Clustering

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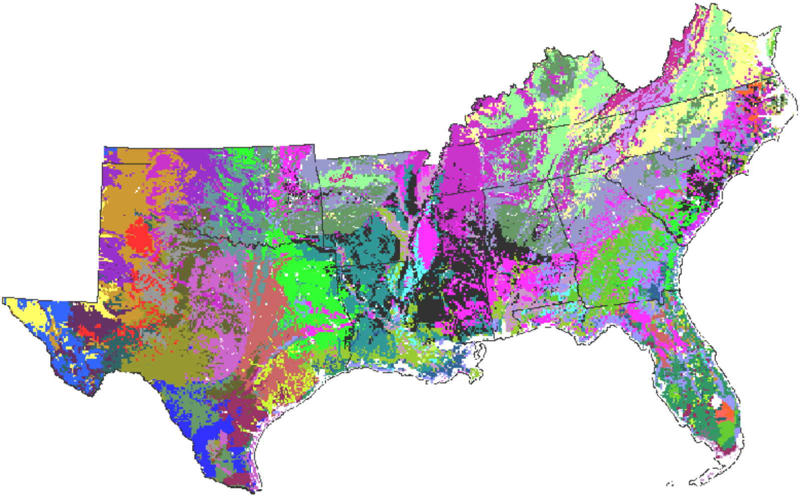
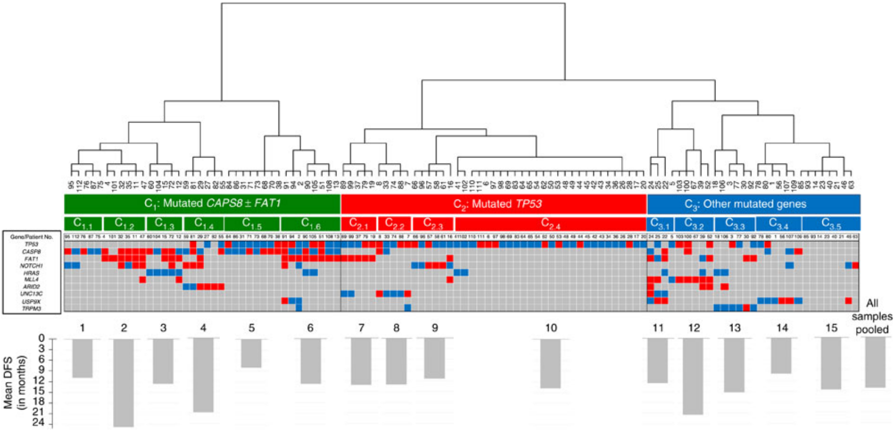
Clustering Application - Geo

13 States Clustered into 51 Custom Ecoregions.



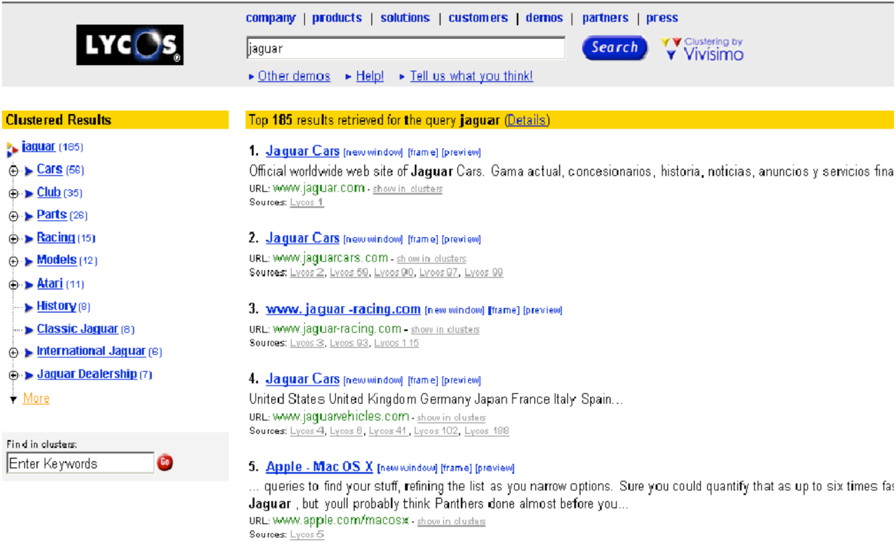
Clustering Application - Cancer Patients

Clustering of gingivo-buccal oral cancer patients based on mutational profiles.

