Music Machine Learning

Master ATIAM - Informatique
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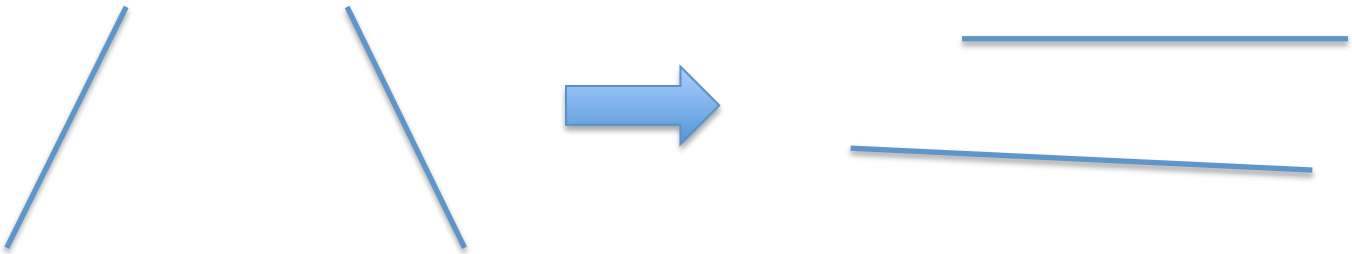
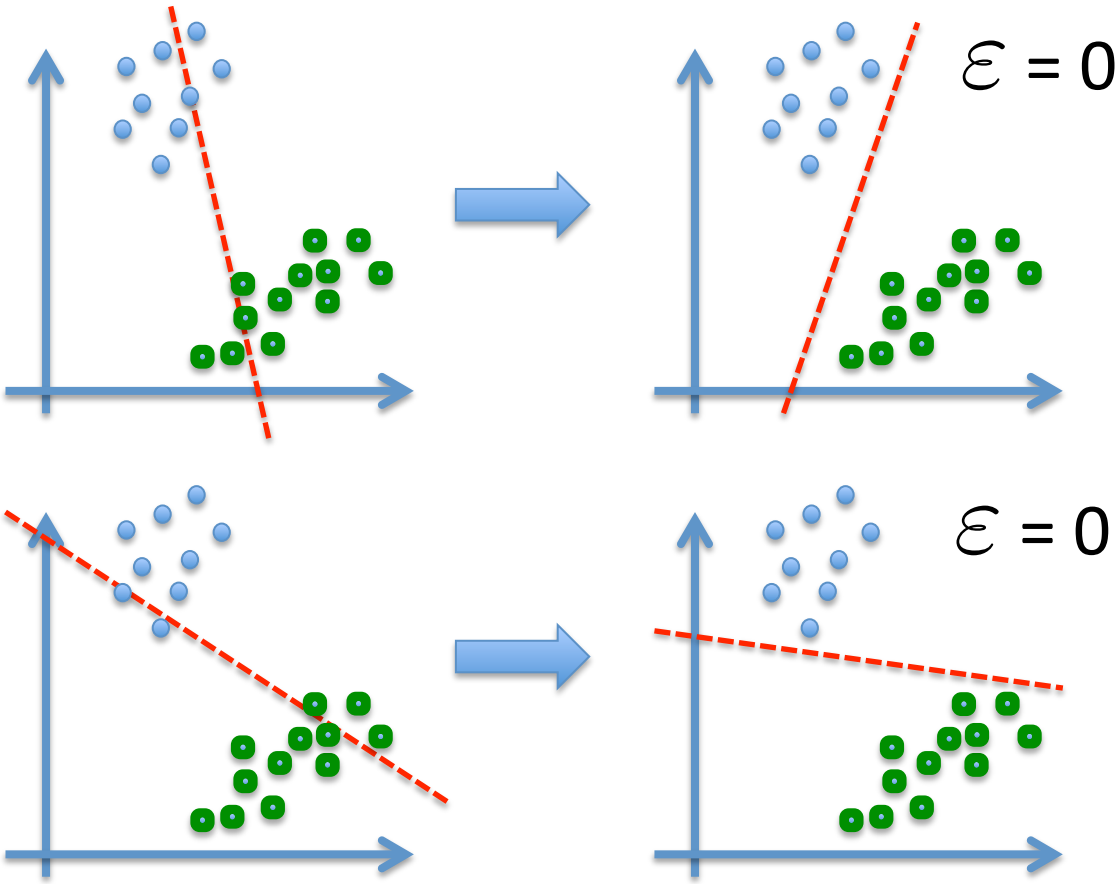
Support Vector Machines

- So all methods sort of divide the space
- But the essential question is **how** to divide the space
  1. Centroïd-based division
  2. Decision tree
- But is this space needs to be fixed?
- How things look from a different angle?
- We can obtain this if we know the geometry of the world



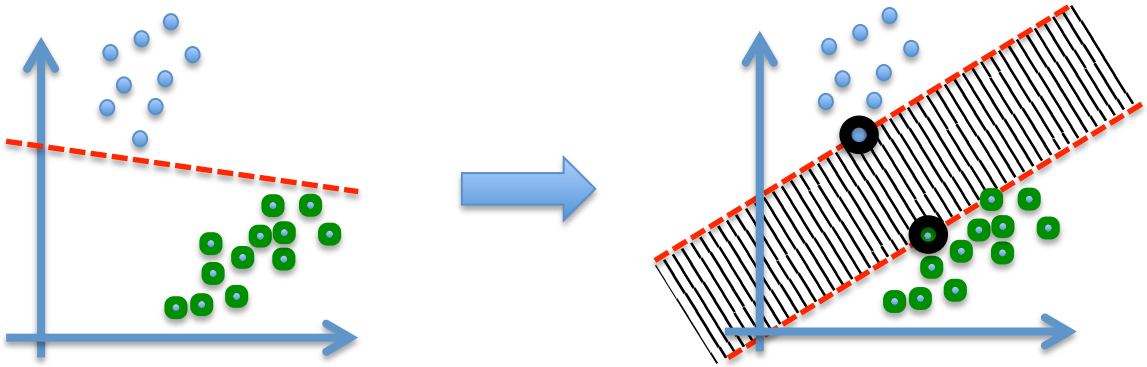
- Rich and powerful through geometrical models
- Neural networks provided a whole **set** of solutions

Support Vector Machines



Support Vector Machines

- Neural networks provided a whole set of solutions
- Each one defines a « street » between two populations
- Can we find the **widest** street (margin) between two populations
- Based on the hypothesis that the widest is the best separation

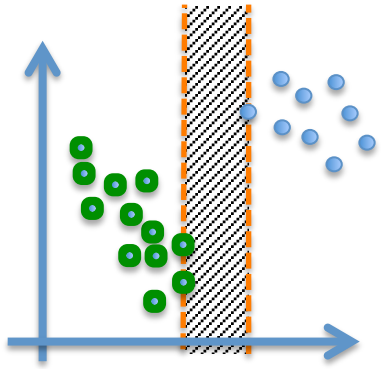


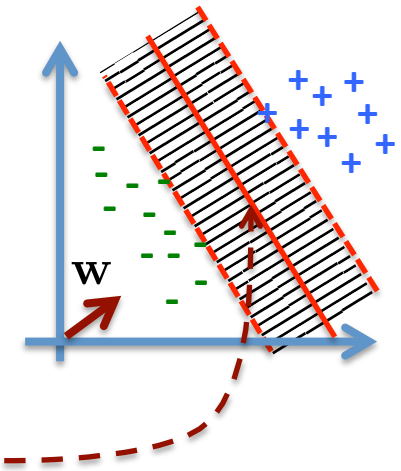
- So how to find this « optimal » separation?
- What is my decision function? (typical optimization question)

Support Vector Machines

So what decision function could separate these two situations ?

narrow



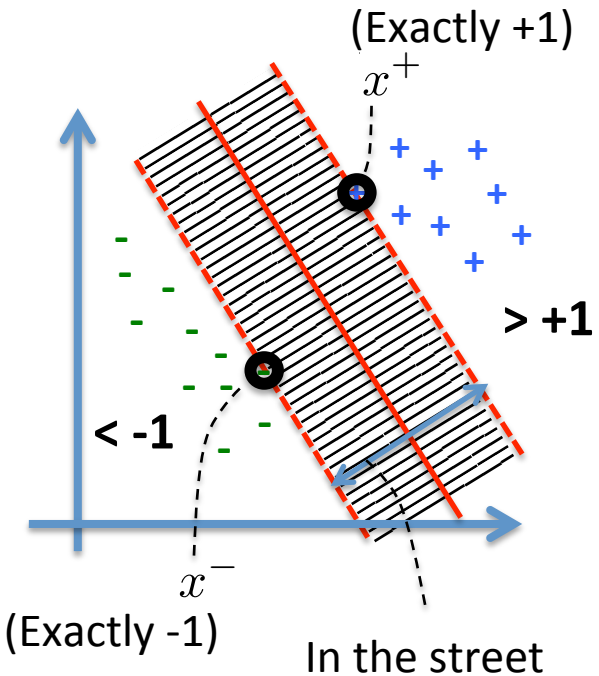


wide

1. Take the **median** of the street
2. Consider a vector $\mathbf{w}$ from origin perpendicular to it
3. Compute for any unknown spot $\mathbf{w} \cdot \mathbf{x} + \mathbf{b} \geq 0$
4. This allows to perform separation
5. So our decision function might look like

$$\mathbf{w} \cdot \mathbf{u} + \mathbf{b} \geq 0$$

Support Vector Machines



Based on our potential decision function

$$\underbrace{\mathbf{w}} \cdot \mathbf{u} + \mathbf{b} \geq 0$$

So far we only know that this is orthogonal to median

- How to ensure that we find **the widest** ?
- We can add two additional constraints

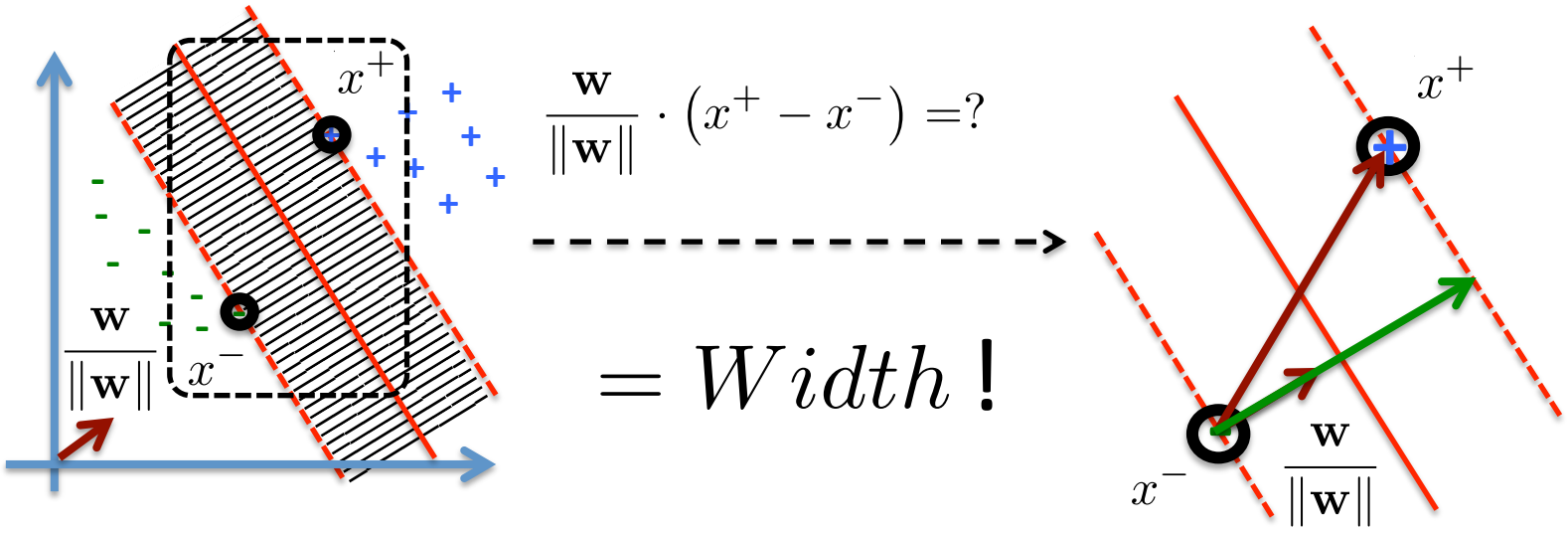
$$\begin{aligned} \mathbf{w} \cdot \mathbf{u}^+ + \mathbf{b} &\geq 1 \\ \mathbf{w} \cdot \mathbf{u}^- + \mathbf{b} &\leq -1 \end{aligned} \quad \Big\} \; y_i = {}^+/_-1$$

- Need a single function to optimize, introduce y_i

$$y_i \left(x_i \cdot \mathbf{w} + \mathbf{b} \right) - 1 \geq 0$$

1. Some elements « on the margin » have to be exactly $^+/_-1$ (labeled x^+ and x^-)
2. In the street the values goes from [-1;1], everything else is < -1 or > 1
3. We can take the x^+ and x^- vectors (*not* perpendicular to the median)

Support Vector Machines



- Dot product projects one on another and gives us the **width** of the street
- If we dot $\mathbf{w}$ with x^+ and with x^-, $\mathbf{b}$ drops if we substract

$$\left.\begin{aligned} \mathbf{w} \cdot \mathbf{x}^+ + \mathbf{b} &= 1 \\ \mathbf{w} \cdot \mathbf{x}^- + \mathbf{b} &= -1 \end{aligned}\right\} \quad \mathbf{w} \cdot (\mathbf{x}^+ - \mathbf{x}^-) = 2$$

$$\frac{\mathbf{w}}{\|\mathbf{w}\|} \cdot (x^+ - x^-) = \frac{2}{\|\mathbf{w}\|} = Width$$

minimize

maximize

Support Vector Machines

- So the goal is to solve $min\ \|\mathbf{w}\|$ under $+/-1$ constraints
- Looks like a form of Lagrange multipliers
- However Lagrange use equalities (instead of inequalities)
- Hence we need a search that can be written as the **primal formulation**

$$min\left(P\left(\mathbf{w},b\right)\right)=\frac{\|\mathbf{w}\|}{2}+t.\sum_{i}\varepsilon_{i}$$

Tradeoff error / margin minimization — **Minimize error**

- If we go through the Lagrange formulation, we find (*cf. 2nd part of this course*)

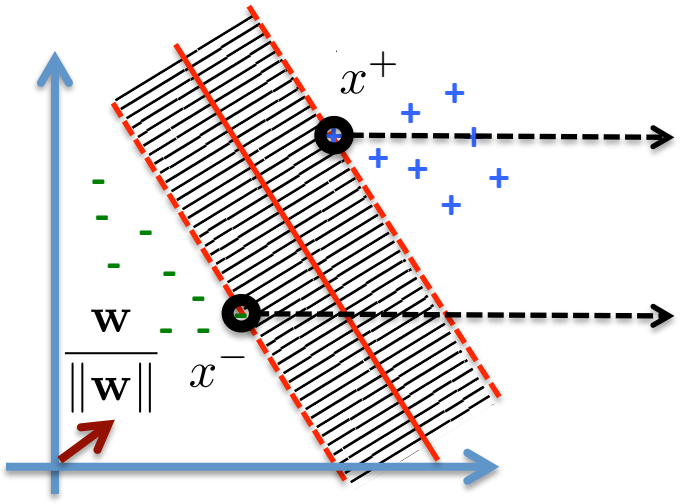
$$\mathbf{w}=\sum_{i}c_{i}\cdot x_{i}$$

Dual formulation (cf. end slides)

- So we can answer our problem, and all we need is
  - To optimize the c_i
  - Only requires the dot product

Support Vector Machines

- Based on our new formulation, a marvelous property appears $\mathbf{w} = \sum c_i \cdot x_i$
- Compared to neural nets, the space we are spanning is gloriously **convex**
- There is only **a global maximum**, no local ones
- You also discover that most $c_i = 0$ (so most points are useless)
- Only points on the fronteers *dictates* the value of $\mathbf{w}$



These points « support » the separation

=> Called **support vectors**

Support Vector Machines

- In order to obtain the complete problem to optimize
- We need to transform the problem to its **dual formulation**

$$max\left(w\left(\alpha\right)\right) = \sum_i \alpha_i - \frac{1}{2}\sum_i \sum_j \alpha_i \alpha_j y_i y_j x_i^T x_j$$

- Under the constraints

$$\sum_i \alpha_i y_i = 0 \quad \text{and} \quad \alpha_i \geq 0$$

- So we have a final equation in the form of

$$\mathbf{w} = \sum_{i=0}^{n} \alpha_i y_i x_i$$

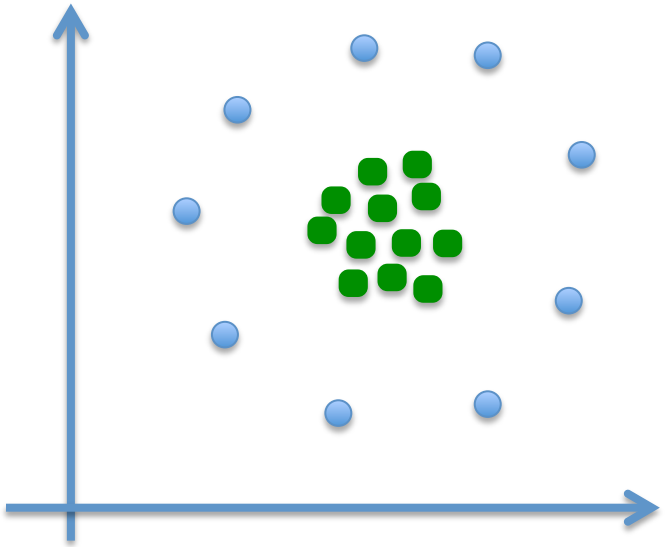
We need to optimize this

Value of decision

Coordinates in the space

Support Vector Machines

- Support Vector Machines (SVM) can find the **best straight line**
- And that is absolutely all that the SVM can do !...
- Unfortunately our world can rarely be separated by a straight line
- So **what to do when the data is non-linearly separable ?...**
- I am **stating** that the following groups can be separated by a single straight line



HOW ?

