Clustering

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Clustering Problem: Galaxies

- A catalog of 2 billion "sky objects" represents objects by their radiation in 7 dimensions (frequency bands).
- **Problem:** Cluster into similar objects, e.g., galaxies, nearby stars, quasars, etc.
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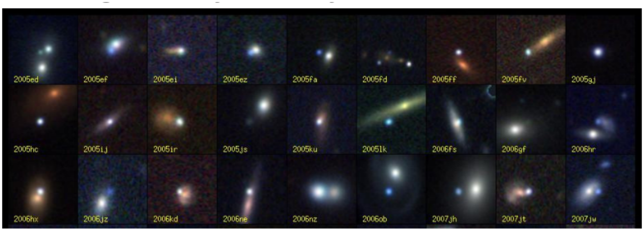

Finding topics:

- Represent a document by a vector $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ iff the i-th word (in some order) appears in the document
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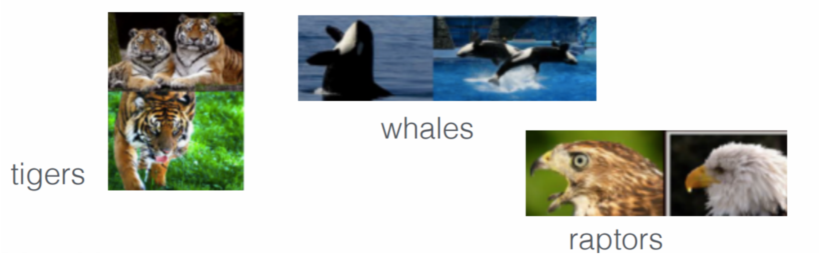
Clustering Problem: Images

Goal: partitioning data in maximally homogeneous, maximally distinguished subsets.

- **Internal criterion:** members of the cluster should be similar to each other (**inter-cluster compactness**).



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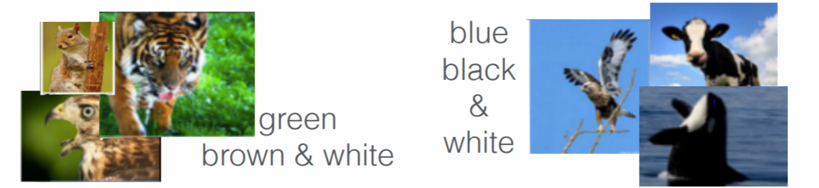
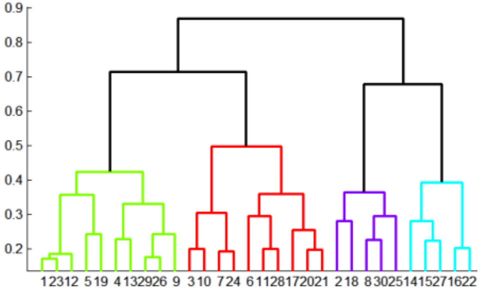


- **Agglomerative (bottom up)**:
  - Initially, each point is a cluster;
  - Repeatedly combine the two "nearest" clusters into one.
- **Divisive (top down)**:
  - Start with one cluster and recursively split it.



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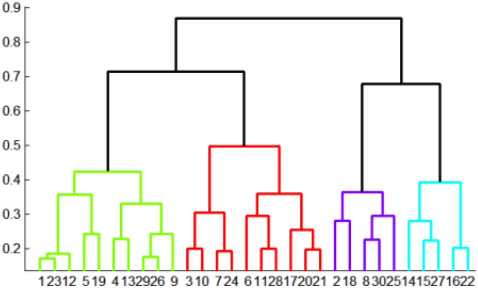
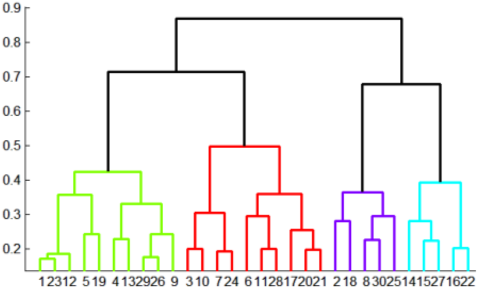


Key operation: Repeatedly combine two nearest clusters.

Three important questions:

1. How do you represent a cluster of more than one point?
2. How do you determine the "nearness" of clusters?
3. When to stop combining clusters?



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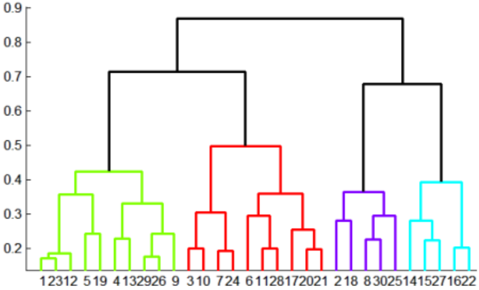

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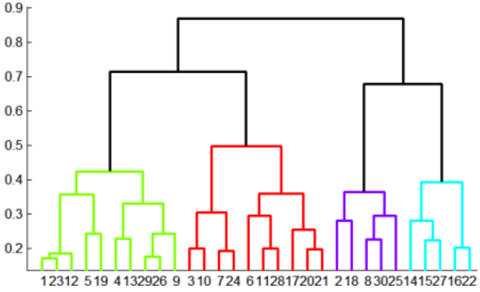

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   - **Key problem:** As you merge clusters, how do you represent the "location" of each cluster, to tell which pair of clusters is closest?
   - **Euclidean case**: each cluster has a centroid = average of its points
2. How do you determine the "nearness" of clusters?
   - Measure cluster distances by distances of centroids

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Minkowski family of distances:

$$D(x,y) = \sqrt[p]{|x_1 - y_1|^p + |x_2 - y_2|^p + \cdots + |x_n - y_n|^p}.$$

It can be checked that for any $p \geq 1$:

- $D(x,y) \geq 0$,
- $D(x,x) = 0$,
- $D(x,y) = D(y,x)$,
- $D(x,y) \leq D(x,z) + D(z,y)$.