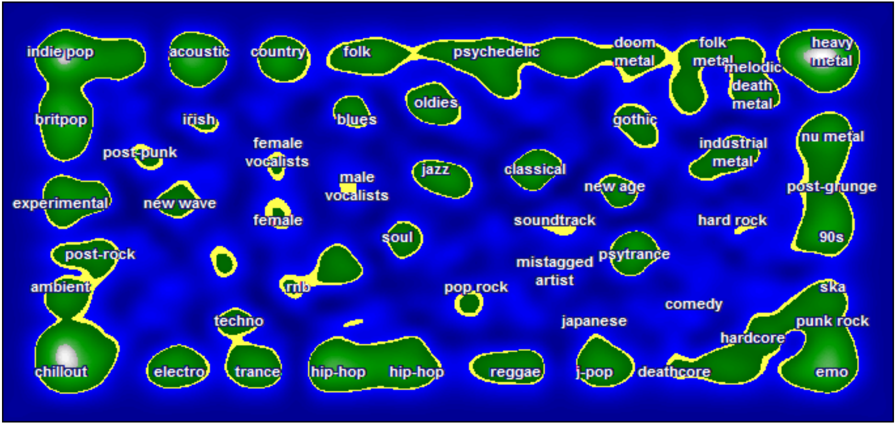


Mutational landscape of gingivo-buccal oral squamous cell carcinoma reveals new recurrently-mutated genes and molecular subgroups, Nature Communications, 2013

Clustering Application - Search Result Clustering

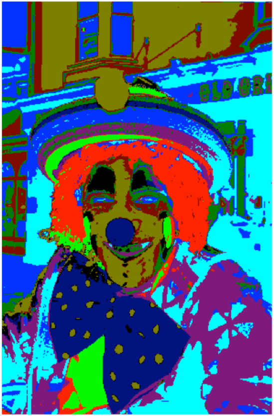


Clustering Application - Island of Music

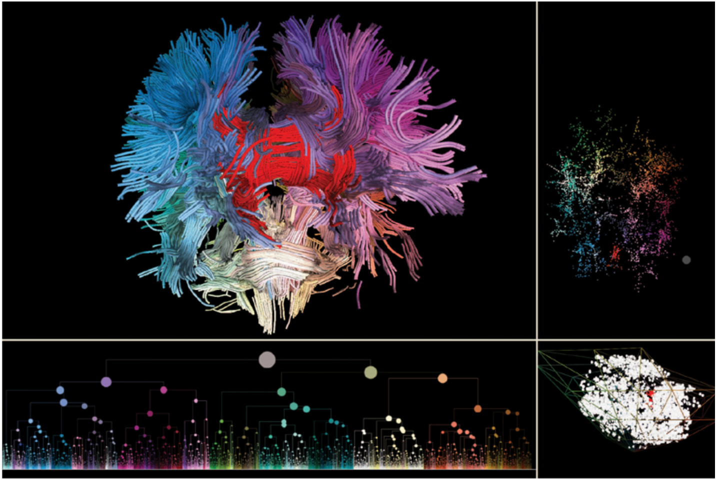


Pampalk, Elias, Andreas Rauber, and Dieter Merkl. "Content-based organization and visualization of music archives." Proceedings of the tenth ACM international conference on Multimedia. ACM, 2002.