Support Vector Machines

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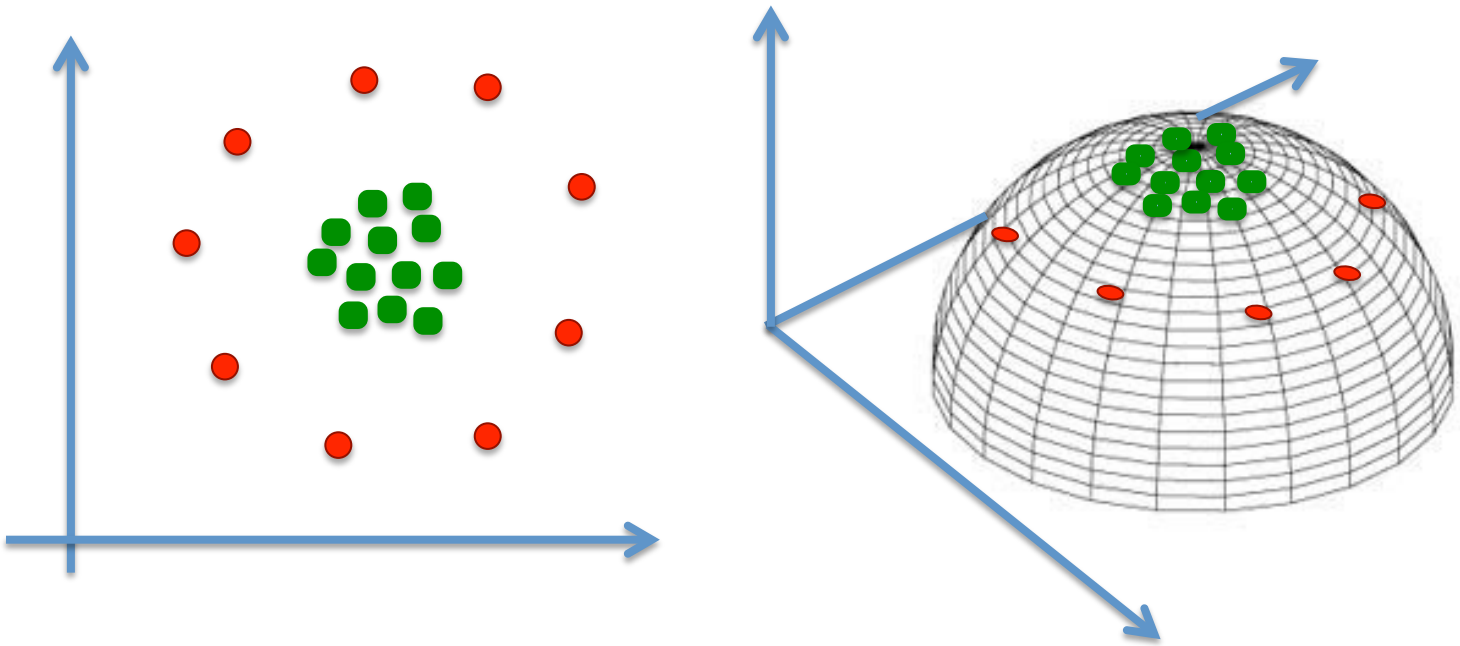
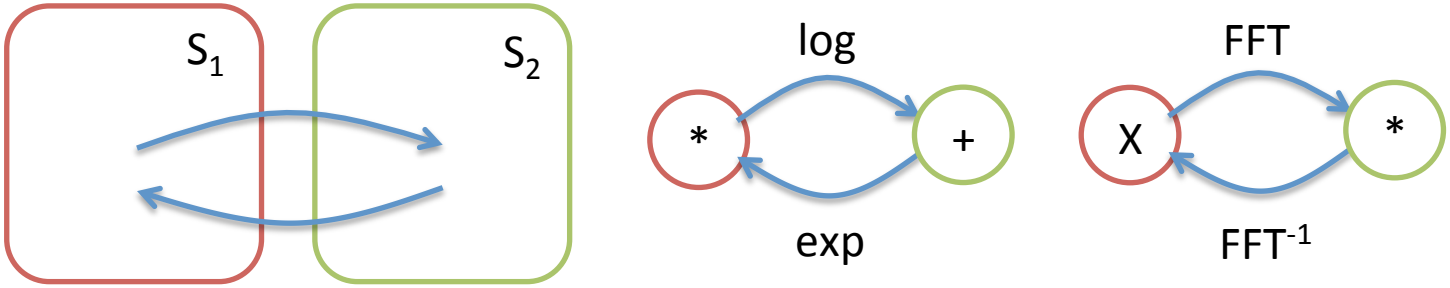
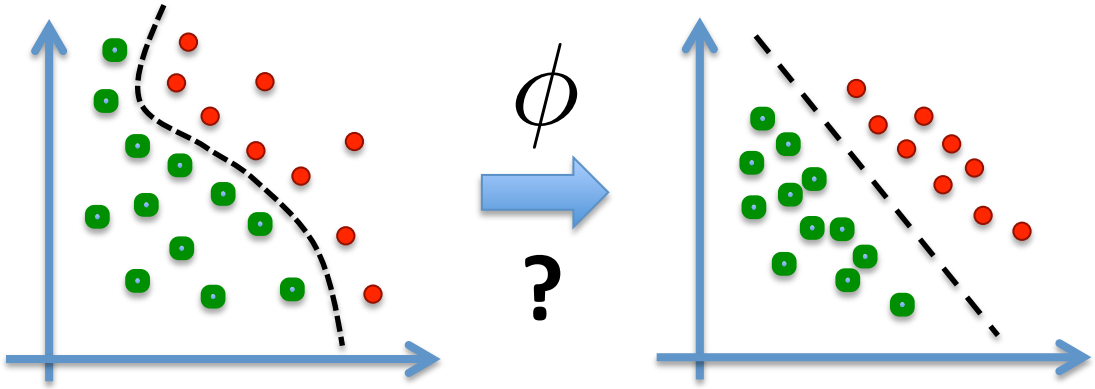


Support Vector Machines

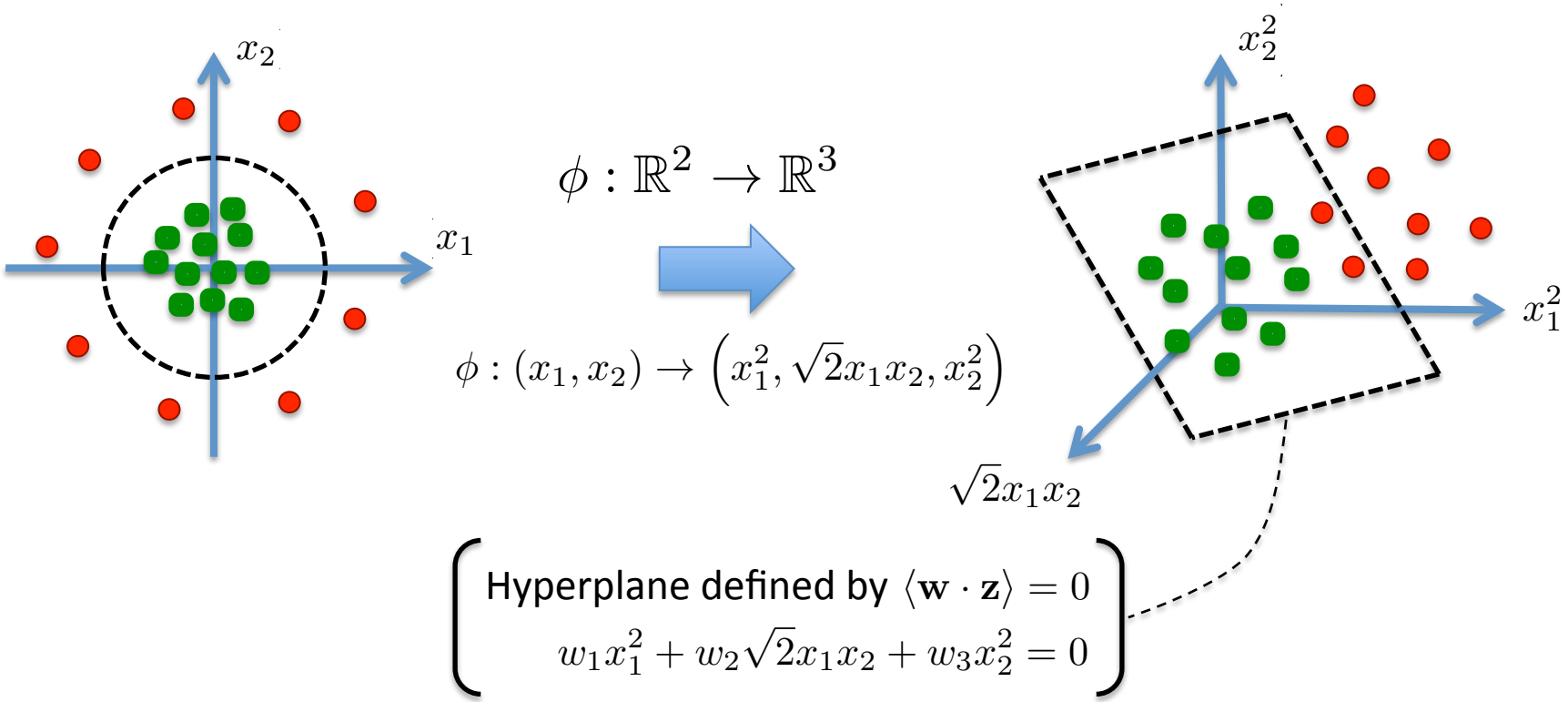
- If a problem is hard in a given space S_1
- It is usual to go to a second space S_2 where it is easier to solve
- And then apply the inverse transformation (going back from S_2 to S_1)



- Same here, if we don't have a straight line in S_1 maybe we have one in S_2



Support Vector Machines



Problem: The dimensionality of ϕ can be very large

- Vector $\mathbf{w}$ is hard to keep in memory with larger dimensions
- Quadratic programming is also hard to solve
- Instead of optimizing $\mathbf{w}$ directly, could we optimize only the α_i ?

Support Vector Machines

Reminder: We have been using the *primal formulation*

$$min\left(\frac{1}{2}\|\mathbf{w}\|^2\right) \quad \text{with constraint} \quad \forall i \; d_i\left(w \cdot x_i + w_0\right) \geq 1$$

- Both objectives are strictly convex
- Hence, we can express this as a Lagrangian

$$L\left(w, w_0, \alpha\right) = \frac{\|\mathbf{w}\|^2}{2} - \sum_i \alpha_i \left(d_i\left(w \cdot x_i + w_0\right) - 1\right)$$

- Remember that we want to maximize the margin, which means

$$\frac{\delta L}{\delta w_0} = 0 \Leftrightarrow \sum_i \alpha_i d_i \; = 0$$
$$\frac{\delta L}{\delta w} = 0 \Leftrightarrow w - \sum_i \alpha_i d_i x_i = 0 \Leftrightarrow w = \sum_i \alpha_i d_i x_i$$

- If we plug back this $\mathbf{w}$ into the primal formulation (as a Lagrangian)

$$L\left(w, w_0, \alpha\right) = \frac{1}{2}\left\langle \sum_i \alpha_i d_i x_i, \sum_j \alpha_j d_j x_j \right\rangle - \sum_i \alpha_i d_i \left(\sum_j \alpha_j d_j x_j\right) x_i - w_0 \sum_i \alpha_i d_i + \sum_i \alpha_i$$

$$= \qquad\qquad = 0$$

Support Vector Machines

We obtain the **dual formulation** of the SVM optimization

$$L(w, w_0, \alpha) = \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i d_i \alpha_j d_j \langle x_i, x_j \rangle$$

- Why should we care about the dual formulation?
- Remember that we want to perform a space transformation ϕ

Primal $F(x) = \sum_i w_i \cdot \phi(x_i) + w_0$

Need to actually do the transform ϕ

Dual $F(x) = \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i d_i \alpha_j d_j \langle \phi(x_i), \phi(x_j) \rangle$

There is no need to perform the transform ϕ
We just need to define the behavior of $K(x_i, x) = \phi(x_i) \cdot \phi(x_j)$

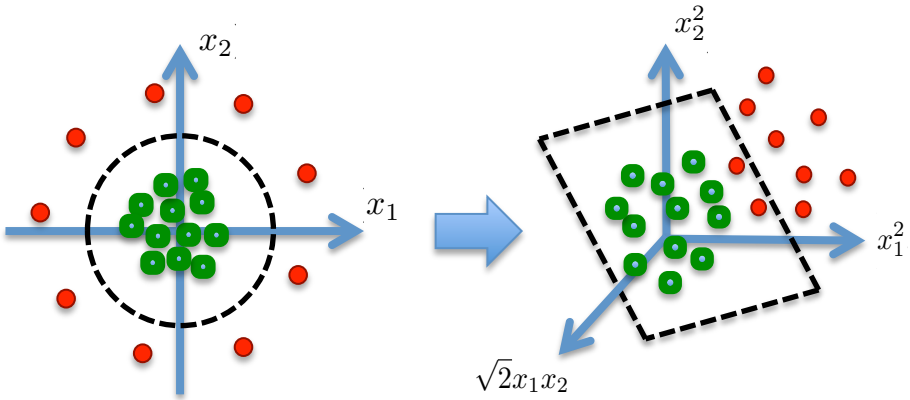
Math magic: We don't need to know what ϕ is but just what $\phi(x_i) \cdot \phi(x_j)$ does

Support Vector Machines

Remember our example transform ϕ ?

$$\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

$$\phi : (x_1, x_2) \rightarrow \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right)$$



What happens if we just introduce

$$K(x, z) = \langle x, z \rangle^2$$

(the square of the dot product)

$$\begin{aligned} K(x, z) &= \langle x, z \rangle^2 = (x_1z_1 + x_2z_2)^2 \\ &= \left(x_1^2z_1^2 + 2x_1z_1x_2z_2 + x_2^2z_2^2\right) \\ &= \left\langle \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right) \cdot \left(z_1^2, \sqrt{2}z_1z_2, z_2^2\right) \right\rangle \\ &= \langle \phi(x) \cdot \phi(z) \rangle \end{aligned}$$

Can be plugged directly into the dual formulation without even having to compute the transform ϕ

Dual

$$F(x) = \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i d_i \alpha_j d_j \langle \phi(x_i), \phi(x_j) \rangle$$

Support Vector Machines

Decision $f(x) = \sum_i \alpha_i \phi(x_i) \cdot \phi(x_j) + b$

Kernel function $K(x_i, x) = \phi(x_i) \cdot \phi(x_j)$

Some of the most used kernel functions are

Polynomial $K(x, y) = \left(x^T y + 1\right)^d$

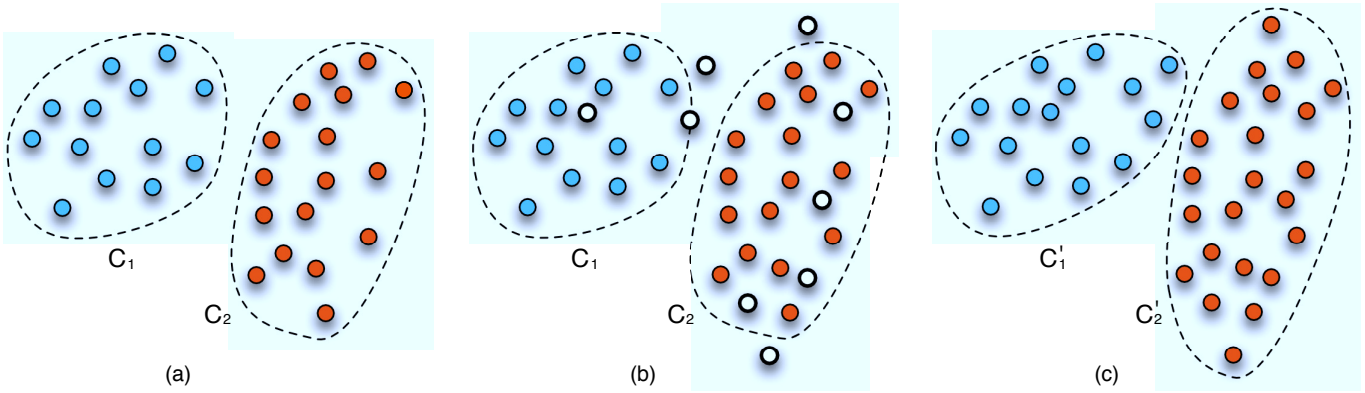
Gaussian $K(x, y) = exp(-\psi(x - y)^2)$

Radial Basis $K(x, y) = exp\left(-\|x-y\|^2/(2\sigma^2)\right)$

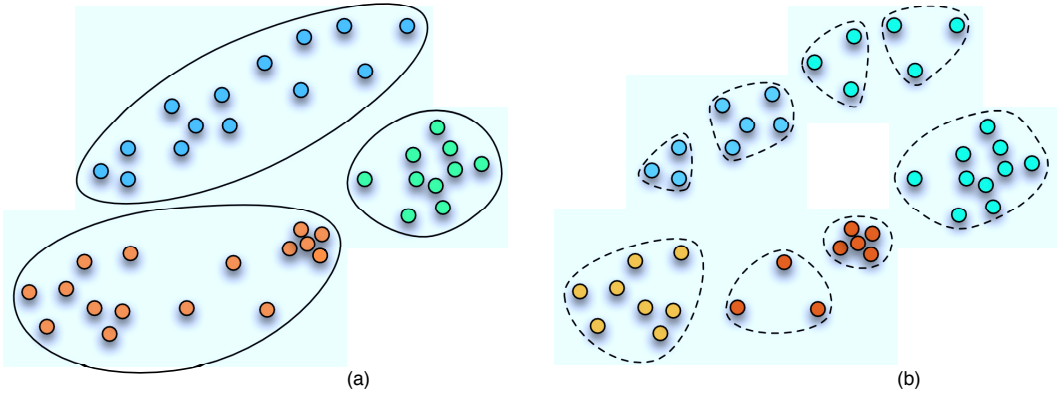
Sigmoïd $K(x, y) = tanh\left(kx^T y + \Theta\right)$