Manhattan distanse

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In case of $p = 1$:

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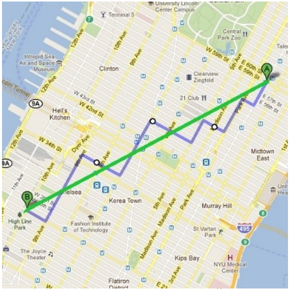
It is nicknamed **Manhattan distance** (blue):



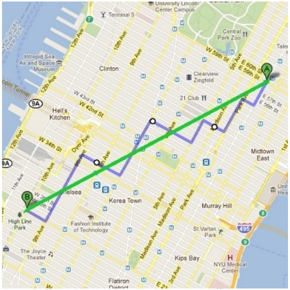
Minkowski family of distances:

$$D(x, y) = \sqrt[p]{|x_1 - y_1|^p + |x_2 - y_2|^p + \cdots + |x_n - y_n|^p}.$$

In case of $p = 2$:

$$\sqrt[2]{|x_1 - y_1|^2 + |x_2 - y_2|^2 + \cdots + |x_n - y_n|^2}.$$

Euclidean distance (green):



- Randomly **initialize** k centers:

$$\mu^0 = (\mu_1^0, \dots, \mu_k^0).$$

- **Classify:** Assign each point $j \in \{1, \dots, m\}$ to nearest center:

$$z^j = \arg\min_i \|\mathbf{x}_j - \mu_i^t\|_2^2.$$

- **Recenter:** μ_i becomes centroid of its points:

$$\mu_i^{t+1} = \arg\min_\mu \sum_{j : z^j = i} \|\mathbf{x}_j - \mu\|_2^2.$$

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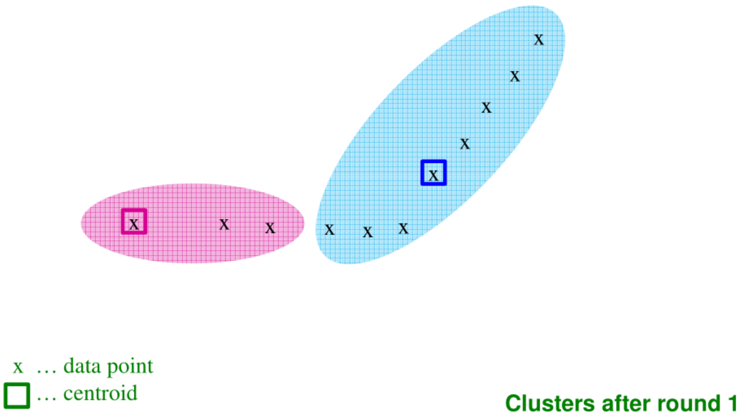
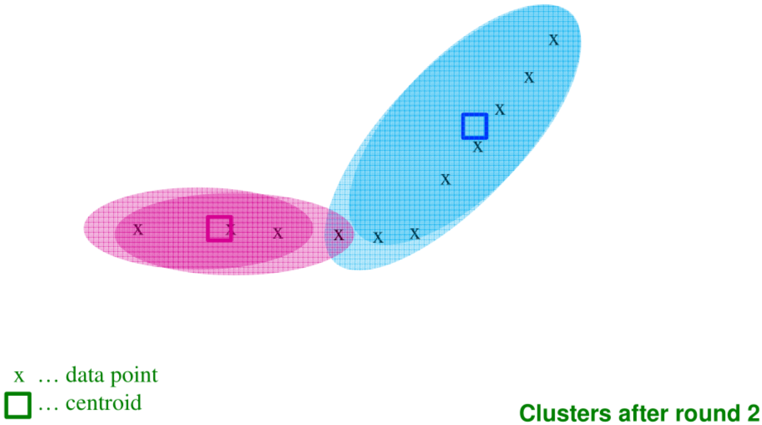
Equivalent to μ_i average of its points!


x ... data point
... centroid
Clusters after round 1


x … data point
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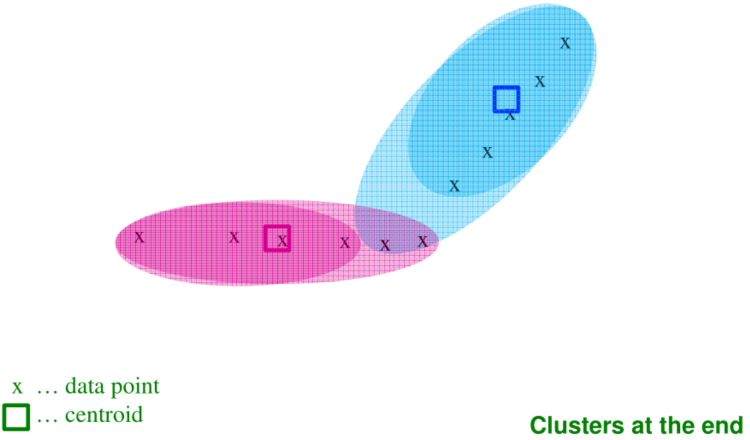
Clusters after round 2


X
X
X
X
X
X
X
X
X
X
X
X
x ... data point
... centroid
Clusters at the end

Assumptions:

- Known number of clusters;
- Clusters of approximately same size and density;
- Spherical form.

