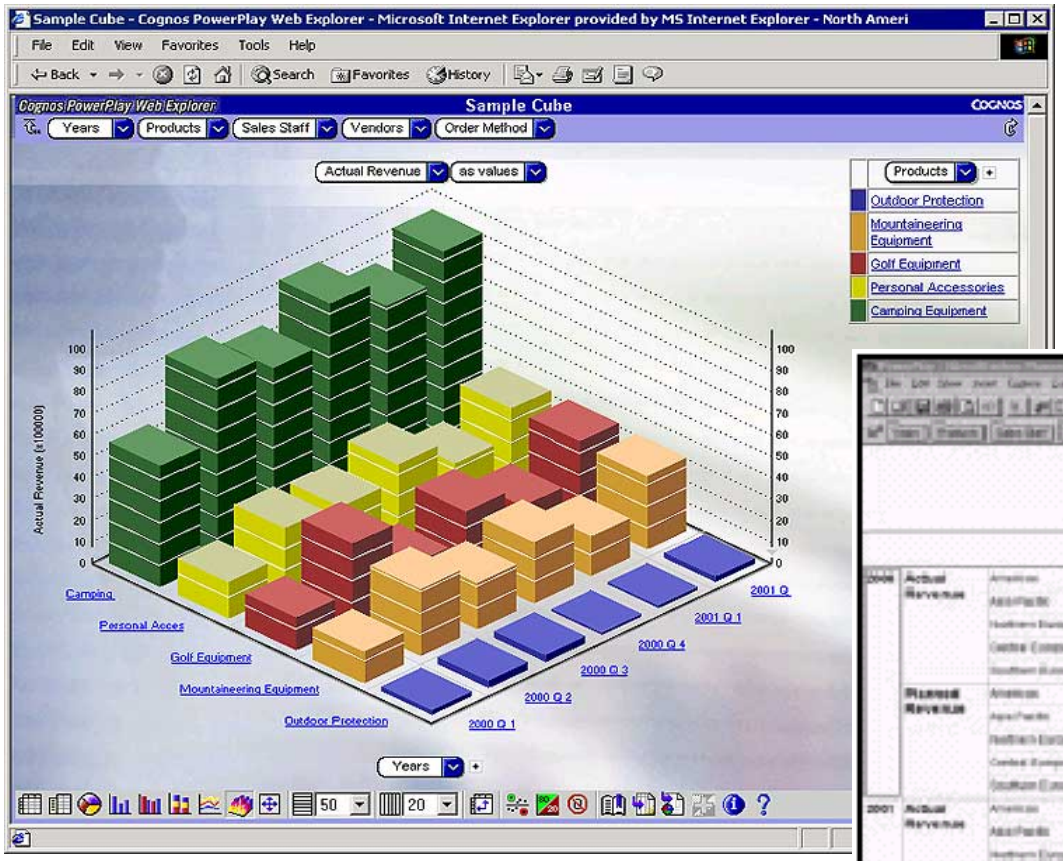
"Less (info) is more (meaning)"

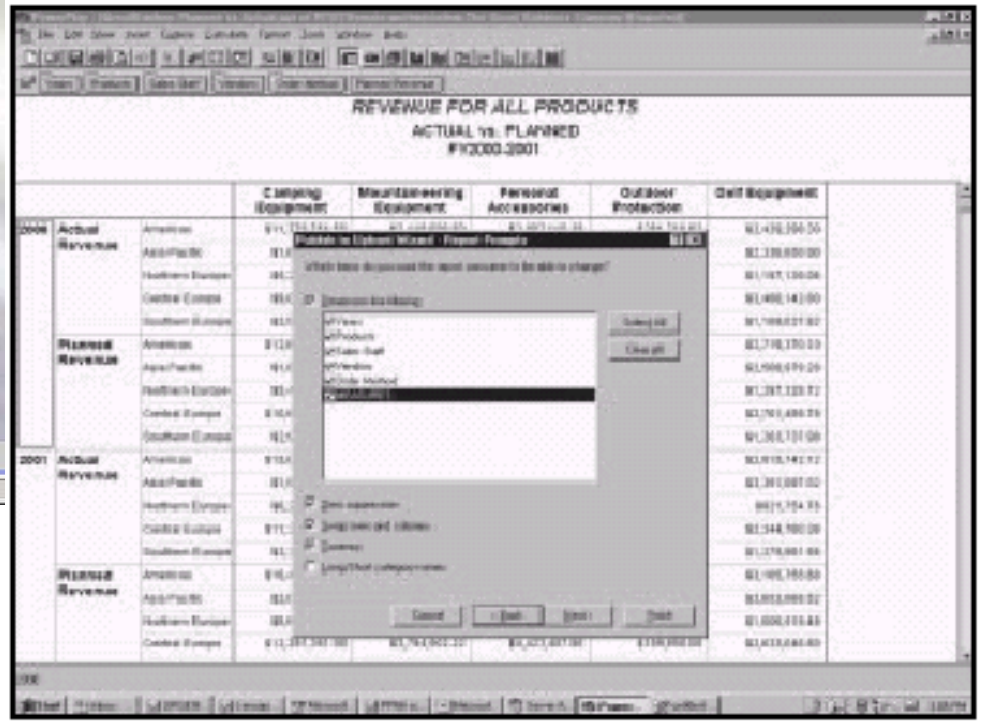
Visualization

VISUALIZATION is the study of the visual representation of the data

Main goal is to communicate the information clearly and effectively through graphical means

Data visualization vs model visualization

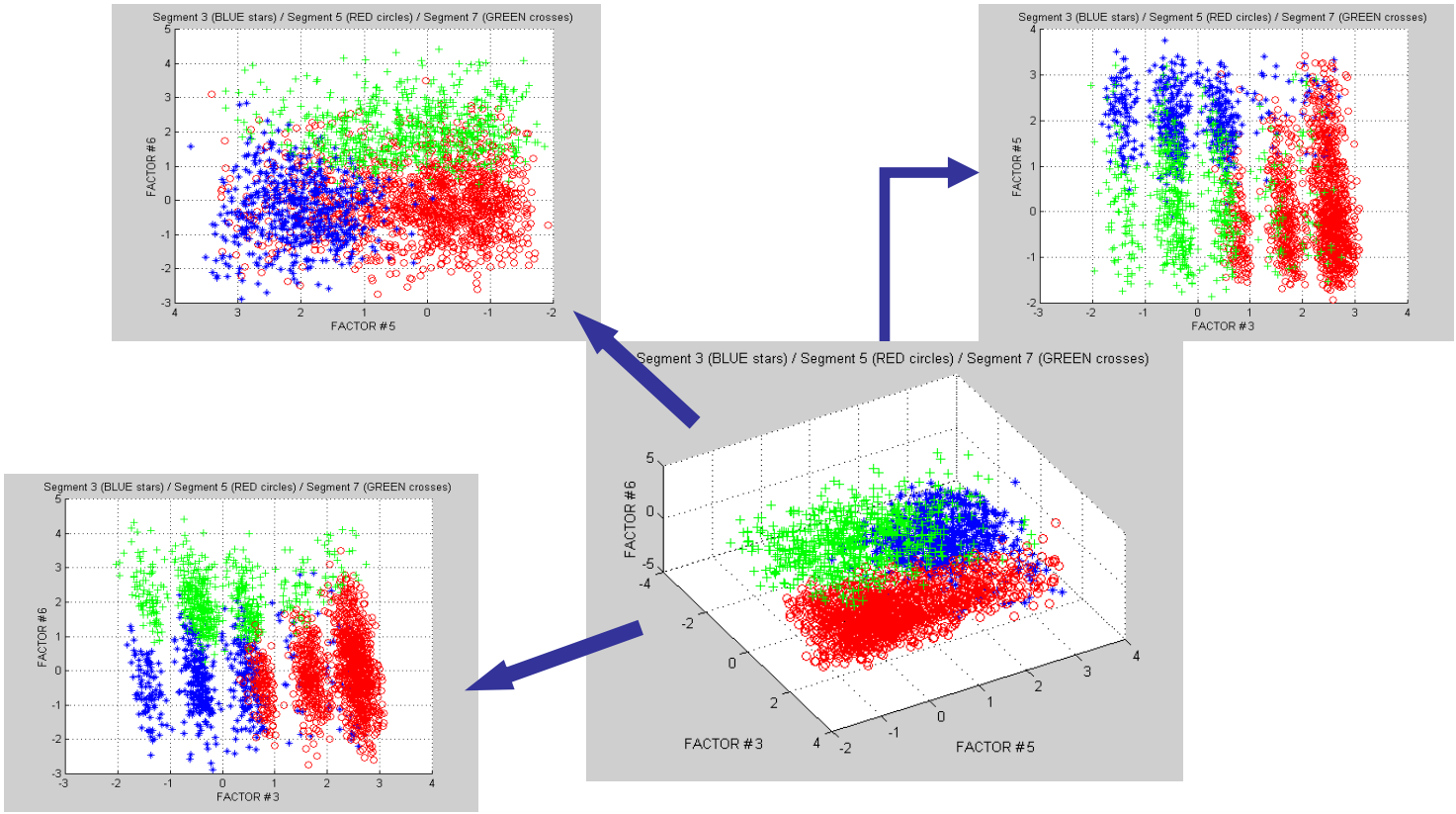




We can visualize the data using a tool, here an OLAP tool

Data visualization vs model visualization

*… or we can visualize a **model**. Here we visualize in 3D three factors of interest in a factor analysis solution*



