

Machine Learning for Signal Processing Clustering

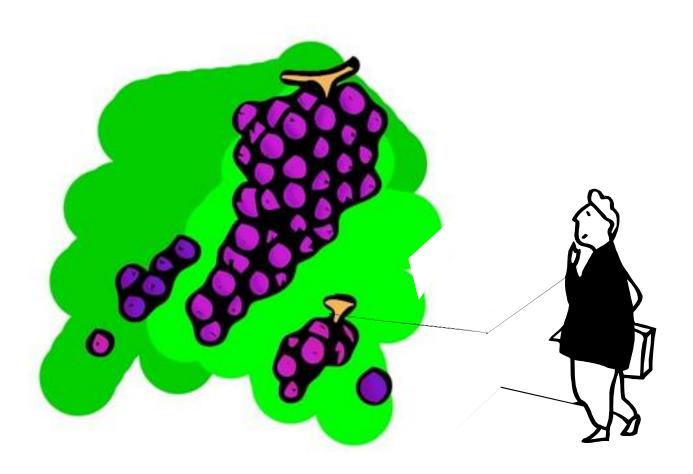
Bhiksha Raj Class 12. 10 Oct 2013



Statistical Modelling and Latent Structure

- Much of statistical modelling attempts to identify *latent* structure in the data
 - Structure that is not immediately apparent from the observed data
 - But which, if known, helps us explain it better, and make predictions from or about it
- Clustering methods attempt to extract such structure from proximity
 - *First-level* structure (as opposed to deep structure)
- We will see other forms of latent structure discovery later in the course







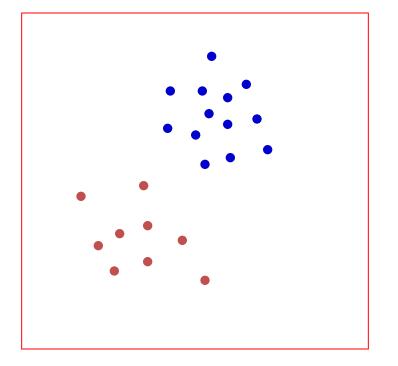
How





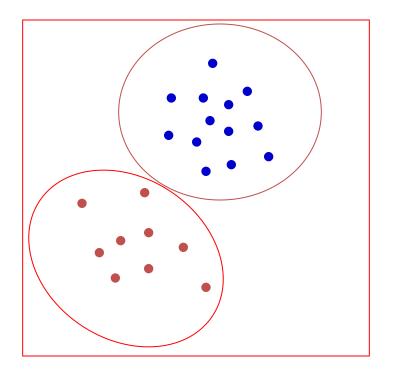


- What is clustering
 - Clustering is the determination of naturally occurring grouping of data/instances (with low withingroup variability and high betweengroup variability)



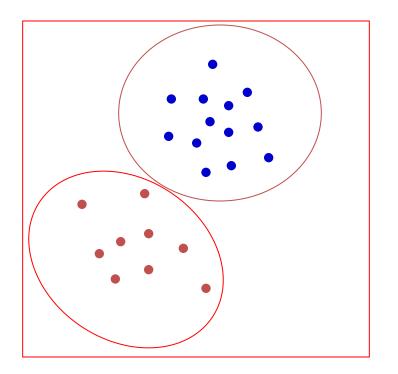


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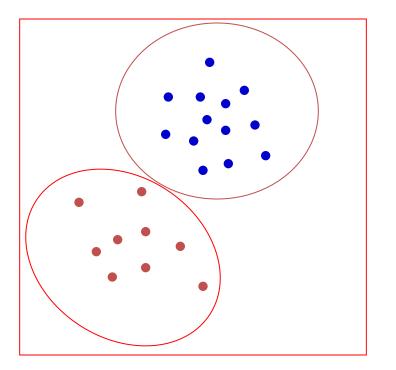


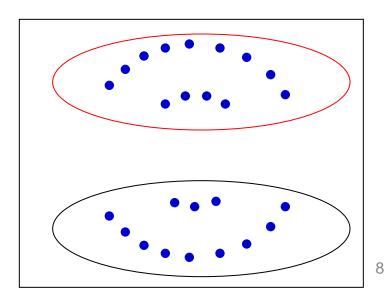
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- How is it done
 - Find groupings of data such that the groups optimize a "within-groupvariability" objective function of some kind





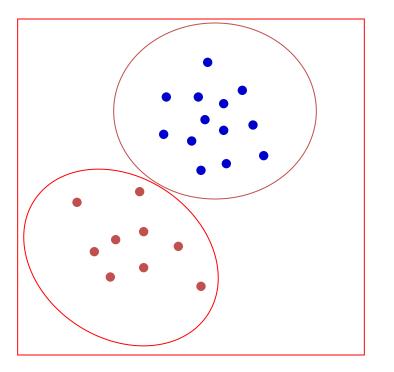
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 - The objective function used affects the nature of the discovered clusters
 - E.g. Euclidean distance vs.
 - Distance from center

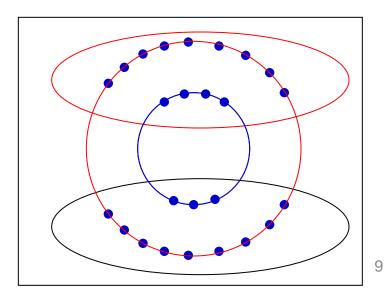






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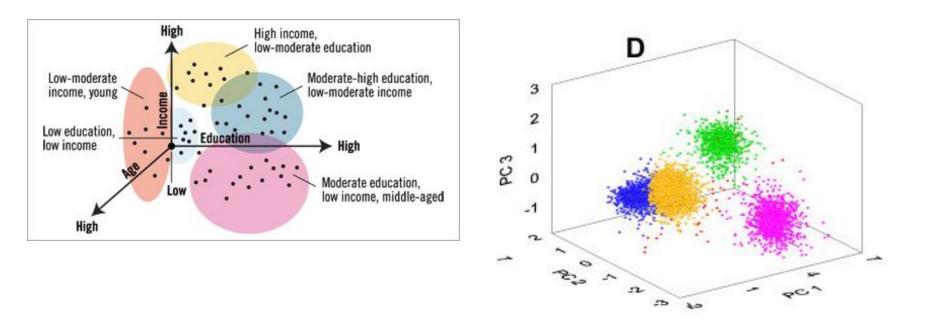
Why Clustering

- Automatic grouping into "Classes"
 - Different clusters may show different behavior
- Quantization
 - All data within a cluster are represented by a single point
- Preprocessing step for other algorithms

 Indexing, categorization, etc.