- For supervised classification we have a variety of measures to evaluate how good our model is: accuracy, precision, recall.
- For cluster analysis, the analogous question is how to evaluate the goodness of the resulting clusters?
- We need measures to compare:
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- **External measure:** used to measure the extent to which cluster labels match externally supplied class labels.
  - Example: entropy
- **Internal measure:** used to measure the goodness of a clustering structure without respect to external information.
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- Partition obtained: $P = \{P_1, \dots, P_K\}$;
- External (true) partition: $C = \{C_1, \dots, C_K\}$;
- m_{ij} is a number of objects in $P_i \cap C_j$;
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- Distribution of objects in P_i:

$$\frac{m_{i1}}{m_{i\cdot}}, \frac{m_{i2}}{m_{i\cdot}}, \ldots, \frac{m_{in}}{m_{i\cdot}}.$$

- Entropy (impurity) of the distribution is

$$\sum_{j=1}^{K} \frac{m_{ij}}{m_{i\cdot}} \log \frac{m_{ij}}{m_{i\cdot}}.$$

- Overall entropy:

$$E = -\sum_{i=1}^{K} \frac{m_{i\cdot}}{m} \sum_{j=1}^{K} \frac{m_{ij}}{m_{i\cdot}} \log \frac{m_{ij}}{m_{i\cdot}}.$$

- The lower the entropy, the better the clustering.

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External measures: Entropy

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- The lower the entropy, the better the clustering.

- Given: to which P_i an object $\mathbf{x}$ belongs
- This fact tells us something about the true class
- The amount information is measured by

$$MI = \sum_{i,j=1}^{K} p_{ij} \log \frac{p_{ij}}{p_i p_j},$$

  where $p_{ij} = \frac{m_{ij}}{m}$, $p_i = \frac{m_{i.}}{m}$, $p_j = \frac{m_{.j}}{m}$.
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- Higher mutual information implies a higher clustering quality

$$J = \frac{a}{a+b+c},$$

where

- a is the number of pairs of points with the same label in C and assigned to the same cluster in P;
- b is the number of pairs with the same label, but in different clusters;
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The index produces a result in the range $[0, 1]$, where a value of 1.0 indicates that C and P are identical

$$RI = \frac{a+d}{a+b+c+d},$$

where

- a, b, c are as above
- d denotes the number of pairs with a different label in C that were assigned to a different cluster in P
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Consider an i-th individual point

- $a(i)$ = average distance of the i-th point to the points in its cluster.
- $b(i)$ = min (average) distance of the i-th point to points in other clusters.
- The silhouette coefficient for the point is then given by

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}.$$

- Property: $-1 \leq s(i) \leq 1$.

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- If $s(i)$ is close to 1, sample i is well-clustered and it was assigned to a very appropriate cluster
- If $s(i)$ is close to zero, sample i could be assign to another closest cluster as well, and the sample lies equally far away from both clusters
- If $s(i)$ is close to -1, sample i is misclassified.
- We can consider average $\frac{\sum_i s(i)}{m}$ of $s(i)$ for all objects in the whole dataset:
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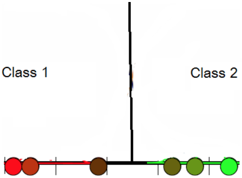
- K-means performs hard assignment
- Each data point is assigned to one and only one cluster
- Appropriate for points close to cluster centroids
- Not appropriate for points midway between the two cluster centroids



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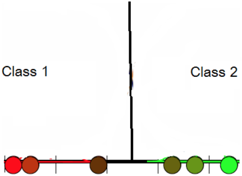

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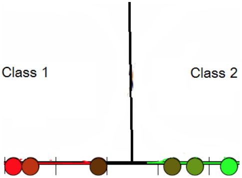

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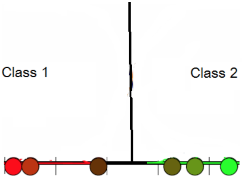
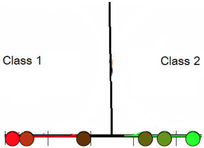
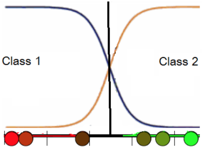


- Each data point is (partially) assigned to clusters with certain probabilities
- One point might be (partially) assigned to multiple clusters
- The midway point is assigned to either cluster with probability 0.5





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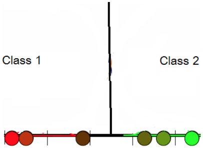

