Clustering

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Outline

- 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.
- **Sloan Digital Sky Survey**:

Finding topics:

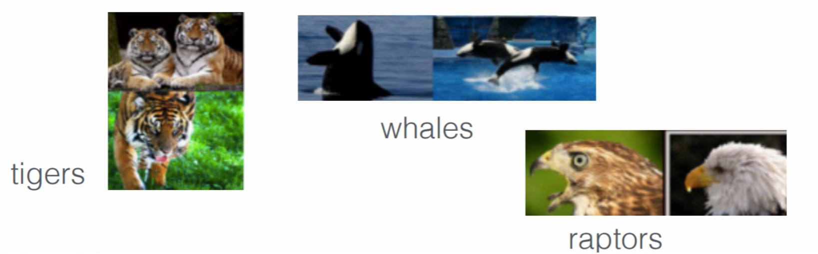
- Represent a document by a vector $(x_1, x_2, \ldots, x_k)$, where $x_i = 1$ iff the i-th word (in some order) appears in the document
- Documents with similar sets of words may be about the same topic

Clustering Problem: Images

What is a cluster?

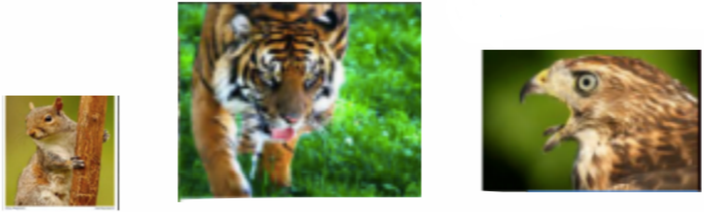
Goal: partitioning data in maximally homogeneous, maximally distinguished subsets.

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



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

- **External criterion**: objects outside the cluster should be dissimilar from the objects inside the cluster (**intra-cluster distance**).



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

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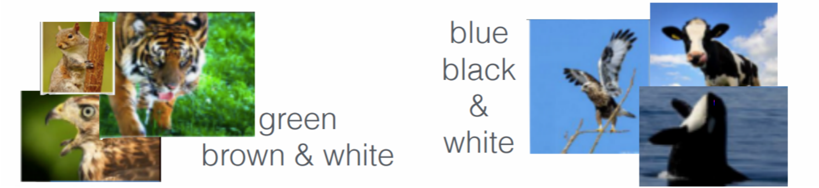
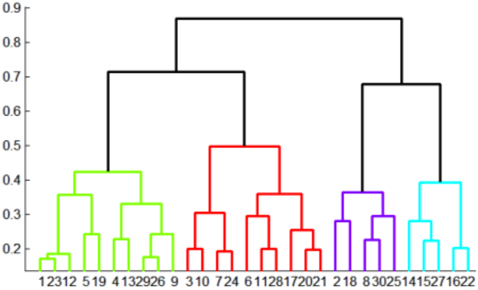


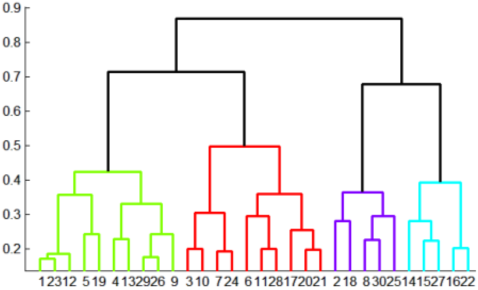
- **Agglomerative (bottom up)**:
  - Initially, each point is a cluster;
  - Repeatedly combine the two "nearest" clusters into one.
- **Divisive (top down)**:
  - Start with one cluster and recursively split it.



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?