Clustering

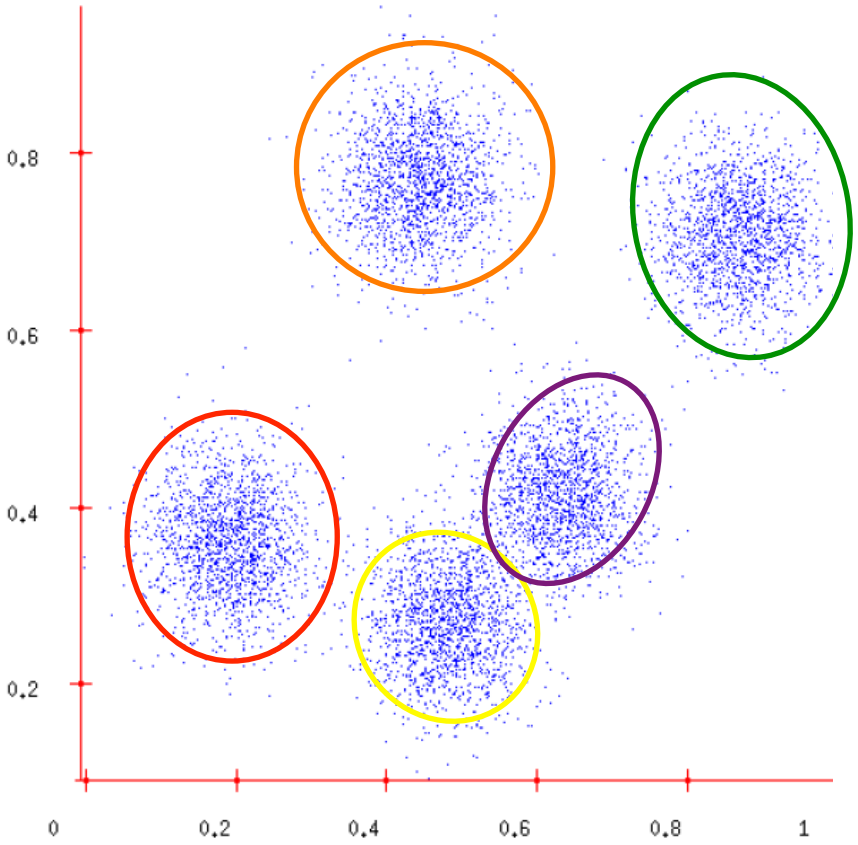
- So far we have dealt with the **classification** problem
- Based on labeled training data, we want to find the class of unlabeled



- But what happens if we don't have any prior knowledge on the data?

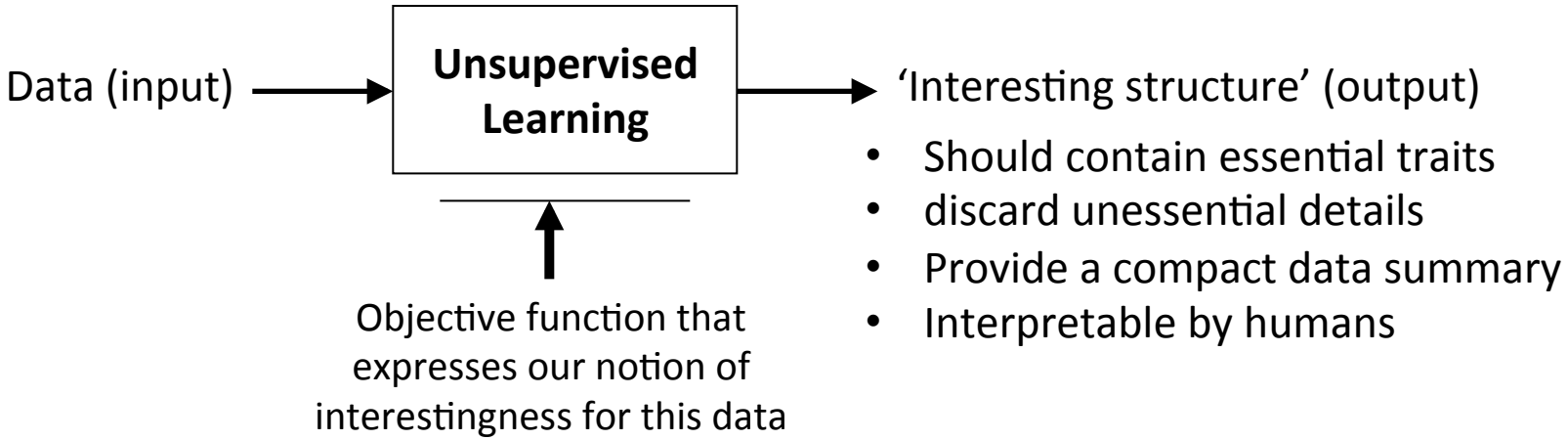


Clustering example



Clustering

- Attach label to each observation or data points in a set
- You can say this is "unsupervised classification"
- Clustering is alternatively called as "grouping"
- You want to assign same label to data points that are "close"
- Thus, clustering algorithms rely on a distance metric between data points
- Sometimes, it is said that the for clustering, the distance metric is more important than the clustering algorithm



What we need for clustering

Data matrix

$$\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}$$

Dissimilarity matrix

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & & \\ d(n,1) & d(n,2) & \cdots & \cdots & 0 \end{bmatrix}$$

(Dis)similarity between objects

- Distances are normally used to measure the similarity or dissimilarity between two data objects
- Some popular ones include: *Minkowski distance*:

$$d(i,j) = \sqrt[q]{(|x_{i_1} - x_{j_1}|^q + |x_{i_2} - x_{j_2}|^q + \ldots + |x_{i_p} - x_{j_p}|^q)}$$

where $i = (x_{i1}, x_{i2}, \ldots, x_{ip})$ and $j = (x_{j1}, x_{j2}, \ldots, x_{jp})$ are two p-dimensional data objects, and q is a positive integer

- If $q = 1$, d is Manhattan distance

$$d(i,j) = |x_{i_1} - x_{j_1}| + |x_{i_2} - x_{j_2}| + \ldots + |x_{i_p} - x_{j_p}|$$

- *If* $q = 2$, d is Euclidean distance

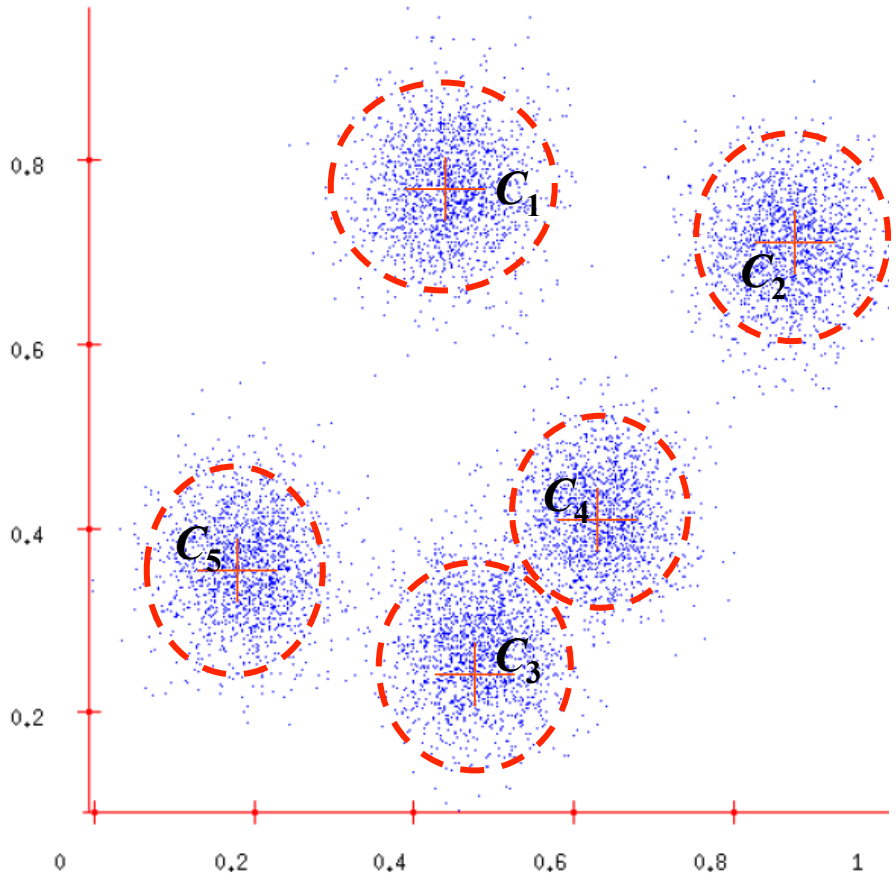
$$d(i,j) = \sqrt{(|x_{i_1} - x_{j_1}|^2 + |x_{i_2} - x_{j_2}|^2 + \ldots + |x_{i_p} - x_{j_p}|^2)}$$

- Also one can use weighted distance, parametric Pearson product moment correlation, or other disimilarity measures.

Distance-based clustering

- Assign a distance measure between data
- Find a partition such that:
  - Distance between objects within partition (I.e. same cluster) is minimized
  - Distance between objects from different clusters is maximised
- Issues :
  - Requires defining a distance (similarity) measure in situation where it is unclear how to assign it
  - What relative weighting to give to one attribute vs another?
  - Number of possible partition us superexponential

A « good » clustering ?



We can evaluate the distance **within-clusters**

$$argmin_{C_j, m_{i,j}} (\sum_j \sum_i (x_i - C^j))$$

based on the centroid of each

With the membership functions and the conditions

$$m_{i,j} = \begin{cases} 1 & x_i \in \text{the j-th cluster} \\ 0 & x_i \notin \text{the j-th cluster} \end{cases}$$

$$\sum_j m_{i,j} = 1$$

$\rightarrow$ any $x_i \in$ a single cluster

How to efficiently cluster ?

$$argmin_{C_j, m_{i,j}} \left(\sum_j \sum_i (x_i - C^j) \right)$$

based on the centroid of each

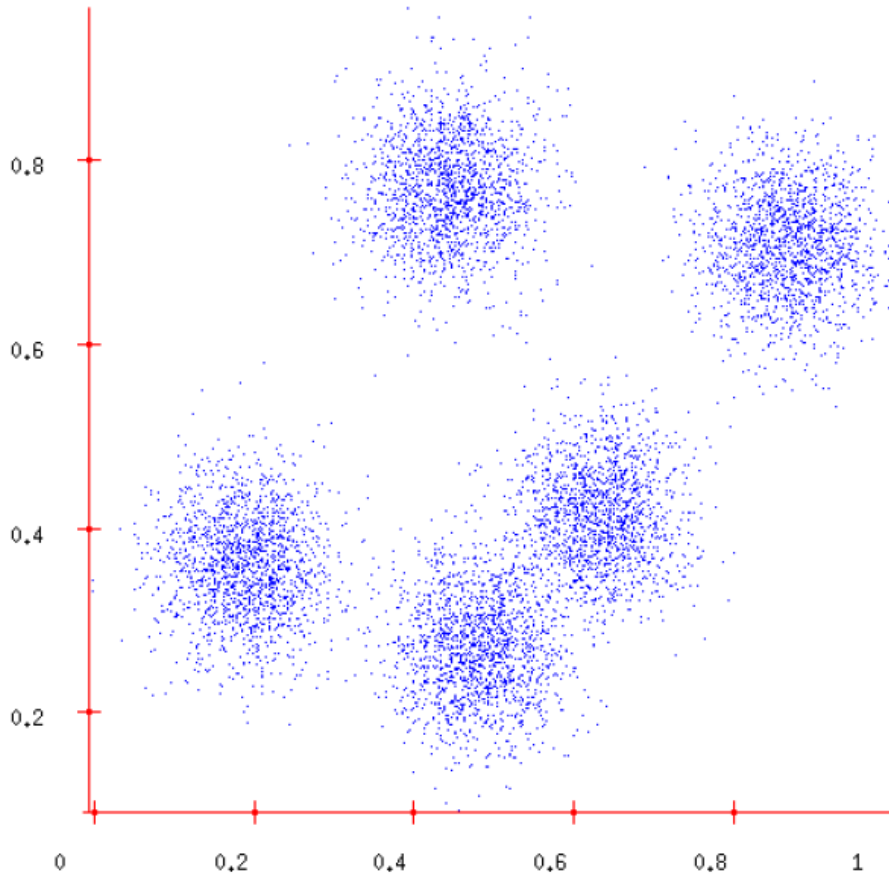
Memberships $\{m_{i,j}\}$ and centroids $\{C_j\}$ are correlated.

So we could somehow reverse the paradigm

$$\text{Given centroids } \{C_j\},\ m_{i,j} = \begin{cases} 1 & j = \arg\min_k (x_i - C_j)^2 \\ 0 & \text{otherwise} \end{cases}$$

$$\text{Given memberships } \{m_{i,j}\},\ C_j = \frac{\sum_{i=1}^{n} m_{i,j} x_i}{\sum_{i=1}^{n} m_{i,j}}$$

K-Means for clustering



- **K-means algorithm**

1. Start with a random guess of cluster centers
2. Determine the membership of each data points
3. Adjust the cluster centers

Loop with stop criterion based on
1. Iterations number
2. Quality criterion
3. Evolution of quality

Formalising *stop criterions*

- Define a **measure of cluster compactness** (total distance from the cluster mean)

$$\sum_{\mathbf{x}_n \in \mathcal{C}_k} ||\mathbf{x}_n - \mathbf{m}_k||^2 = \sum_{n=1}^{N} z_{kn} ||\mathbf{x}_n - \mathbf{m}_k||^2$$

where the cluster mean is defined as

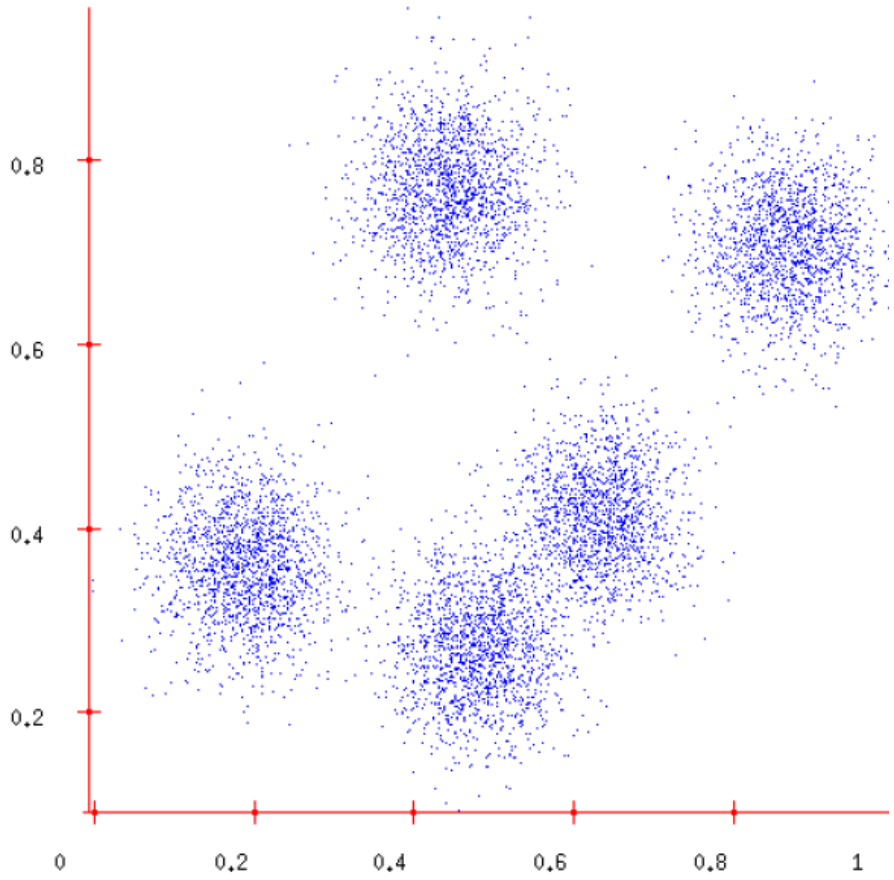
$$\mathbf{m}_k = \frac{1}{N_k} \sum_{\mathbf{x}_n \in \mathcal{C}_k} \mathbf{x}_n$$

and $N_k = \sum_{n=1}^{N} z_{kn}$ is the total number of points allocated to cluster K

- Define a **measure of cluster quality**

$$\mathcal{E}_K = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{kn} ||\mathbf{x}_n - \mathbf{m}_k||^2$$