Finding natural structure in data



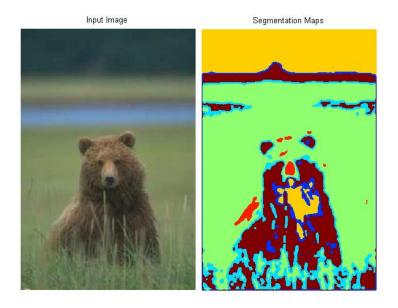
- Find natural groupings in data for further analysis
- Discover *latent* structure in data



Some Applications of Clustering

Image segmentation



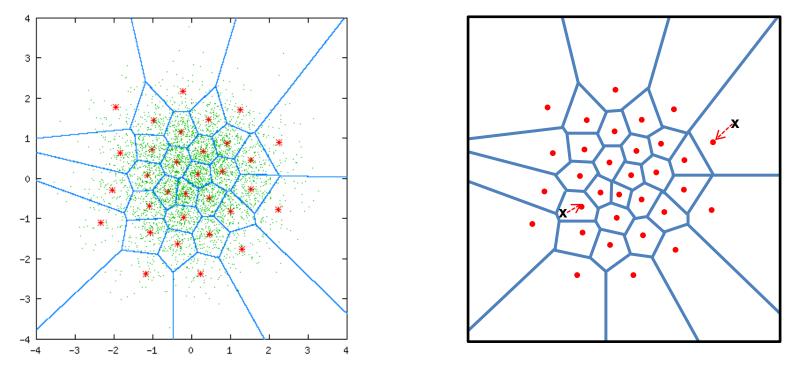




Representation: Quantization

TRAINING

QUANTIZATION



- *Quantize* every *vector* to one of K (vector) values
- What are the optimal K vectors? How do we find them? How do we perform the quantization?
- LBG algorithm



Representation: BOW



- How to retrieve all music videos by this guy?
- Build a classifier
 - But how do you *represent* the video?

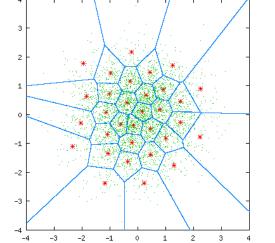
10 Oct 2013



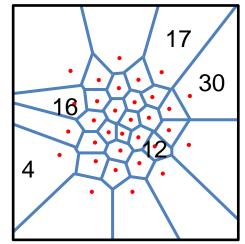
Representation: BOW



Training: Each point is a video frame



Representation: Each number is the #frames assigned to the codeword



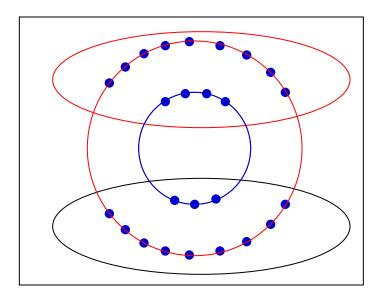
Bag of words representations of video/audio/data



Obtaining "Meaningful" Clusters

- Two key aspects:
 - 1. The feature representation used to characterize your data
 - 2. The "clustering criteria" employed







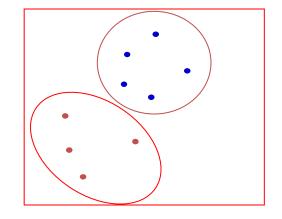
Clustering Criterion

- The "Clustering criterion" actually has two aspects
- Cluster compactness criterion
 - Measure that shows how "good" clusters are
 - The objective function
- Distance of a point from a cluster

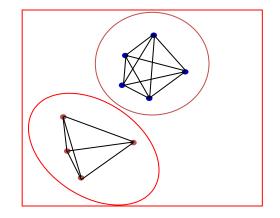
- To determine the cluster a data vector belongs to



- Distance based measures
 - Total distance between each element in the cluster and every other element in the cluster

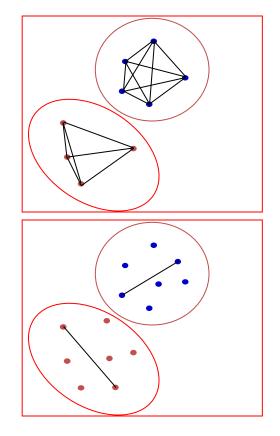


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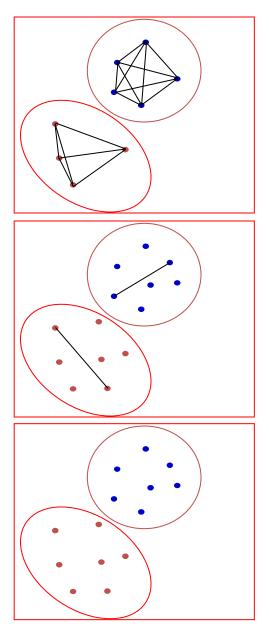


- Distance based measures
 - Total distance between each element in the cluster and every other element in the cluster
 - Distance between the two farthest points in the cluster



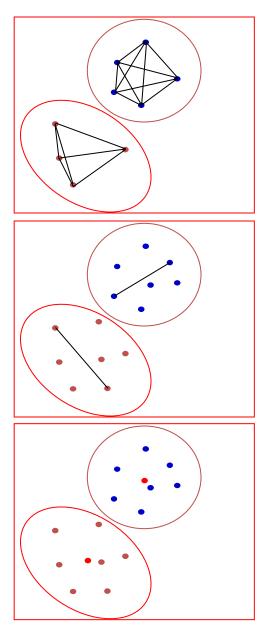


- Distance based measures
 - Total distance between each element in the cluster and every other element in the cluster
 - Distance between the two farthest points in the cluster
 - Total distance of every element in the cluster from the centroid of the cluster



