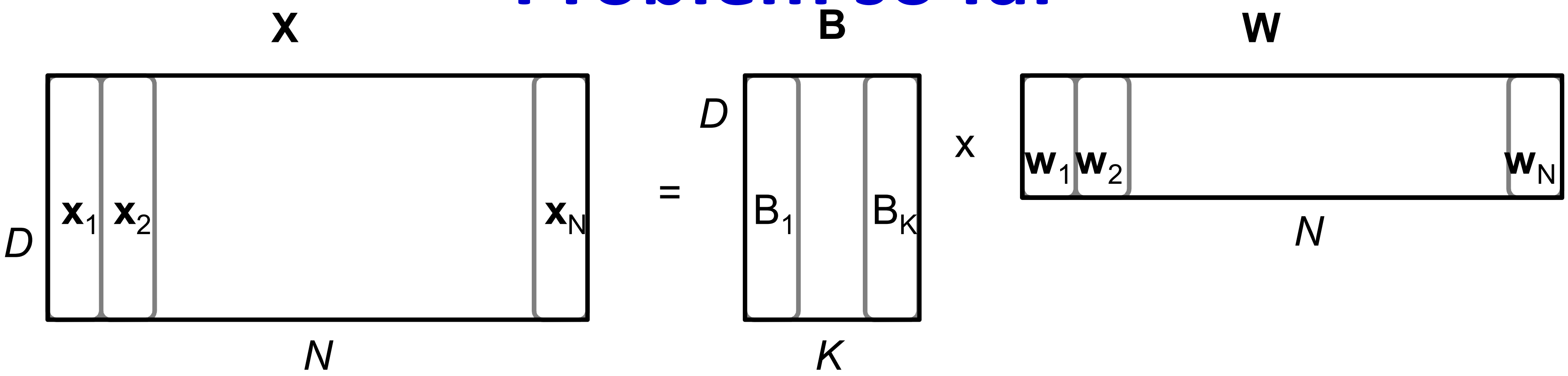
Machine Learning for Signal Processing

Quantization and Clustering

Bhiksha Raj

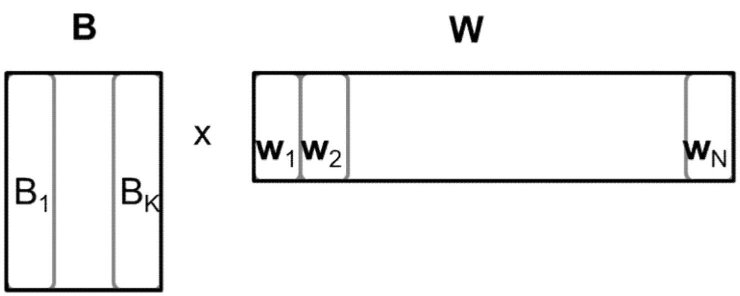
Learning Representations: Problem so far

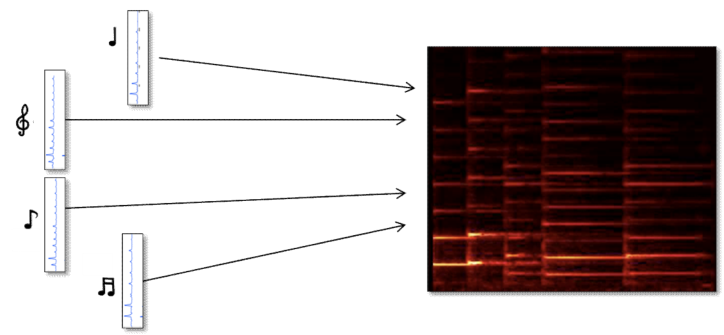


$\boldsymbol{x}_i = \boldsymbol{B}\boldsymbol{w}_i$ ⟹ $\boldsymbol{x}_i = w_{11}B_1 + \cdots + w_{1K}B_K$

- **Problem:** Given a collection of data $\boldsymbol{X}$, find a set of "bases" $\boldsymbol{B}$, such that each vector $x_{\boldsymbol{i}}$ can be expressed as a weighted combination of the bases

Why is this important?





- With the right set of bases, the weights represent the data most effectively
  - We can now use the weights to represent the data
  - E.g. with notes as bases, the weights would be the score

- If the bases are agreed upon, we can also *communicate* the information about the data most efficiently
  - Just communicate the weights
  - E.g. enough to store eigen face weights to reconstruct face
  - E.g. just reading the score is sufficient for anyone to recreate music

What is the most accurate way to represent data

 ...