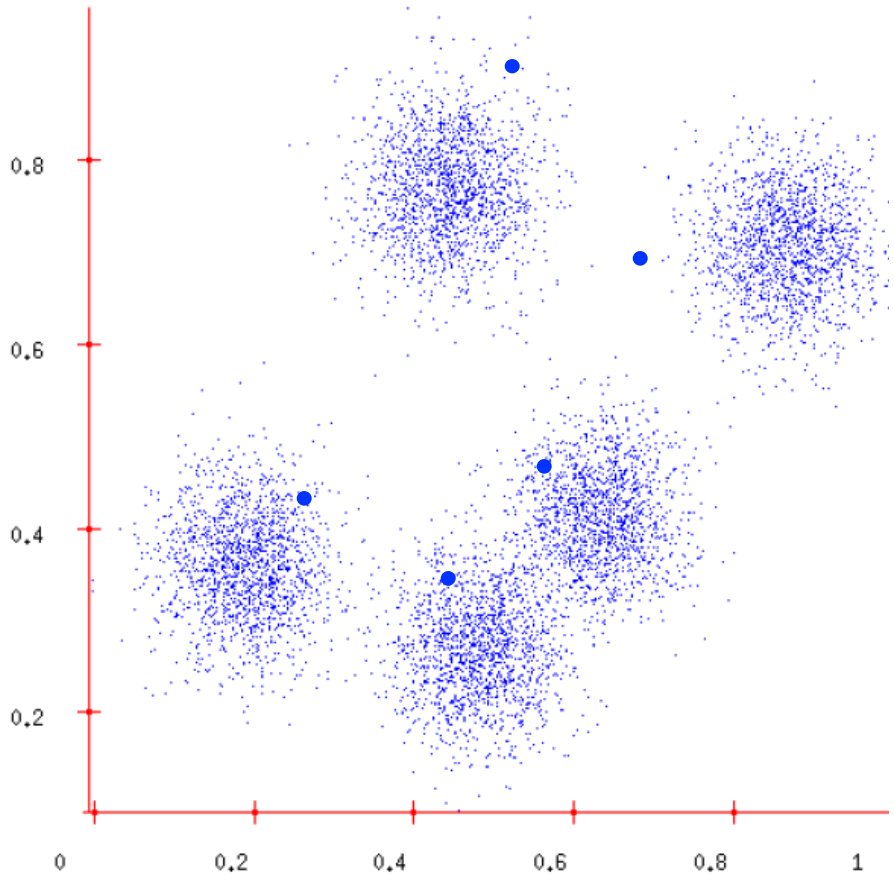
K-Means for clustering



- **K-means algorithm**

  1. Ask user how many clusters (here we set K=5)

K-Means for clustering



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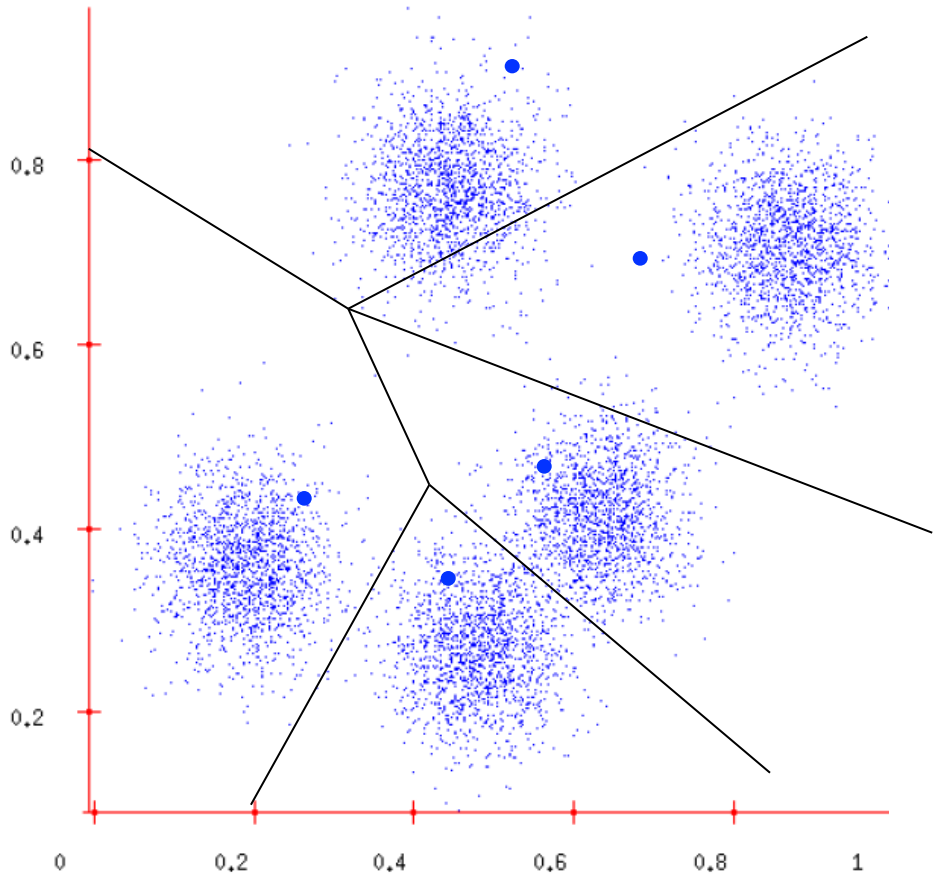

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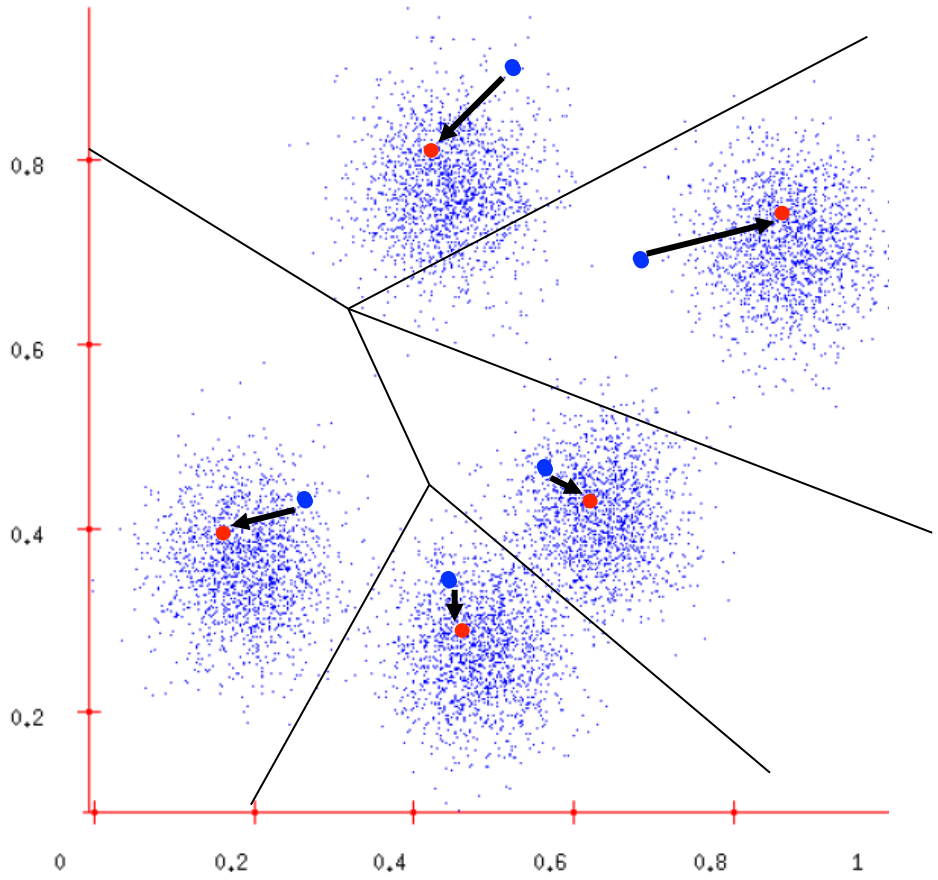
3. Each datapoint finds out which Center its closest to. (each Center "owns" a set of points)

K-Means for clustering



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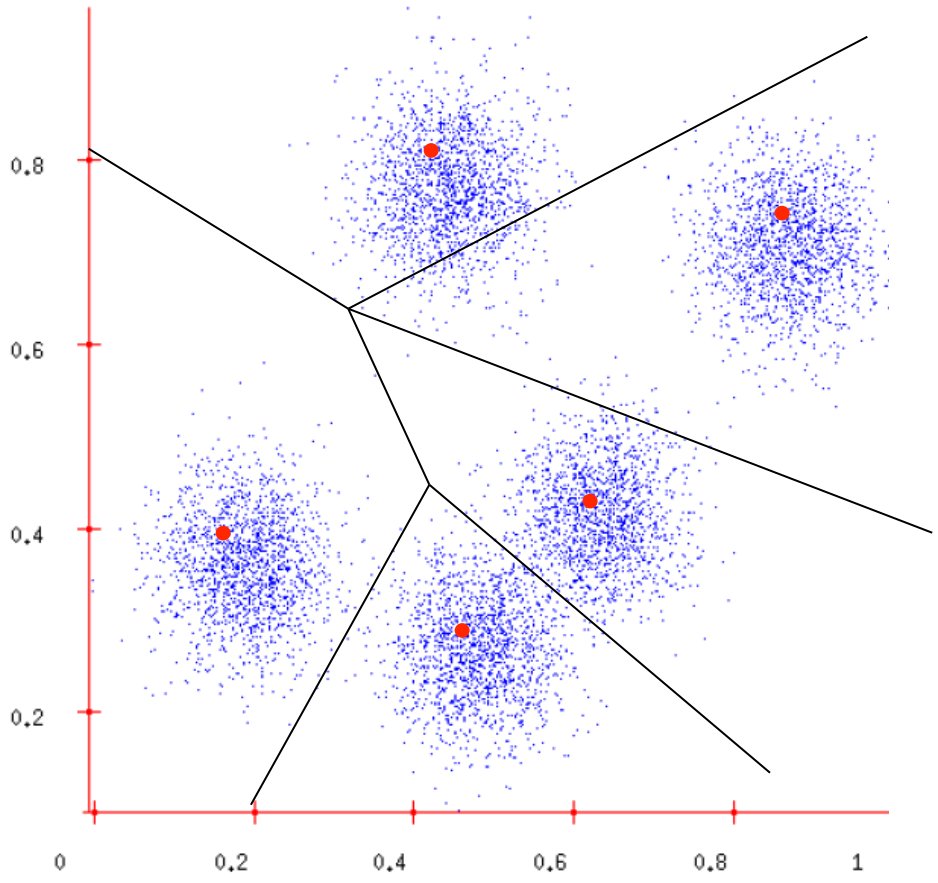
K-Means for clustering



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Computational Complexity: O(N) where N is the number of points?

Problems of K-means

1. Obviously the number of clusters K
2. But even with the right number, will we find a good optima?

3. Also highly depends on the random start
4. We could perform several runs of K-means

K-Means for clustering

- Strength
  - *Relatively efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, $k, t << n$.
  - Often terminates at a *local optimum*. The *global optimum* may be found using techniques such as: *deterministic annealing* and *genetic algorithms*
- Weakness
  - Applicable only when *mean* is defined, then what about categorical data?
  - Need to specify *k,* the *number* of clusters, in advance
  - Unable to handle noisy data and *outliers*
  - Not suitable to discover clusters with *non-convex shapes*

Variations of K-means

- A few variants of the *k-means* which differ in
  - Selection of the initial *k* means
  - Dissimilarity calculations
  - Strategies to calculate cluster means
- Handling categorical data: *k-modes* (Huang'98)
  - Replacing means of clusters with modes
  - Using new dissimilarity measures to deal with categorical objects
  - Using a frequency-based method to update modes of clusters
  - A mixture of categorical and numerical data: *k-prototype* method

K-medoids clustering

- *K*-means is appropriate when we can work with Euclidean distances
- Thus, *K*-means can work only with numerical, quantitative variable types
- Euclidean distances do not work well in at least two situations
  - Some variables are categorical
  - Outliers can be potential threats
- A general version of *K*-means algorithm called *K*-medoids can work with any distance measure
- *K*-medoids clustering is computationally more intensive

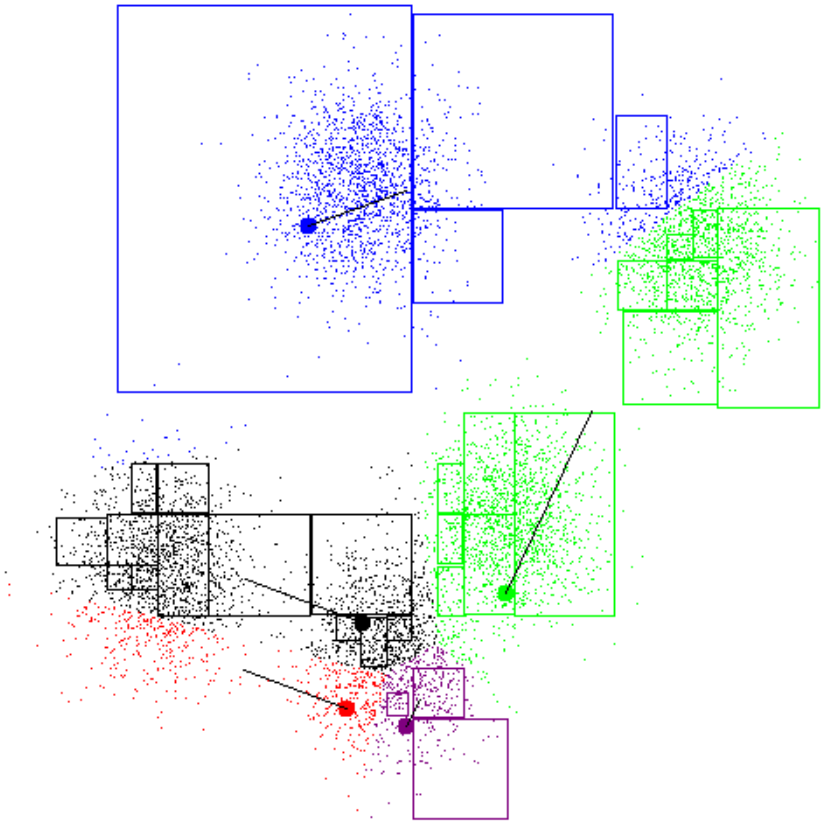
K-medoids algorithm

- Step 1: For a given cluster assignment C, find the observation in the cluster minimizing the total distance to other points in that cluster: $i_k^* = \underset{\{i:C(i)=k\}}{\arg\min} \sum_{C(j)=k} d(x_i, x_j).$
- Step 2: Assign $m_k = x_{i_k^*}, \; k = 1,2,\ldots,K$
- Step 3: Given a set of cluster centers $\{m_1, \ldots, m_K\}$, minimize the total error by assigning each observation to the closest (current) cluster center:

$$C(i) = \underset{1 \le k \le K}{\arg\min} \, d(x_i, m_k), \; i = 1,\ldots,N$$

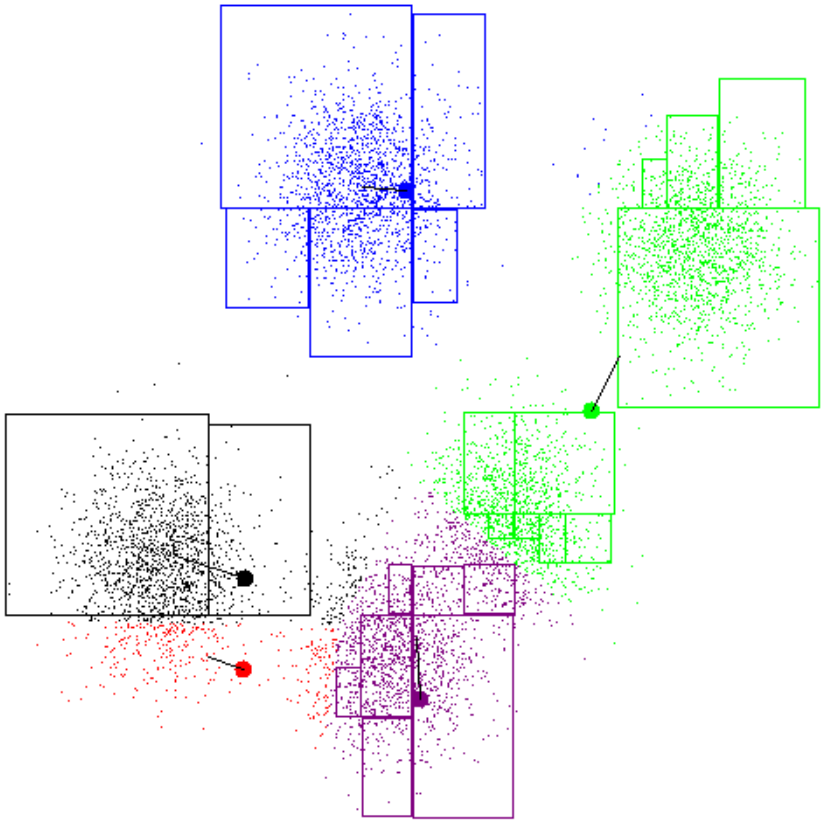
- Iterate steps 1 to 3

Improving K-means



- Group points by region
  - KD tree
  - SR tree
- **Key difference**
  - Find the closest center for each rectangle
  - Assign all the points within a rectangle to one cluster