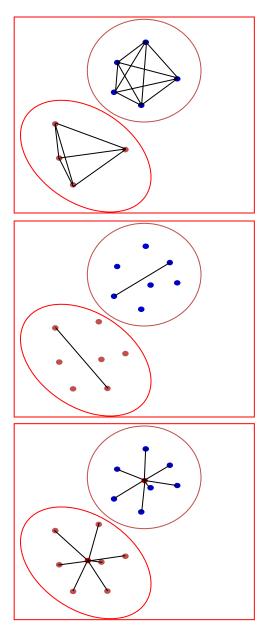


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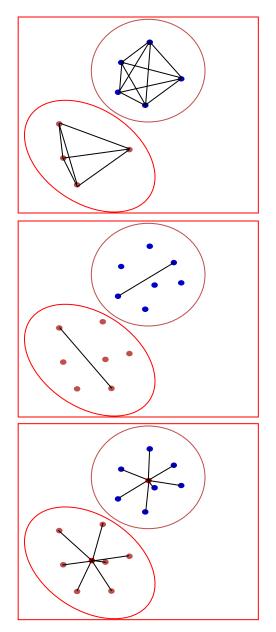
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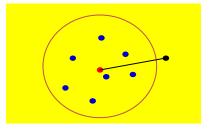
- Distance based measures
 - Total distance between each element in the cluster and every other element in the cluster
 - Distance between the two farthest points in the cluster
 - Total distance of every element in the cluster from the centroid of the cluster
 - Distance measures are often weighted Minkowski metrics

$$dist = \sqrt[n]{w_1|a_1 - b_1|^n + w_2|a_2 - b_2|^n + \dots + w_M|a_M - b_M|^n}$$



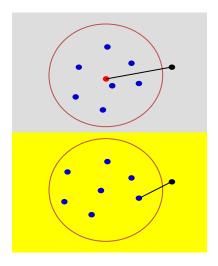


- How far is a data point from a cluster?
 - Euclidean or Minkowski distance from the centroid of the cluster



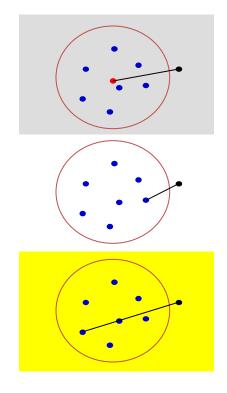


- How far is a data point from a cluster?
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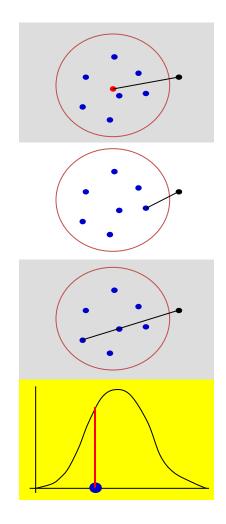


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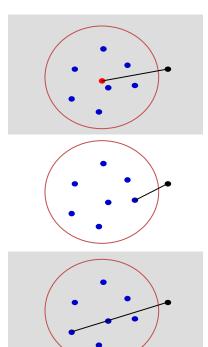


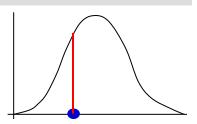
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 - Euclidean or Minkowski distance from the centroid of the cluster
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 - Distance from the farthest point in the cluster
 - Probability of data measured on cluster distribution





- How far is a data point from a cluster?
 - Euclidean or Minkowski distance from the centroid of the cluster
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 - Distance from the farthest point in the cluster
 - Probability of data measured on cluster distribution
 - Fit of data to cluster-based regression





Optimal clustering: Exhaustive enumeration

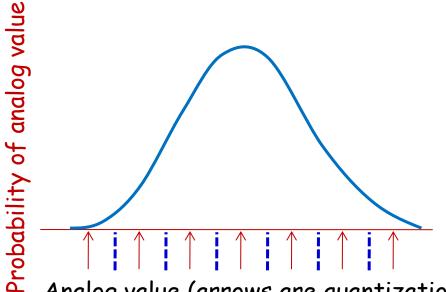
- All possible combinations of data must be evaluated
 - If there are M data points, and we desire N clusters, the number of ways of separating M instances into N clusters is

$$\frac{1}{M!}\sum_{i=0}^{N}(-1)^{i}\binom{N}{i}(N-i)^{M}$$

- Exhaustive enumeration based clustering requires that the objective function (the "Goodness measure") be evaluated for every one of these, and the best one chosen
- This is the only correct way of optimal clustering
 - Unfortunately, it is also computationally unrealistic



Not-quite non sequitur: Quantization



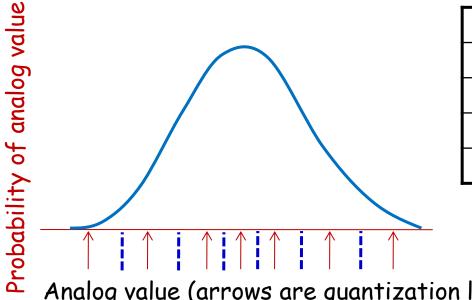
Signal Value	Bits	Mapped to
S >= 3.75v	11	3 * const
3.75v > S >= 2.5v	10	2 * const
2.5v > S >= 1.25v	01	1 * const
1.25v > S >= 0v	0	0

Analog value (arrows are quantization levels)

- Linear quantization (uniform quantization):
 - Each digital value represents an equally wide range of analog values
 - Regardless of distribution of data
 - Digital-to-analog conversion represented by a "uniform" table



Not-quite non sequitur: Quantization



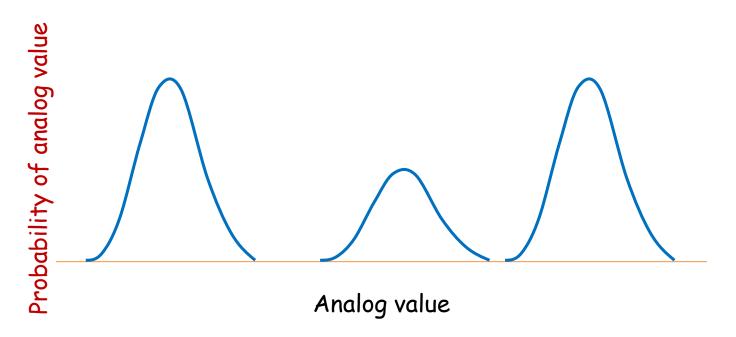
Signal Value	Bits	Mapped to
S >= 4v	11	4.5
4v > S >= 2.5v	10	3.25
2.5v > S >= 1v	01	1.25
1.0v > S >= 0v	0	0.5

Analog value (arrows are quantization levels)

- Non-Linear quantization:
 - Each digital value represents a different range of analog values
 - Finer resolution in high-density areas
 - Mu-law / A-law assumes a Gaussian-like distribution of data
 - Digital-to-analog conversion represented by a "non-uniform" table