Clustering Application - Image Compression

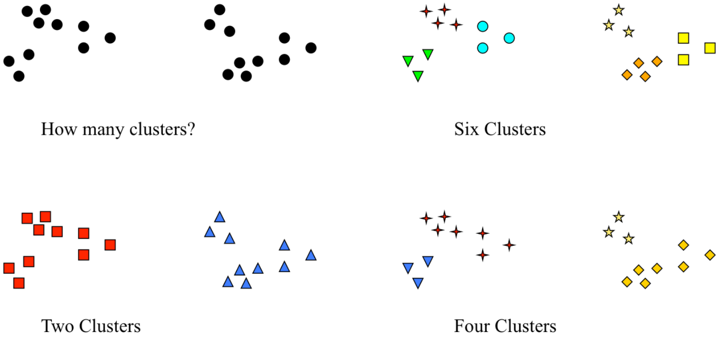


Clustering Application - MRI TDI Fibers



"Exploring 3D DTI fiber tracts with linked 2D representations." Visualization and Computer Graphics, IEEE Transactions on 15.6 (2009): 1449-1456.

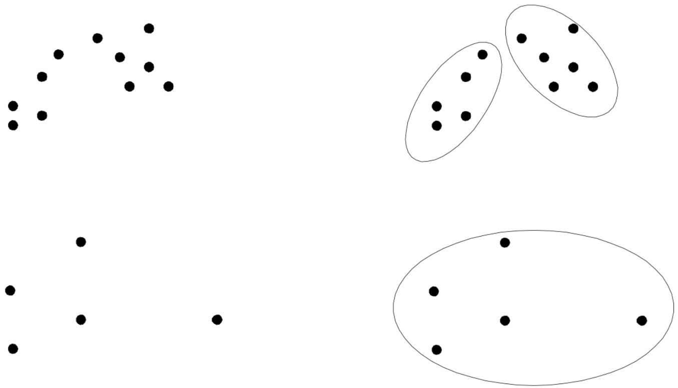
Notion of a Cluster can be Ambiguous



Types of Clustering

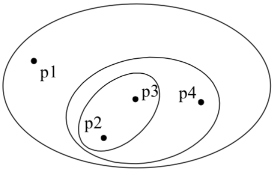
- A clustering is a set of clusters.
- Important distinction between hierarchical and partitional sets of clusters
  - **Partitional Clustering**
    A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
  - **Hierarchical clustering**
    A set of nested clusters organized as a hierarchical tree

Partitional Clustering

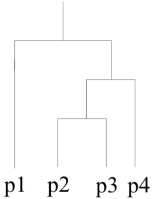


Original Points **A Partitional Clustering**

Hierarchical clustering



Traditional Hierarchical Clustering



Traditional Dendrogram

K-means for Clustering

K-means Clustering

- Partitional clustering approach
- Each cluster is associated with a **centroid** (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K, must be specified
- Optimization objective

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$$\arg\min_{\{c_j, m_{i,j}\}} \sum_{j=1}^{K} \sum_{i=1}^{n} m_{i,j} \|x_i - c_j\|^2$$

where memberships $\{m_{i,j}\}$ and centers $\{C_j\}$ are correlated.

K-means Clustering Algorithm

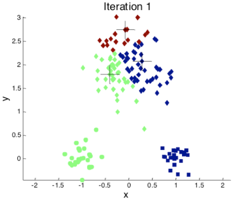
$$\arg\min_{\{c_j, m_{i,j}\}} \sum_{j=1}^{K} \sum_{i=1}^{n} m_{i,j} \|x_i - C_j\|^2$$

- Given centroids $\{c_j\}$, $m_{i,j} = \begin{cases} 1 & j = \arg\min_{j \in [1 \dots K]} \|x_i - c_j\|^2 \\ 0 & \text{otherwise} \end{cases}$
- Given memberships $\{m_{i,j}\}$, $c_j = \frac{\sum_{i=1}^{n} m_{i,j} x_i}{\sum_{i=1}^{n} m_{i,j}}$

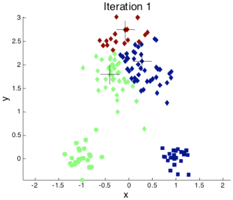
The alternating procedure leads to the following algorithm.