Key operation: Repeatedly combine two nearest clusters

1. How do you represent a cluster of more than one point?
    - **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

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 $p \geq 1$:

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

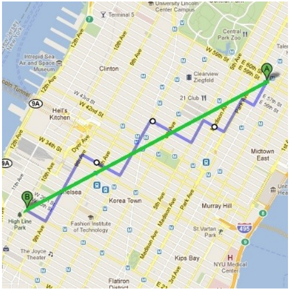
Minkowski family of distances:

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

In case of $p = 1$:

$$D(x, y) = |x_1 - y_1| + |x_2 - y_2| + \cdots + |x_n - y_n|.$$

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



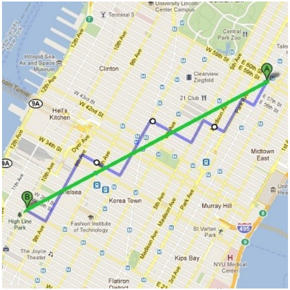
Minkowski family of distances:

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

In case of $p = 2$:

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

Euclidean distance (green):



- Randomly **initialize** k centers:

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

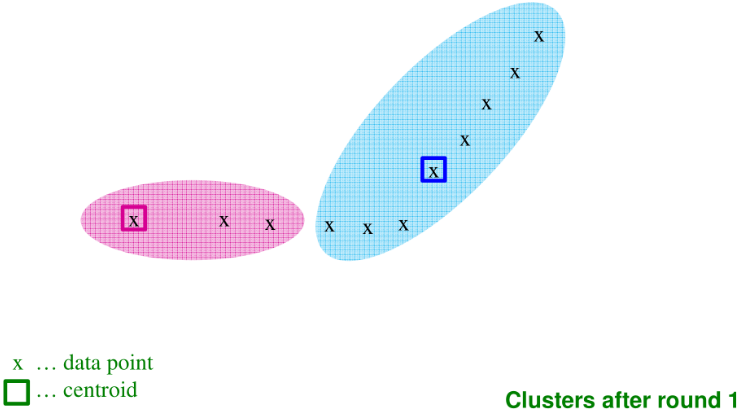
- **Classify:** Assign each point $j \in \{1, \ldots, m\}$ to nearest center:

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

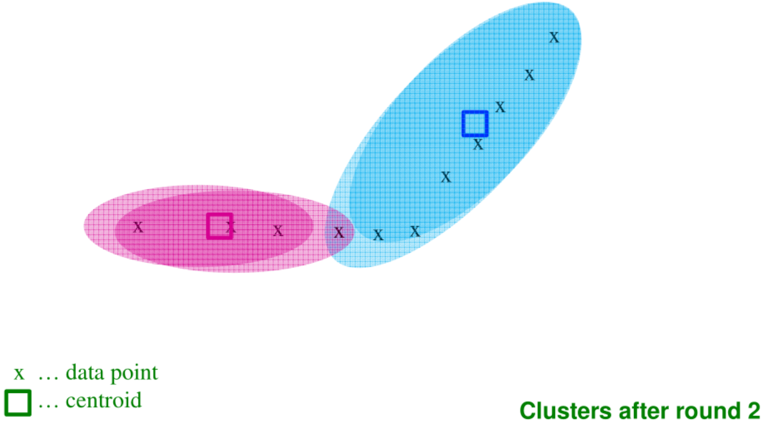
- **Recenter:** μ_i becomes centroid of its points:

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

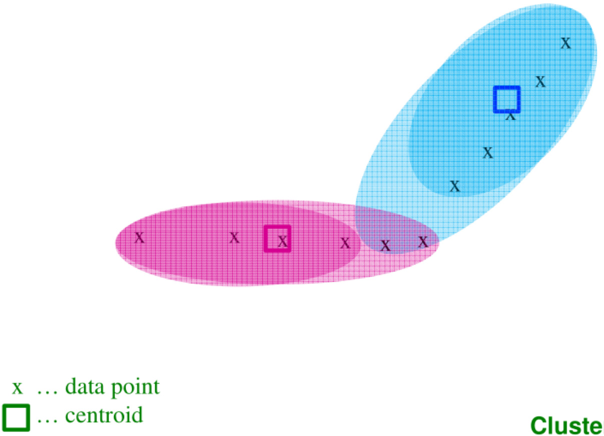
Equivalent to μ_i average of its points!


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

K-means



K-means



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:
  - clustering algorithms;
  - two sets of clusters.

- **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.
  - Example: Sum of Squared Errors (SSE)

- 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 $P_i \cap C_j$;
- $m_{i\cdot} = \sum_{j=1}^{K} m_{ij}$.

- 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.

- 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 $p_{ij} = \frac{m_{ij}}{m}$, $p_i = \frac{m_{i.}}{m}$, $p_j = \frac{m_{.j}}{m}$.