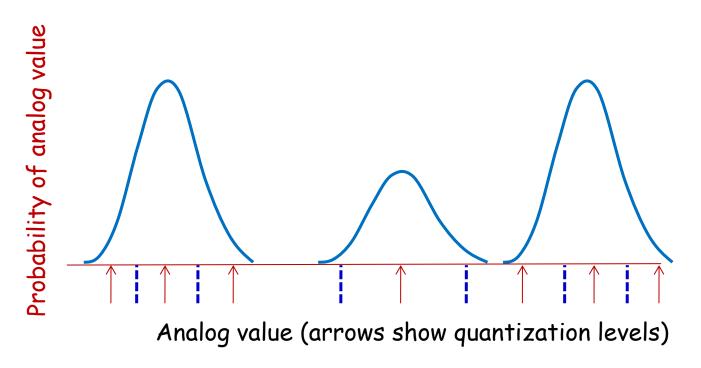
Non-uniform quantization



- If data distribution is not Gaussian-ish?
 - Mu-law / A-law are not optimal
 - How to compute the optimal ranges for quantization?
 - Or the optimal table



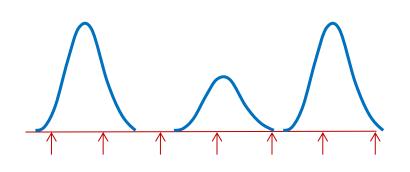
The Lloyd Quantizer



- Lloyd quantizer: An iterative algorithm for computing optimal quantization tables for non-uniformly distributed data
- Learned from "training" data



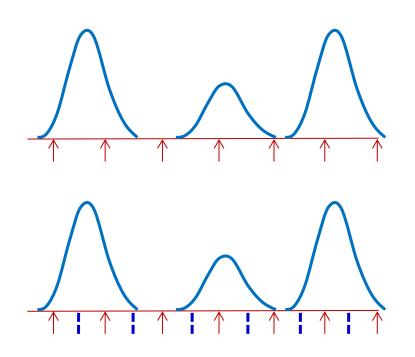
Lloyd Quantizer



- Randomly initialize quantization points
 - Right column entries of quantization table



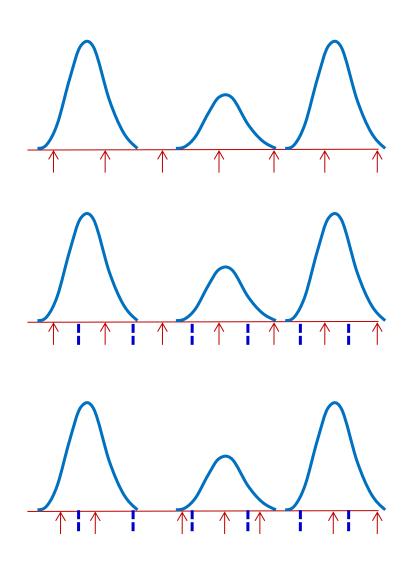
Lloyd Quantizer



- Randomly initialize quantization points
 - Right column entries of quantization table
- Assign all training points to the nearest quantization point
 - Draw boundaries



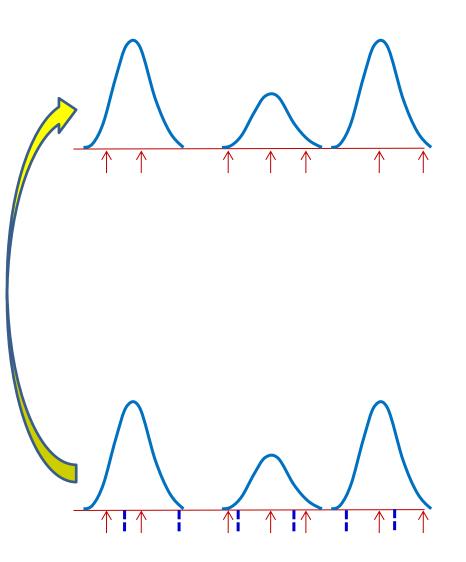
Lloyd Quantizer



- Randomly initialize quantization points
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- Reestimate quantization points



Lloyd Quantizer



- Randomly initialize quantization points
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 - Draw boundaries
- Reestimate quantization points
- Iterate until convergence



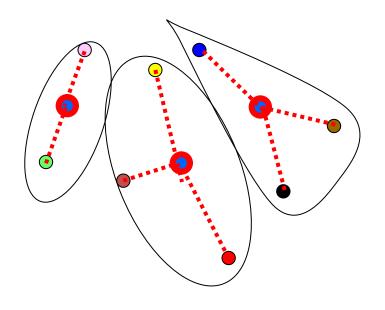
Generalized Lloyd Algorithm: K–means clustering

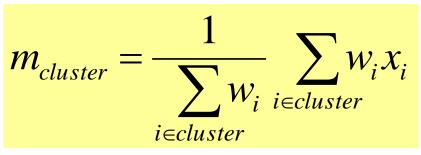
- K means is an iterative algorithm for clustering *vector* data
 - McQueen, J. 1967. "Some methods for classification and analysis of multivariate observations." Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability, 281-297
- General procedure:
 - Initially group data into the required number of clusters somehow (initialization)
 - Assign each data point to the closest cluster
 - Once all data points are assigned to clusters, redefine clusters
 - Iterate



K–means

- Problem: Given a set of data vectors, find natural clusters
- Clustering criterion is scatter: distance from the centroid
 - Every cluster has a centroid
 - The centroid represents the cluster
- **Definition**: The **centroid** is the weighted mean of the cluster
 - Weight = 1 for basic scheme





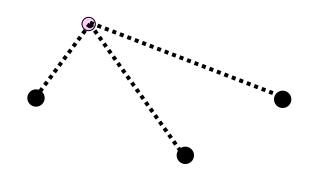




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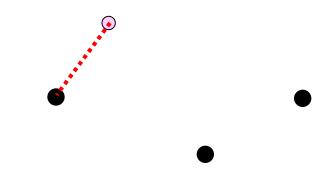


- 1. Initialize a set of centroids randomly
- 2. For each data point x, find the distance from the centroid for each cluster
 - $d_{cluster} = \text{distance}(x, m_{cluster})$



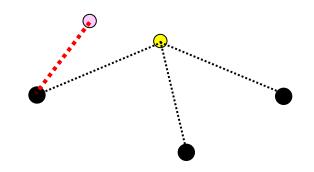


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 - Cluster for which **d**_{cluster} is minimum