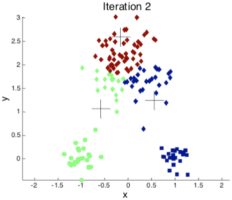
1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

k-means illustration

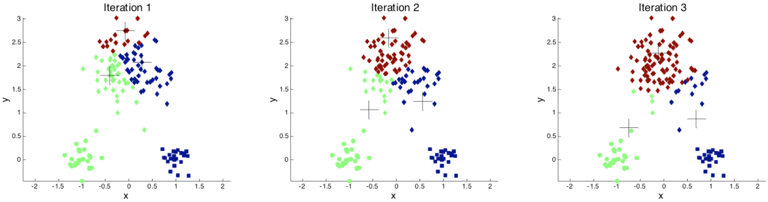


k-means illustration





k-means illustration



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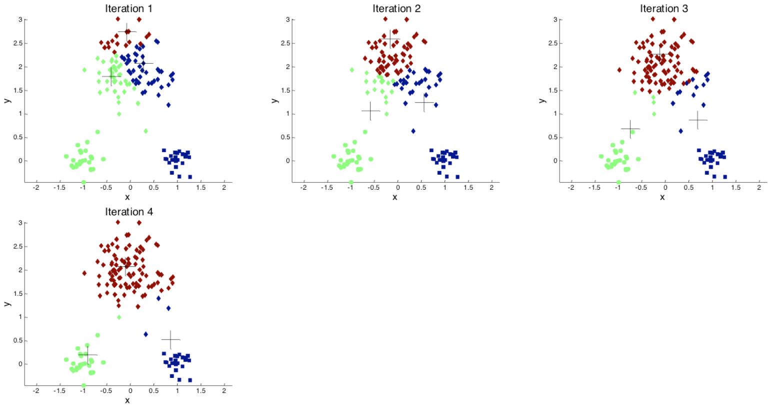

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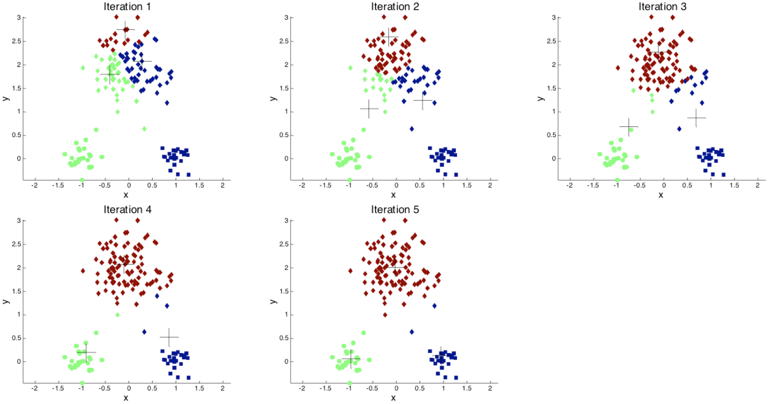
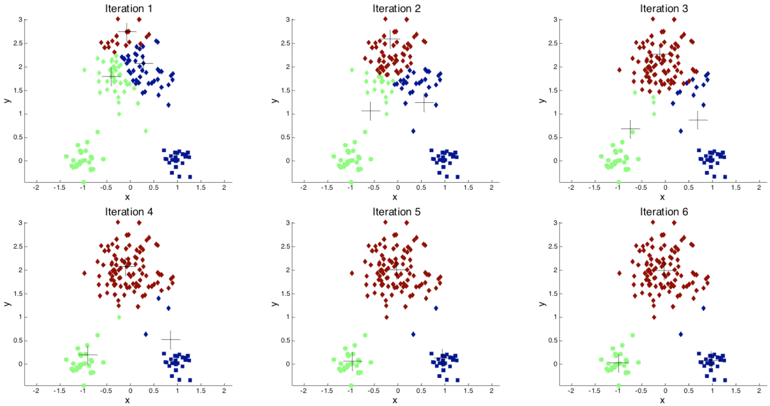


k-means illustration



k-means Clustering Details

- Initial centroids are often chosen randomly.
- The centroid is (typically) the mean of the points in the cluster.
- Closeness is measured by Euclidean distance, cosine similarity, correlation, etc.
- K-means will converge for common similarity measures mentioned above.
- Most of the convergence happens in the first few iterations. Often the stopping condition is changed to "Until relatively few points change clusters"
- Let $n =$ number of points, $K =$ number of clusters, $I =$ number of iterations, $d =$ number of attributes, complexity is