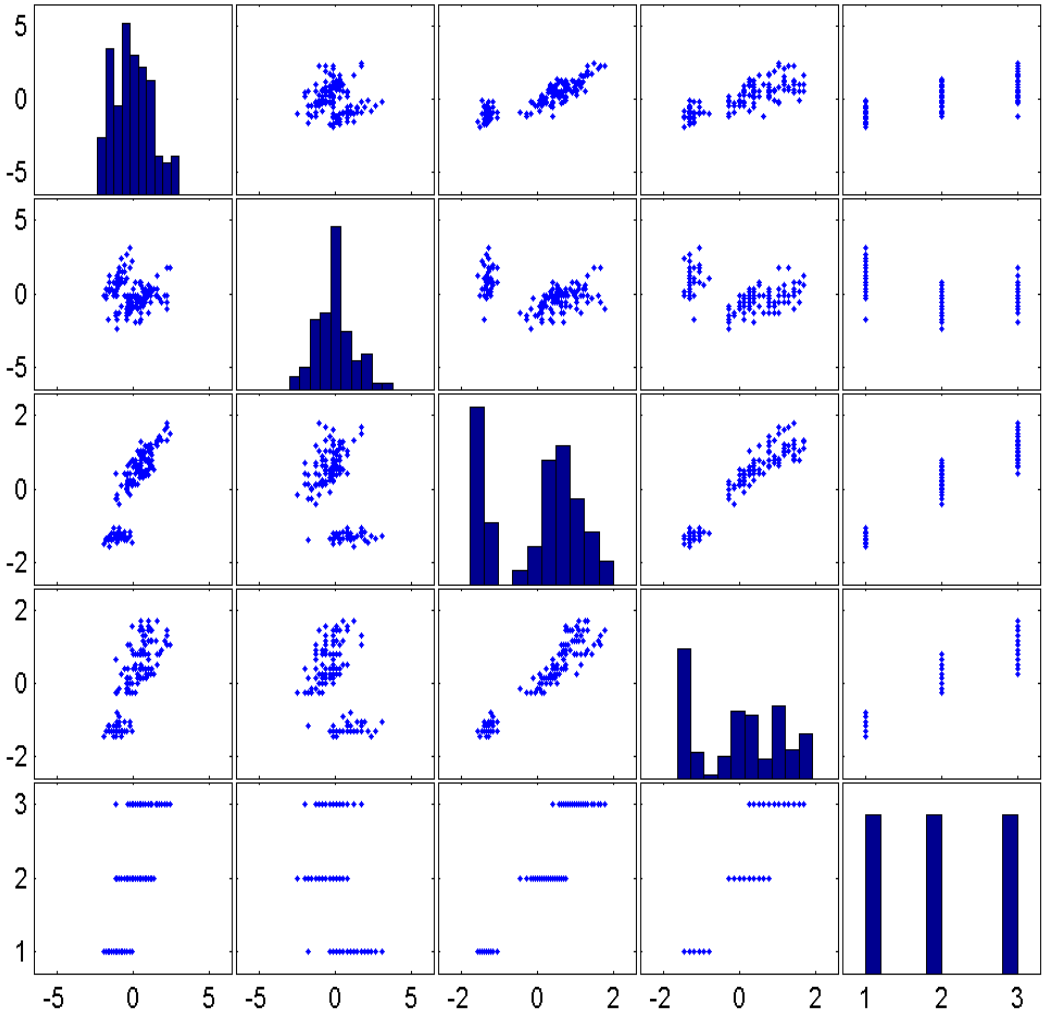
Introduction to visualization

How do we visualize data of high (or even very high) dimensionality?

- Eliminate dimensions (data variables): those which are redundant and/or uninformative (at least you manage to alleviate part of the problem…)
- Divide & conquer: a classic approach where you create multiple visualizations of low dimensionality
- Latent and projection models

Multiple visualization of Iris data

This is a divide & conquer approach



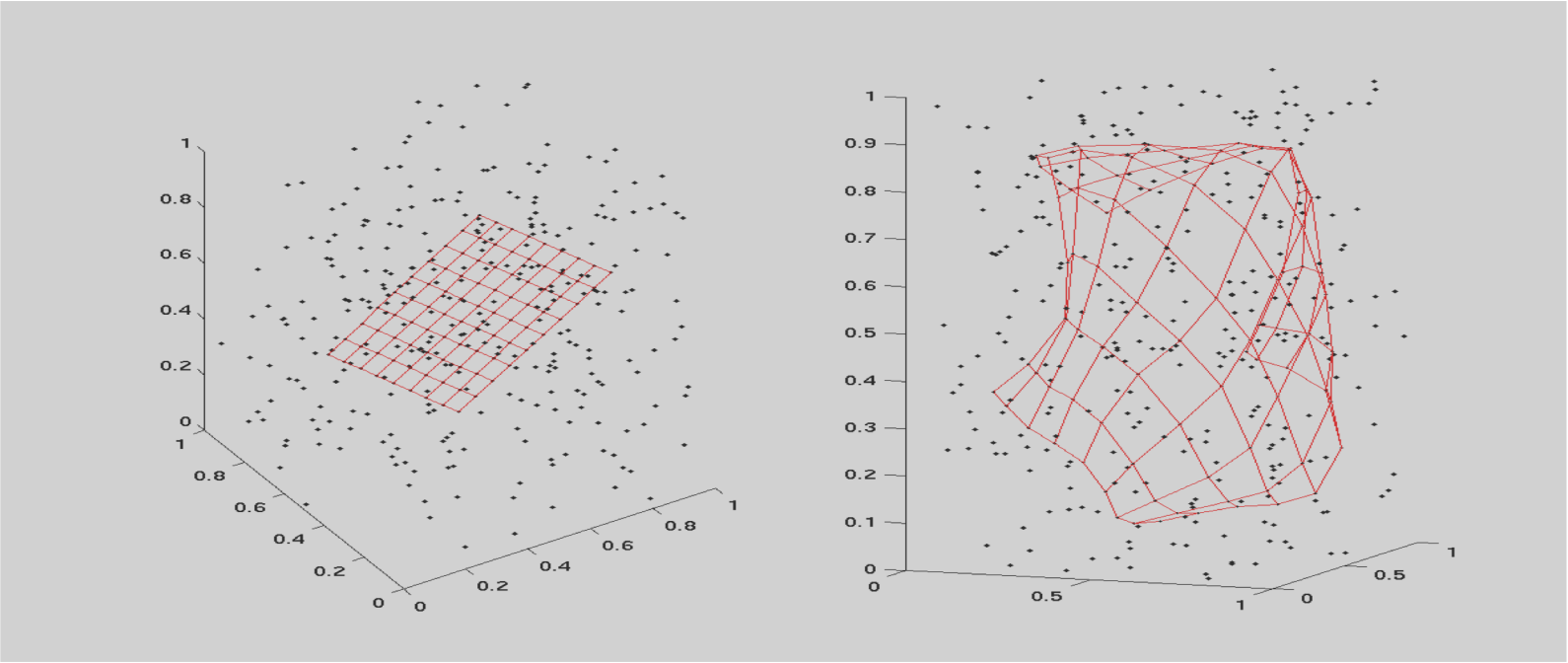
www.ics.uci.edu/~mlearn/MLRepository.html

Latency and projection

- **Projection**
  - Dimensionality compression
    - **Multi-dimensional Scaling**
  - Similitude information coding
- **Clustering**
  - Finding grouping structure in data
    - E.g., **Principal Components Analysis**
  - Similitude information coding
- ***Self-Organizing Map* (SOM) & *Generative Topographic Mapping* (GTM)**
  - They combine latent representation and clustering

Projection

- **Representation in <4-D, so that the distance-neighborhood relations between multi-dimensional points are faithfully preserved**
  - **It is impossible** to preserve information integrally
  - Some scale normalization is required
- **Linear vs. non-linear projections**



Projection methods

- **Methods based on inter-point distances, where:**

  dx = distance in the original space

  dy = distance in the projection space

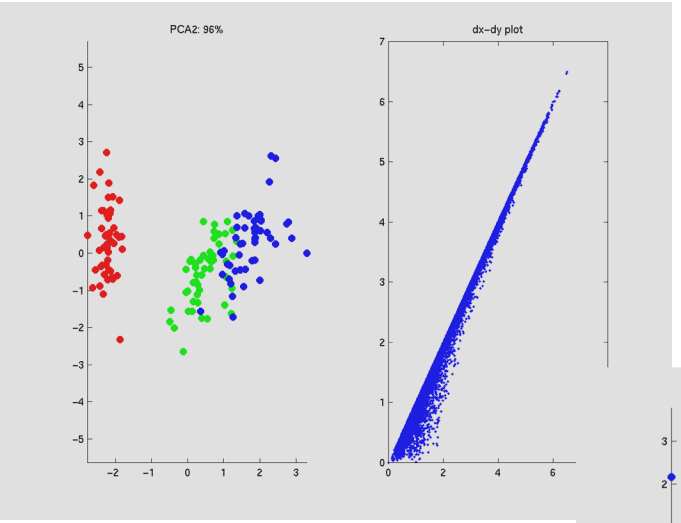
  h = neighborhood function

$E = \Sigma (dx - dy)^2$	**MDS, PCA**
$E = \Sigma (dx - dy)^2 / dx$	**Sammon's projection**
$E = \Sigma (dx - dy)^2 e^{-dy}$	**CCA**
$E = \Sigma dx^2 h(dy)$	**SOM**

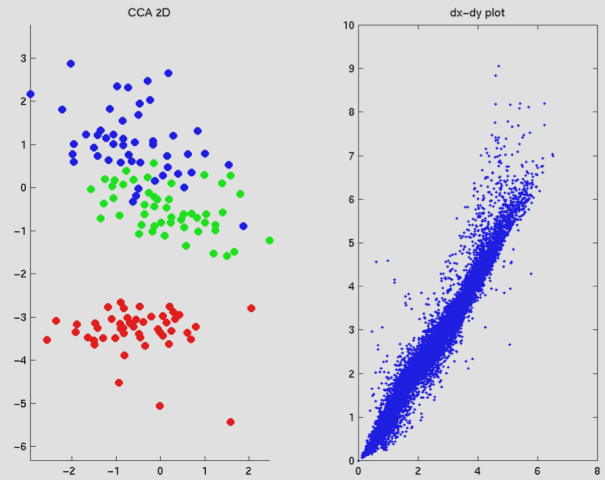
... and in which we aim to minimize an inherent projection distortion (E)