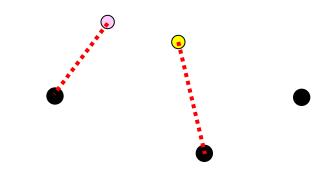


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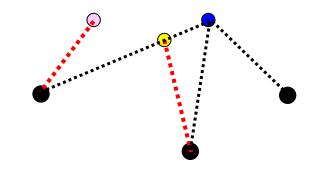


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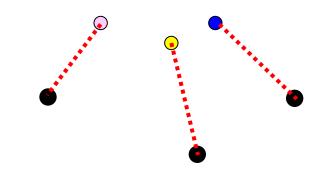
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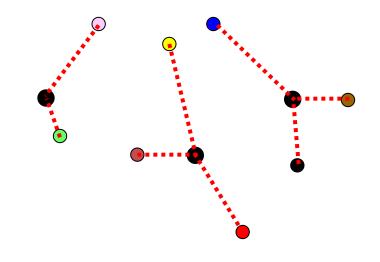
K–means

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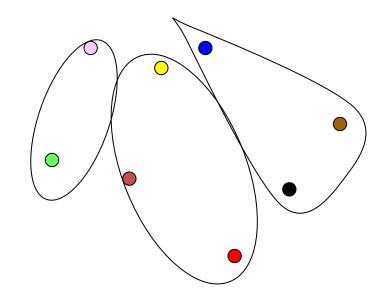


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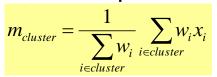


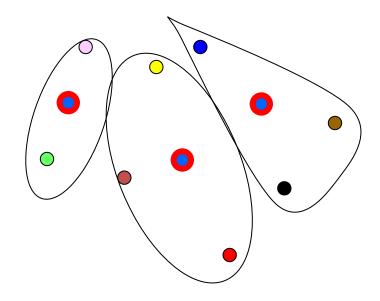
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 - Cluster for which **d**_{cluster} is minimum
- 4. When all data points are clustered, recompute centroids

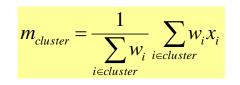




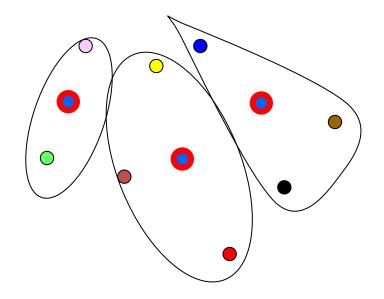


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5. If not converged, go back to 2





K-Means comments

- The distance metric determines the clusters
 - In the original formulation, the distance is L_2 distance
 - Euclidean norm, w_i = 1

distance_{cluster} $(x, m_{cluster}) = ||x - m_{cluster}||_2$

$$m_{cluster} = \frac{1}{N_{cluster}} \sum_{i \in cluster} x_i$$

- If we replace every x by $m_{cluster}(x)$, we get *Vector Quantization*
- K-means is an instance of *generalized* EM
- Not guaranteed to converge for all distance metrics

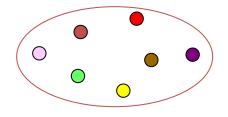


Initialization

- Random initialization
- Top-down clustering
 - Initially partition the data into two (or a small number of) clusters using K means
 - Partition each of the resulting clusters into two (or a small number of) clusters, also using K means
 - Terminate when the desired number of clusters is obtained

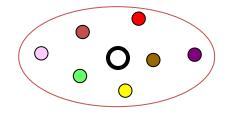


1. Start with one cluster



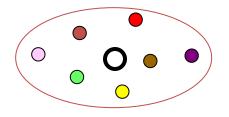


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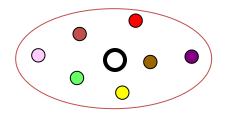


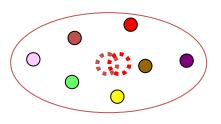
- 1. Start with one cluster
- 2. Split each cluster into two:
 - Perturb centroid of cluster slightly (by < 5%) to generate two centroids





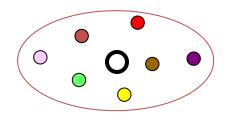
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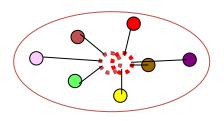






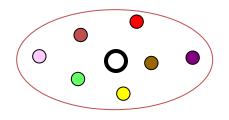
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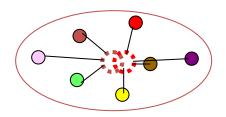


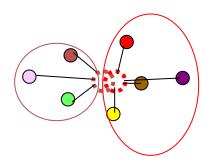




- 1. Start with one cluster
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 - Perturb centroid of cluster slightly (by < 5%) to generate two centroids
- Initialize K means with new set of centroids
- 4. Iterate Kmeans until convergence

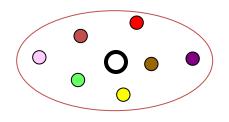


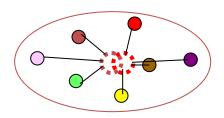


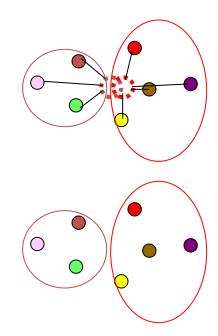




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- 2. Split each cluster into two:
 - Perturb centroid of cluster slightly (by < 5%) to generate two centroids
- 3. Initialize K means with new set of centroids
- 4. Iterate Kmeans until convergence

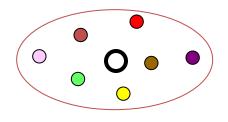


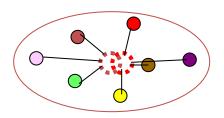


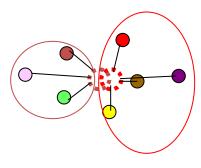


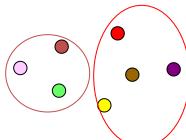


- 1. Start with one cluster
- 2. Split each cluster into two:
 - Perturb centroid of cluster slightly (by < 5%) to generate two centroids
- 3. Initialize K means with new set of centroids
- 4. Iterate Kmeans until convergence
- 5. If the desired number of clusters is not obtained, return to 2