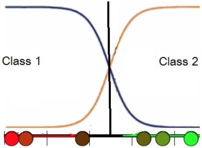

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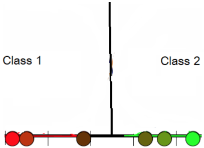
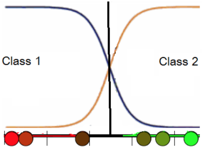
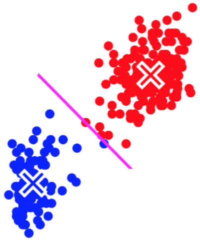
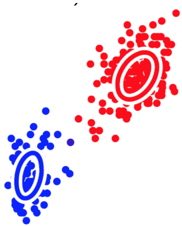




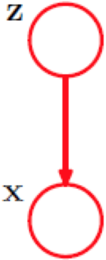
Hard/Soft Assignment: 2D example



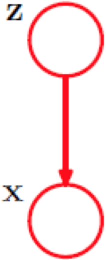
Hard Assignment



Soft Assignment
(Ellipses: contour of probability functions).



- K clusters: $1, 2, \ldots, K$
- Randomly drawn object
  - $\mathbf{x}$: attribute values of the object, observed.
  - z: class of the object, latent variable (not observed)
- $P(z)$: distribution of z
  - $\pi_k = P(z = k)$: probability that the object is from class k
- $p(\mathbf{x}|z)$: conditional distribution of attribute values
  - $p(\mathbf{x}|z = k)$: distribution for objects from class k



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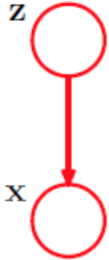

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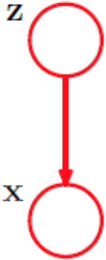

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- Distribution of data:

$$p(\mathbf{x}) = \sum_{k=1}^{K} P(z = k) p(\mathbf{x}|z = k) = \sum_{k=1}^{K} \pi_k p(\mathbf{x}|z = k)$$

- It is a mixture of the distributions for individual classes
- Each $p(\mathbf{x}|z = k)$ is a component in the mixture
- Gaussian mixtures: each component is a Gaussian distribution

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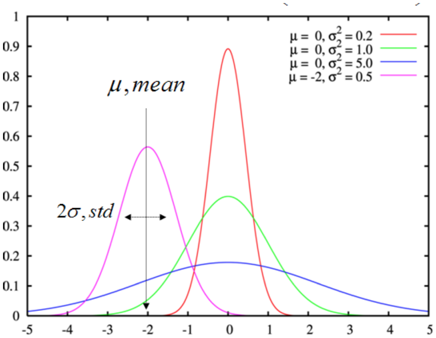
- Gaussian distribution: $\mathcal{N}(x|\mu, \sigma)$
- Probability density function:

$$p(\mathbf{x}|\mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$



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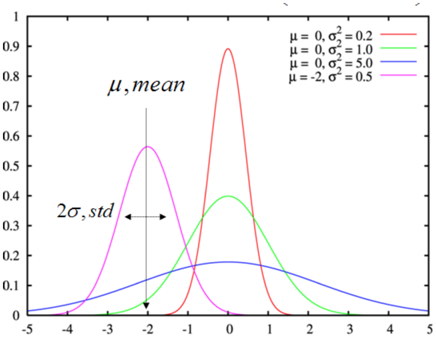
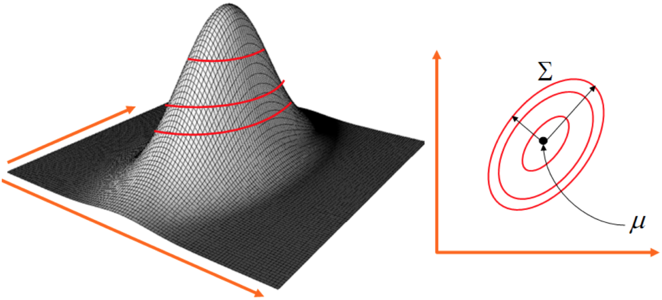


$$p(\mathbf{x}|\boldsymbol{\mu}, \Sigma) = \frac{1}{\sqrt{(2\pi)^d \det(\boldsymbol{\Sigma})}} \exp\left[-\frac{(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}{2}\right],$$

where

- d: dimension;
- $\mathbf{x}$: vector of d random variables, representing data;
- $\boldsymbol{\mu}$: vector of means;
- $\boldsymbol{\Sigma}$: covariance matrix.

- $\boldsymbol{\mu}$: center of contour lines
- $\boldsymbol{\Sigma}$: orientation and size of contour lines



- Mixture distribution:

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k p(\mathbf{x}|z = k).$$

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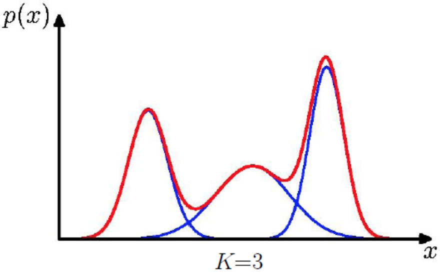