Example of Projection

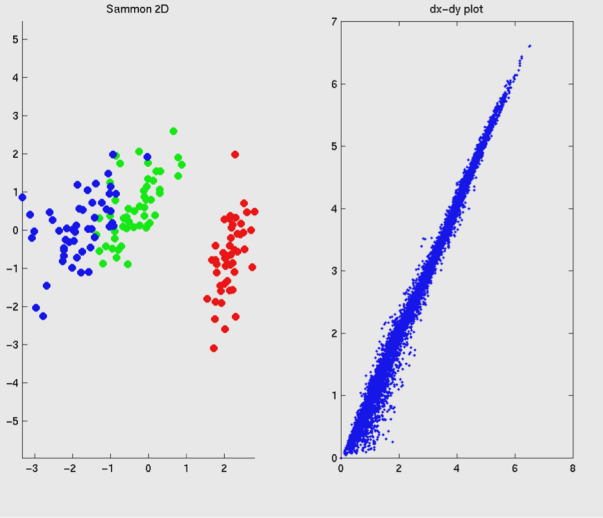
PCA



CCA



Sammon's projection



Self-Organizing Maps (SOM)

Look at the videos

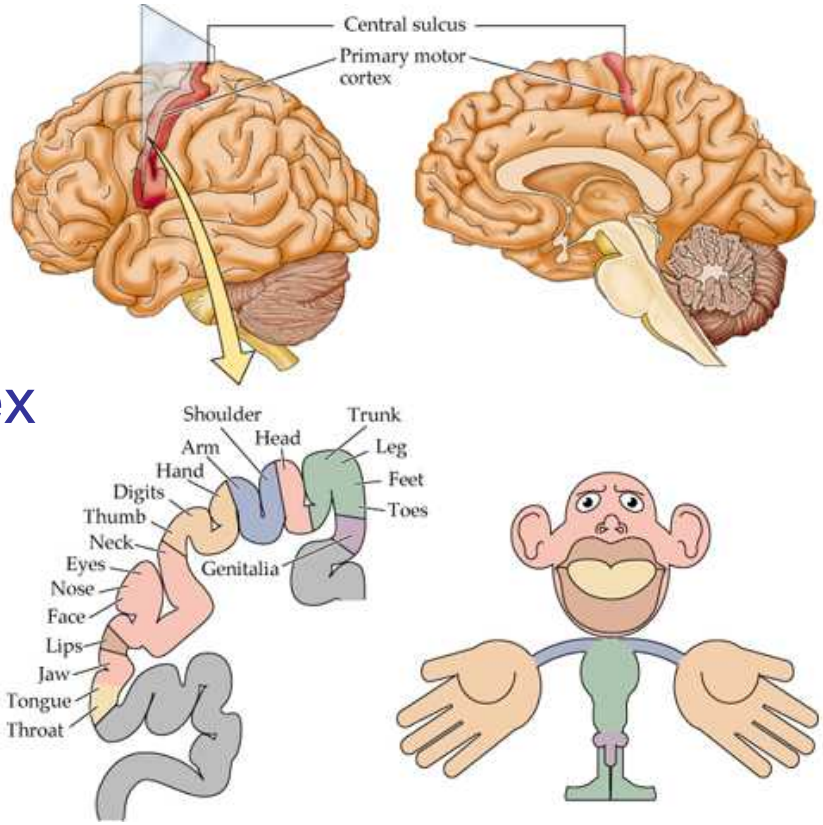
https://youtu.be/K4WuE7zlOZo

https://youtu.be/0qtvb_Nx2tA

Introduction to Self-Organizing Maps

- T. Kohonen proposes SOM in 1982

- **SOM are simplified models of cortical maps in the brain**
- Things that are near in the outside world link to areas near in the cortex
- These areas are represented by two-dimensional maps
- Neighboring areas in these maps represent neighboring areas in the sensory input space

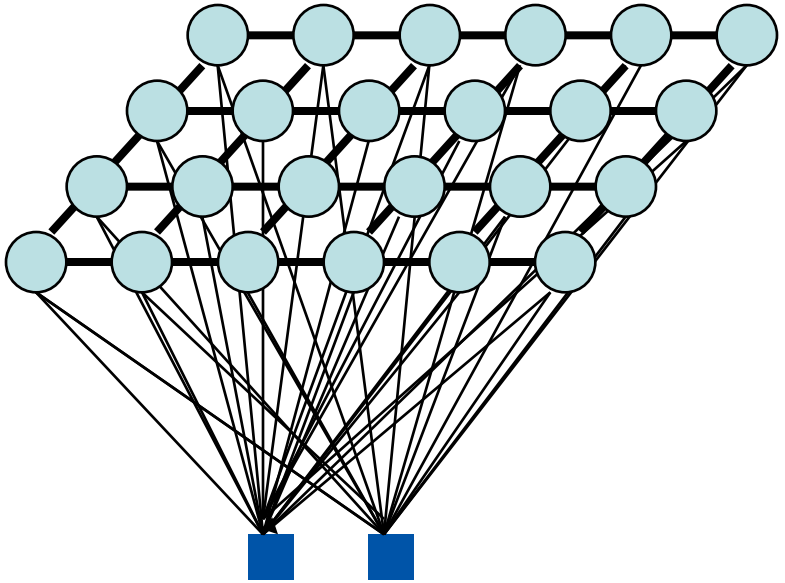


Introduction to Self-Organizing Maps

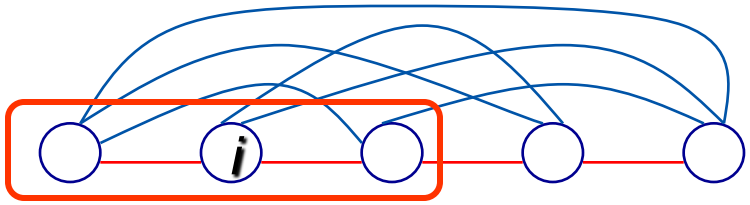
- Kohonen describes SOM as "**visualization and analysis tool for high dimensional data**"
- It is an unsupervised ANN
- Belongs to the category of competitive learning networks
- Applications
  - Clustering
  - Dimensionality reduction
  - Classification
  - Feature extraction (Self-Organized Feature Map)
  - Visualization

Self organizing maps

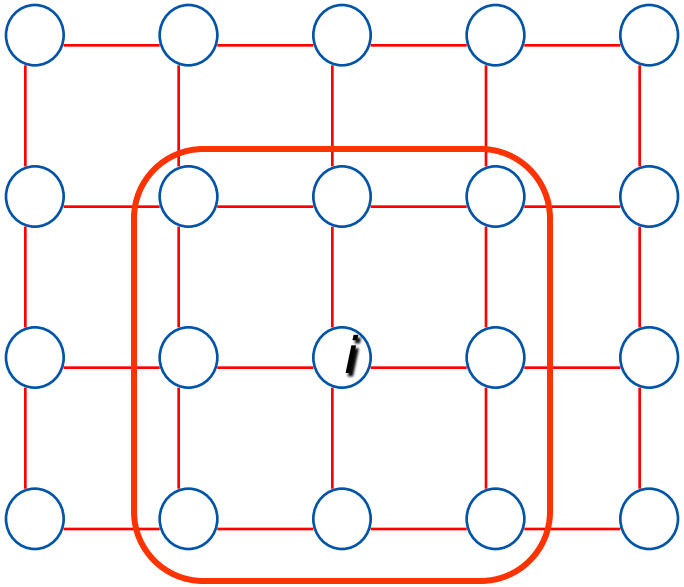
- The purpose of SOM is to map a multi-dimensional input space onto a **topology preserving** map of neurons
  - Preserve a topological so that neighboring neurons respond to «*similar*» input patterns
  - The topological structure is often a 2 or 3 dimensional space



Commonly output-layer structures



One-dimensional
(completely interconnected for determining “winner” unit)

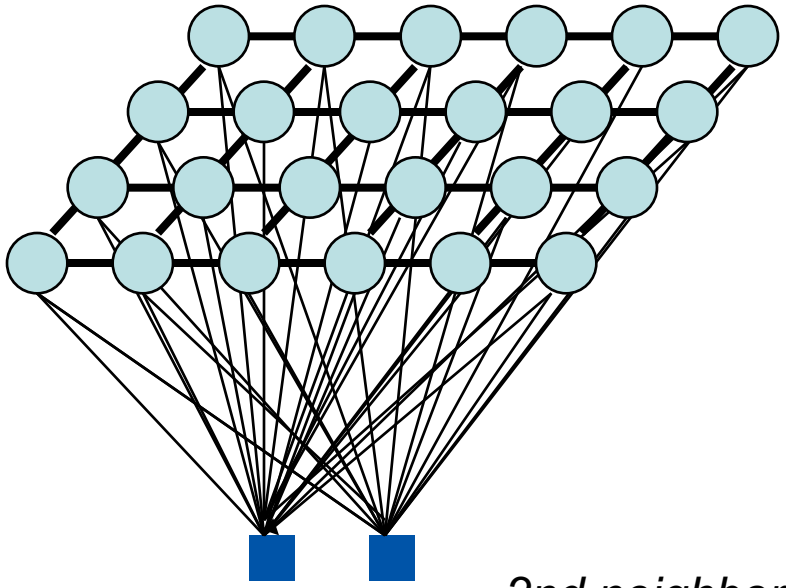


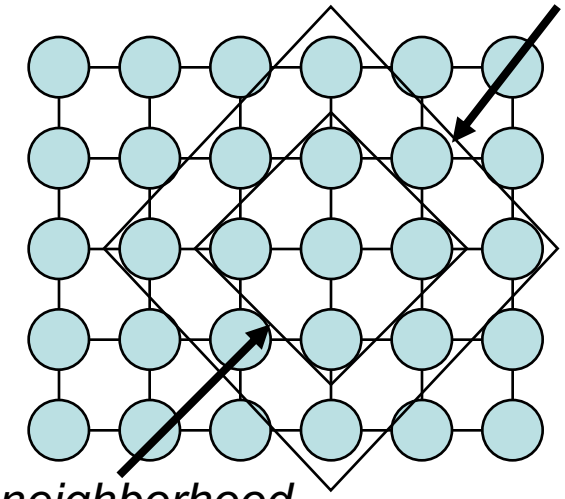
Two-dimensional
(connections omitted, only neighborhood relations shown [green])