D

$$f = \sum_i w_i d_i$$

$$w_k = 1, \; w_j = 0 \; for \; j \neq k$$

Selecting the kth face in the collection

f

- If, instead of bases, we had a *dictionary* of all possible data
  - A matrix that included every possible data vector as a column
  - And the weights vector simply selected the correct data instance
  - I.e. $\boldsymbol{w}$ was *one-sparse* vector

$$|\boldsymbol{w}|_0 = 1$$

(actually a one-hot vector because the one non-zero entry of $\boldsymbol{w}$ = 1, i.e. $\sum_i w_i = 1$)

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  - And the weights vector simply selected the correct data instance

- **Problem:** Infeasible to construct such a dictionary!
  - Will require infinite entries
    - And our $\boldsymbol{w}$ vector too will require infinite bits to represent
  - Alternately, will require storing the entire training data
    - And will not be useful to represent data outside the training set

Approximate representation with a dictionary

 ...

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- **Problem:** Infeasible to construct a perfect dictionary
  - Will require too many (potentially infinite) entries

- **Solution:** Can we instead construct a smaller *finite* dictionary such that all data can be approximated well by one of the entries in the dictionary?
  - E.g. "The guy looks a lot like the 7th face in the dictionary"
  - E.g. The vector $\boldsymbol{x}$ looks a lot like the $\boldsymbol{d_i}$, the i-th entry in the dictionary.
- **Questions:**
  - What do we mean by "looks a lot like"
  - How do we construct the dictionary?

Approximate representation with a dictionary

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Quantifying the error

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Selecting the kth face in the collection

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- Different error metrics will result in different solutions
- Lets generically represent the error as $div()$

$$\hat{f} = D\boldsymbol{w}, \qquad |\boldsymbol{w}|_0 = 1, \sum_i w_i = 1$$

$$Error(f) = div(f, \hat{f})$$

- A common choice is the L2 error

$$Error(f) = |f - \hat{f}|^2$$

Approximate representation with a dictionary

 $\cdots$

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Learning the Dictionary

- $\boldsymbol{V} = [V_1, V_2, V_3, \dots]$ are the data for which the dictionary is being learned
- $\boldsymbol{D} = [d_1, d_2, \dots, d_K]$ is the matrix of dictionary vectors
- $\boldsymbol{W} = [\mathrm{w}_1, \mathrm{w}_2, \mathrm{w}_3, \dots]$ is a set of *one-hot* vectors
- Learning: Learn $\boldsymbol{D}$ and $\boldsymbol{W}$ to minimize total error on $\boldsymbol{V}$

$$\widehat{\boldsymbol{D}}, \widehat{\boldsymbol{W}} = \underset{\boldsymbol{D},\boldsymbol{W}}{\operatorname{argmin}}\, div(\boldsymbol{V}, \boldsymbol{D}\boldsymbol{W}) = \underset{\boldsymbol{D},\boldsymbol{W}}{\operatorname{argmin}} \sum_i div(V_i, \boldsymbol{D}\mathrm{w}_i),$$

$$s.t.\, \mathrm{w}_i = one\ hot$$

- If we're only interested in learning the dictionary

$$\widehat{\boldsymbol{D}} = \underset{\boldsymbol{D}}{\operatorname{argmin}} \min_{\boldsymbol{W}} \sum_i div(V_i, \boldsymbol{D}\mathrm{w}_i), \qquad s.t.\, \mathrm{w}_i = one\ hot$$

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- $\widehat{\boldsymbol{D}} = \underset{\boldsymbol{D}}{\operatorname{argmin}} \min_{\boldsymbol{W}} \sum_i div(V_i, \boldsymbol{D}\mathrm{w}_i)$

$$= \underset{\boldsymbol{D}}{\operatorname{argmin}} \sum_i \min_{\mathrm{w}_i} \; div(V_i, \boldsymbol{D}\mathrm{w}_i)$$

- Generally does not have a closed form solution, but can solved with the following iteration that provably reduces error in each step

$$\mathrm{w}_i = \underset{\mathrm{w}}{\operatorname{argmin}} \, div(V_i, \boldsymbol{D}\mathrm{w})$$

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Learning the Dictionary

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For $div(.) = \|V_i - \boldsymbol{D}\mathrm{w}_i\|^2$ this gives us the well-known K-means algorithm

$$= \underset{\boldsymbol{D}}{\text{argmin}} \sum_i \min_{\mathrm{w}_i} div(V_i, \boldsymbol{D}\mathrm{w}_i)$$