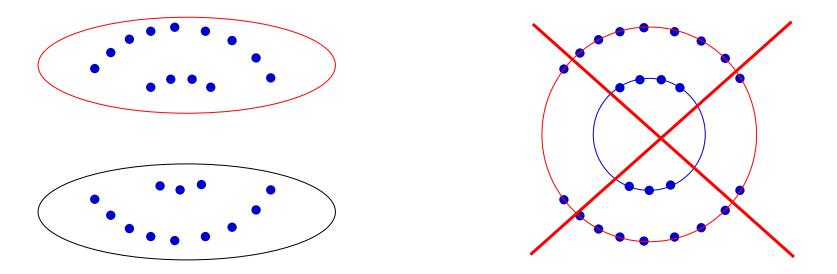








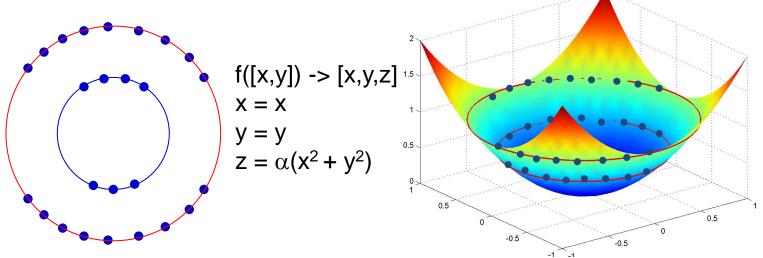
Non-Euclidean clusters



- Basic K-means results in good clusters in Euclidean spaces
 - Alternately stated, will only find clusters that are "good" in terms of Euclidean distances
- Will not find other types of clusters

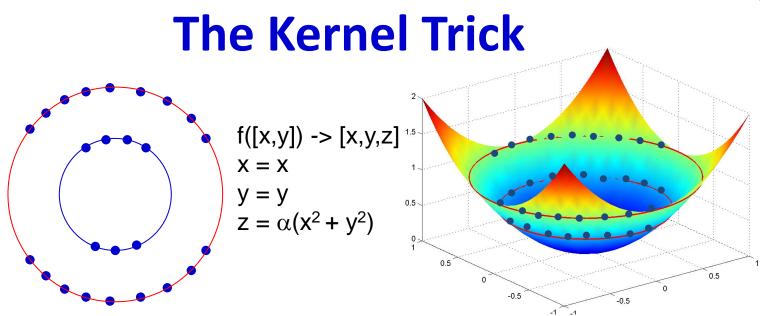


Non-Euclidean clusters



- For other forms of clusters we must modify the distance measure
 E.g. distance from a circle
- May be viewed as a distance in a higher dimensional space
 - I.e *Kernel* distances
 - Kernel K-means
- Other related clustering mechansims:
 - Spectral clustering
 - Non-linear weighting of adjacency
- Normalized cuts..





- Transform the data into a synthetic higher-dimensional space where the desired patterns become natural clusters
 - E.g. the quadratic transform above
- Problem: What is the function/space?
- Problem: Distances in higher dimensional-space are more expensive to compute

Yet only carry the same information in the lower-dimensional space
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Distance in higher-dimensional space

 Transform data x through a *possibly unknown* function Φ(x) into a higher (potentially infinite) dimensional space

 $-z = \Phi(x)$

 The distance between two points is computed in the higher-dimensional space

$$-d(\mathbf{x}_1, \mathbf{x}_2) = ||\mathbf{z}_1 - \mathbf{z}_2||^2 = ||\Phi(\mathbf{x}_1) - \Phi(\mathbf{x}_2)||^2$$

d(x₁, x₂) can be computed without computing z
 – Since it is a direct function of x₁ and x₂



Distance in higher-dimensional space

 Distance in lower-dimensional space: A combination of dot products

$$- ||z_1 - z_2||^2 = (z_1 - z_2)^{\mathsf{T}}(z_1 - z_2) = z_1 \cdot z_1 + z_2 \cdot z_2 - 2 z_1 \cdot z_2$$

- Distance in higher-dimensional space $- d(\mathbf{x}_1, \mathbf{x}_2) = ||\Phi(\mathbf{x}_1) - \Phi(\mathbf{x}_2)||^2$ $= \Phi(\mathbf{x}_1) \cdot \Phi(\mathbf{x}_1) + \Phi(\mathbf{x}_2) \cdot \Phi(\mathbf{x}_2) - 2 \Phi(\mathbf{x}_1) \cdot \Phi(\mathbf{x}_2)$
- d(x₁, x₂) can be computed without knowing Φ(x) if:
 Φ(x₁). Φ(x₂) can be computed for any x₁ and x₂ without knowing Φ(.)



The Kernel function

- A kernel function K(x₁,x₂) is a function such that:
 K(x₁,x₂) = Φ(x₁). Φ(x₂)
- Once such a kernel function is found, the distance in higher-dimensional space can be found in terms of the kernels

$$-d(\mathbf{x}_{1}, \mathbf{x}_{2}) = ||\Phi(\mathbf{x}_{1}) - \Phi(\mathbf{x}_{2})||^{2}$$

= $\Phi(\mathbf{x}_{1})$. $\Phi(\mathbf{x}_{1}) + \Phi(\mathbf{x}_{2})$. $\Phi(\mathbf{x}_{2}) - 2 \Phi(\mathbf{x}_{1})$. $\Phi(\mathbf{x}_{2})$
= $K(\mathbf{x}_{1}, \mathbf{x}_{1}) + K(\mathbf{x}_{2}, \mathbf{x}_{2}) - 2K(\mathbf{x}_{1}, \mathbf{x}_{2})$

• But what is $K(\mathbf{x}_1, \mathbf{x}_2)$?



A property of the dot product

- For any vector \mathbf{v} , $\mathbf{v}^{\mathsf{T}}\mathbf{v} = ||\mathbf{v}||^2 \ge 0$
 - This is just the length of v and is therefore nonnegative
- For any vector $\mathbf{u} = \sum_{i} a_{i} \mathbf{v}_{i}$, $||\mathbf{u}||^{2} \ge 0$ => $(\sum_{i} a_{i} \mathbf{v}_{i})^{\mathsf{T}} (\sum_{i} a_{i} \mathbf{v}_{i}) \ge 0$ => $\sum_{i} \sum_{j} a_{i} a_{j} \mathbf{v}_{i} \cdot \mathbf{v}_{j} \ge 0$
- This holds for ANY real $\{a_1, a_2, ...\}$