- 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;
- c is the number of pairs in the same cluster, but with different class labels.

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
- The index produces a result in the range $[0, 1]$, where a value of 1.0 indicates that C and P are identical.
- A high value for this measure generally indicates a high level of agreement between a clustering and the true classes.

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

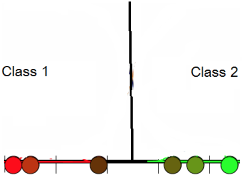
$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}.$$

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

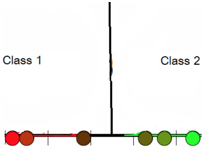
$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$

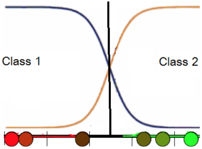
- If $s(i)$ is close to 1, sample i is well-clustered and it was assigned to a very appropriate cluster
- If $s(i)$ is close to zero, sample i could be assign to another closest cluster as well, and the sample lies equally far away from both clusters
- If $s(i)$ is close to -1, sample i is misclassified.
- We can consider average $\frac{\sum_i s(i)}{m}$ of $s(i)$ for all objects in the whole dataset:
  - the larger it is, the better the clustering is

- 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

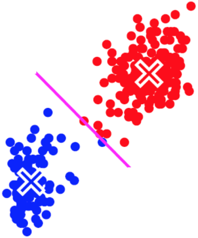


- Each data point is (partially) assigned to clusters with certain probabilities
- One point might be (partially) assigned to multiple clusters
- The midway point is assigned to either cluster with probability 0.5

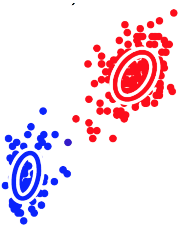




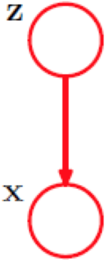
Hard/Soft Assignment: 2D example



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

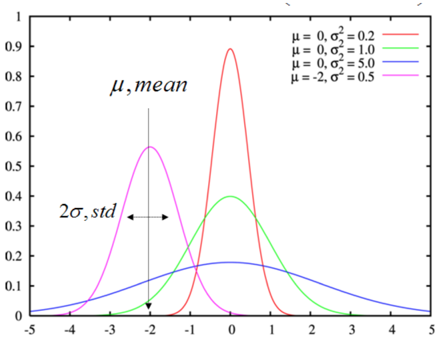
- Distribution of data:

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

- 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

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

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

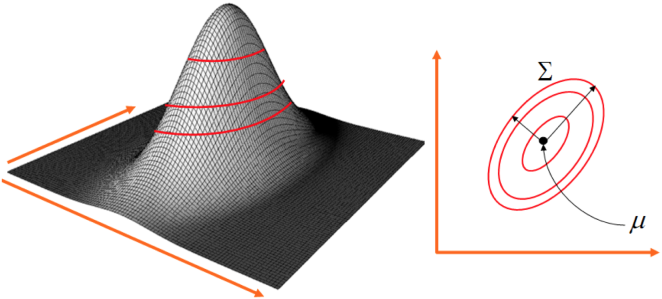


$$p(\mathbf{x}|\boldsymbol{\mu}, \Sigma) = \frac{1}{\sqrt{(2\pi)^d \det(\boldsymbol{\Sigma})}} \exp\left[-\frac{(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}{2}\right],$$

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

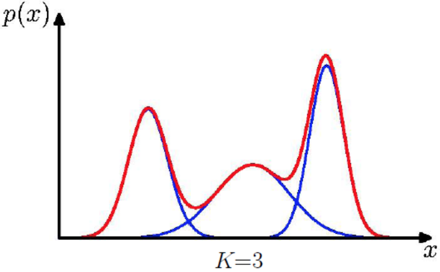


- Mixture distribution:

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

- Each component is a Gaussian distribution:

$$p(\mathbf{x}|z = k) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$

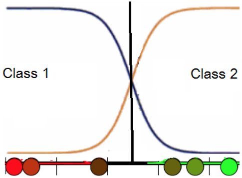


- Given mixture model:

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

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

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

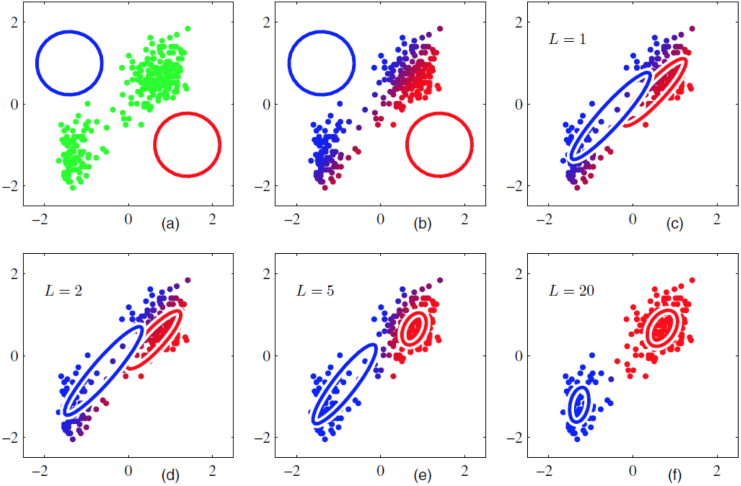


- Given
  - unlabeled data $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$;
  - number of clusters K
- Find a K-component Gaussian mixture model:
  - mixing coefficients $\{\pi_1, \ldots, \pi_K\}$;
  - components parameters $\{(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\}_{k=1}^K$

  by maximizing data likelihood

- Choose initial values for $\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$, $k = 1, \dots, K$
- repeat:
  - Expectation: for each training example $\mathbf{x}_n$
    (a) Compute $r_{nk} = P(z = k|\mathbf{x}_n)$, $k = 1, \dots, K$
    (b) Break data into K parts according to the probabilities
    $$\mathbf{x}_n[r_{nk}],\ k = 1, \dots, K$$
    (c) Assign each part $\mathbf{x}_n[r_{nk}]$ to the corresponding cluster k
  - Maximization: Re-estimate $\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$, $k = 1, \dots, K$
- Until convergence

EM: 2D illustration



- Main computations are in step (a):

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

- r_{nk} are often called responsibilities.

- Total number of examples, assigned to cluster k:

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

- Re-estimate $\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k$:

$$\pi_k^{new} = \frac{m_k}{m},$$

$$\boldsymbol{\mu}_k^{new} = \frac{1}{m_k} \sum_{i=1}^{m} r_{ki} \mathbf{x}_i,$$

$$\boldsymbol{\Sigma}_k^{new} = \frac{1}{m_k} \sum_{i=1}^{m} r_{ki} (\mathbf{x}_i - \boldsymbol{\mu}_k^{new})(\mathbf{x}_i - \boldsymbol{\mu}_k^{new})^{\mathrm{T}}$$

- Choose initial values for π_k, $\boldsymbol{\mu}_k$, $\boldsymbol{\Sigma}_k$.
- Repeat until convergence
  - Expectation: for each training example $\mathbf{x}_n$ compute
$$r_{nk} = \frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{s=1}^{K} \pi_s \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_s, \boldsymbol{\Sigma}_s)}, \ k = 1, 2, \ldots, K.$$
  - Maximization: Re-estimate π_k, $\boldsymbol{\mu}_k$, $\boldsymbol{\Sigma}_k$:
$$\pi_k^{new} = \frac{m_k}{m}, \ \boldsymbol{\mu}_k^{new} = \frac{1}{m_k} \sum_{i=1}^{m} r_{ki} \mathbf{x}_i,$$
$$\boldsymbol{\Sigma}_k^{new} = \frac{1}{m_k} \sum_{i=1}^{m} r_{ki} (\mathbf{x}_i - \boldsymbol{\mu}_k^{new})(\mathbf{x}_i - \boldsymbol{\mu}_k^{new})^{\mathrm{T}},$$
where $m_k = \sum_{i=1}^{m} r_{ki}$

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

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

- Data: $\boldsymbol{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_m\}$
- Log-Likelihood as function of model parameters:

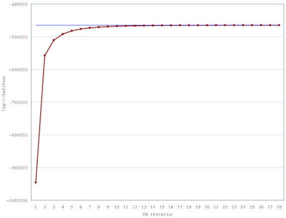
$$l(\boldsymbol{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \log \prod_{i=1}^{m} p(\mathbf{x}_i|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{i=1}^{m} \log p(\mathbf{x}_i|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