Neighborhood of neuron i

Topological structure

- The activation of the neuron is spread in its direct neighborhood
  - neighbors become sensitive to the same input patterns
- Block distance
- The size of the neighborhood is initially large but reduce over time
  - Specialization of the network



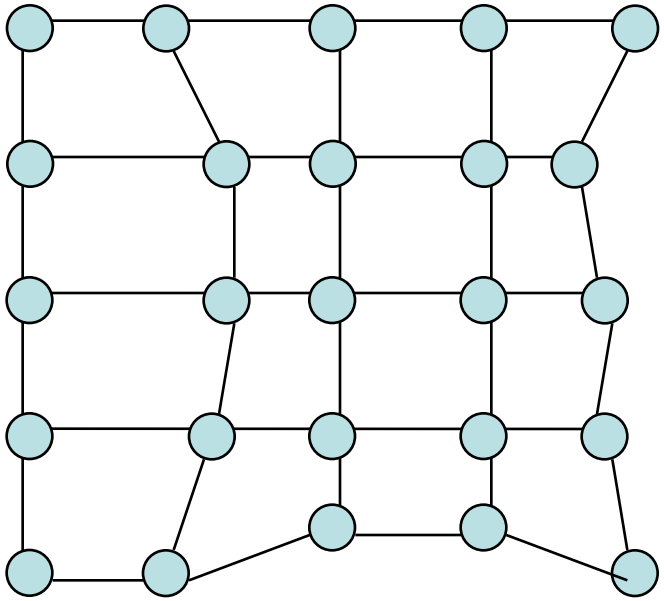


Neurons in Self organizing maps

- SOM maps a multi-dimensional input space onto a topology preserving **map of neurons**
- Each neuron is assigned a weight vector with the same dimensionality of the input space
- Each Input pattern is compared to each weight vector
  - Distance is calculated between the input pattern and each neuron in the network (e.g. *Euclidean Distance*)
- Selects the neuron that is closest as the winning neuron

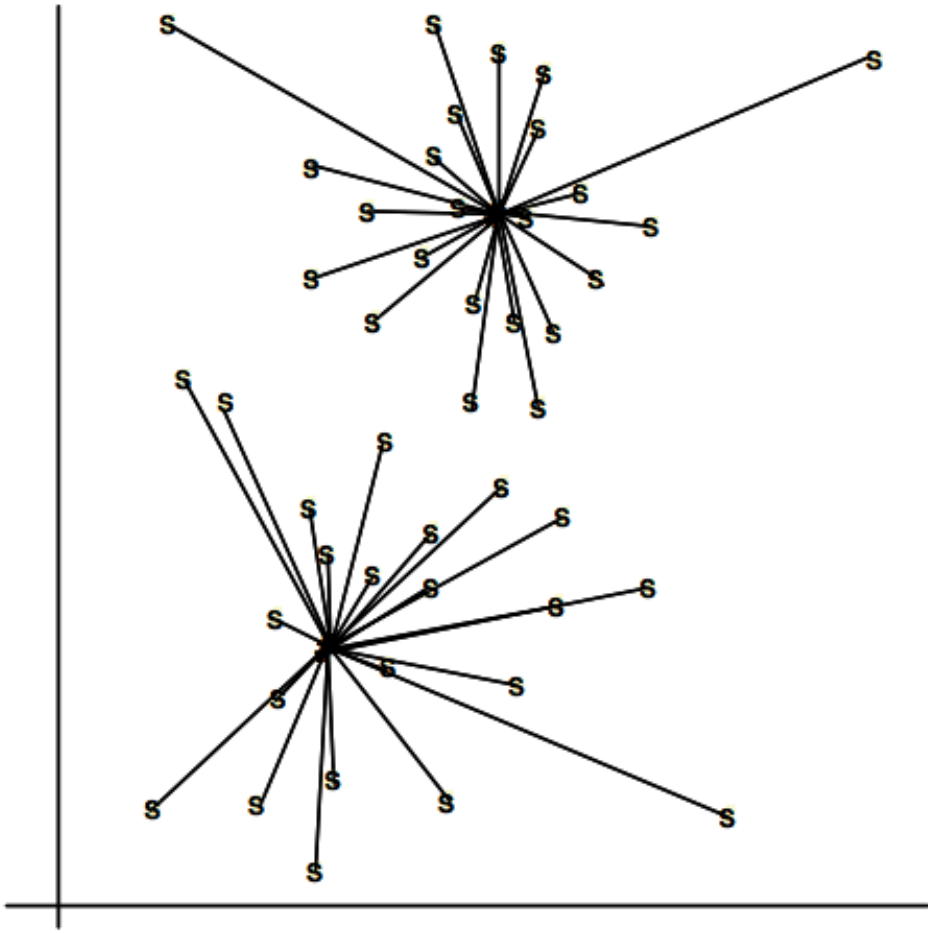
Adaptation in SOM

- During **training**, the "winner" neuron and its neighborhood adapts to make their weight vector more similar to the input pattern that caused the activation
- The neurons are moved closer to the input pattern
- The magnitude of the adaptation is controlled via a **learning parameter** which decays over time



Quantization error

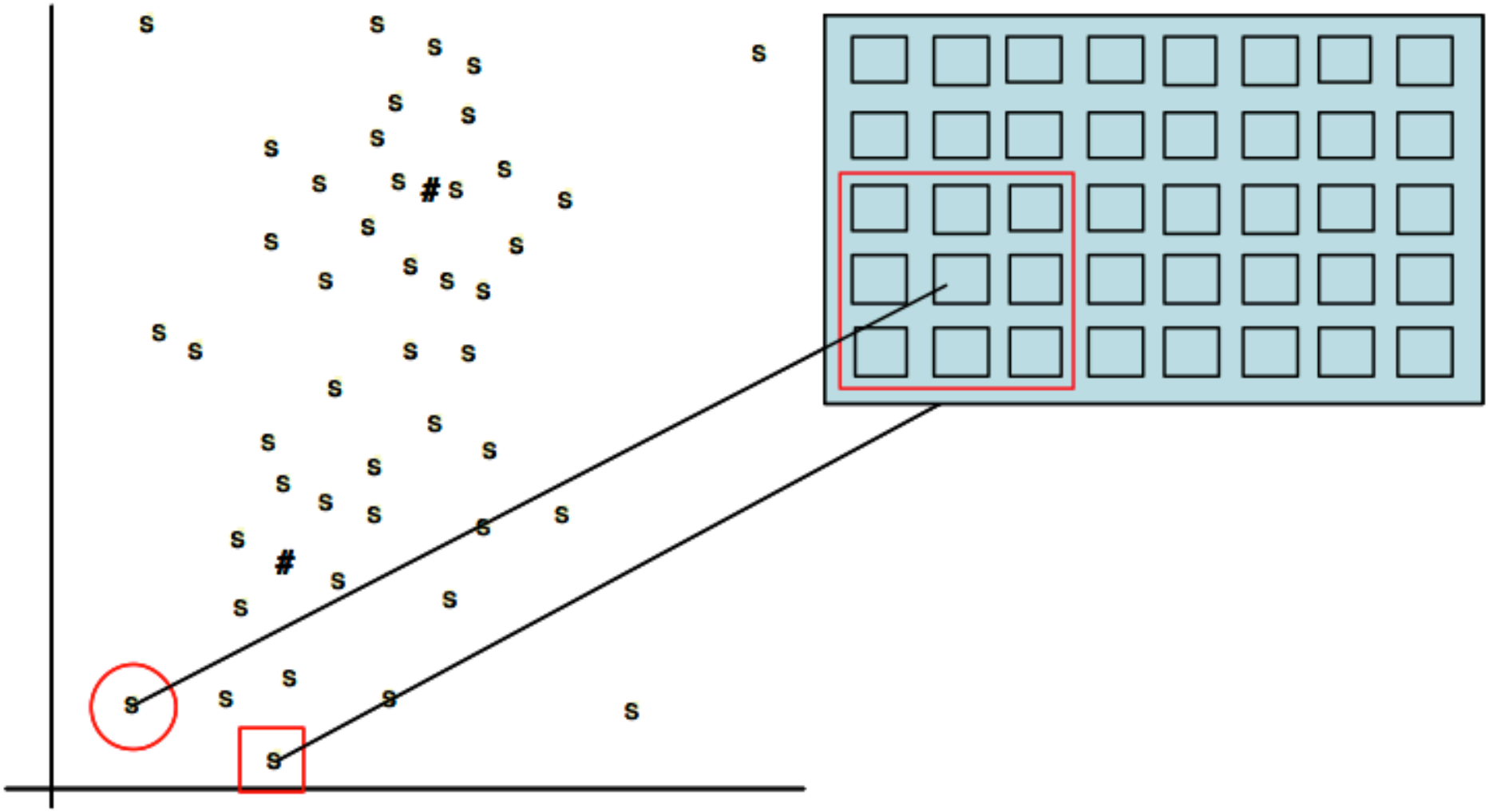
- Measures how well our neurons represent the input patterns
  - Note that there will be always some difference between the input pattern and the neuron it is mapped to
- It is calculated by summing all the distances between each input pattern and the neuron to which is mapped.