Improving K-means



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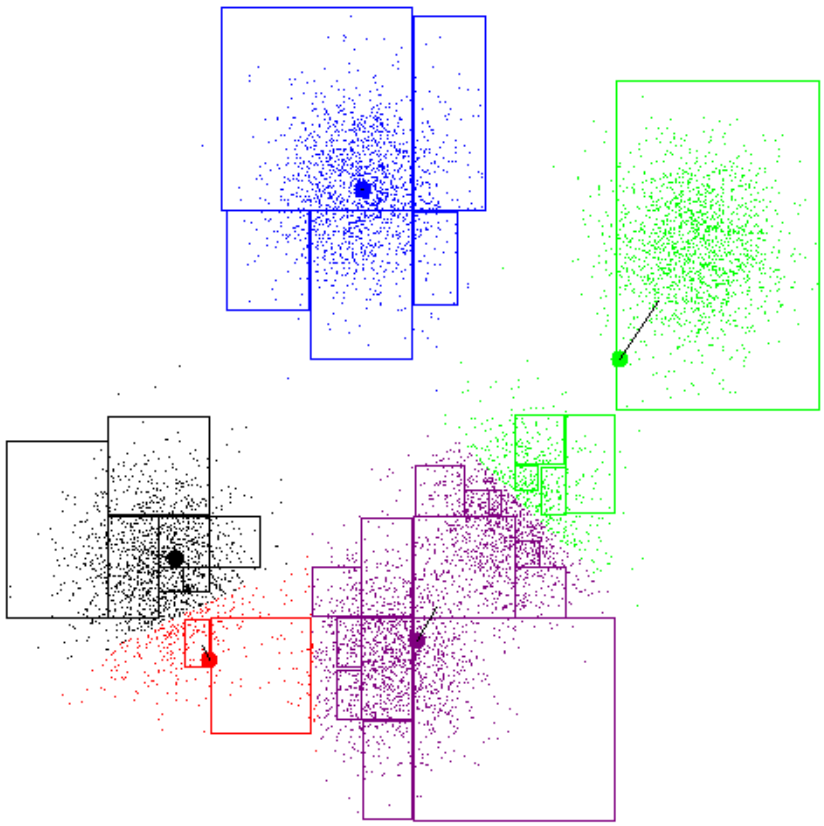

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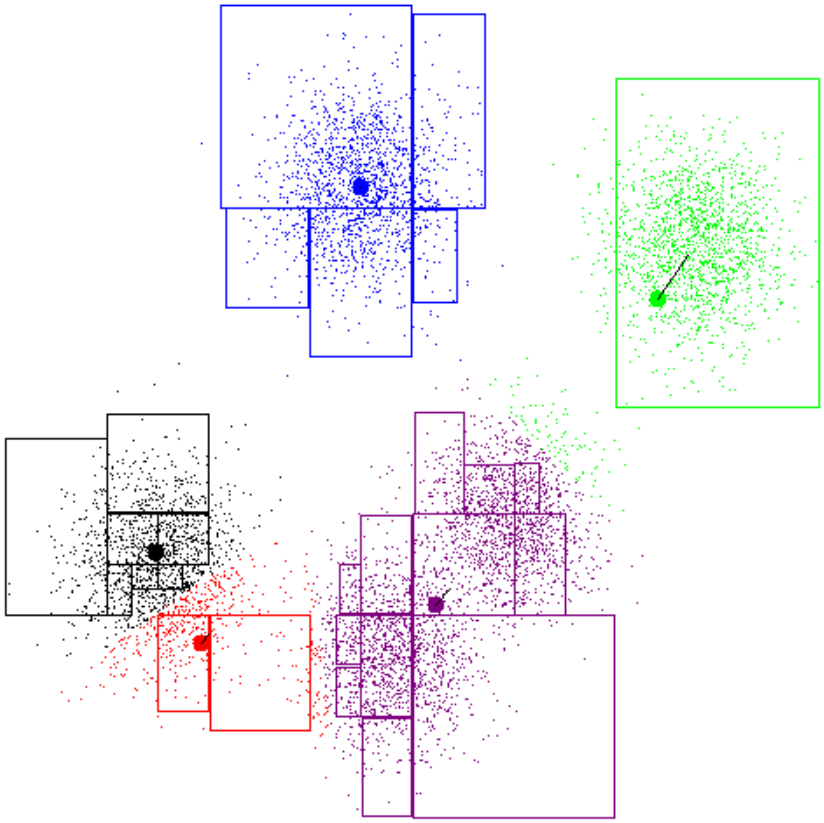

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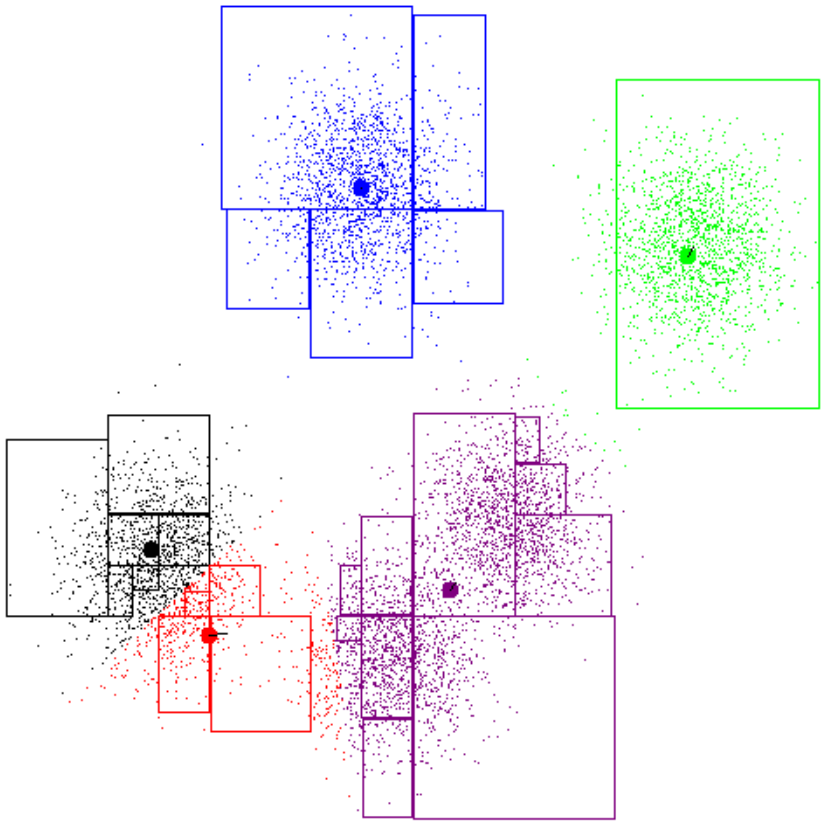

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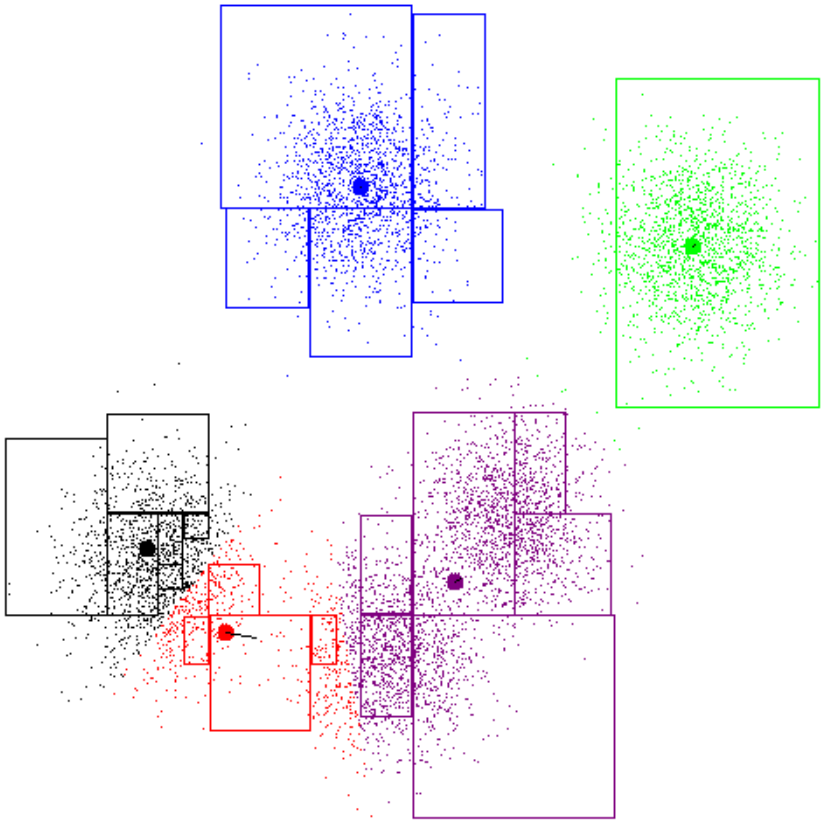

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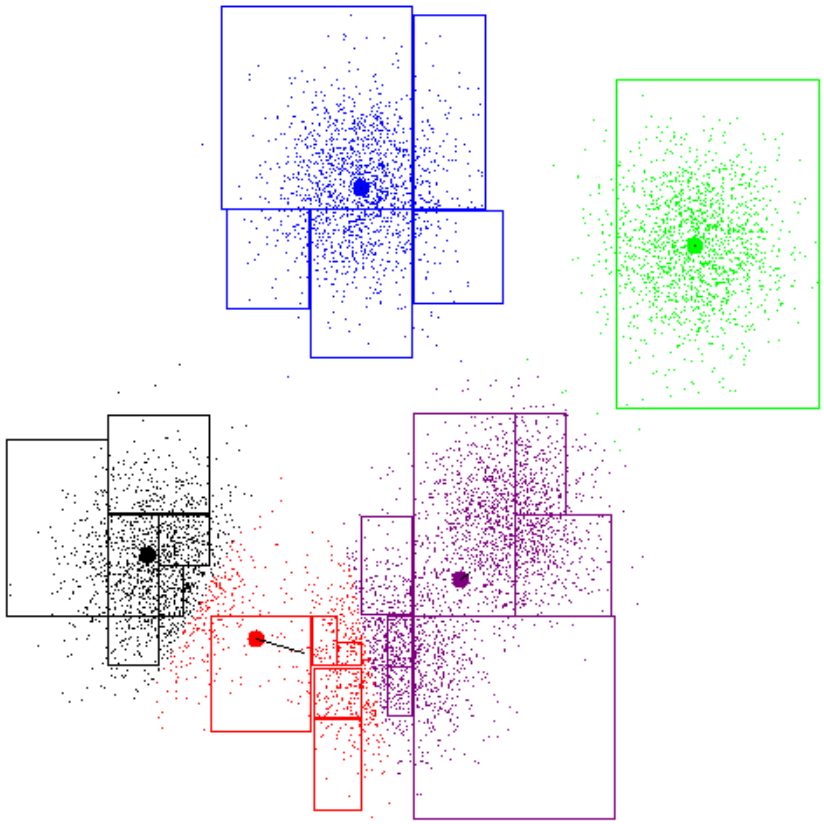

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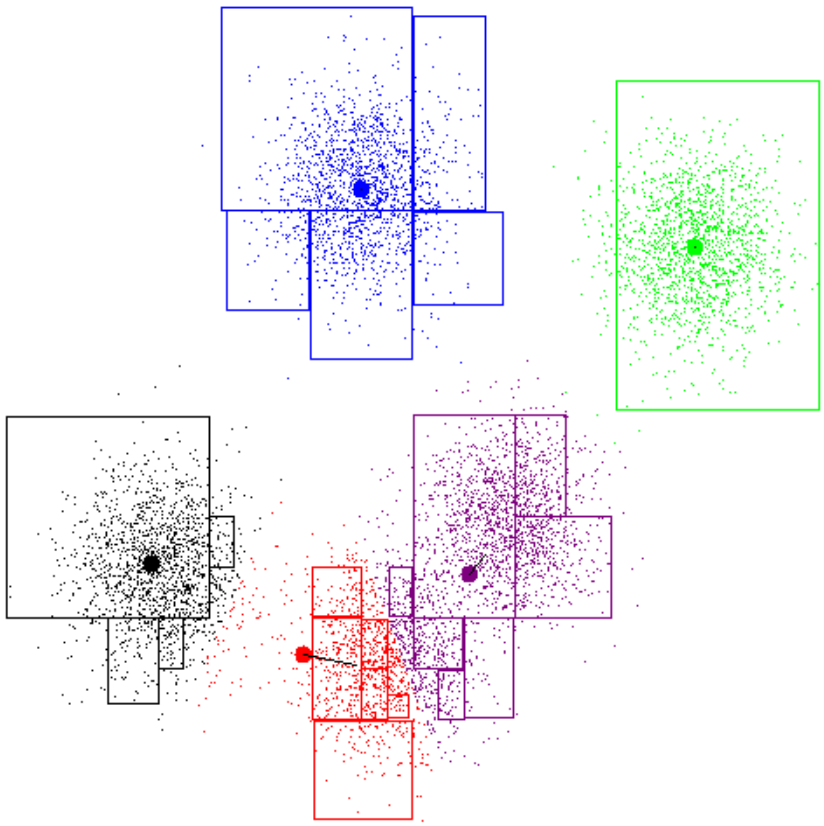

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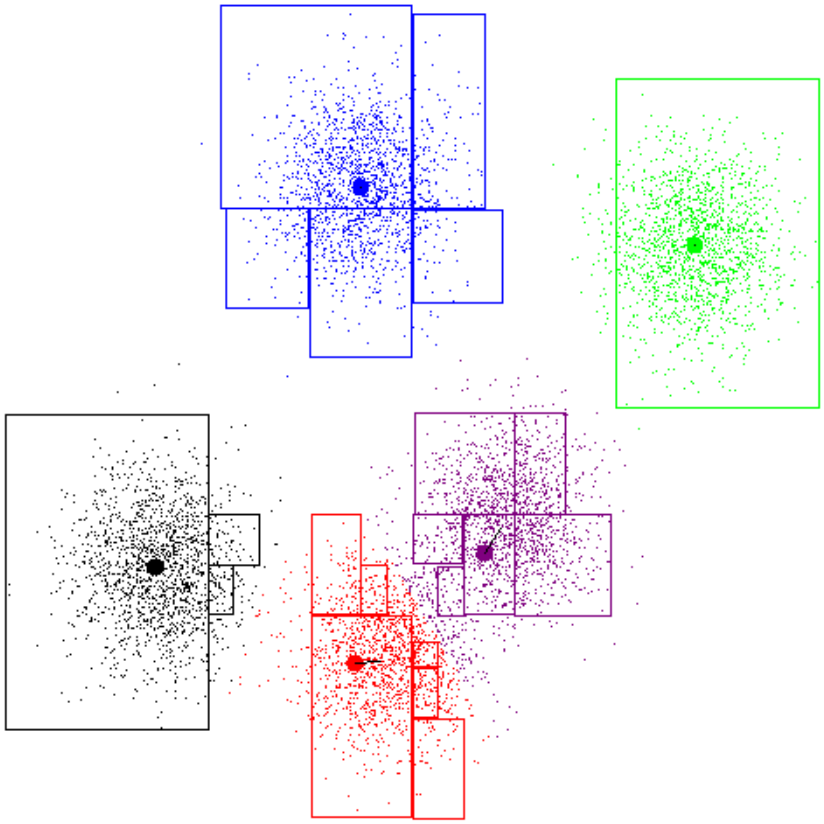

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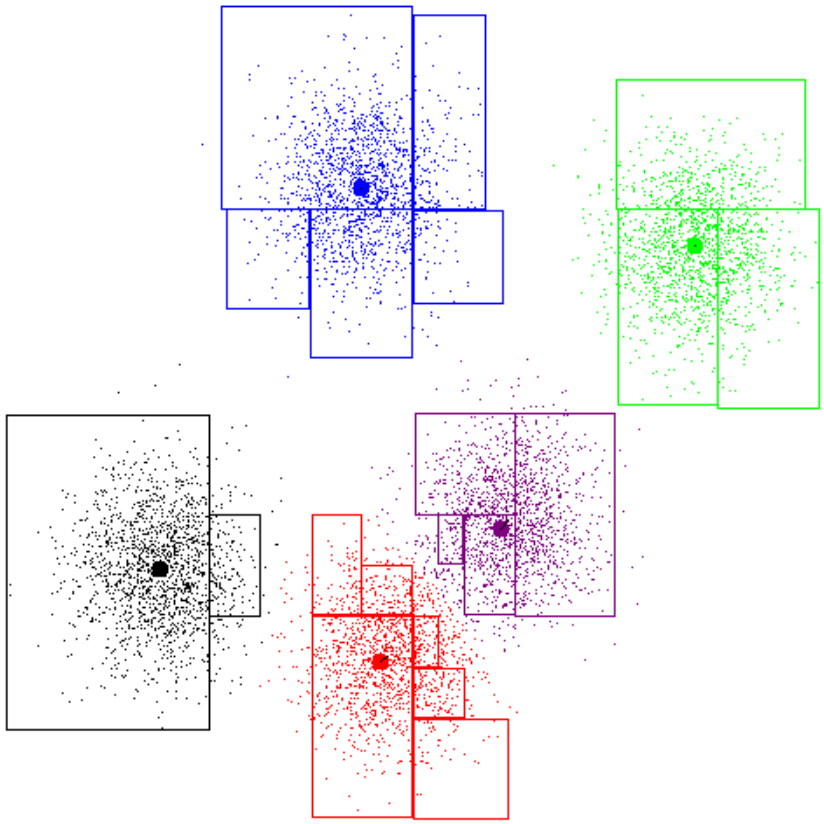

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Choice of K?