EM Convergence

- EM aims at computing the maximum likelihood estimation (MLE) of the parameters

$$(\boldsymbol{\pi}^*, \boldsymbol{\mu}^*, \boldsymbol{\Sigma}^*) = \arg \max_{\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}} l(\boldsymbol{X} | \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

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

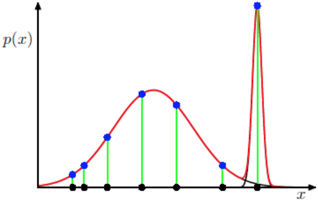


EM Convergence: Singularity

- The maximum value of log-likelihood might be infinite:

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

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



- Solution: Bound the eigenvalues of covariance matrix
- To avoid local maximum: multiple restart

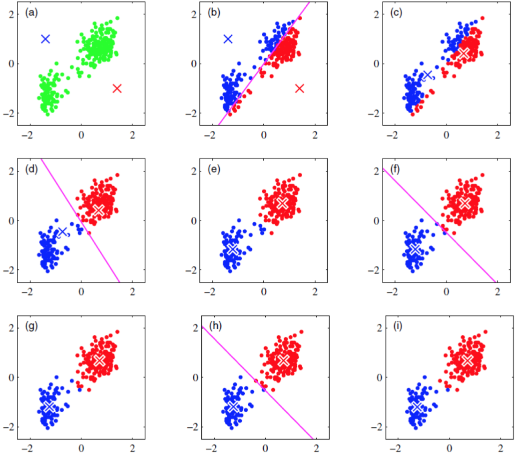
Hard Assignment:

- 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

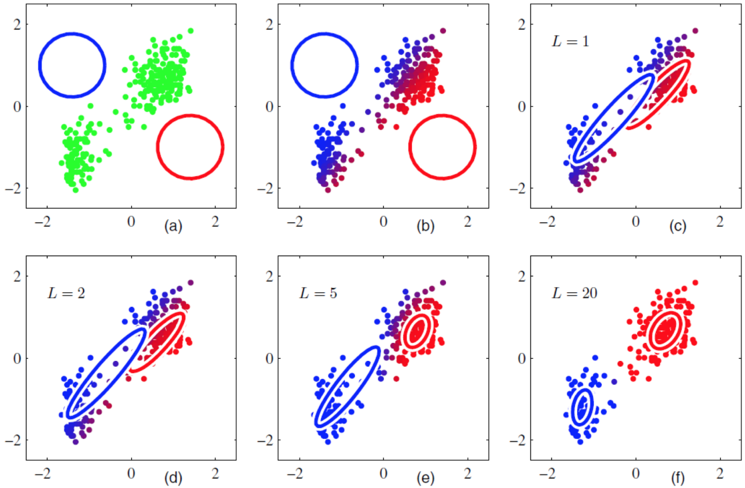
Soft Assignment:

- 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

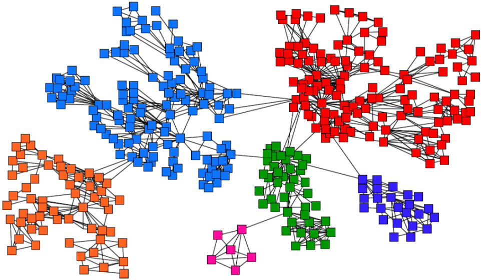
K-means example



EM example



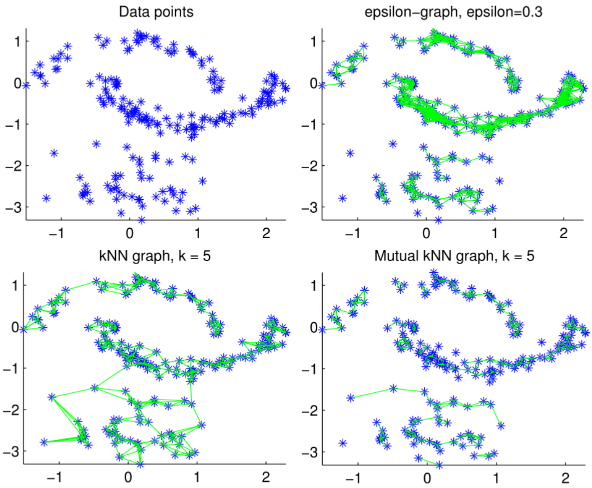
- **Graph** $G(E, V)$:
  - Nodes v_j
  - Edge weights $w_{ij} > 0$
- **Problem**: Want to partition graph such that edges between groups have low weights