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- Grouping V_i by the dictionary entries they are assigned to (w_i) results in *clustering*

error in each step

$$\mathrm{w}_i = \underset{\mathrm{w}}{\operatorname{argmin}}\, div(V_i, \boldsymbol{D}\mathrm{w})$$

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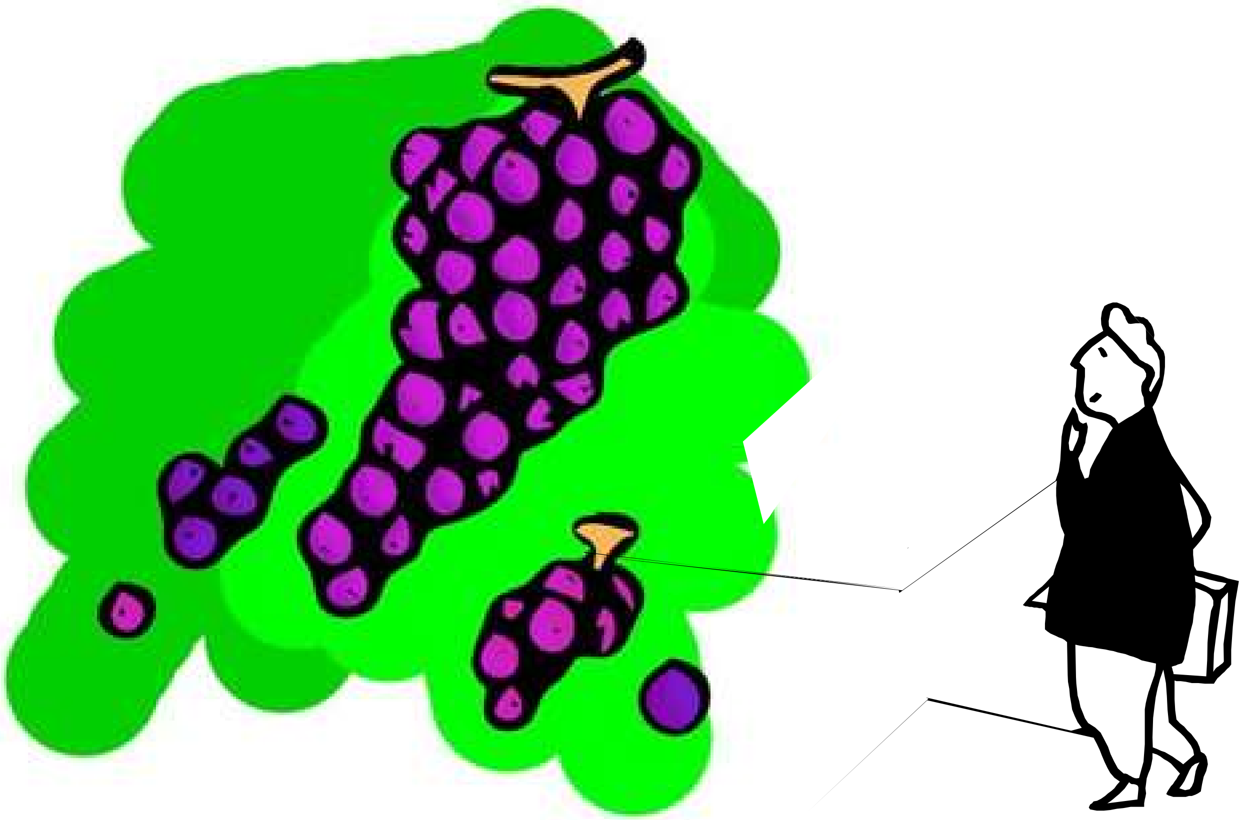
So lets look at clustering

- From a more naïve, procedural perspective..

Clustering



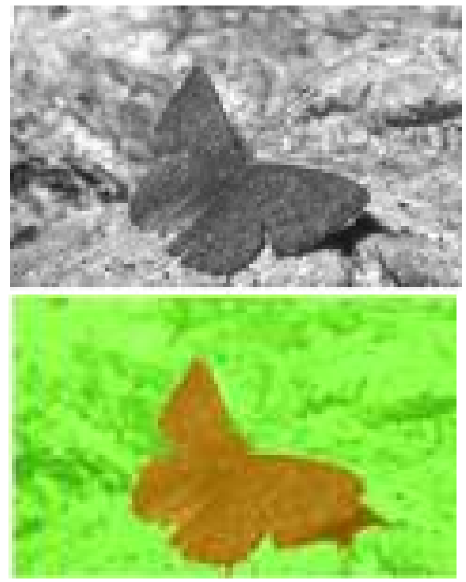
Statistical Modelling and Latent Structure