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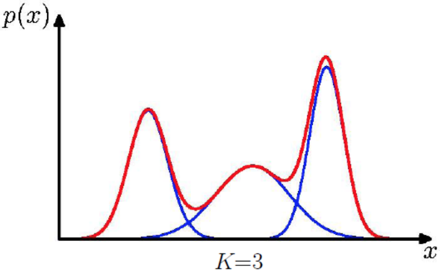
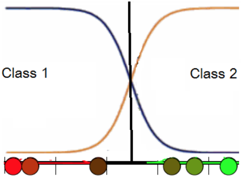


- Given mixture model:

$$p(\mathbf{x}) = \sum_{k=1}^{K} P(z = k) p(\mathbf{x}|z = k) = \sum_{k=1}^{K} \pi_k p(\mathbf{x}|z = k)$$

- Object $\mathbf{x}$ belongs to class k with probability

$$P(z = k|\mathbf{x}) = \frac{P(z = k) p(\mathbf{x}|z = k)}{p(\mathbf{x})} = \frac{\pi_k p(\mathbf{x}|z = k)}{\sum_{s=1}^{K} \pi_s p(\mathbf{x}|z = s)}$$



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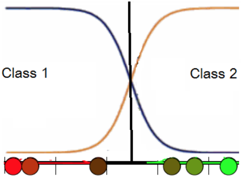

- Given
  - unlabeled data $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$;
  - number of clusters K
- Find a K-component Gaussian mixture model:
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  by maximizing data likelihood

- Choose initial values for $\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$, $k = 1, \ldots, K$
- repeat:
  — Expectation: for each training example $\mathbf{x}_n$
    (a) Compute $r_{nk} = P(z = k|\mathbf{x}_n)$, $k = 1, \ldots, K$
    (b) Break data into K parts according to the probabilities

$$\mathbf{x}_n[r_{nk}],\ k = 1, \ldots, K$$

    (c) Assign each part $\mathbf{x}_n[r_{nk}]$ to the corresponding cluster k

  — Maximization: Re-estimate $\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$, $k = 1, \ldots, K$
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Expectation-Maximization (EM) algorithm

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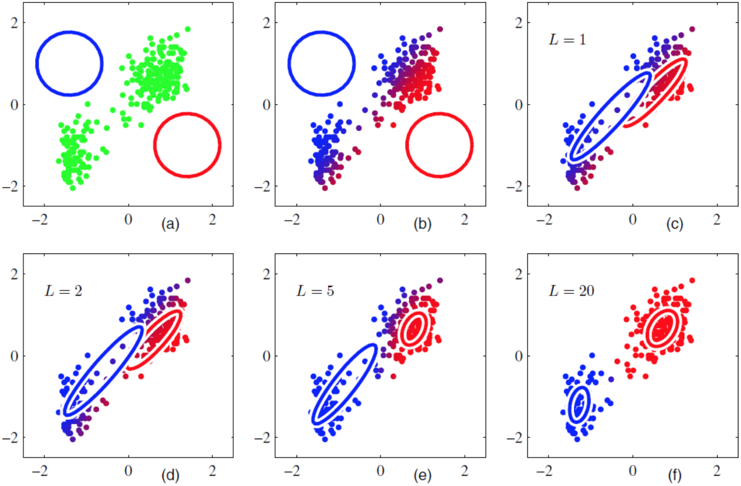
EM: 2D illustration



- Main computations are in step (a):

$$r_{nk} = P(z = k|\mathbf{x}_n) = \frac{P(z = k)p(\mathbf{x}_n|z = k)}{\sum_{k=1}^{K} P(z = k)p(\mathbf{x}_n|z = k)} = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{s=1}^{K} \pi_s \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_s, \boldsymbol{\Sigma}_s)}.$$

- r_{nk} are often called responsibilities.

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- r_{nk} are often called responsibilities.

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$$m_k = \sum_{i=1}^{m} r_{ki}$$

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- Choose initial values for π_k, $\boldsymbol{\mu}_k$, $\boldsymbol{\Sigma}_k$.
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$$l(\boldsymbol{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \log \prod_{i=1}^{m} p(\mathbf{x}_i|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{i=1}^{m} \log p(\mathbf{x}_i|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

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$$l(\boldsymbol{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \log \prod_{i=1}^{m} p(\mathbf{x}_i|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{i=1}^{m} \log p(\mathbf{x}_i|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- Let $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_K)$, $\boldsymbol{\mu} = (\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K)$, $\boldsymbol{\Sigma} = (\boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_K)$
- Specification of $\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}$ defines a probability density functions over features $\mathbf{x}$:

$$p(\mathbf{x}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

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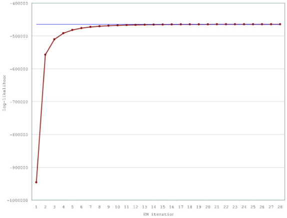
- Let $l(t)$ be the log-likelihood after iteration t
- The series $l(1), l(2), \ldots$ increases monotonically with t
- Terminate EM when $l(t+1) - l(t)$ falls below a threshold



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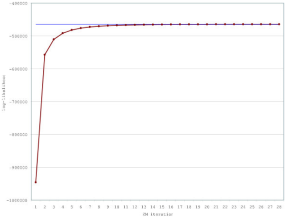

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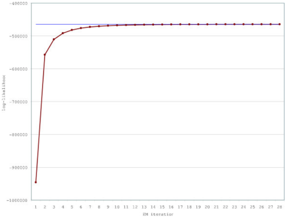