The Mercer Condition

- If $\mathbf{z} = \Phi(\mathbf{x})$ is a high-dimensional vector derived from \mathbf{x} then for all real $\{a_1, a_2, ...\}$ and any set $\{\mathbf{z}_1, \mathbf{z}_2, ...\} = \{\Phi(\mathbf{x}_1), \Phi(\mathbf{x}_2), ...\}$ $- \sum_i \sum_j a_i a_j \mathbf{z}_i . \mathbf{z}_j \ge 0$ $- \sum_i \sum_j a_i a_j \Phi(\mathbf{x}_i) . \Phi(\mathbf{x}_j) \ge 0$
- If $K(\mathbf{x}_1, \mathbf{x}_2) = \Phi(\mathbf{x}_1)$. $\Phi(\mathbf{x}_2)$ => $\sum_i \sum_j \mathbf{a}_i \mathbf{a}_j \mathbf{K}(\mathbf{x}_i, \mathbf{x}_j)$ >= 0
- Any function K() that satisfies the above condition is a valid kernel function



The Mercer Condition

- $K(\mathbf{x}_1, \mathbf{x}_2) = \Phi(\mathbf{x}_1) \cdot \Phi(\mathbf{x}_2)$ => $\Sigma_i \Sigma_j a_i a_j K(\mathbf{x}_i, \mathbf{x}_j) >= 0$
- A corollary: If any kernel K(.) satisfies the Mercer condition
 - $d(\mathbf{x}_1, \mathbf{x}_2) = K(\mathbf{x}_1, \mathbf{x}_1) + K(\mathbf{x}_2, \mathbf{x}_2) 2K(\mathbf{x}_1, \mathbf{x}_2)$ satisfies the following requirements for a "distance"

$$-d(x,x) = 0$$

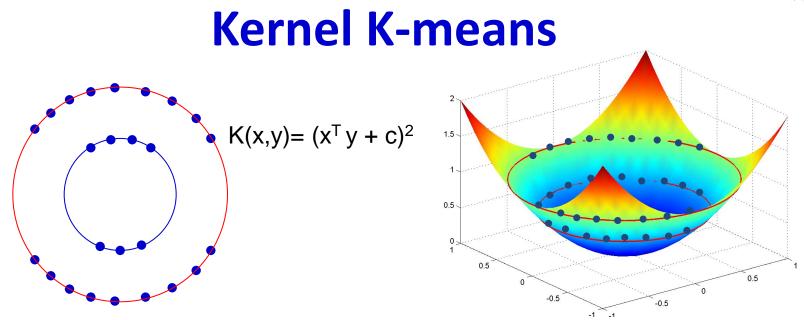
 $-d(x,y) \ge 0$
 $-d(x,w) + d(w,y) \ge d(x,y)$



Typical Kernel Functions

- Linear: $K(x,y) = x^Ty + c$
- Polynomial $K(\mathbf{x},\mathbf{y}) = (\mathbf{a}\mathbf{x}^{\mathsf{T}}\mathbf{y} + \mathbf{c})^{\mathsf{n}}$
- Gaussian: $K(x,y) = \exp(-||x-y||^2/\sigma^2)$
- Exponential: $K(\mathbf{x}, \mathbf{y}) = \exp(-||\mathbf{x}-\mathbf{y}||/\lambda)$
- Several others
 - Choosing the right Kernel with the right parameters for your problem is an artform





• Perform the K-mean in the Kernel space

- The space of $z = \Phi(x)$

• The algorithm..



The mean of a cluster

• The average value of the points in the cluster *computed in the high-dimensional space*

$$m_{cluster} = \frac{1}{N_{cluster}} \sum_{i \in cluster} \Phi(x_i)$$

• Alternately the weighted average

$$m_{cluster} = \frac{1}{\sum_{i \in cluster}} \sum_{i \in cluster} w_i \Phi(x_i) = C \sum_{i \in cluster} w_i \Phi(x_i)$$



The mean of a cluster

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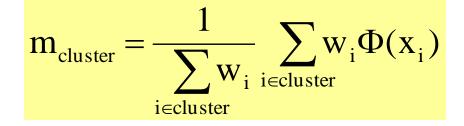
RECALL: We may never actually be able to compute this mean because $\Phi(x)$ is not known

• Alternately the weighted average

$$m_{cluster} = \frac{1}{\sum_{i \in cluster} W_i} \sum_{i \in cluster} W_i \Phi(x_i) = C \sum_{i \in cluster} W_i \Phi(x_i)$$



- Initialize the clusters with a random set of K points
 - Cluster has 1 point



For each data point x, find the closest cluster

 $cluster(\mathbf{x}) = \min_{cluster} d(\mathbf{x}, cluster) = \min_{cluster} \| \Phi(\mathbf{x}) - m_{cluster} \|^{2}$ $d(\mathbf{x}, cluster) = \| \Phi(\mathbf{x}) - m_{cluster} \|^{2} = \left(\Phi(\mathbf{x}) - C \sum_{i \in cluster} w_{i} \Phi(\mathbf{x}_{i}) \right)^{T} \left(\Phi(\mathbf{x}) - C \sum_{i \in cluster} w_{i} \Phi(\mathbf{x}_{i}) \right)$ $= \left(\Phi(\mathbf{x})^{T} \Phi(\mathbf{x}) - 2C \sum_{i \in cluster} w_{i} \Phi(\mathbf{x})^{T} \Phi(\mathbf{x}_{i}) + C^{2} \sum_{i \in cluster} \sum_{j \in cluster} w_{i} w_{j} \Phi(\mathbf{x}_{i})^{T} \Phi(\mathbf{x}_{j}) \right)$ $= K(\mathbf{x}, \mathbf{x}) - 2C \sum_{i \in cluster} w_{i} K(\mathbf{x}, \mathbf{x}_{i}) + C^{2} \sum_{i \in cluster} \sum_{j \in cluster} w_{i} w_{j} K(\mathbf{x}_{i}, \mathbf{x}_{j})$

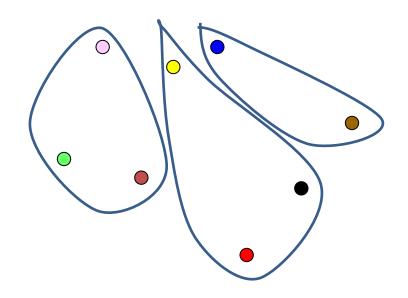
Computed entirely using only the kernel function!