- 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)

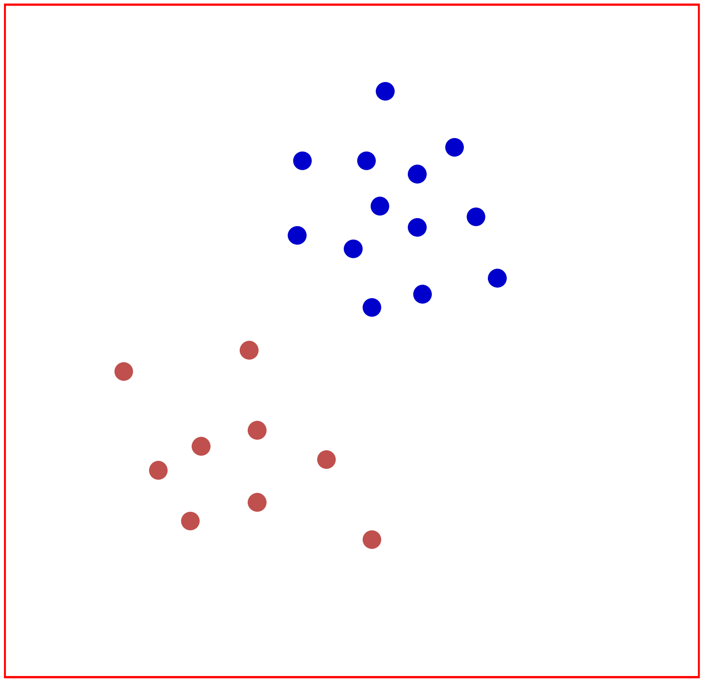
- We will see still other forms of latent structure discovery later in the course

How



Clustering

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



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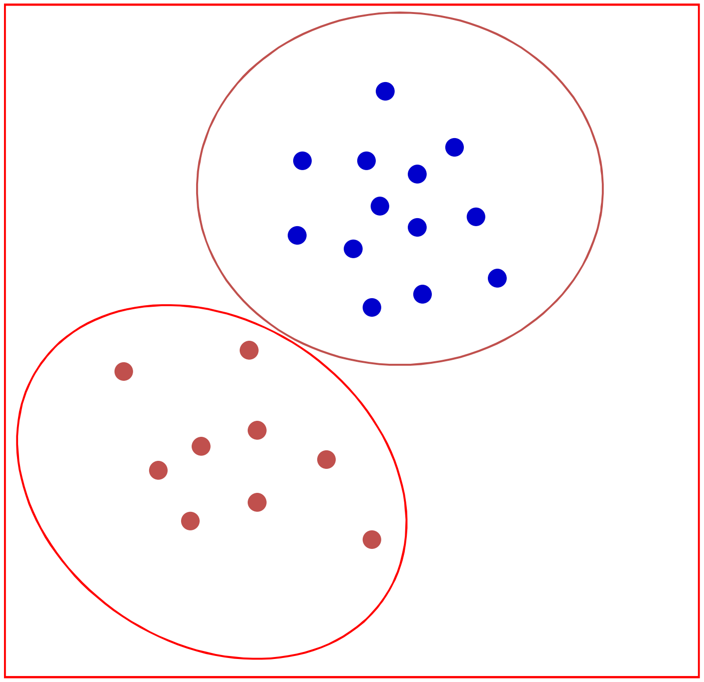