- Can $W_K(C)$, *i.e.*, the within cluster distance as a function of K serve as any indicator?
- Note that $W_K(C)$ decreases monotonically with increasing K. That is the within cluster scatter decreases with increasing centroids.
- Instead look for gap statistics (successive difference between $W_K(C)$):

$$\{W_K - W_{K+1} : K < K^*\} >> \{W_K - W_{K+1} : K \geq K^*\}$$

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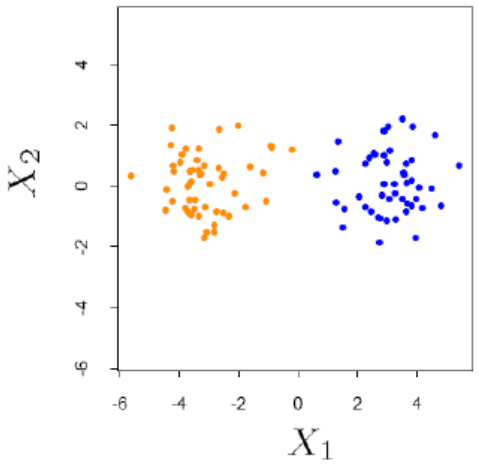
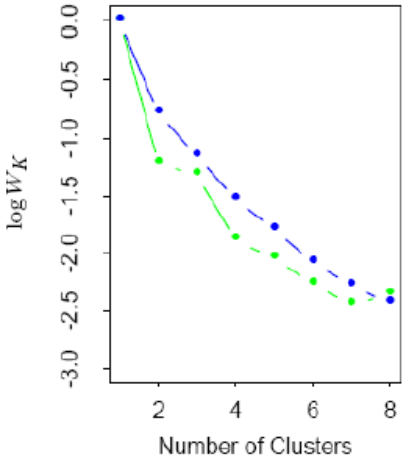
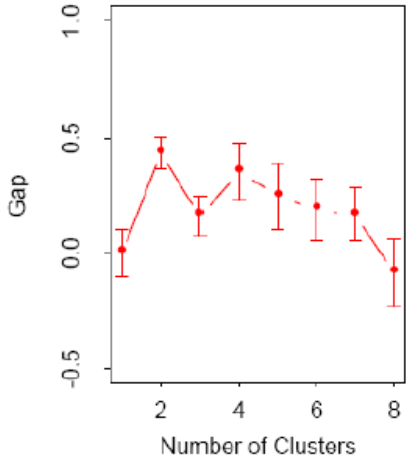


Data points simulated from two pdfs



Log(W_K) curve



Gap curve

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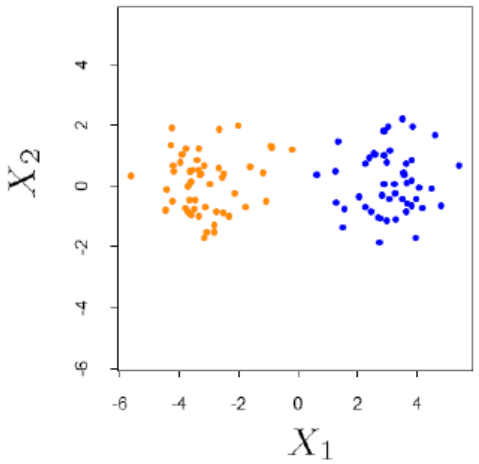

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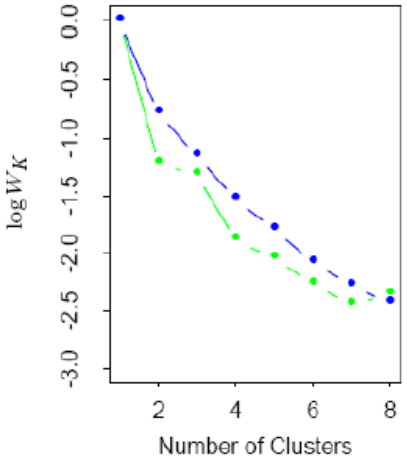

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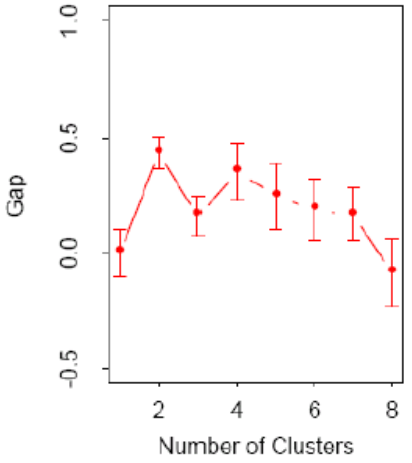
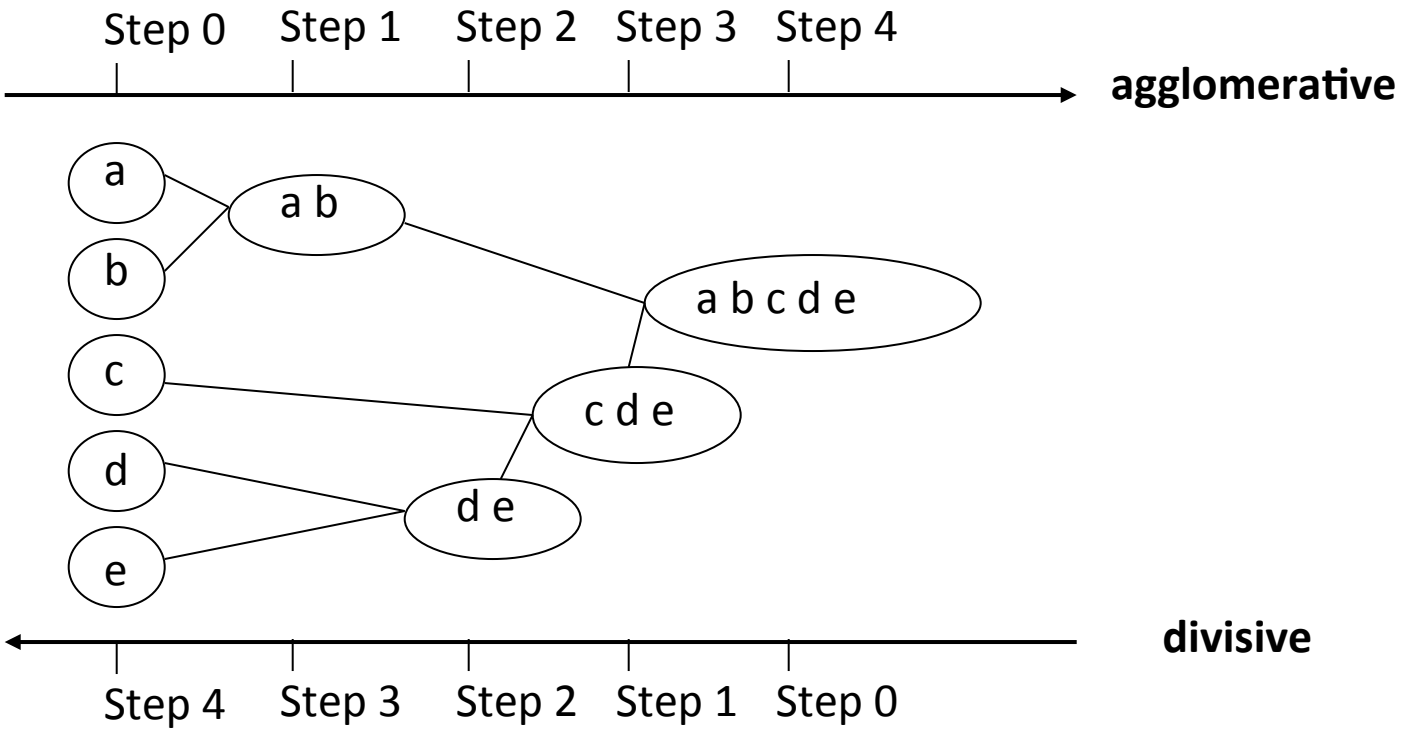


Gap curve

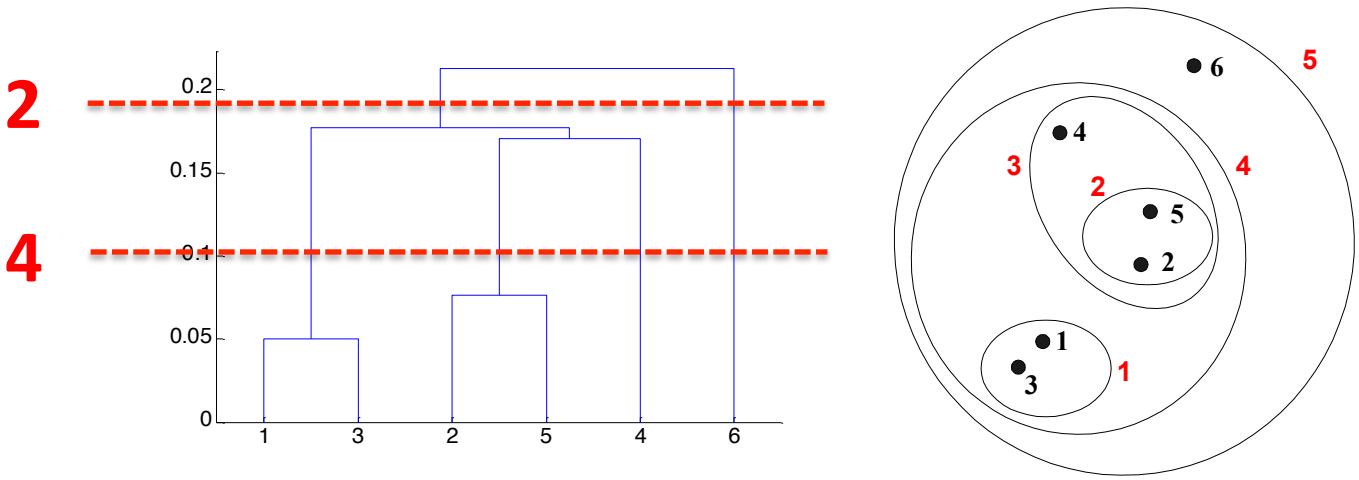
Hierarchical clustering

- Use distance matrix as clustering criteria. This method does not require the number of clusters ***k*** as an input, but needs a termination condition



Hierarchical clustering

- Produces set of ***nested clusters*** organized as hierarchical tree
- Can be visualized as a **dendrogram**
  - A tree-like diagram that records the sequences of merges or splits
  - A clustering can be obtained by trimming the tree



Hierarchical clustering

- Two main types of hierarchical clustering
  - **Agglomerative:**
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or **k** clusters) left
  - **Divisive:**
    - Start with one, all-inclusive cluster
    - At each step, split a cluster until each cluster contains a point (or there are **k** clusters)
- Traditional hierarchical algorithms use a similarity or distance matrix
  - Merge or split one cluster at a time

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- Produces set of ***nested clusters*** organized as hierarchical tree
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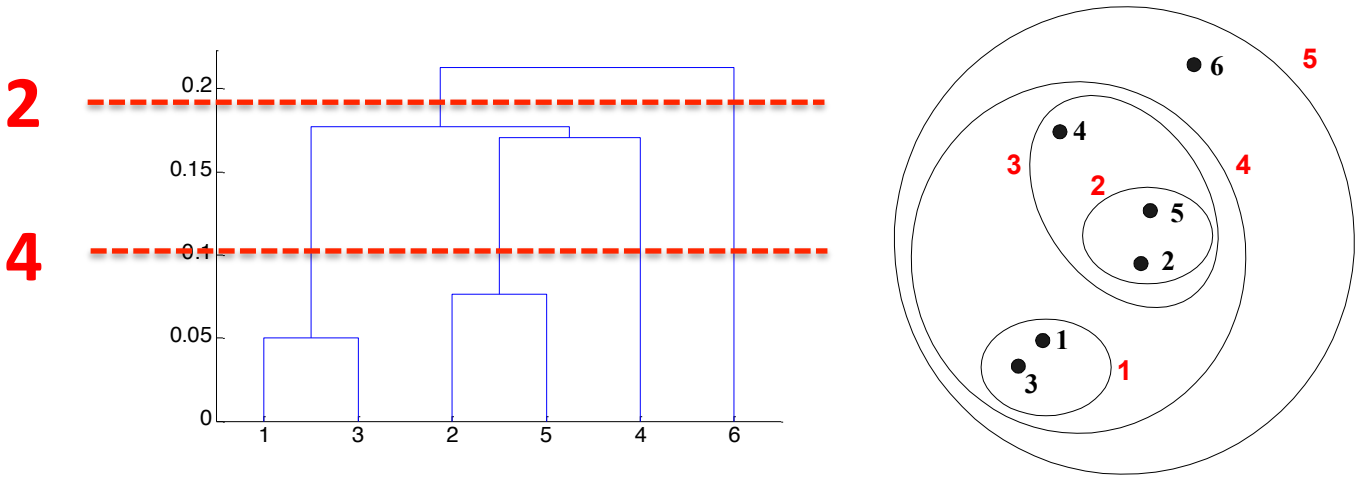


Hierarchical clustering

Strength

- No assumptions on the number of clusters
  - Any desired number of clusters can be obtained by 'cutting' the dendogram at the proper level
- Hierarchical clusterings may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., phylogeny reconstruction, etc), web (e.g., product catalogs) etc

Complexity

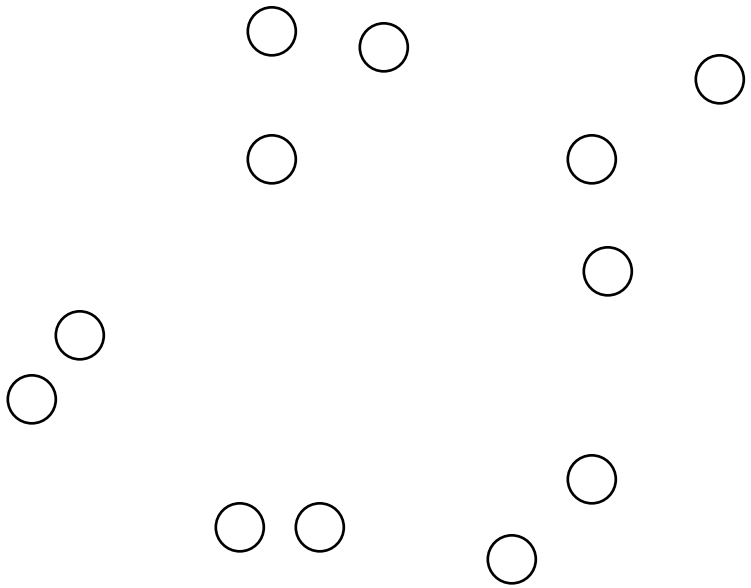
- Distance matrix is used for deciding which clusters to merge/split
- At least quadratic in the number of data points
- Not usable for large datasets

Agglomerative clustering

- Most popular hierarchical clustering technique
- Basic algorithm
  1. Compute the distance matrix between the input data points
  2. Let each data point be a cluster
  3. **Repeat**
  4. Merge the two closest clusters
  5. Update the distance matrix
  6. **Until** only a single cluster remains
- Key operation is the computation of the distance between two clusters
  - Different definitions of the distance between clusters lead to different algorithms

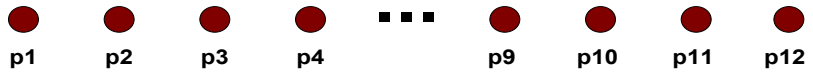
Hierarchical clustering

- Start with clusters of individual points and a distance/proximity matrix



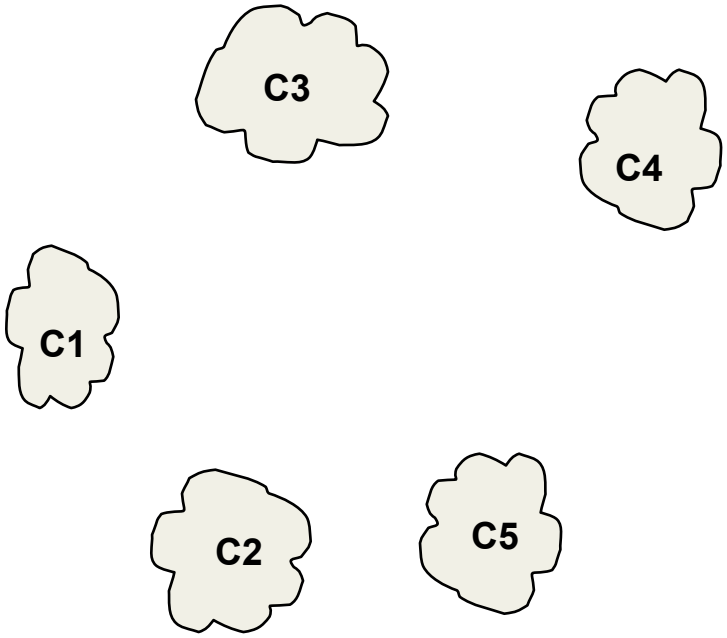
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						

Distance/Proximity Matrix



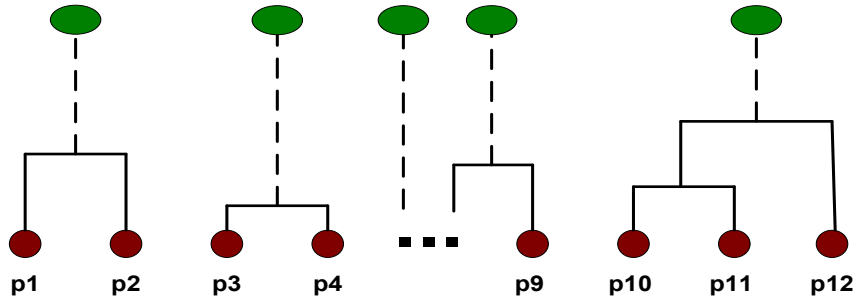
Hierarchical clustering

- After some merging steps, we have some clusters



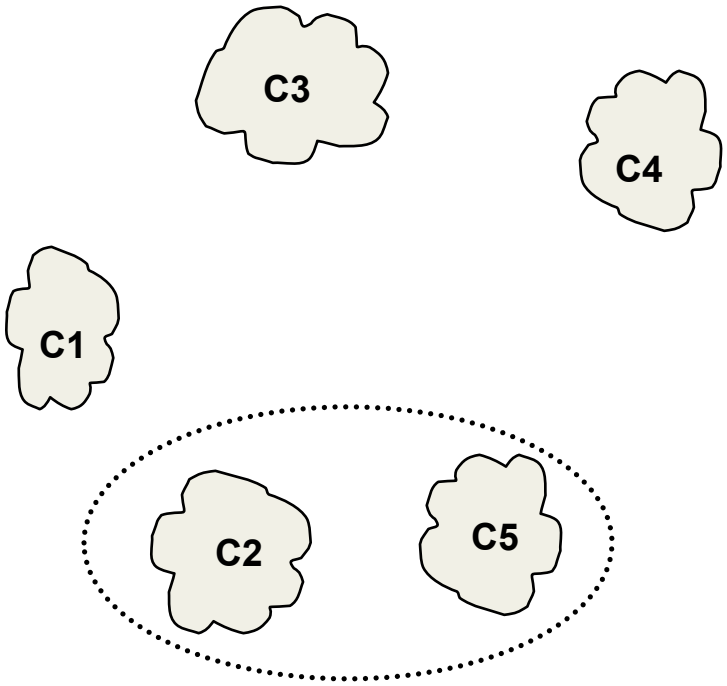
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Distance/Proximity Matrix



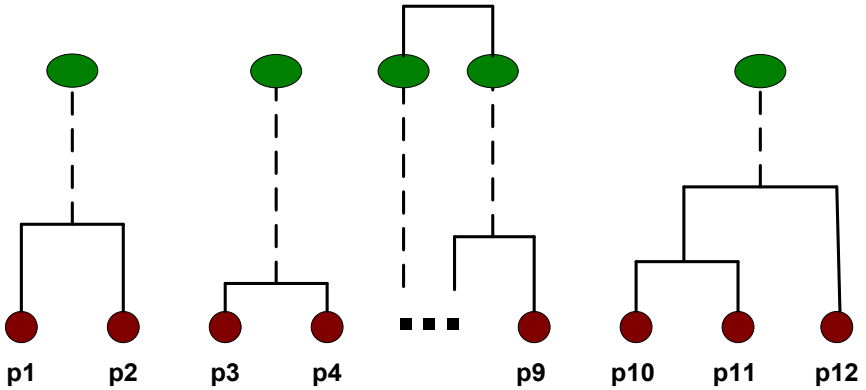
Hierarchical clustering

- Merge the two closest clusters (C2 and C5) and update the distance matrix.