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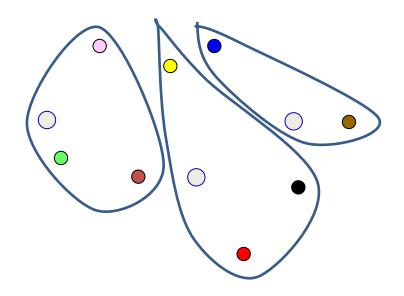
1. Initialize a set of *clusters* randomly







1. Initialize a set of *clusters* randomly



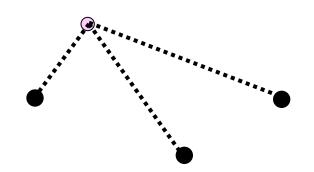
The centroids are *virtual:* we don't actually compute them explicitly!

$$m_{cluster} = \frac{1}{\sum_{i \in cluster} W_i} \sum_{i \in cluster} W_i x_i$$

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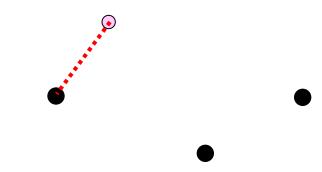


- 1. Initialize a set of clusters randomly
- 2. For each data point x, find the distance from the centroid for each cluster
 - $d_{cluster} = \text{distance}(x, m_{cluster})$



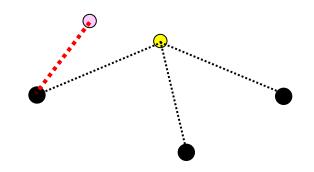


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- 2. For each data point x, find the distance from the centroid for each cluster
 - $d_{cluster} = \text{distance}(x, m_{cluster})$
- 3. Put data point in the cluster of the closest centroid
 - Cluster for which **d**_{cluster} is minimum



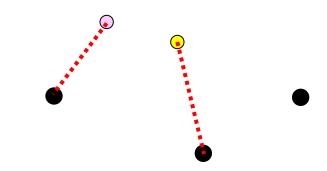


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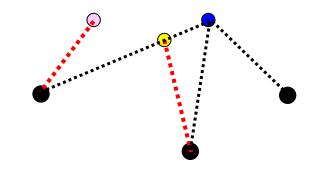


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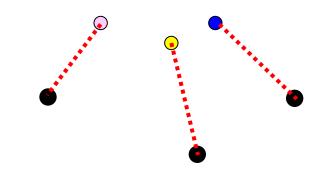


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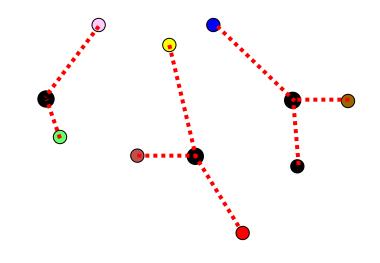


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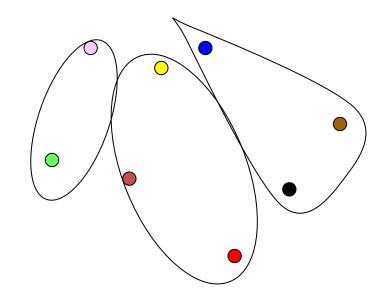


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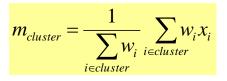


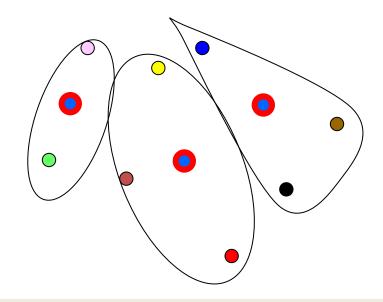
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- 4. When all data points are clustered, recompute centroids



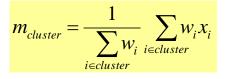


- We do not explicitly compute the means
- May be impossible we do not know the high-dimensional space
- We only know how to compute inner products in it

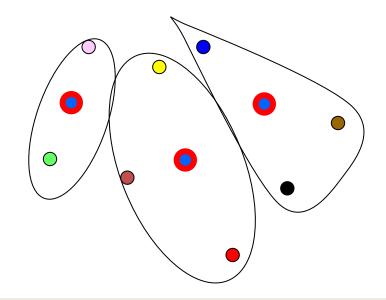


Kernel K–means

- 1. Initialize a set of clusters randomly
- 2. For each data point x, find the distance from the centroid for each cluster
 - $d_{cluster} = \text{distance}(x, m_{cluster})$
- 3. Put data point in the cluster of the closest centroid
 - Cluster for which **d**_{cluster} is minimum
- 4. When all data points are clustered, recompute centroids



5. If not converged, go back to 2



- We do not explicitly compute the means
- May be impossible we do not know the high-dimensional space
- We only know how to compute inner products in it



How many clusters?

- Assumptions:
 - Dimensionality of kernel space > no. of clusters
 - Clusters represent separate *directions* in Kernel spaces
- Kernel correlation matrix ${\bf K}$

$$-\mathbf{K}_{ij} = K(\mathbf{x}_{i}, \mathbf{x}_{j})$$

- Find Eigen values Λ and Eigen vectors ${\bf e}$ of kernel matrix

- No. of clusters = no. of dominant λ_i (1^T e_i) terms



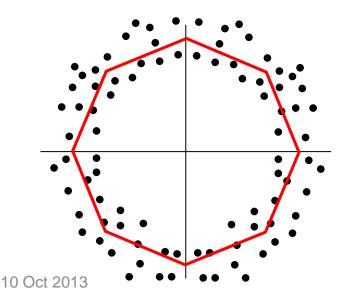
Spectral Methods

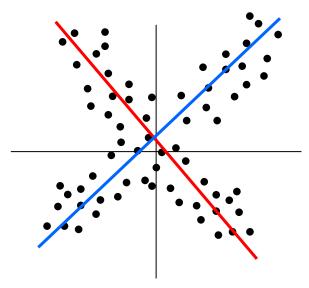
- "Spectral" methods attempt to find "principal" subspaces of the high-dimensional kernel space
- Clustering is performed in the principal subspaces
 - Normalized cuts
 - Spectral clustering
- Involves finding Eigenvectors and Eigen values of Kernel matrix
- Fortunately, provably analogous to Kernel Kmeans



Other clustering methods

- Regression based clustering
- Find a regression representing each cluster
- Associate each point to the cluster with the best regression
 - Related to kernel methods







Clustering..

- Many many other variants
- Many applications..

- Important: Appropriate choice of feature
 - Appropriate choice of feature may eliminate need for kernel trick..

- Google is your friend.