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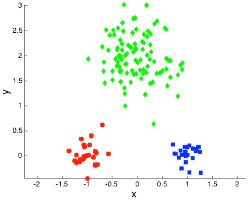
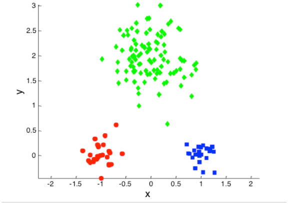
k-means revisited

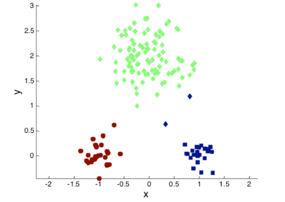


Original Points

k-means revisited

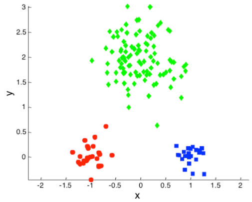


Original Points

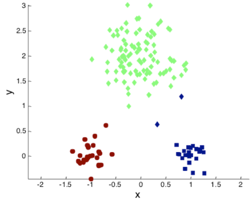


Optimal Clustering

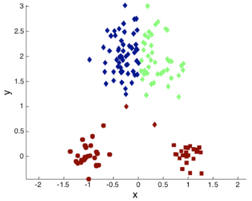
k-means revisited



Original Points



Optimal Clustering



Sub-optimal Clustering

Problems with Selecting Initial Points

If there are K "real" clusters then the chance of selecting one centroid from each cluster is small.

- Chance is relatively small when K is large
- If clusters are the same size, n, then the probability is

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- If clusters are the same size, n, then the probability is

$$P = \frac{\text{ways to select one centroid from each cluster}}{\text{ways to select K centroids}} = \frac{K!n^K}{(Kn)^K} = \frac{K!}{K^K}$$

- For example, if $K = 10$, then probability $= 10!/10 = 0.00036$
- Sometimes the initial centroids will readjust themselves in "right" way, and sometimes they don't.

Solutions to Initial Centroids Problem

- Multiple runs
  Helps, but probability is not on your side
- Sample and use hierarchical clustering to determine initial centroids
- Select more than k initial centroids and then select among these initial centroids
- Bisecting K-means
  1. Pick a cluster to split.
  2. Find 2 sub-clusters using the basic k-Means algorithm (Bisecting step)
  3. Repeat step 2, the bisecting step, for ITER times and take the split that produces the clustering with the highest overall similarity.
  4. Repeat steps 1, 2 and 3 until the desired number of clusters is reached.

  Not as susceptible to initialization issues

Evaluating K-means Clusters

Most common measure is Sum of Squared Error (SSE)

- For each point, the error is the distance to the nearest cluster
- To get SSE, we square these errors and sum them.

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} d^2(m_i, x)$$

- x is a data point in cluster C_i and m_i is the representative point (center/mean) for cluster C_i.
- Given two clusters, we can choose the one with the smaller error
- One easy way to reduce SSE is to increase K, the number of clusters
  - A good clustering with smaller K can have a lower SSE than a poor clustering with higher K.

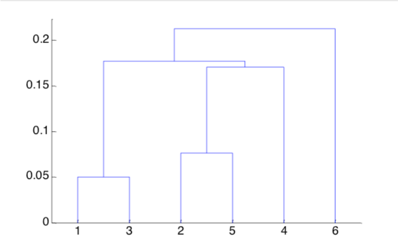
Limitations of K-means

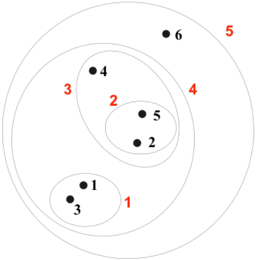
- K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes
- K-means has problems when the data contains outliers.
- The number of clusters (K) is difficult to determine.