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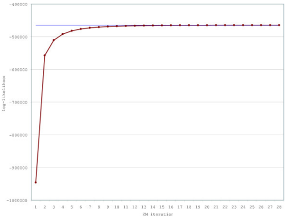

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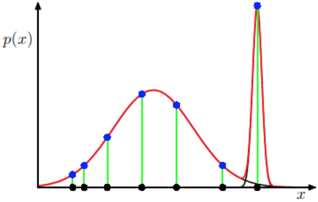
- Such singularity in likelihood function happens often in case of outliers and repeated points



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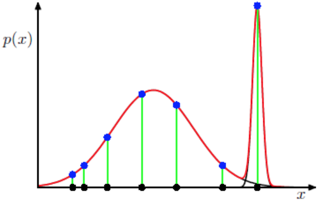

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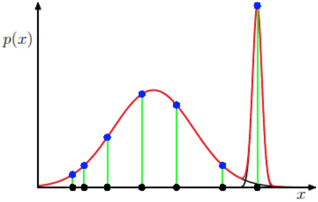

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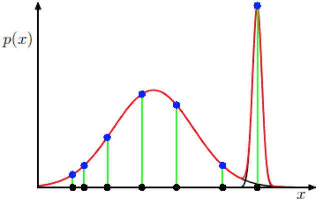

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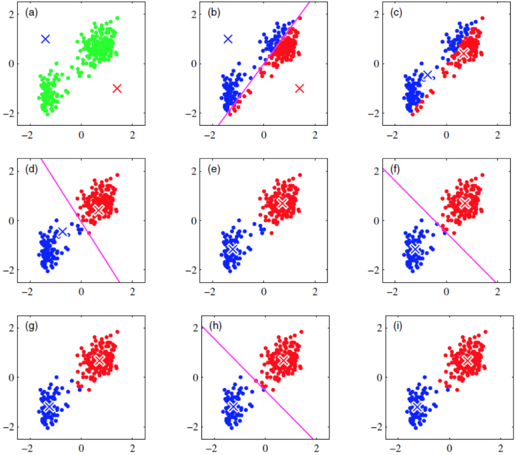
Hard Assignment:

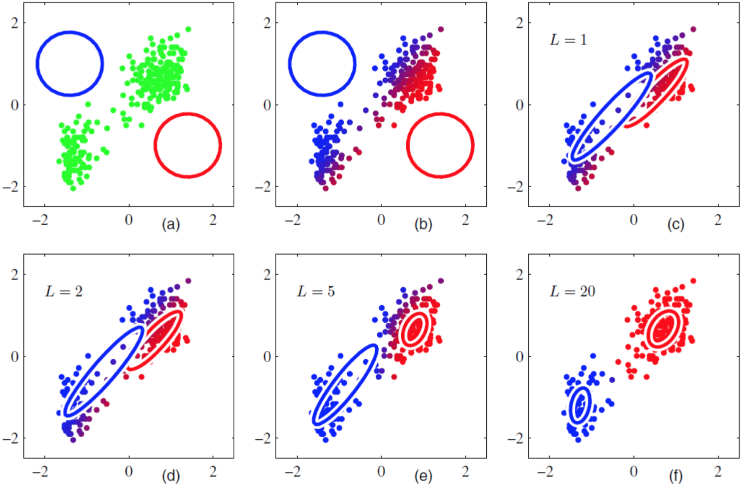
- Select K points as the initial centroids
- Repeat
  - for K clusters by assigning all points to the closest centroid;
  - recompute the centroid of each cluster
- until the centroids don't change

Soft Assignment:

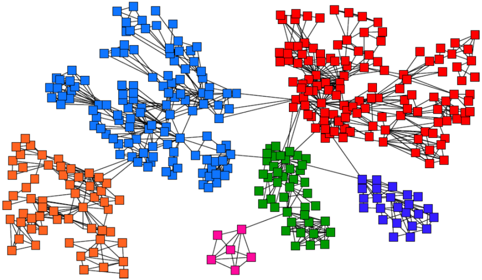
- Choose initial values for π_k, $\boldsymbol{\mu}_k$, $\boldsymbol{\Sigma}_k$
- Repeat
  - Expectation:
    (a) Compute $r_{nk} = P(z = k|\mathbf{x}_n)$ for $k = 1, \ldots, K$;
    (b) Break it into K fractional examples according to the probabilities;
    (c) Assign each fractional examples to the corresponding cluster k
  - Maximization: Re-estimate π_k, $\boldsymbol{\mu}_k$, $\boldsymbol{\Sigma}_k$
- until convergence


(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)

EM example



- **Graph** $G(E, V)$:
  - Nodes v_j
  - Edge weights $w_{ij} > 0$
- **Problem**: Want to partition graph such that edges between groups have low weights



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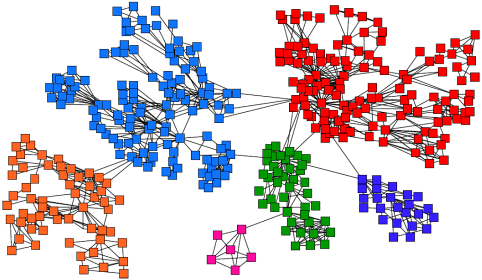

Types of graphs:

- ϵ-**neighborhood**:
  - Only include edges with distances $< \epsilon$;
  - Treat as unweighted: $w_{ij} = Const$
- **k-NN**:
  - Connect v_i and v_j if v_j is a k-NN of v_i
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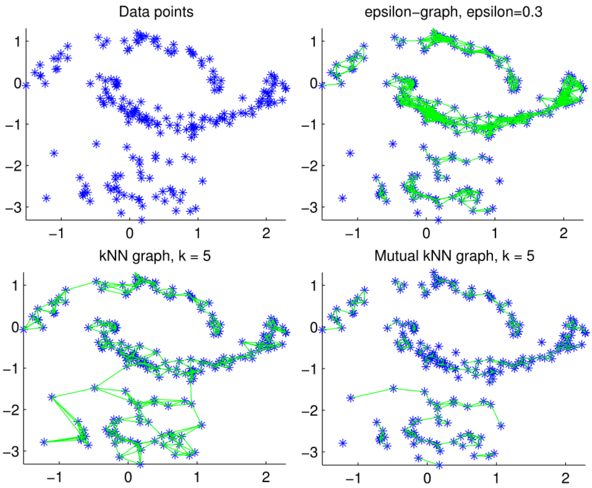
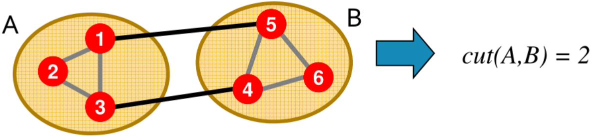

Data points
epsilon−graph, epsilon=0.3
kNN graph, k = 5
Mutual kNN graph, k = 5
1
0
−1
−2
−3
−1
0
1
2

- **Problem:** Partition graph such that edges between groups have low weights
- **Define:** $W(A,B) = \sum_{i \in A, j \in B} w_{ij}$
- **MinCut problem:** $Cut(A_1, \dots, A_k) = \sum_{i=1}^{k} W(A_i, \overline{A}_i)$
- **Choose:** $A_1, \dots, A_k = \arg\min_{A_1, \dots, A_k} Cut(A_1, \dots, A_k)$



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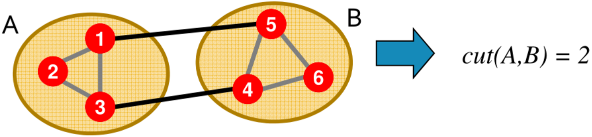

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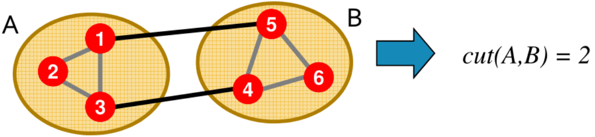

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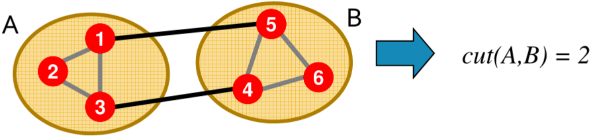
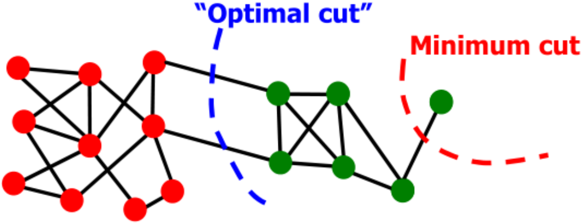


Problem: MinCut favors isolated clusters.



Solution:

- Ratio cuts (RatioCut);
- Normalized cuts (Ncut);
- Lead to "balanced" clusters.

Two measures of size of a subset:

- Cardinality:

$$|A| = \# \text{ of vertices in } A$$

- Volume:

$$vol(A) = \sum_{i \in A} \sum_{j=1}^{N} w_{ij}$$

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- Ratio cuts (RatioCut)
  - $k = 2:\ RatioCut(A, \overline{A}) = Cut(A, \overline{A})\left(\frac{1}{|A|} + \frac{1}{|\overline{A}|}\right).$
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Segmentation of Lena

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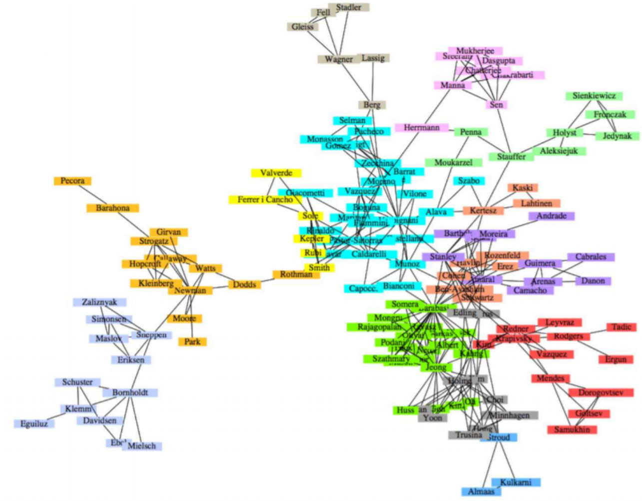
Citation network



Objects of study:

- social networks,
- citation/co-authorship networks,
- designing network protocols,
- biological networks,
- ...

$$Q = \frac{1}{2m} \sum_{(i,j)\in E} \left(w_{ij} - \frac{d_i d_j}{2m} \right) \delta(C_i, C_j),$$

where

- d_i is a degree of node i;
- C_i is a community of node i;
- $\delta(C_i, C_j)$ is a delta function;
- $m = |E|$ is a total number of edges in a graph

Interpretation: difference between the fraction of edges inside the community and its expectation in random graph with fixed node degrees.