Topological error

- Evaluates the complexity of the output space
- Measures the number of times the second closest neighbor in the input space is not mapped into the neighbourhood of the neuron in the output space
- A high topological error may indicate that the classification problem is complex or may suggest that the training was not adequate and the network is folded

Topological error

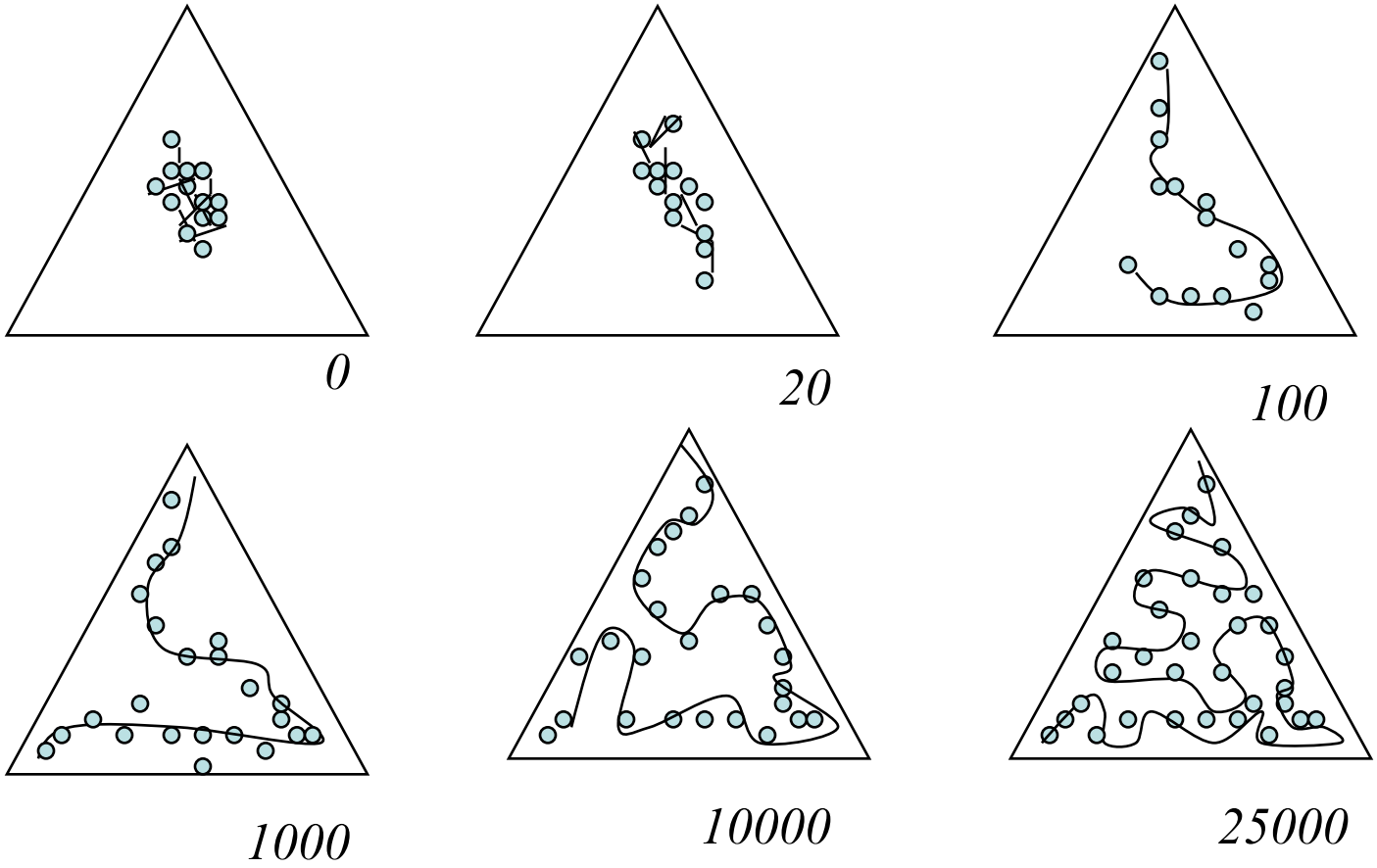


SOM training proces

- Before training, neurons may be initialized ramdomly
- **Part 1. Unfolding phase**
  - Neurons are “spread out” and pulled towards the general area (in the input space) where they will stay
- **Part 2. Fine tuning phase**
  - SOM match the neurons as far as possible to the input patterns, thus decreasing the quantization error

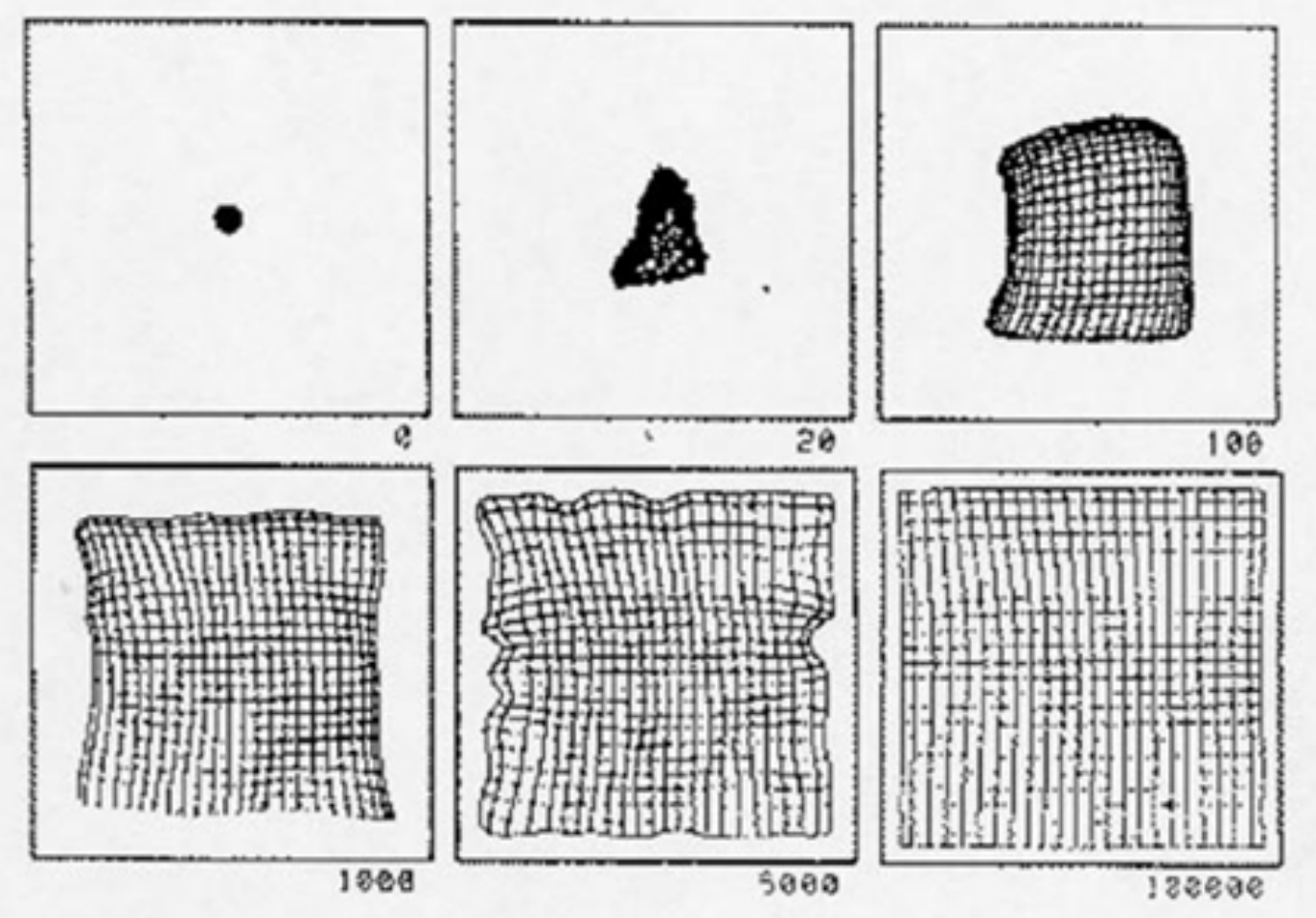
Example 1 when training SOM

Learning a one-dimensional representation of a two-dimensional (triangular) input space:



Example 2 when training a SOM

Learning a two-dimensional representation of a two-dimensional (square) input space:



SOM algorithm

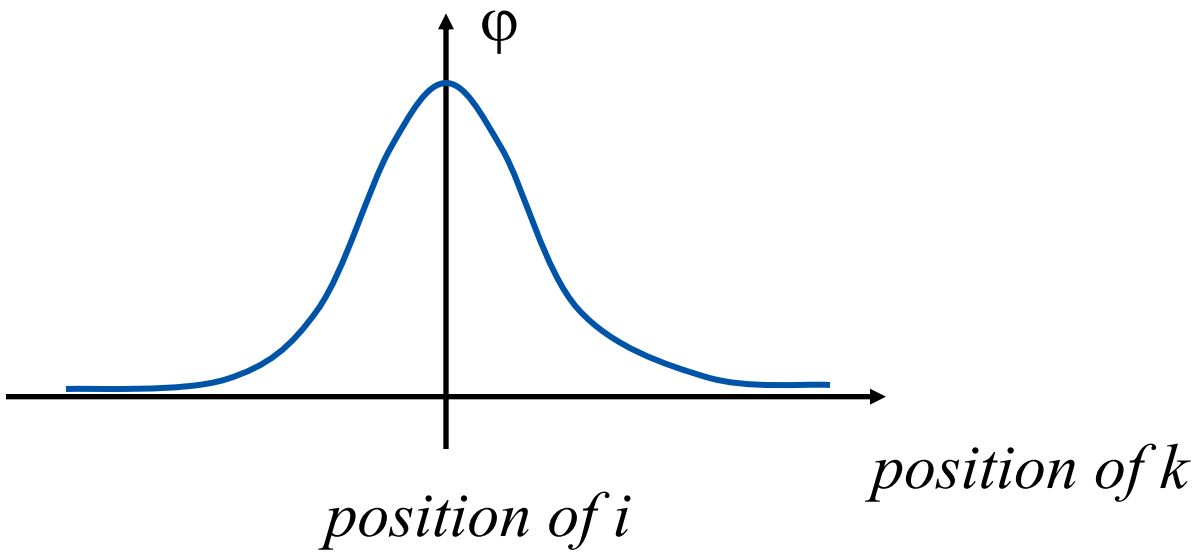
For *n*-dimensional input space and *m* output neurons:

1. Choose random weight vector w_i for neuron i, i = 1, ..., m
2. For each input, choose random input x and do 2, 3, 4, and 5
3. Calculate the distance between the pattern and all neurons (usually the Euclidean distance)
4. Determine winner neuron k:
   $||w_k - x|| = \min_i ||w_i - x||$
5. Update all weight vectors of all neurons i in the neighborhood of neuron k: $w_i := w_i + \eta \cdot \varphi(i, k) \cdot (x - w_i)$
   (w_i is shifted towards x)
6. If convergence criterion met, STOP.
   Otherwise, narrow neighborhood function φ and learning parameter η and go to (2).