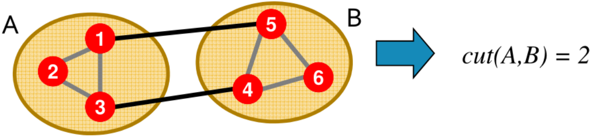
Types of graphs:

- 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
  - Weighted by similarity $w_{ij} = s_{ij}$
  - Directed or undirected
- **Mutual k-NN**:
  - Same as k-NN, but only include mutual k-NN

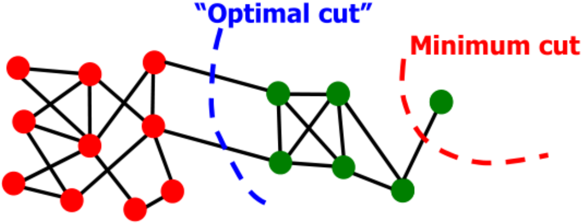
Similarity graphs



- **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:** $Cut(A_1, \ldots, A_k) = \sum_{i=1}^{k} W(A_i, \overline{A}_i)$
- **Choose:** $A_1, \ldots, A_k = \arg\min_{A_1, \ldots, A_k} Cut(A_1, \ldots, A_k)$



Problem: MinCut favors isolated clusters.



Solution:

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

Two measures of size of a subset:

- Cardinality:

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

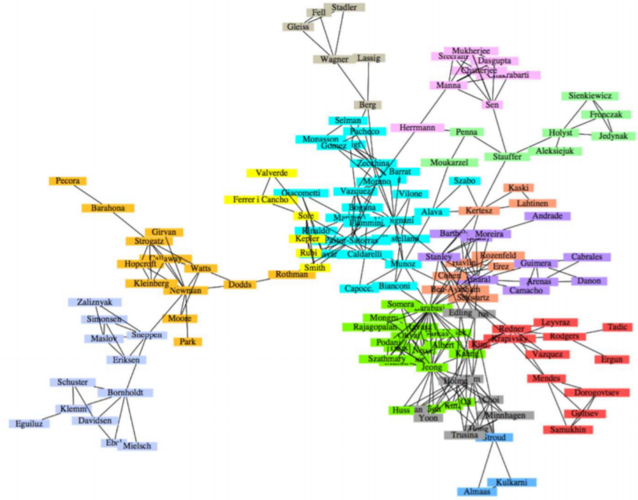
- Volume:

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

- Ratio cuts (RatioCut)
  - $k = 2: \; RatioCut(A, \overline{A}) = Cut(A, \overline{A}) \left(\frac{1}{|A|} + \frac{1}{|\overline{A}|} \right).$
  - General $k: \; RatioCut(A_1, \ldots, A_k) = \frac{1}{2} \sum_{i=1}^{k} \frac{Cut(A_i, \overline{A_i})}{|A_i|}.$
- Normalized cuts (Ncut)
  - $k = 2: \; NCut(A, \overline{A}) = Cut(A, \overline{A}) \left(\frac{1}{Vol(A)} + \frac{1}{Vol(\overline{A})} \right).$
  - General $k: \; NCut(A_1, \ldots, A_k) = \frac{1}{2} \sum_{i=1}^{k} \frac{Cut(A_i, \overline{A_i})}{Vol(A_i)}$
- Problem is NP-hard!
- We need to look at relaxation (solution = Spectral clustering)