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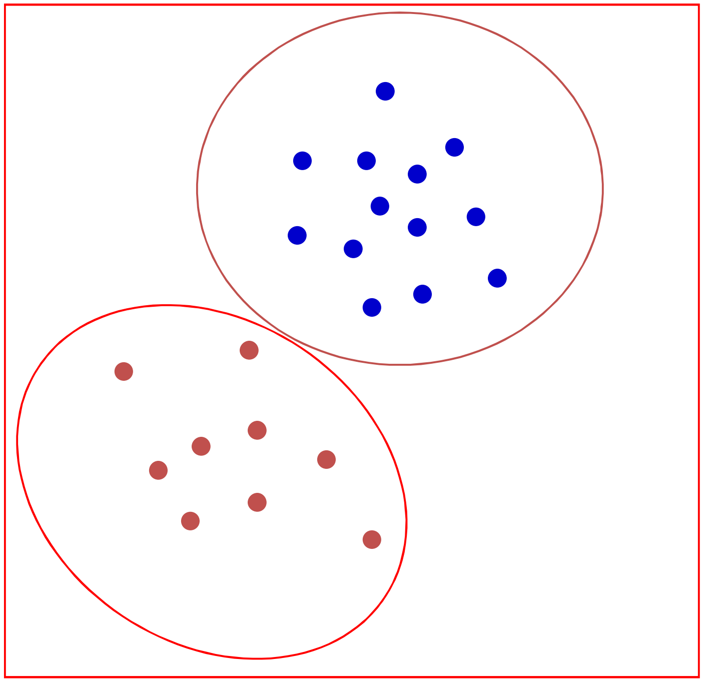
  - Find groupings of data such that the groups optimize a “within-group-variability” objective function of some kind



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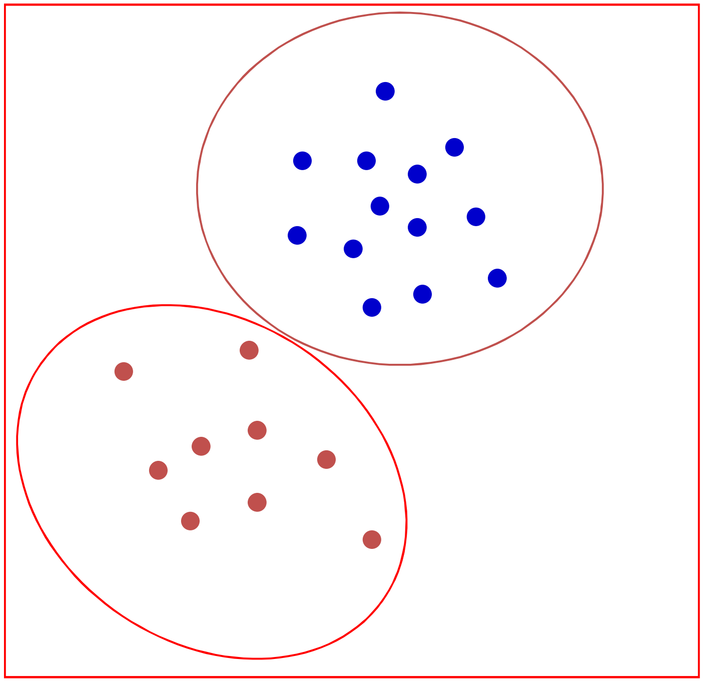

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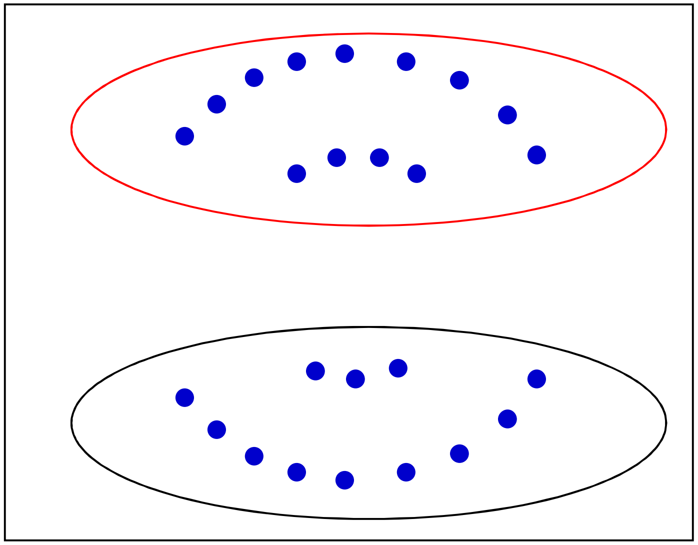
  - The objective function used affects the nature of the discovered clusters
    - E.g. Euclidean distance vs.