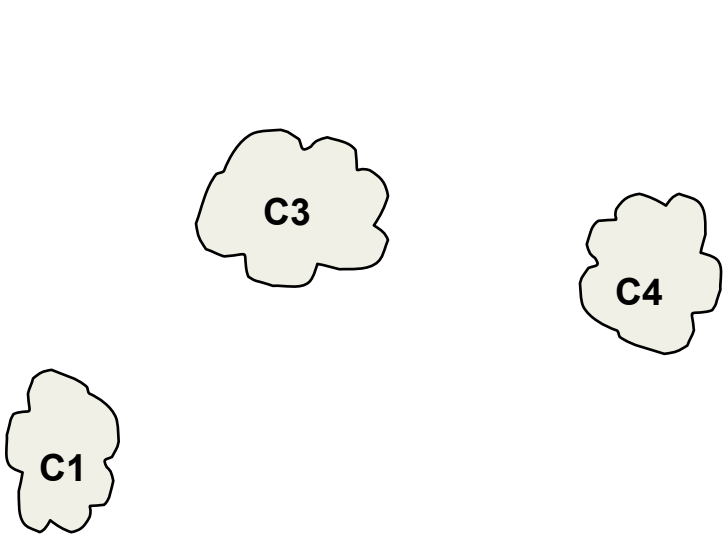
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Distance/Proximity Matrix

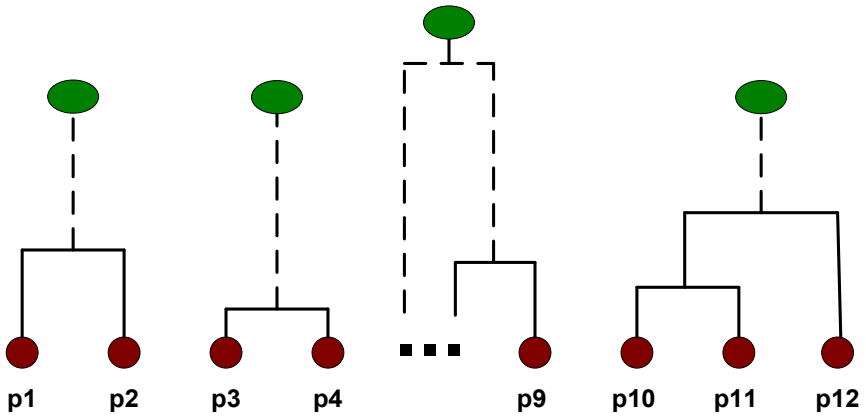


Hierarchical clustering

- "How do we update the distance matrix?"



	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		



Single-link

- **Single-link distance** between clusters C_i and C_j is the ***minimum distance*** between any object in C_i and any object in C_j

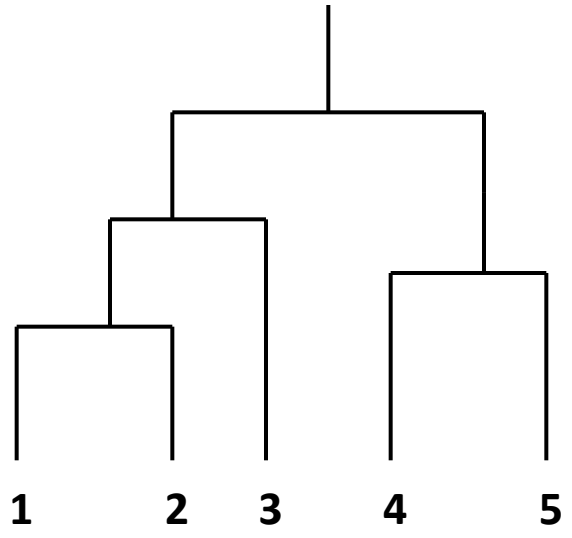
- The distance is **defined by the two most similar objects**

$$D_{sl}(C_i, C_j) = \min_{x,y} \left\{ d(x,y) \middle| x \in C_i, y \in C_j \right\}$$

Single-link: example

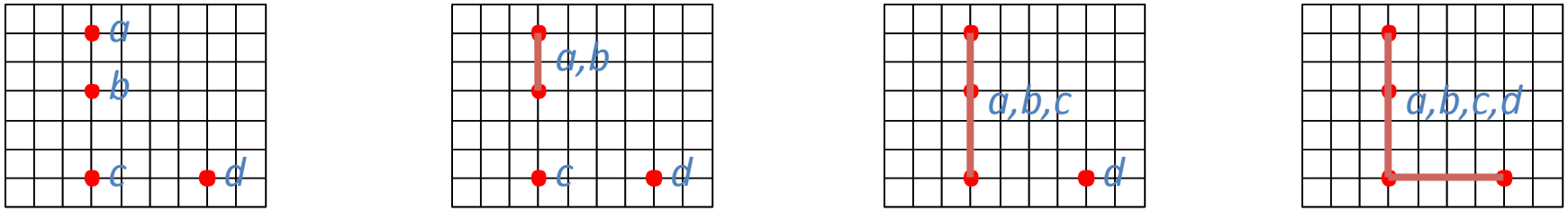
- Determined by one pair of points, i.e., by one link in the proximity graph.

	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



Single-link: evolution

Euclidean Distance



(1) (2) (3)

	b	c	d
a	2	5	6
b		3	5
c			4

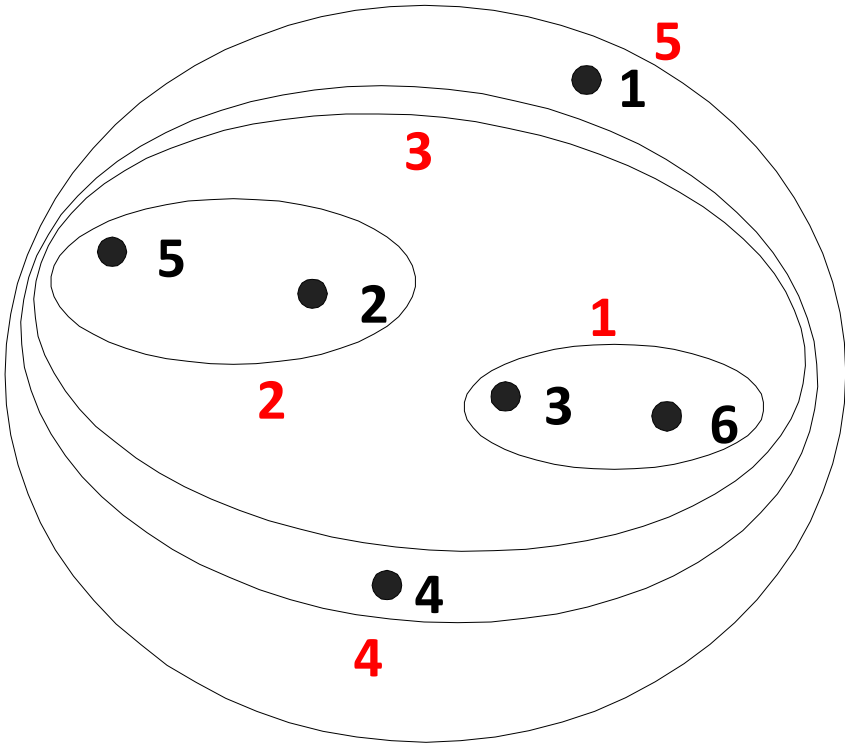
	b	c	d
a	2	5	6
b		3	5
c			4

	c	d
a,b	3	5
c		4

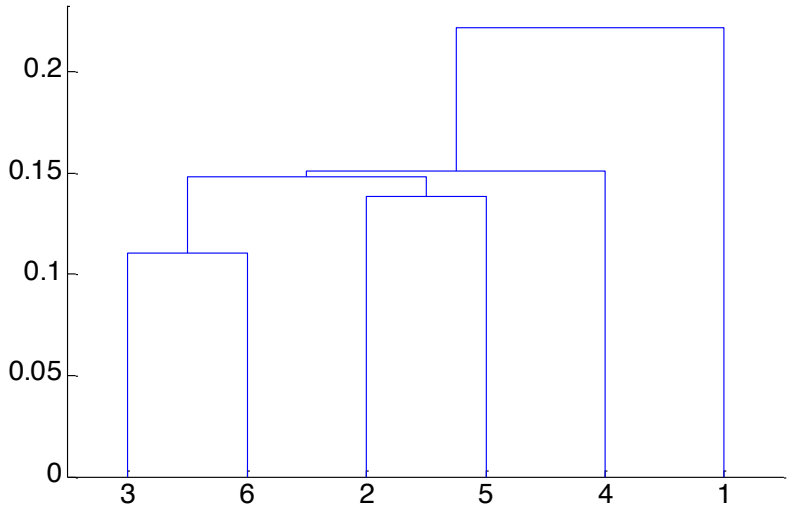
	d
a,b,c	4

Distance Matrix

Single-link: example

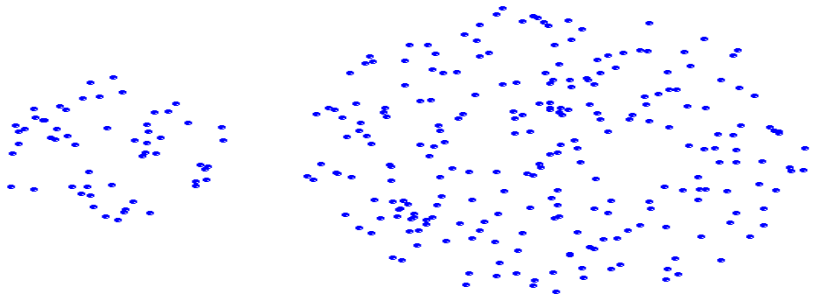


Nested Clusters

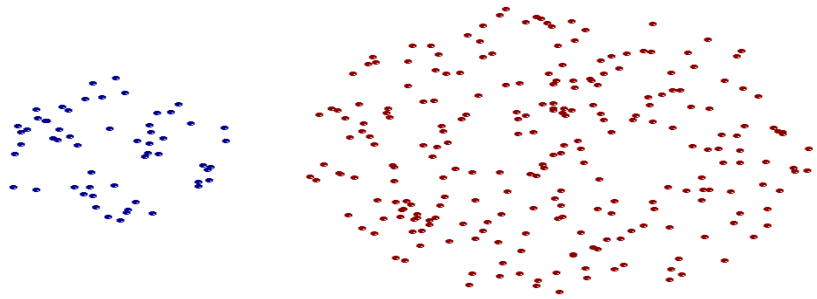


Dendrogram

Single-link: strength



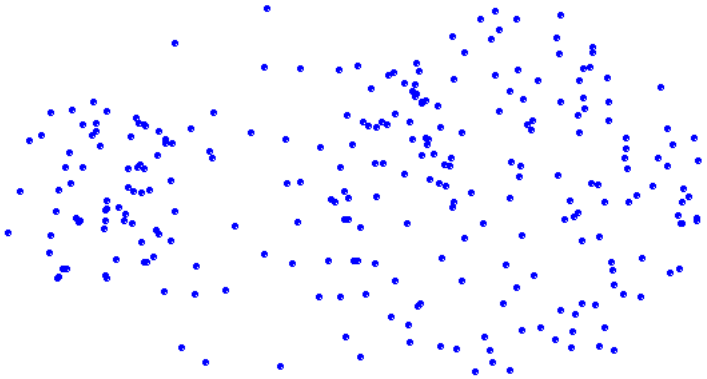
Original Points



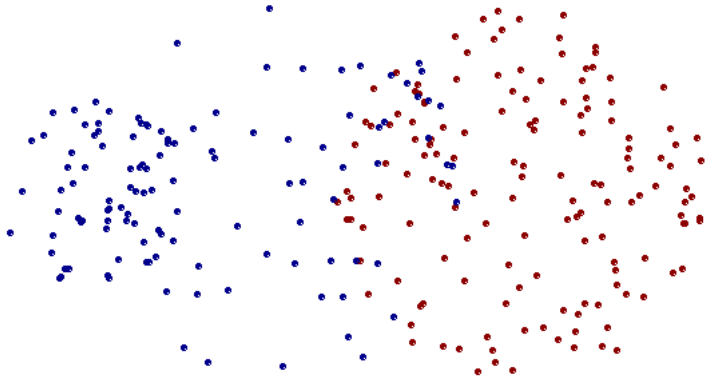
Two Clusters

- **Can handle non-elliptical shapes**

Single-link: limitations



Original Points



Two Clusters

- **Sensitive to noise and outliers**
- **It produces long, elongated clusters**

Complete-link

- **Complete-link distance** between clusters C_i and C_j is the ***maximum distance*** between any object in C_i and any object in C_j

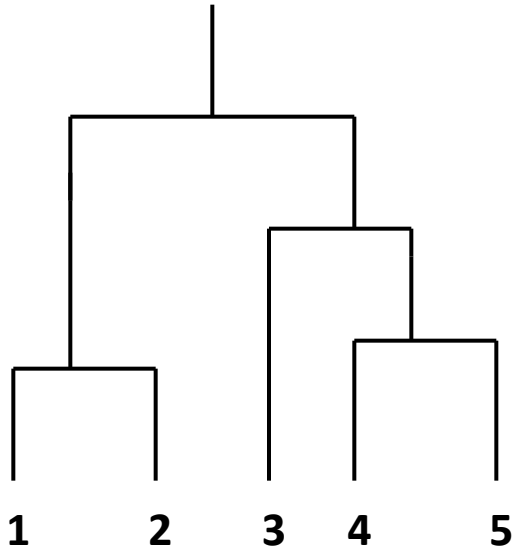
- The distance is **defined by the two most dissimilar objects**

$$D_{cl}(C_i, C_j) = \max_{x,y} \left\{ d(x,y) \middle| x \in C_i, y \in C_j \right\}$$

Complete-link: example

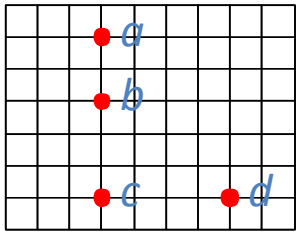
- Distance between clusters is determined by the two most distant points in the different clusters

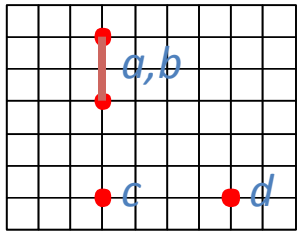
	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



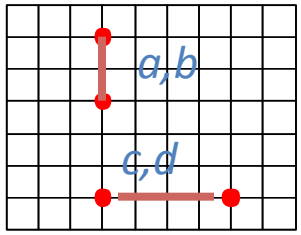
Complete-link: example

Euclidean Distance

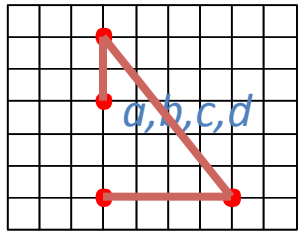




(1)



(2)