Neighbourhood function

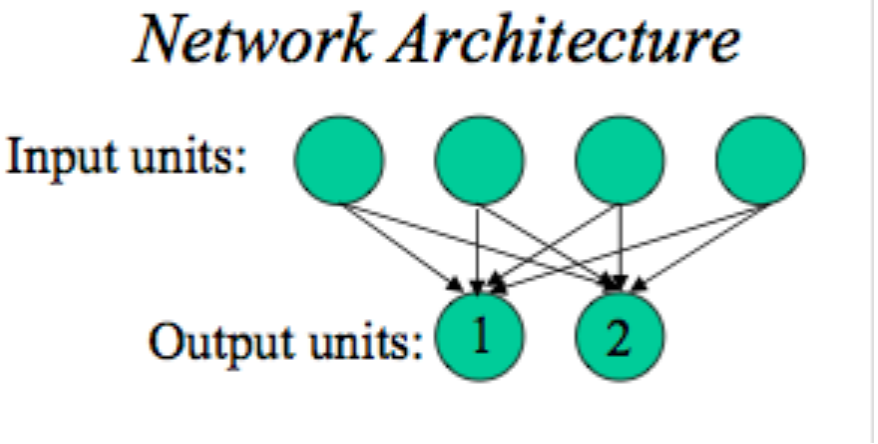
A neighborhood function φ(i, k) indicates how closely neurons i and k in the output layer are connected to each other.

Usually, a Gaussian function on the distance between the two neurons in the layer is used:



Example SOM

- From Fausett (1994)
- n = 4, m = 2
- Training samples
  - i1: (1, 1, 0, 0)
  - i2: (0, 0, 0, 1)
  - i3: (1, 0, 0, 0)
  - i4: (0, 0, 1, 1)



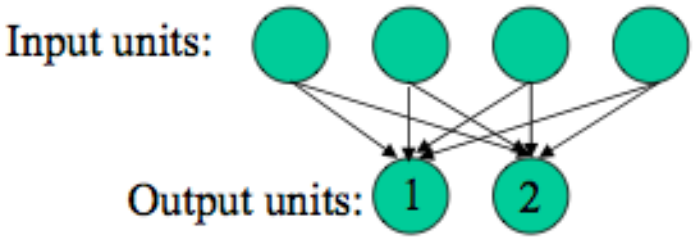
What should we expect as outputs?

Distances between data samples

- Use Minkowski distance with r = 1
- Training samples
  - i1: (1, 1, 0, 0)
  - i2: (0, 0, 0, 1)
  - i3: (1, 0, 0, 0)
  - i4: (0, 0, 1, 1)

	i1	i2	i3	i4
i1	0			
i2	3	0		
i3	1	2	0	
i4	4	1	3	0

Network Architecture



What might we expect from the SOM?

Example details

- Let Neighbourhood, $\varphi(i, k) = 0$
- Learning rate η

$$\eta(t) = 0.6;\ 1 <= t <= 4$$
$$\eta(t) = 0.5\ \eta(1);\ 5 <= t <= 8$$
$$\eta(t) = 0.5\ \eta(5);\ 9 <= t <= 12$$

- Initial weight matrix
  - Neuron 1, N1 [.2, .6, .5, .9]
  - Neuron 2, N2 [.8, .4, .7, .3]
- Weight update: $w_i(t+1) := w_i(t) + \eta(t) \cdot (x - w_i)$

- **Problem**: Calculate the weights updates for the first four steps

First weight update

- Training sample i1
- Distances (Euclidean) input pattern to all neurons
  - D(1) = $(.2-1)^2 + (.6-1)^2 + (.5-0)^2 + (.9-0)^2 = 1.86$
  - D(2) = $(.8-1)^2 + (.4-1)^2 + (.7-0)^2 + (.3-0)^2 = .98$
  - Neuron 2 (N2) wins
- Weights on winning neuron are updated
  - $w_i(t+1) := w_i(t) + .6 \cdot (x - w_i) = .4w_i(t) + .6x$

  - N1 [.2, .6, .5, .9]
  - N2 [.92, .76, .28, .12]

Second weight update

- Training sample i2
- Distances input pattern to all neurons
  - D(1) = $(.2-0)^2 + (.6-0)^2 + (.5-0)^2 + (.9-1)^2 = .66$
  - D(2) = $(.92-0)^2 + (.76-0)^2 + (.28-0)^2 + (.12-1)^2 = 2.28$
  - N1 wins
- Weights on winning neuron are updated
  - $w_i(t+1) := w_i(t) + .6 \cdot (x - w_i) = .4w_i(t) + .6x$
  - N1 [.08, .24, .20, .96]
  - N2 [.92, .76, .28, .12]

TODO: Complete the example with training i3 and i4

At the end of the example

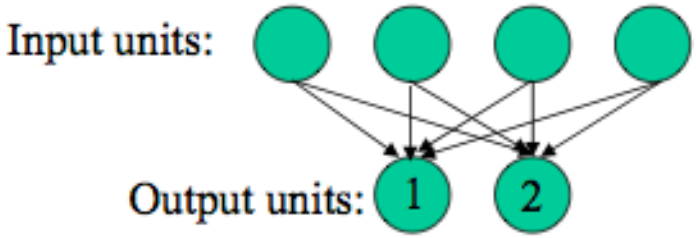
- Once finished the first iteration (also known as epoch) the learning rate is updated, it will be .3
- Next, second iteration will start
- The process finishes when the number of iterations is reached
- After many iterations through the data set
  - N1 [0, 0, .5, 1]
  - N2 [1, .5, 0, 0]

Did we get the clustering we expected?

Solution

- Training samples
  - i1: (1, 1, 0, 0)
  - i2: (0, 0, 0, 1)
  - i3: (1, 0, 0, 0)
  - i4: (0, 0, 1, 1)
- Weights
- N1 [0, 0, .5, 1]
- N2 [1, .5, 0, 0]

Network Architecture



Sample: i1

- Distance from unit1 weights
  - $(1-0)^2 + (1-0)^2 + (0-.5)^2 + (0-1.0)^2 = 1+1+.25+1=3.25$
- Distance from unit2 weights
  - $(1-1)^2 + (1-.5)^2 + (0-0)^2 + (0-0)^2 = 0+.25+0+0=.25$ (winner)

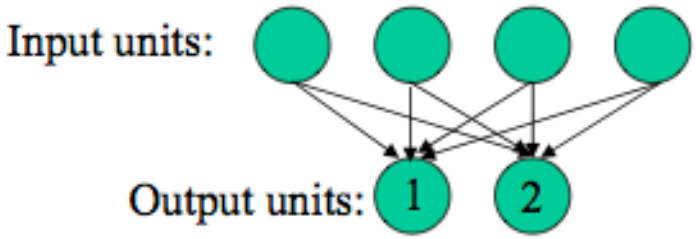
Sample: i2

- Distance from unit1 weights
  - $(0-0)^2 + (0-0)^2 + (0-.5)^2 + (1-1.0)^2 = 0+0+.25+0$ (winner)
- Distance from unit2 weights
  - $(0-1)^2 + (0-.5)^2 + (0-0)^2 + (1-0)^2 = 1+.25+0+1=2.25$

Solution

- Training samples
  - i1: (1, 1, 0, 0)
  - i2: (0, 0, 0, 1)
  - i3: (1, 0, 0, 0)
  - i4: (0, 0, 1, 1)
- Weights
- N1 [0, 0, .5, 1]
- N2 [1, .5, 0, 0]

Network Architecture



Sample: i3

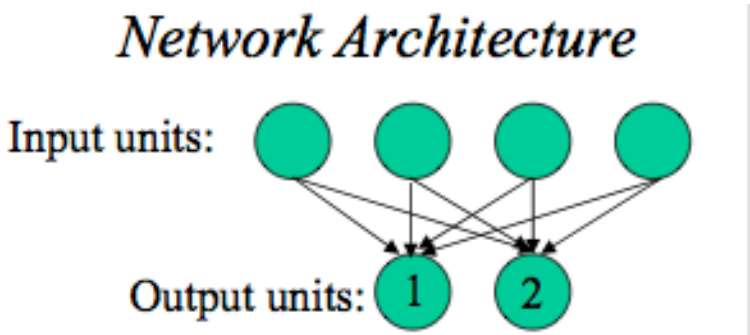
- Distance from unit1 weights
  - $(1-0)^2 + (0-0)^2 + (0-.5)^2 + (0-1.0)^2 = 1+0+.25+1=2.25$
- Distance from unit2 weights
  - $(1-1)^2 + (0-.5)^2 + (0-0)^2 + (0-0)^2 = 0+.25+0+0=.25$ (winner)

Sample: i4

- Distance from unit1 weights
  - $(0-0)^2 + (0-0)^2 + (1-.5)^2 + (1-1.0)^2 = 0+0+.25+0$ (winner)
- Distance from unit2 weights
  - $(0-1)^2 + (0-.5)^2 + (1-0)^2 + (1-0)^2 = 1+.25+1+1=3.25$

At the end of the example

- Training samples
  - i1: (1, 1, 0, 0)
  - i2: (0, 0, 0, 1)
  - i3: (1, 0, 0, 0)
  - i4: (0, 0, 1, 1)
- Weights
  - N1 [0, 0, .5, 1]
  - N2 [1, .5, 0, 0]



- Samples i1, i3 clusters with neuron 2
- Samples i2, i4 clusters with neuron 1

Summary of SOM

- **Also known as Kohonen Maps**
  - **It is an unsupervised ANN**
  - Cooperative learning (through neighbourhood function)
  - Competitive learning (*winner takes most –if not all-*)
  - Discretization (in the form of network grids) and projection are simultaneously performed
  - SOM provides a topology preserving mapping from the high dimensional space to map units
  - A SOM has the capability to generalize
  - ***k-means*** is an special case of **SOM**

What else?