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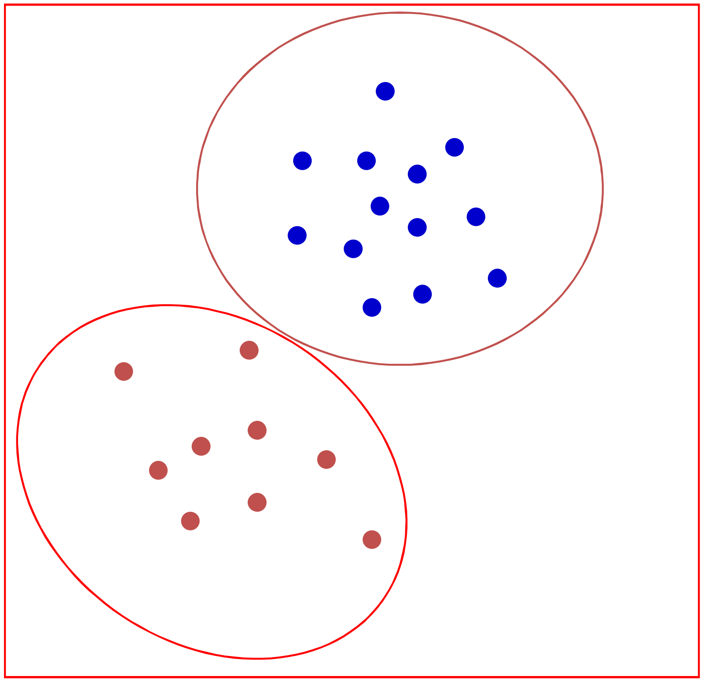

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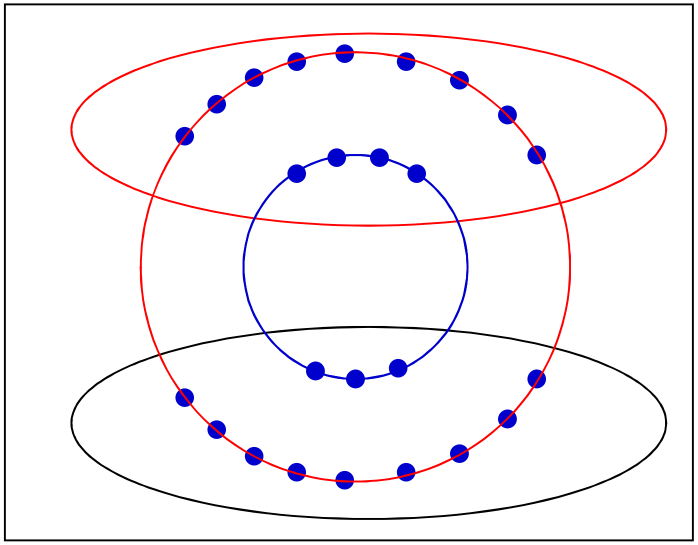
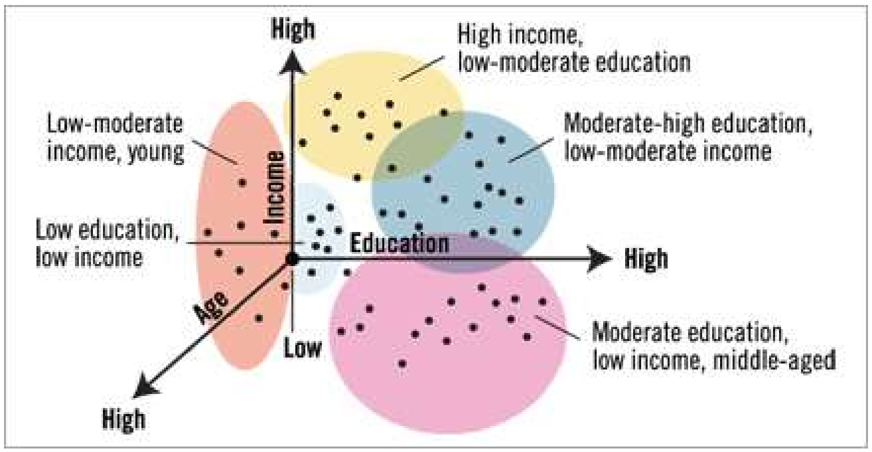
    - Distance from center