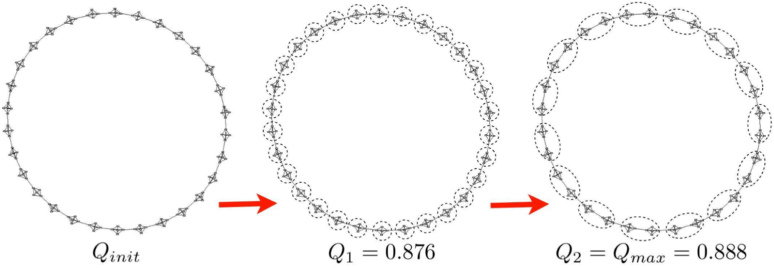
Louvain

Modularity:

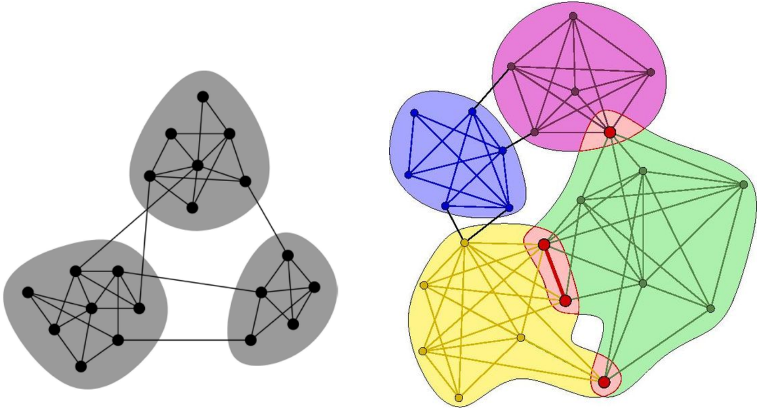
$$Q = \frac{1}{2m} \sum_{(i,j)\in E} \left(w_{ij} - \frac{d_i d_j}{2m} \right) \delta(C_i, C_j),$$

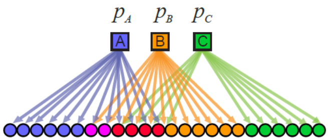
- **Idea:** optimize modularity (discrete optimization problem).
- **Efficient implementation:** Louvain community detection algorithm.
- **Problem:** low resolution.

Low resolution of modularity



Non-overlapping vs. overlapping communities





AGM generates the links:

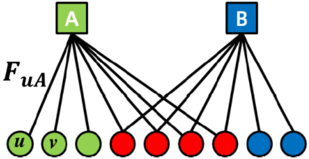
- For each pair of nodes in community A we connect them with probability p_A.
- The overall edge probability is:

$$P(u, v) = 1 - \prod_{c \in M_u \cap M_v} (1 - p_c),$$

where M_z is a set of communities node z belongs to.

- If u, v share no communities: $P(u, v) = \epsilon$.

Relaxation: Memberships have strengths



- F_{uA}: The membership strength of node u to community A ($F_{uA} = 0$: no membership).
- Each community A links nodes independently:

$$P_A(u, v) = 1 - \exp\{-F_{uA}F_{vA}\}.$$

- Community membership strength matrix: $F = (F_{uA}, u \in V, A \in \mathcal{C})$.
- Community A links nodes u, v independently:

$$P_A(u,v) = 1 - \exp\{-F_{uA} \cdot F_{vA}\}.$$

- Then probability at least one common C links them:

$$P(u,v) = 1 - \prod_{C \in \mathcal{C}} (1 - P_C(u,v)) = 1 - \exp\{-F_u F_v^T\}.$$

Task: Given a network $G(V, E)$, estimate F.

- Find F that maximizes the likelihood:

$$\arg\max_F \prod_{(u,v)\in E} P(u,v) \prod_{(u,v)\notin E} \big(1 - P(u,v)\big),$$

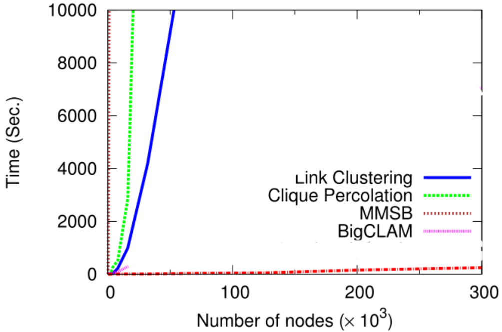
where $P(u,v) = 1 - \exp\{-F_u F_v^T\}$.

Goal: Find F that maximizes log-likelihood:

$$\ell(F) = \sum_{(u,v)\in E} \log\big(1 - \exp\{-F_u F_v^T\}\big) - \sum_{(u,v)\notin E} F_u F_v^T.$$

Note: Non-convex optimization problem!

BigCLAM performance



- BigCLAM takes 5 minutes for 300k node nets (other methods take 10 days).
- Can process networks with 100M edges!