Arriving at this point:

TO READ

An introduction to Self-Organizing Maps

- Read from page 299 to 315

In general all the chapter is interesting.

- You do not need to memorize the formulas, just to understand the concepts and what SOM is doing in its algorithm (the same contents that I have introduced you in the slides)

Multi-Dimensional Scaling (MDS)

Introduction

- *“ If you are interested in how certain objects relate to each other … and if you would like to present these relationships in the form of a map then MDS is the technique you need ”*

- **The goal** of an MDS analysis is to find a spatial configuration of objects when all that is known is some measure of their general (dis)similarity.

Multidimensional Scaling

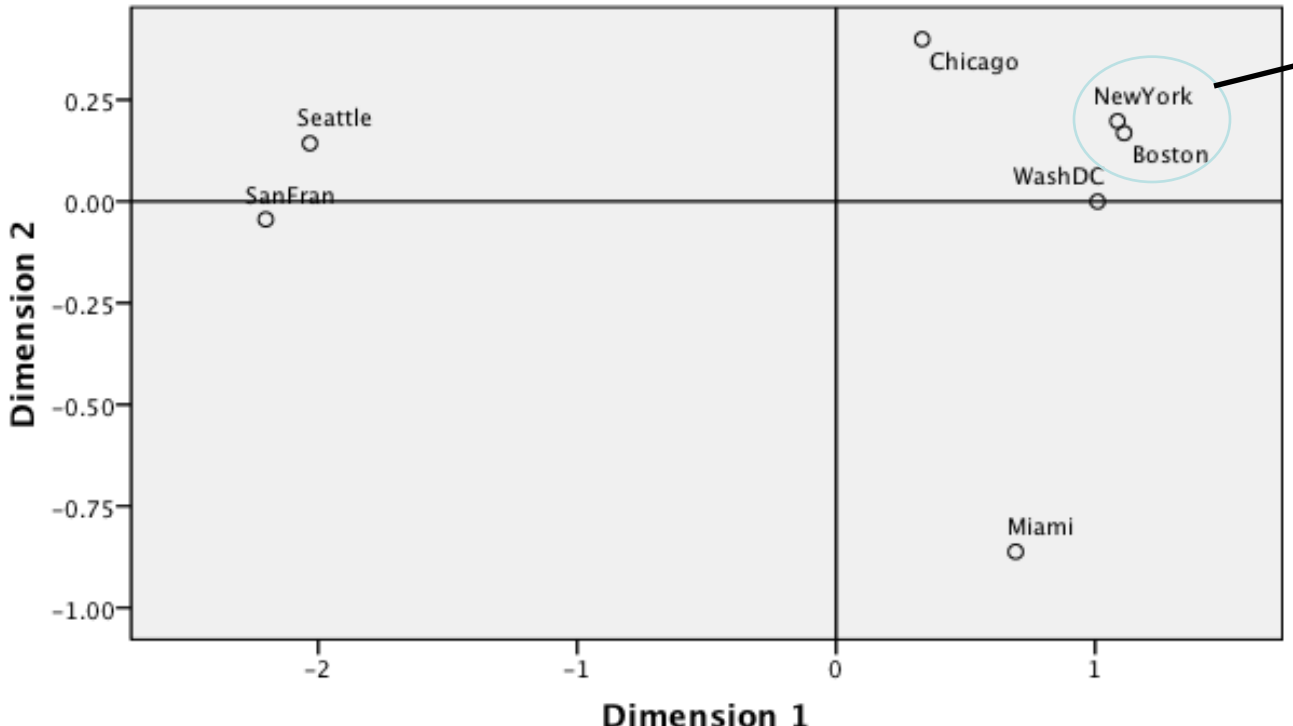
- Generally regarded as **exploratory data analysis**
- **Reduces large amounts of data** into easy-to-visualize structures
- Attempts to **find structure** (visual representation) in a set of distance measures, e.g. dis/similarities, between objects/instances
    - Shows how variables/objects are related perceptually

- **How**? By assigning instances to specific locations in space
- Distances between points in space match dis/similarities as closely as possible:
  - Similar objects: Close points
  - Dissimilar objects: Far apart points

MDS Example: City Distances

***Distances Matrix**: Symmetric*

		1 BOST	2 NY	3 DC	4 MIAM	5 CHIC	6 SEAT	7 SF	8 LA	9 DENV
1	BOSTON	0	206	429	1504	963	2976	3095	2979	1949
2	NY	206	0	233	1308	802	2815	2934	2786	1771
3	DC	429	233	0	1075	671	2684	2799	2631	1616
4	MIAMI	1504	1308	1075	0	1329	3273	3053	2687	2037
5	CHICAGO	963	802	671	1329	0	2013	2142	2054	996
6	SEATTLE	2976	2815	2684	3273	2013	0	808	1131	1307
7	SF	3095	2934	2799	3053	2142	808	0	379	1235
8	LA	2979	2786	2631	2687	2054	1131	379	0	1059
9	DENVER	1949	1771	1616	2037	996	1307	1235	1059	0



Cluster

Spatial Map

Dimensions

1: North/South

2: East/West

The Process of MDS: The Data

- Data of MDS: **similarities**, **dissimilarities**, **distances**, or **proximities** reflects amount of dis/similarity or distance between pairs of objects.

- Distinction between similarity and dissimilarity data dependent on type of scale used:
  - **Dissimilarity** scale: Low #=high similarity & High #=high dissimilarity.
  - **Similarity** scale: Opposite of dissimilarity.

    E.g. On a scale of 1-9 (1 being the same and 9 completely different) how similar are chocolate bars A and B? Dissimilarity scale.

Types of MDS

MDS model classified according to:

1) Type of proximities:

- **Metric/quantitative**: Quantitative information/interval data about objects' proximities e.g. city distance
- **Non-metric/qualitative**: Qualitative information/nominal data about proximities e.g. rank order

2) Number of proximity matrices (distance, dis/similarity matrix).

- Proximity matrix is the input for MDS
- The above criteria yield:
  - 1) **Classical** MDS: One proximity matrix (metric or non-metric)
  - 2) **Replicated** MDS: Several matrices
  - 3) **Weighted MDS/Individual Difference Scaling**: Aggregate proximities and individual differences in a common MDS space

Focus of MDS

This course we will concentrate on the classical MDS. The next slides and the example come from this reading

TO READ

An introduction to MDS

- From page 4 to page 12 (Introduction, Section 1, Introduction Section 2, and Section 2.1)

The remaining of the article is OPTIONAL.

The MDS Model

- **Classical MDS** uses Euclidean principles to model data proximities in geometrical space, where distance (d_{ij}) between points *i* and *j* is defined as:

$$d_{ij} = \sqrt{\sum (x_{ia} - x_{ja})^2}$$

x_i and x_j specify coordinates of points i and j on dimension a, respectively.

- The modeled Euclidean distances are related to the observed proximities, δ_{ij}, by some transformation/function (*f*).
- Most MDS models assume that the data have the form:

$$\delta_{ij} = f(d_{ij}) = \sqrt{\sum (x_{ia} - x_{ja})^2}$$

- All MDS algorithms are a variation of the above

Classical MDS algorithm

We assume known a coordinate matrix X

1. Set up the matrix of squared proximities, $P^{(2)} = [p^2]$
2. Apply the double centering: $B = -\frac{1}{2} J P^{(2)} J$
   using the matrix $J = I - n^{-1} 11'$
   where n is the number of objects.
3. Extract the *m* largest positive eigenvalues of B and the corresponding *m* eigenvectors
4. A *m*-dimensional spatial configuration of the **n** objects is derived from the coordinate matrix $X = E_m \Lambda_m^{1/2}$
   where $\mathbf{E_m}$ is the matrix of m eigenvectors and Λ_m is the diagonal matrix of m eigenvalues

Classical MDS example

- Proximity matrix
  - Distances between 4 cities

	cph	aar	ode	aal
cph	0	93	82	133
aar	93	0	52	60
ode	82	52	0	111
aal	133	60	111	0

- Step 1 – Matrix of squared proximities

$$\mathbf{P^{(2)}} = \begin{bmatrix} 0 & 8649 & 6724 & 17689 \\ 8649 & 0 & 2704 & 3600 \\ 6724 & 2704 & 0 & 12321 \\ 17689 & 3600 & 12321 & 0 \end{bmatrix}$$

Classical MDS example

- Step 2- Apply the double centering

$$\mathbf{J} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} - 0.25 \times \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 0.75 & -0.25 & -0.25 & -0.25 \\ -0.25 & 0.75 & -0.25 & -0.25 \\ -0.25 & -0.25 & 0.75 & -0.25 \\ -0.25 & -0.25 & -0.25 & 0.75 \end{bmatrix}.$$

Applying $\mathbf{J}$ to $\mathbf{P^{(2)}}$ yields the double centered matrix $\mathbf{B}$

$$\mathbf{B} = -\tfrac{1}{2}\mathbf{J}\mathbf{P^{(2)}}\mathbf{J} = \begin{bmatrix} 5035.0625 & -1553.0625 & 258.9375 & -3740.938 \\ -1553.0625 & 507.8125 & 5.3125 & 1039.938 \\ 258.9375 & 5.3125 & 2206.8125 & -2471.062 \\ -3740.9375 & 1039.9375 & -2471.0625 & 5172.062 \end{bmatrix}.$$

Classical MDS example

- Step 3- Extract the two largest eigenvalues and the corresponding eigenvectors

$$\lambda_1 = 9724.168,\ \lambda_2 = 3160.986$$

$$\mathbf{e_1} = \begin{pmatrix} -0.637 \\ 0.187 \\ -0.253 \\ 0.704 \end{pmatrix},\ \mathbf{e_2} = \begin{pmatrix} -0.586 \\ 0.214 \\ 0.706 \\ -0.334 \end{pmatrix}$$