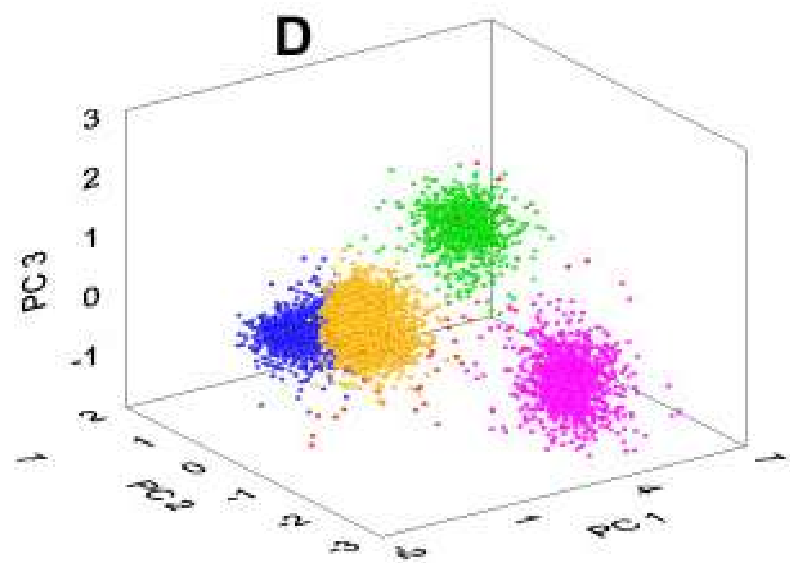


Why Clustering

- Automatic grouping into “Classes”
  – Different clusters may show different behavior
- Representation: 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

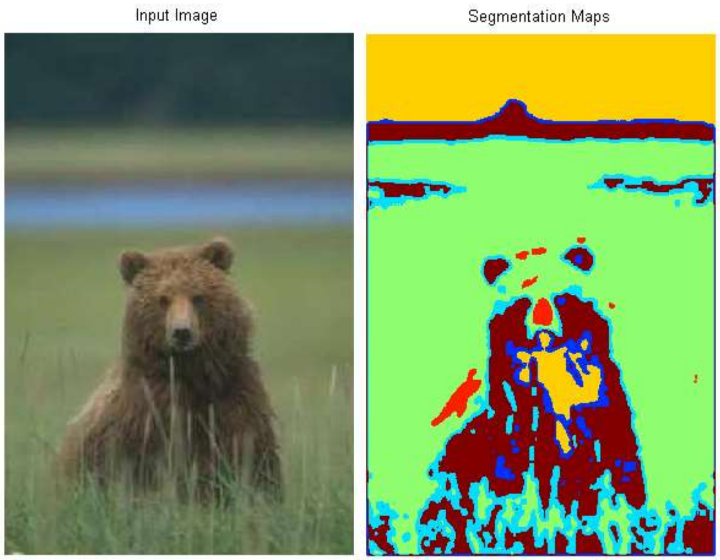




- Find natural groupings in data for further analysis
- Discover *latent* structure in data