Hierarchical Clustering

Hierarchical Clustering

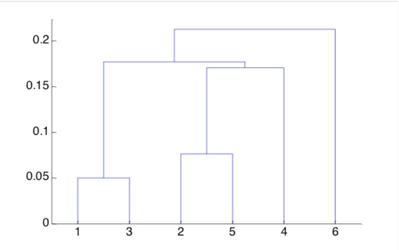
- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram
  - A tree like diagram that records the sequences of merges or splits

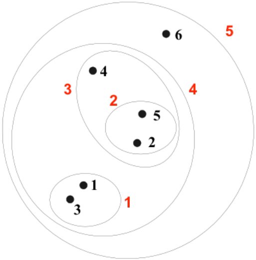




Strengths of Hierarchical Clustering

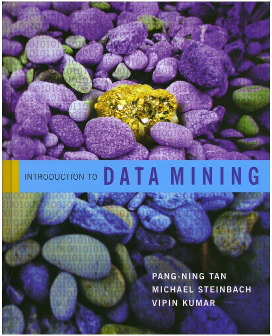
- Do not have to assume any particular number of clusters
  - Any desired number of clusters can be obtained by “cutting” the dendogram at the proper level
- They may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, movie genre, etc.)





Hierarchical Clustering

- Tan, Seinbach, and Kumar, *Introduction to Data Mining*, Addison-Wesley, 2006.
- Chapter 8, Cluster Analysis.
- http://www-users.cs.umn.edu/~kumar/dmbook/ch8.pdf

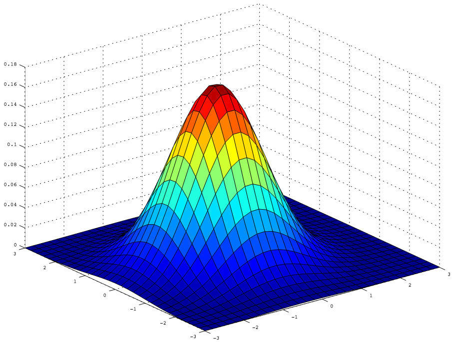


Gaussian Mixture

Multivariate Gaussian

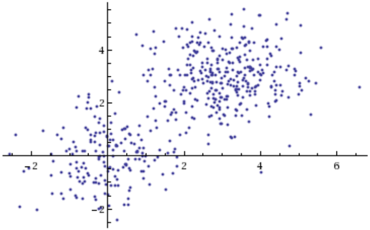
- A generative model specified by a center μ and a covariance Σ

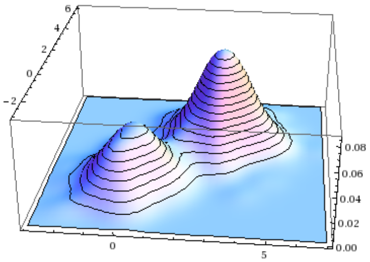
$$p(x) = \frac{1}{\sqrt{(2\pi)^d|\Sigma|}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$



A Gaussian Mixture Model for Clustering

- Assume that data are generated from a mixture of Gaussian distributions
- For each Gaussian distribution
  - Center μ_i
  - Variance: Σ_i
- For each data point
  - Determine membership
- z_{ij}: if x_i belongs to the j-th cluster





Learning a Gaussian Mixture (with known covariance)

- 1-dimensional case.
- Probability $p(x = x_i)$

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$$p(x = x_i) = \sum_{\mu_j} p(x = x_i, \mu = \mu_j) = \sum_{\mu_j} p(\mu = \mu_j) p(x = x_i | \mu = \mu_j)$$
$$= \sum_{\mu_j} p(\mu = \mu_j) \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right)$$

- Log likelihood of data

Learning a Gaussian Mixture (with known covariance)

- 1-dimensional case.
- Probability $p(x = x_i)$

$$p(x = x_i) = \sum_{\mu_j} p(x = x_i, \mu = \mu_j) = \sum_{\mu_j} p(\mu = \mu_j) p(x = x_i | \mu = \mu_j)$$
$$= \sum_{\mu_j} p(\mu = \mu_j) \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{1}{2\sigma^2} (x - \mu)^2 \right)$$