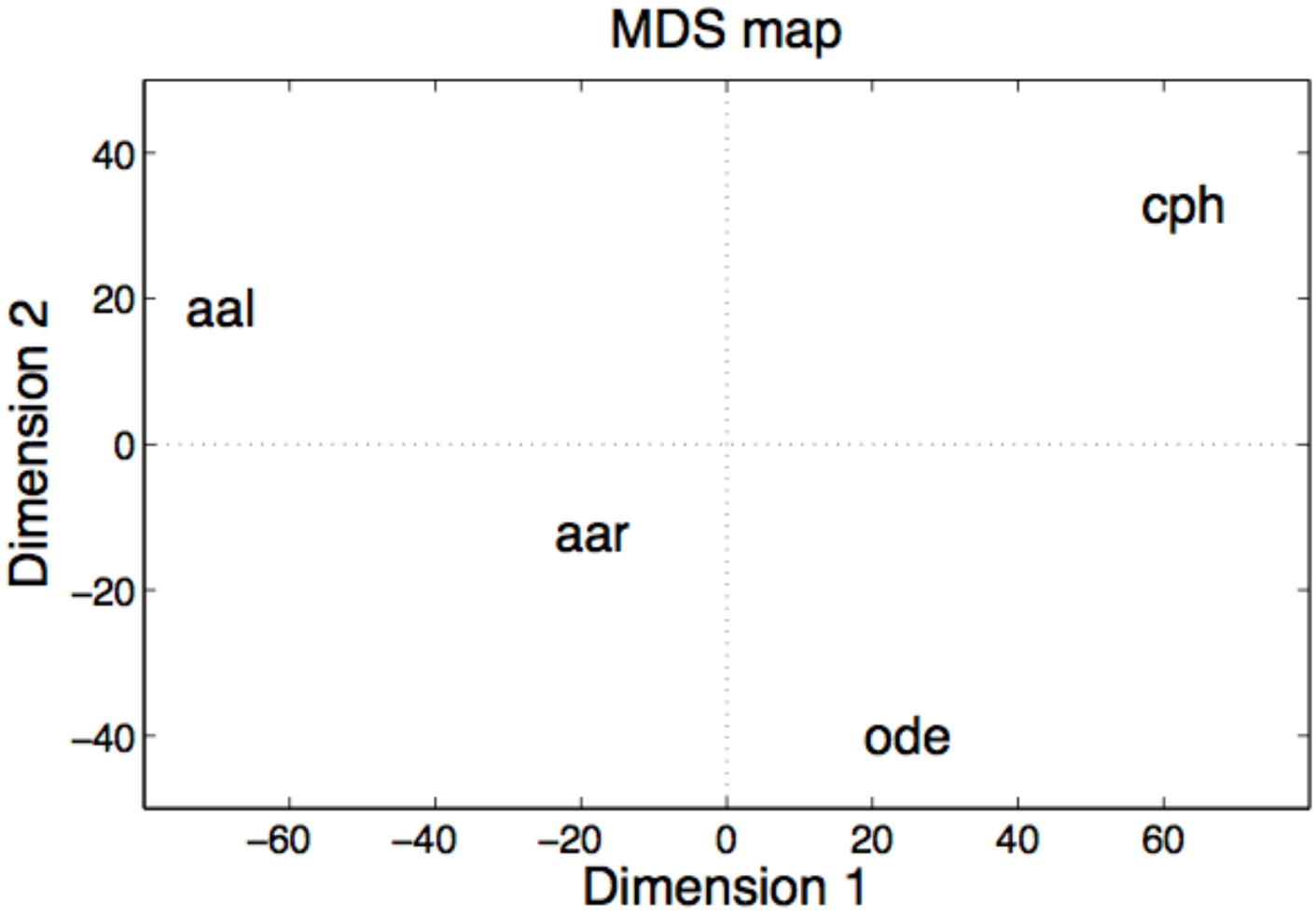
Classical MDS example

- Step 4- the coordinates of the cities are obtained by multiplying eigenvalues and vectors

$$\mathbf{X} = \begin{bmatrix} -0.637 & -0.586 \\ 0.187 & 0.214 \\ -0.253 & 0.706 \\ 0.704 & -0.334 \end{bmatrix} \begin{bmatrix} \sqrt{9724.168} & 0 \\ 0 & \sqrt{3160.986} \end{bmatrix} = \begin{bmatrix} -62.831 & -32.97448 \\ 18.403 & 12.02697 \\ -24.960 & 39.71091 \\ 69.388 & -18.76340 \end{bmatrix}$$

Classical MDS Example

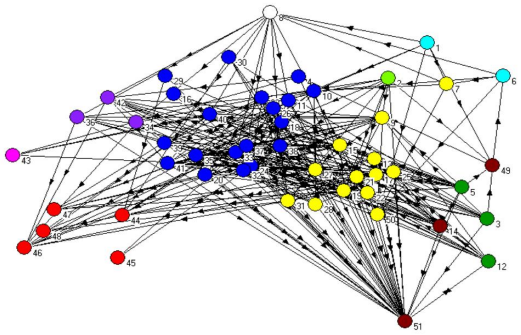
- The result is ....



Output of MDS

MDS Map/Perceptual Map/Spatial Representation:

1) **Clusters:** Groupings in a MDS spatial representation.
   - These may represent a domain/subdomain.
2) **Dimensions**: Hidden structures in data. Ordered groupings that explain similarity between items.
   - Axes are meaningless and orientation is arbitrary.
   - In theory, there is no limit to the number of dimensions.
   - In reality, the number of dimensions that can be perceived and interpreted is limited.



"Advantages" of MDS

- Does not require assumptions of linearity, metricity, or multivariate normality
- Can be used to model nonlinear relationships
- Dimensionality "solution" can be obtained from individuals; gives insight into how individuals differ from aggregate data
- Reveals dimensions without the need for defined attributes
- Dimensions that emerge from MDS can be incorporated into regression analysis to assess their relationship with other variables

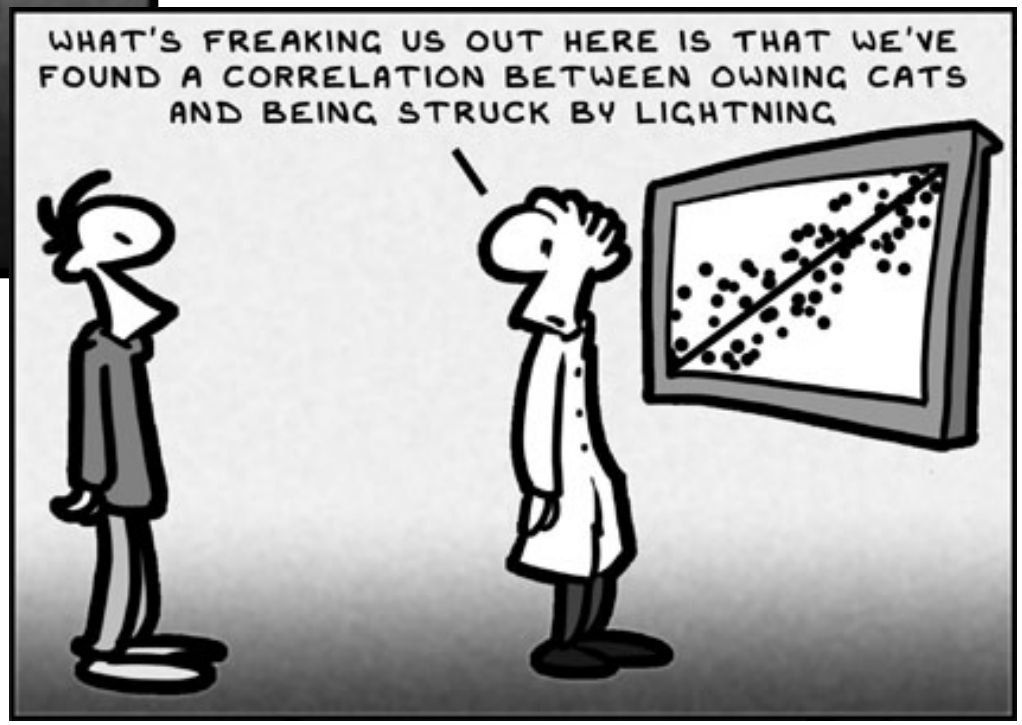
"Disadvantages" of MDS

- Provides a global measure of dis/similarity but does not provide much insight into subtleties
- Increased dimensionality: Difficult to represent and decreases intuitive understanding of the data. As such, the model of the data becomes as complicated as the data itself.
- Determination of meanings of dimensions is subjective.

Summary

- **MDS:** technique used in data visualisation for exploring similarities or dissimilarities in data. An MDS algorithm starts with a matrix of item-item similarities, then assigns a location of each item in a low-dimensional space, suitable for graphing or 3D visualisation.
- **Taxonomy:**
  - Metric multidimensional scaling -- assumes the input matrix is just an item-item distance matrix. Analogous to PCA, an eigenvector problem is solved to find the locations that minimize distortions to the distance matrix. Its goal is to find a Euclidean distance approximating a given distance.
  - Generalized multidimensional scaling (GMDS) -- A superset of metric MDS that allows for the target distances to be non-Euclidean.
  - Non-metric multidimensional scaling -- It finds a non-parametric monotonic relationship between the dissimilarities in the item-item matrix and the Euclidean distance between items, and the location of each item in the low-dimensional space


EVERYBODY WHO WENT TO THE MOON HAS EATEN CHICKEN!
GOOD GRIEF. CHICKEN MAKES YOU GO TO THE MOON!


WHAT'S FREAKING US OUT HERE IS THAT WE'VE FOUND A CORRELATION BETWEEN OWNING CATS AND BEING STRUCK BY LIGHTNING

Questions?

UNIVERSITAT DE BARCELONA

Week 5

Course. Introduction to Machine Learning

Theory 5. Visualization

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