Segmentation of Lena

Segmentation of Lena


Stadler
Fell
Gleiss
Wagner
Lassig
Berg
Mukherjee
Dasgupta
Manna
Sen
Sienkiewicz
Fronczak
Holyst
Jedynak
Aleksiejuk
Herrmann
Penna
Stauffer
Moukarzel
Selman
Pacheco
Monasson
Zecchina
Barrat
Valverde
Ferrer i Cancho
Giacometti
Vazquez
Vilone
Szabo
Kaski
Lahtinen
Pecora
Barahona
Alava
Kertesz
Andrade
Boguna
Sole
Moreira
Girvan
Strogatz
Kepler
Pastor-Satorras
Caldarelli
Stanley
Rozenfeld
Cabrales
Rubi
Smith
Munoz
Guimera
Hopcroft
Callaway
Watts
Rothman
Erez
Amaral
Arenas
Danon
Kleinberg
Newman
Dodds
Capocc.
Bianconi
Camacho
Zaliznyak
Somera
Edling
Simonsen
Mongru
Moore
Leyvraz
Tadic
Sneppen
Rajagopalan
Redner
Maslov
Krapivsky
Rodgers
Park
Podani
Albert
Eriksen
Szathmary
Vazquez
Ergun
Jeong
Schuster
Mendes
Bornholdt
Dorogovtsev
Klemm
Choi
Huss
Goltsev
Eguiluz
Davidsen
Yoon
Minnhagen
Samukhin
Trusina
Stroud
Mielsch
Kulkarni
Almaas

Objects of study:

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

Modularity

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

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

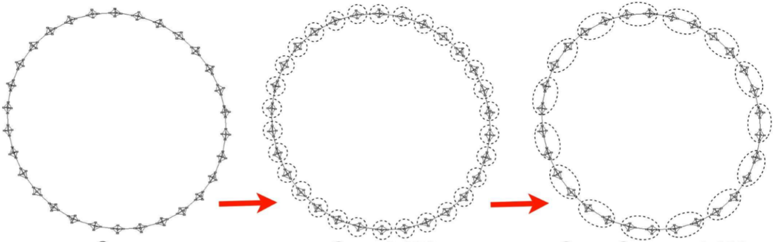
Interpretation: difference between the fraction of edges inside the community and its expectation in random graph with fixed node degrees.

Modularity:

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

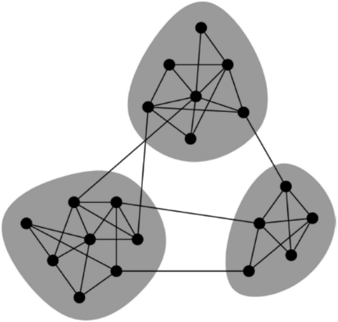
- **Idea:** optimize modularity (discrete optimization problem).
- **Efficient implementation:** Louvain community detection algorithm.
- **Problem:** low resolution.

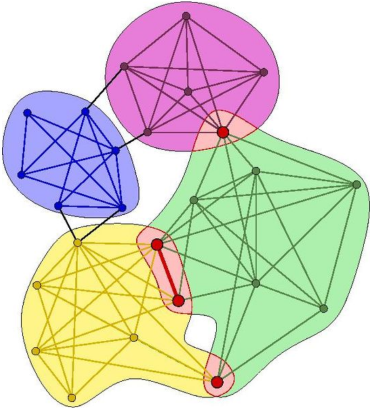
Low resolution of modularity

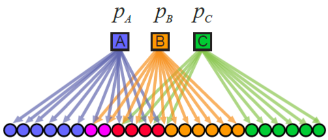


Q_{init} $\quad$ $Q_1 = 0.876$ $\quad$ $Q_2 = Q_{max} = 0.888$

Non-overlapping vs. overlapping communities







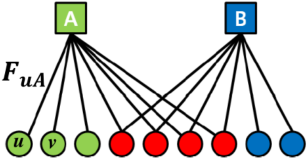
AGM generates the links:

- 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:

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

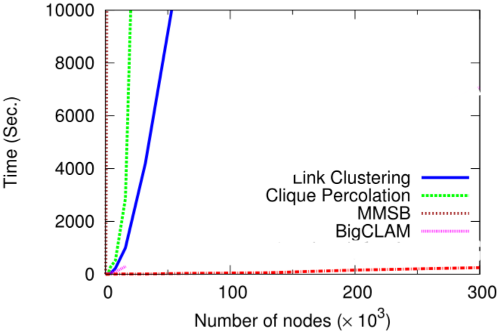
where $P(u,v) = 1 - \exp\{-F_u F_v^T\}$.

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!