- Log likelihood of data

$$\sum_i \log p(x = x_i) = \sum_i \log \left[\sum_{\mu_j} p(\mu = \mu_j) \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{1}{2\sigma^2} (x - \mu)^2 \right) \right]$$

- Apply MLE to find optimal parameters $\{p(\mu = \mu_j), \mu_j\}_j$

Learning a Gaussian Mixture (with known covariance)

E-Step

$$
\begin{aligned}
\mathbb{E}[z_{ij}] &= p(\mu = \mu_j | x = x_i) \\
&= \frac{p(x = x_i | \mu = \mu_j) p(\mu = \mu_j)}{\sum_{k=1}^{K} p(x = x_i | \mu = \mu_k) p(\mu = \mu_k)} \\
&= \frac{\exp\left(-\frac{1}{2\sigma^2}(x_i - \mu_j)^2\right) p(\mu = \mu_j)}{\sum_{k=1}^{K} \exp\left(-\frac{1}{2\sigma^2}(x_i - \mu_k)^2\right) p(\mu = \mu_k)}
\end{aligned}
$$

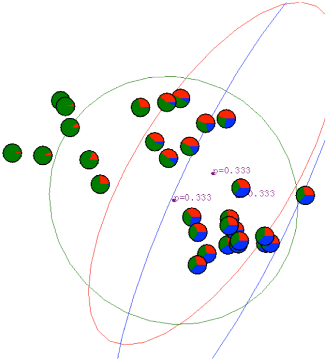
Learning a Gaussian Mixture (with known covariance)

M-Step

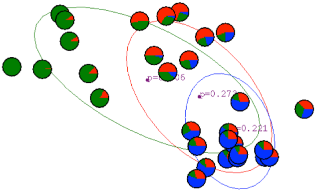
$$\mu_j \Leftarrow \sum_{i=1} \frac{\mathbb{E}[z_{ij}]}{\sum_{i=1} \mathbb{E}[z_{ij}]} x_i = \frac{1}{\sum_{i=1} \mathbb{E}[z_{ij}]} \sum_{i=1} \mathbb{E}[z_{ij}] x_i$$

$$p(\mu = \mu_j) \Leftarrow \frac{1}{m} \sum_{i=1} \mathbb{E}[z_{ij}]$$

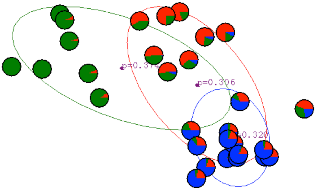
Gaussian Mixture Example: Start



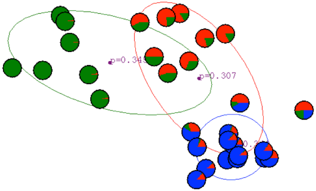
After 1st Iteration



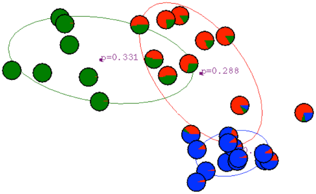
After 2nd Iteration



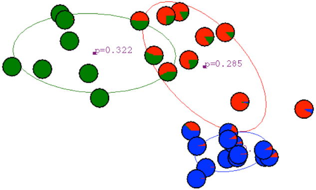
After 3rd Iteration



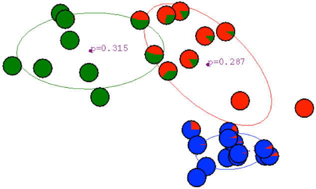
After 4th Iteration



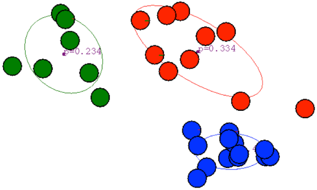
After 5th Iteration



After 6th Iteration



After 20th Iteration



Spectral Clustering

k-means revisited

- We assume that we have n data points $\{x_i\}_{i=1}^n \in \mathbb{R}^m$, which we organize as columns in a matrix

$$X = [x_1, x_2, \cdots, x_n] \in \mathbb{R}^{m \times n}.$$

- Let $\Pi = \{\pi_j\}_{j=1}^k$ denote a partitioning of the data in X into k clusters:

$$\pi_j = \{v \,|\, x_v \text{ belongs to cluster } j\}.$$

- Let the mean, or the centroid, of the cluster be

$$c_j = \frac{1}{n_j} \sum_{v \in \pi_j} x_v,$$

where n_j is the number of elements in π_j.