(3)

	b	*c*	*d*
a	2	5	6
b		3	5
c			4

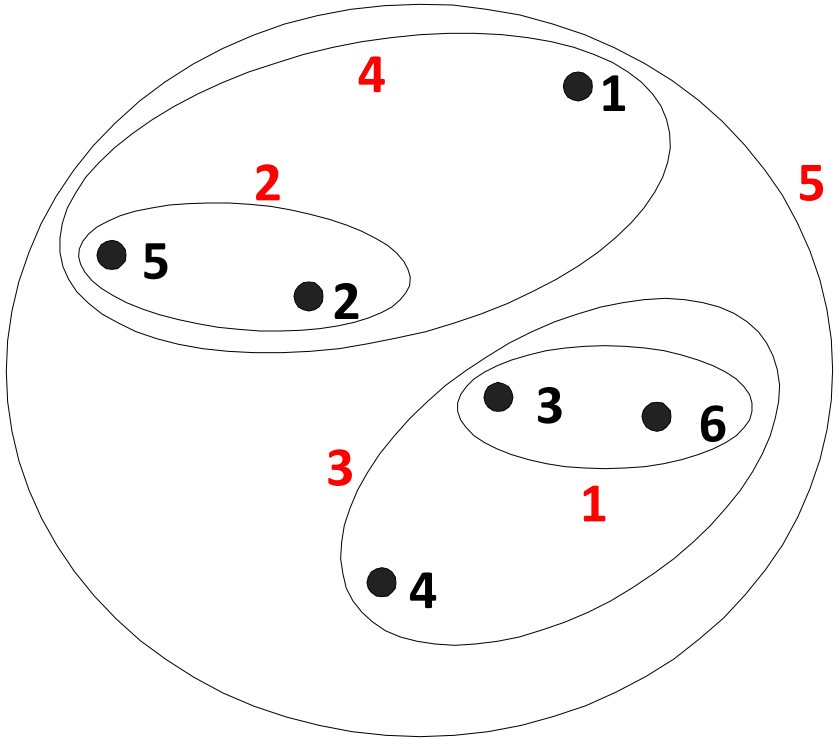
	b	*c*	*d*
a	2	5	6
b		3	5
c			4

	c	*d*
a*,*b	5	6
c		4

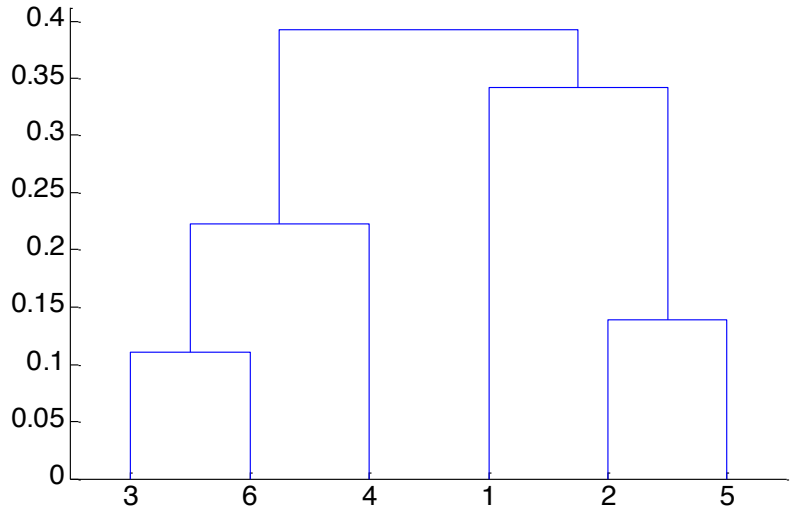
	c,*d*
a*,*b	6

Distance Matrix

Complete-link: example

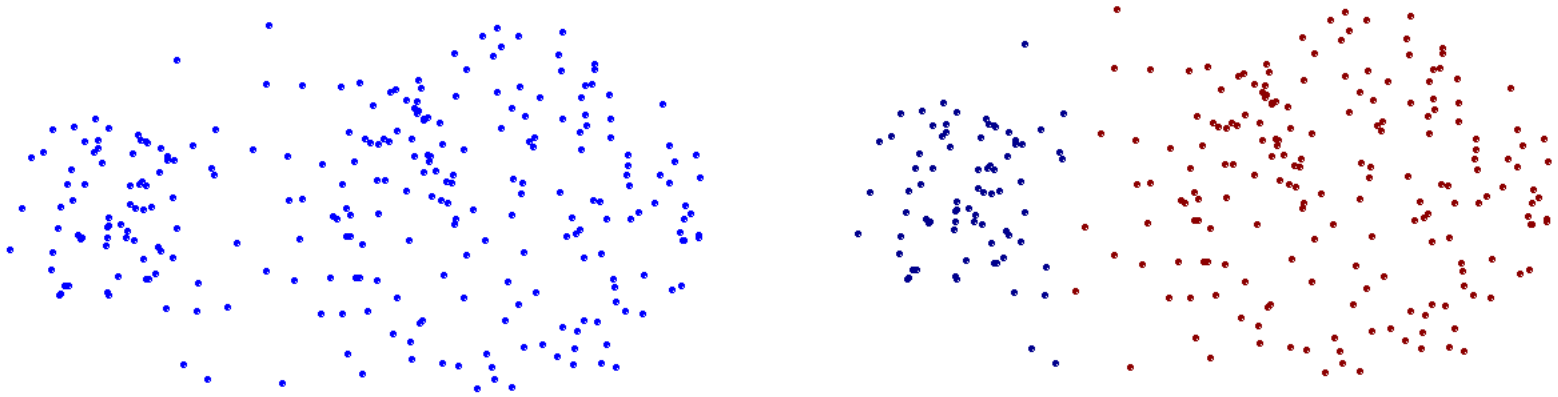


Nested Clusters



Dendrogram

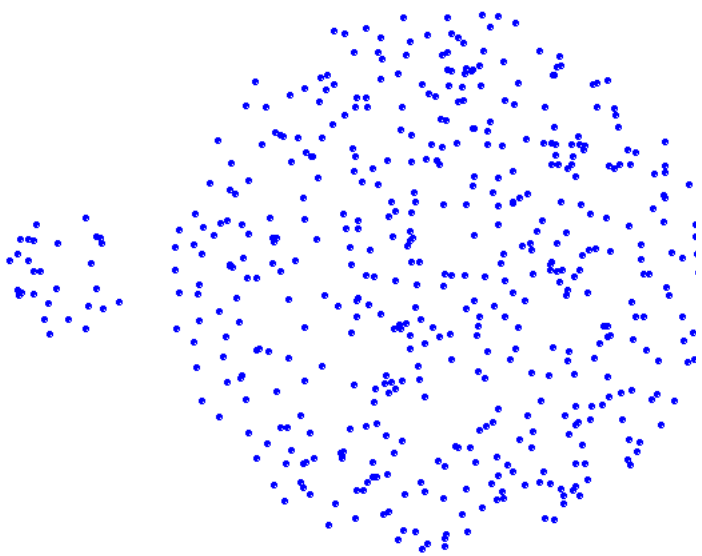
Complete-link: strength



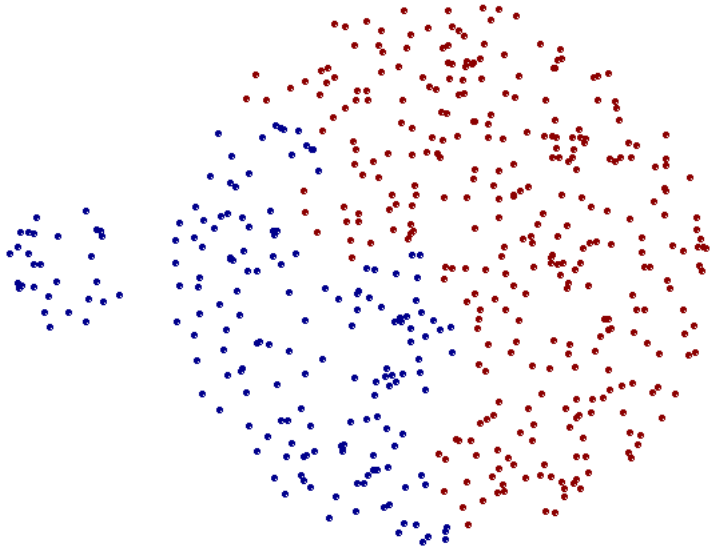
Original Points **Two Clusters**

- **More balanced clusters (with equal diameter)**
- **Less susceptible to noise**

Complete-link: limitations



Original Points



Two Clusters

- **Tends to break large clusters**
- **All clusters tend to have the same diameter – small clusters are merged with larger ones**

Average-link

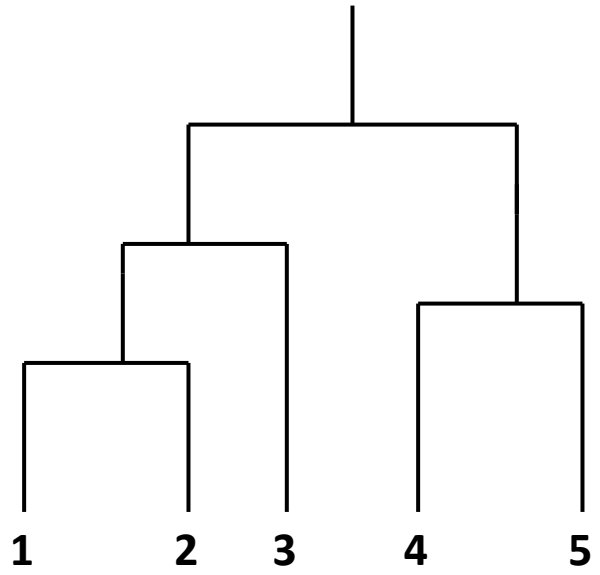
- **Group average distance** between clusters C_i and C_j is the ***average distance*** between any object in C_i and any object in C_j

$$D_{avg}(C_i, C_j) = \frac{1}{|C_i| \times |C_j|} \sum_{x \in C_i, y \in C_j} d(x, y)$$

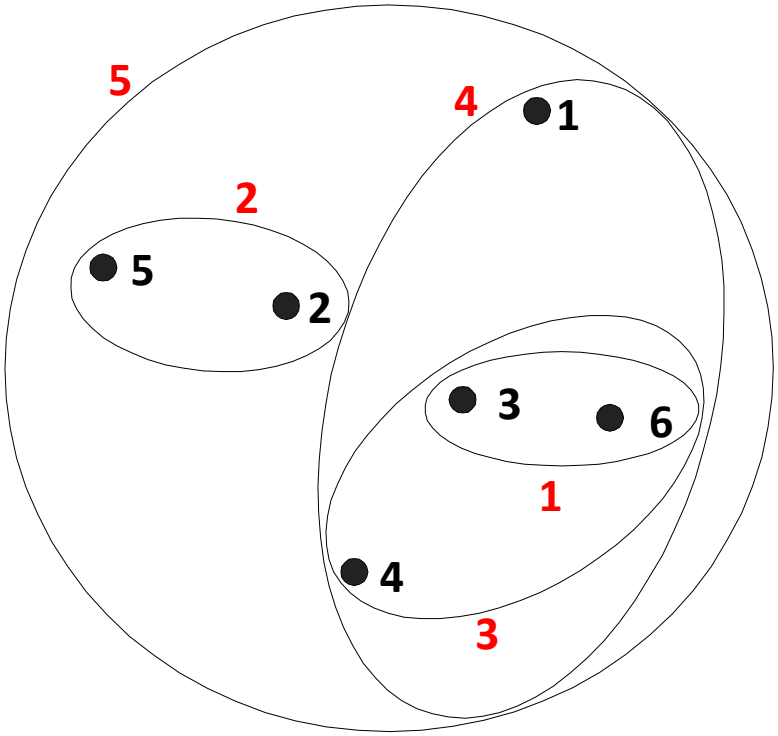
Average-link example

- Proximity of two clusters is the average of pairwise proximity between points in the two clusters.

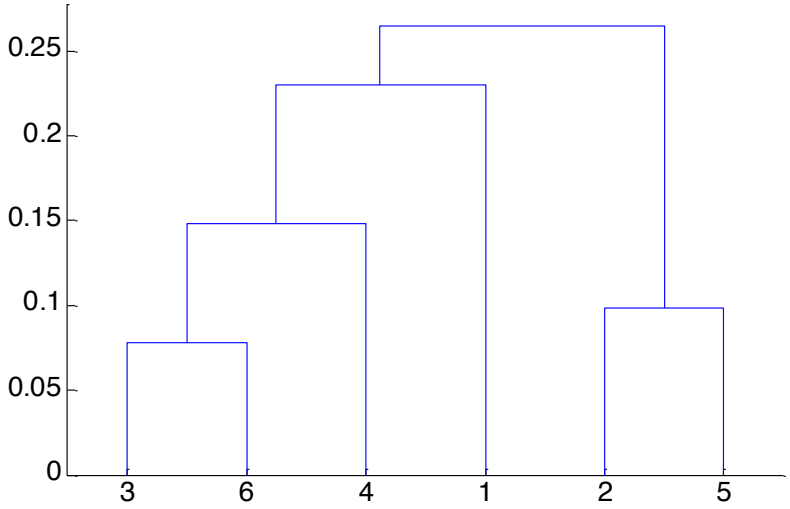
	I1	I2	I3	I4	I5
I1	1.00	0.90	0.10	0.65	0.20
I2	0.90	1.00	0.70	0.60	0.50
I3	0.10	0.70	1.00	0.40	0.30
I4	0.65	0.60	0.40	1.00	0.80
I5	0.20	0.50	0.30	0.80	1.00



Average-link example



Nested Clusters



Dendrogram

Average-link

- Compromise between Single and Complete
- Strengths
  - Less susceptible to noise and outliers
- Limitations
  - Biased towards globular clusters

Centroïd distance

- **Centroid distance** between clusters C_i and C_j is the distance between the centroid r_i of C_i and the centroid r_j of C_j

$$D_{centroids}(C_i, C_j) = d(r_i, r_j)$$

Ward's distance

- **Ward's distance** between clusters C_i and C_j is the ***difference*** between the ***total within cluster sum of squares for the two clusters separately***, and the ***within cluster sum of squares resulting from merging the two clusters*** in cluster C_{ij}

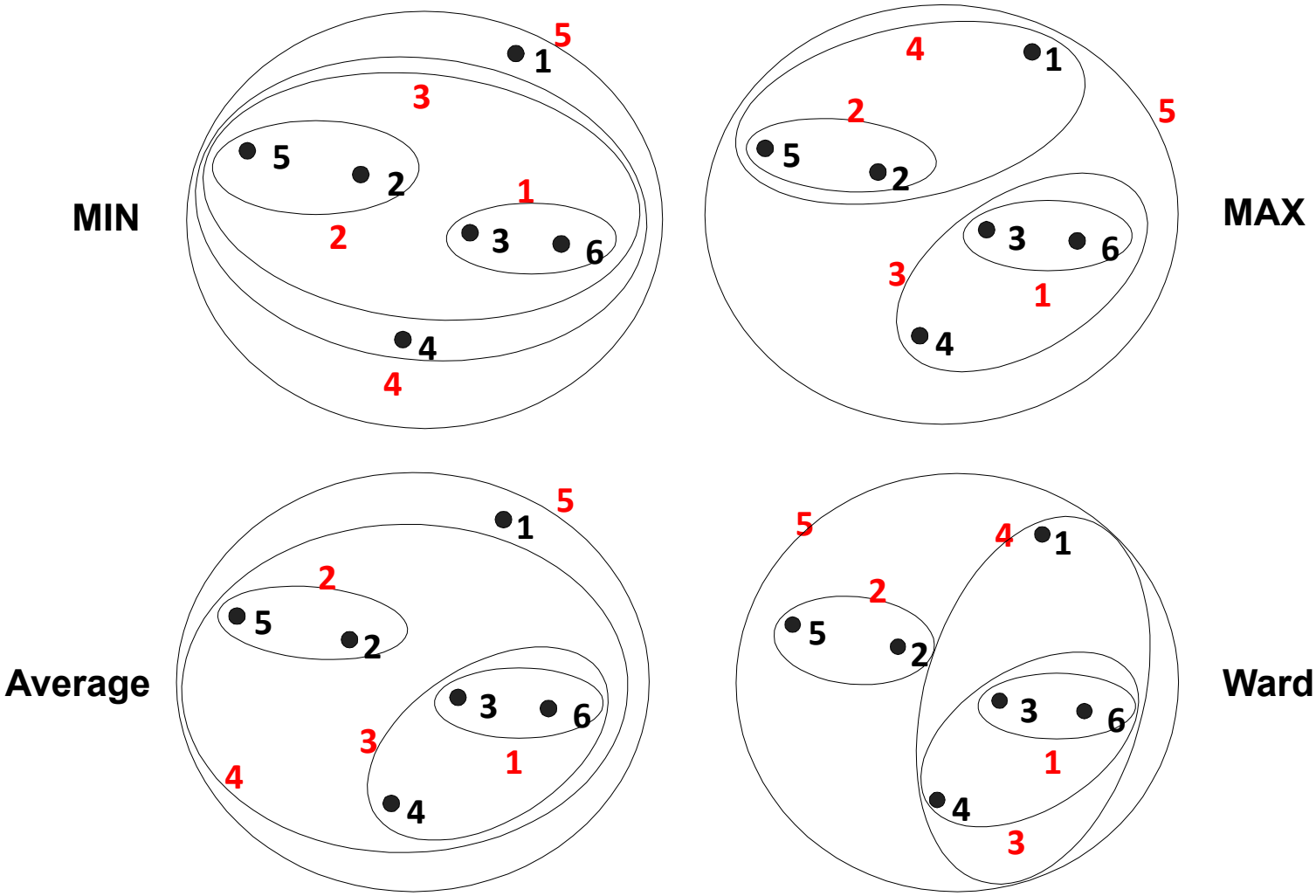
$$D_w(C_i, C_j) = \sum_{x \in C_i} (x - r_i)^2 + \sum_{x \in C_j} (x - r_j)^2 - \sum_{x \in C_{ij}} (x - r_{ij})^2$$

- r_i: centroid of C_i
- r_j: centroid of C_j
- r_{ij}: centroid of C_{ij}

Ward's distance

- Similar to group average and centroid distance
- Less susceptible to noise and outliers
- Biased towards globular clusters
- Hierarchical analogue of k-means
  - Can be used to initialize k-means

Comparisons



Time and space complexity

- For a dataset **X** consisting of **n** points
- **$O(n^2)$ space**; it requires storing the distance matrix
- **$O(n^3)$ time** in most of the cases
  - There are **n** steps and at each step the size n^2 distance matrix must be updated and searched
  - Complexity can be reduced to **$O(n^2 \log(n))$** time for some approaches by using appropriate data structures

Divisive hierarchical clustering

- Start with a single cluster composed of all data points
- Split this into components
- Continue recursively
- *Monothetic* divisive methods split clusters using one variable/dimension at a time
- *Polythetic* divisive methods make splits on the basis of all variables together
- Any intercluster distance measure can be used
- Computationally intensive, less widely used than agglomerative methods

Prim / Kruskal