k-means revisited

- We describe K-means algorithm based on the Euclidean distance measure.
    - The tightness or coherence of cluster π_j can be measured as the sum

$$q_j = \sum_{v \in \pi_j} ||x_v - c_j||^2.$$

- The closer the vectors are to the centroid, the smaller the value of q_j. The quality of a clustering can be measured as the overall coherence,

$$Q(\Pi) = \sum_{j=1}^{k} \sum_{v \in \pi_j} ||x_v - c_j||^2.$$

k-means revisited

- Let e be the vector of all ones with appropriate length. It is easy to see that $c_j = X_j e/n_j$, where X_j is the data matrix of the j-th cluster.
- The sum-of-squares cost function of the j-th cluster is

$$q_j = \sum_{v \in \pi_j} ||x_v - c_j||^2 = ||X_j - c_j e^T||_F^2 = ||X_j(I_{n_j} - ee^T/n_j)||_F^2.$$

- Note that $I_{n_j} - ee^T/n_j$ is a projection matrix and

$$(I_{n_j} - ee^T/n_j)^2 = I_{n_j} - ee^T/n_j.$$

It follows that

$$q_j = \text{trace}\left(X_j(I_{n_j} - ee^T/n_j)X_j^T\right) = \text{trace}\left((I_{n_j} - ee^T/n_j)X_j^T X_j\right).$$

Therefore,

$$Q(\Pi) = \sum\nolimits_{j=1}^k q_j = \sum\nolimits_{j=1}^k \left(\text{trace}\left(X_j^T X_j\right) - \frac{e^T}{\sqrt{n_j}} X_j^T X_j \frac{e}{\sqrt{n_j}}\right).$$

k-means revisited

Define the n-by-k orthogonal matrix Y as follows

$$Y = \begin{pmatrix} e/\sqrt{n_1} & & & \\ & e/\sqrt{n_2} & & \\ & & \vdots & \\ & & & e/\sqrt{n_k} \end{pmatrix} \tag{1}$$

Then

$$Q(\Pi) = \text{trace}\left(X^T X\right) - \text{trace}\left(Y^T X^T X Y\right).$$

The k-means objective, minimization of $Q(\Pi)$, is equivalent to the maximization of trace $\left(Y^T X^T X Y\right)$ with Y is of the form in Eq. (1).

Spectral Clustering

Ignoring the special structure of Y and let it be an arbitrary orthonormal matrix, we obtain a relaxed maximization problem

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It turns out the above trace maximization problem has a closed-form solution.

- Theorem (Ky Fan): Let H be a symmetric matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_n$ and the corresponding eigenvectors $U = [u_1, \cdots, u_n]$. Then

$$\lambda_1 + \cdots \lambda_k = \max_{Y^T Y = I_k} \text{trace}(Y^T H Y).$$

  Moreover, the optimal Y^* is given by $Y^* = [u_1, \cdots, u_k]Q$ with Q an arbitrary orthogonal matrix of size k by k.

- We may derive the following lower bound for the minimum of the sum-of-squares cost function:

$$\min_{\Pi} Q(\Pi) \geq \mathsf{trace}(X^T X) - \max_{Y^T Y = I_k} \mathsf{trace}\left(Y^T X^T X Y\right) = \sum_{i=k+1}^{\min\{m,n\}} \sigma_i^2(X),$$

where $\sigma_i(X)$ is the i-th largest singular value of X.

- Let Y^* be the n-by-k matrix consisting of the k largest eigenvectors of $X^T X$. Each row of Y^* corresponds to a data vector. This can be considered as transforming the original data vectors which lie in a m-dimensional space to new data vectors which now lie in a k-dimensional space.
- **How to get our cluster assignment back?**
One might be attempted to compute the cluster assignment by applying the ordinary K-means method to those data vectors in the reduced dimension space.