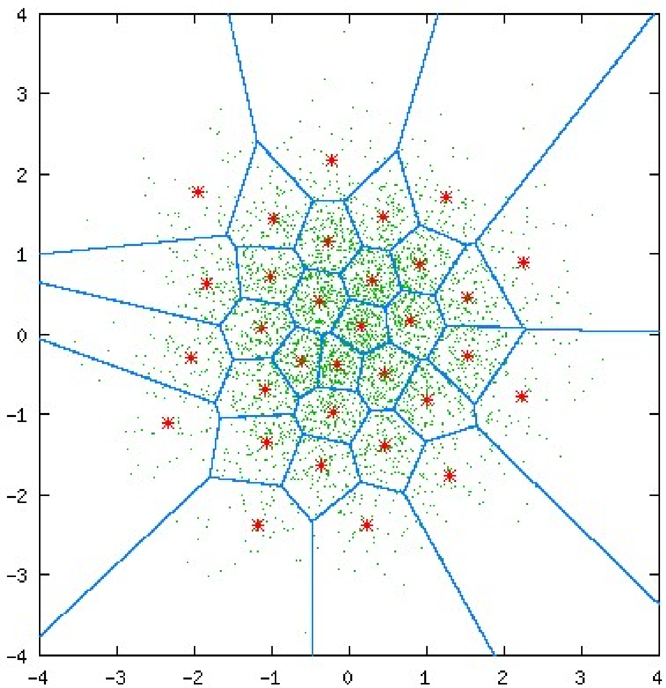
Some Applications of Clustering

- Image segmentation

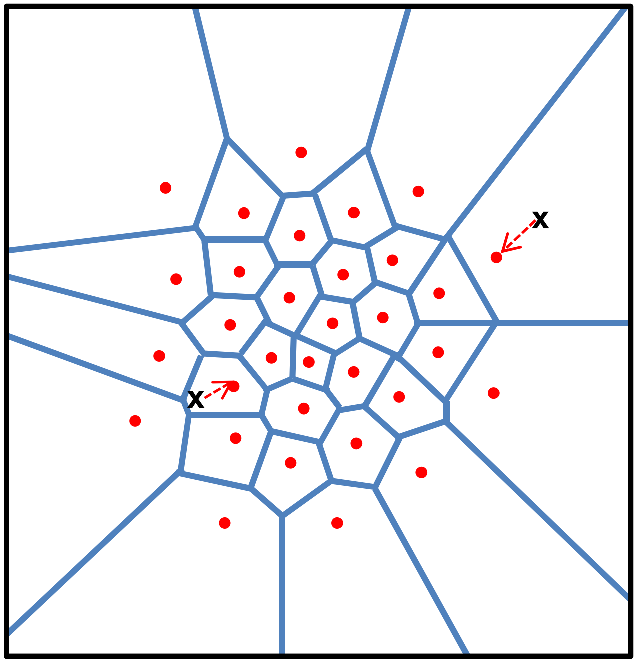


Representation: Quantization

TRAINING



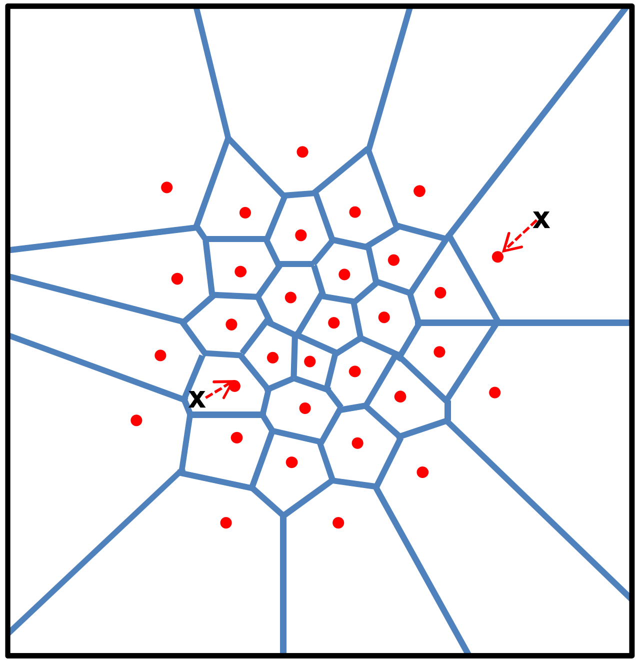
QUANTIZATION



- *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**

Quantization: Formally

$$V = \sum_i w_i d_i$$



$$V = \mathbf{D}\mathbf{w} \qquad |\boldsymbol{w}| = 1$$
$$|\boldsymbol{w}|_0 = 1$$

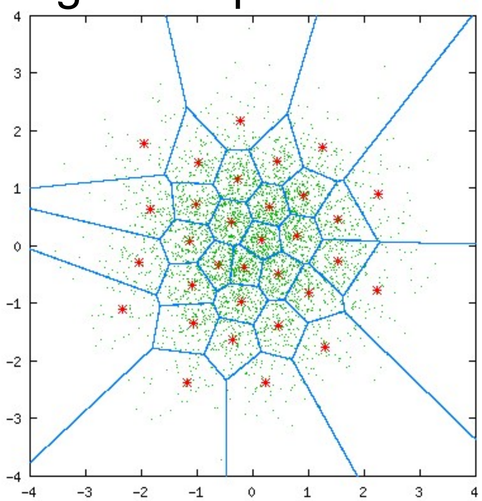
- d_i are the "representative" vectors of each cluster
- Restriction: only one of the w_i is 1, the rest are 0
  - $\sum_i w_i = 0$
  - $\mathbf{w}$ is unit length and one-sparse

Representation: BOW

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

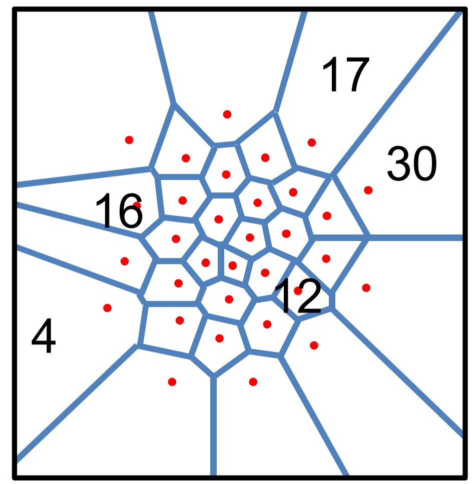
Representation: BOW

Training: Each point is a video frame



$$V_k = \mathbf{D}\mathbf{w}_k \quad f = \sum_k \mathbf{w}_k$$

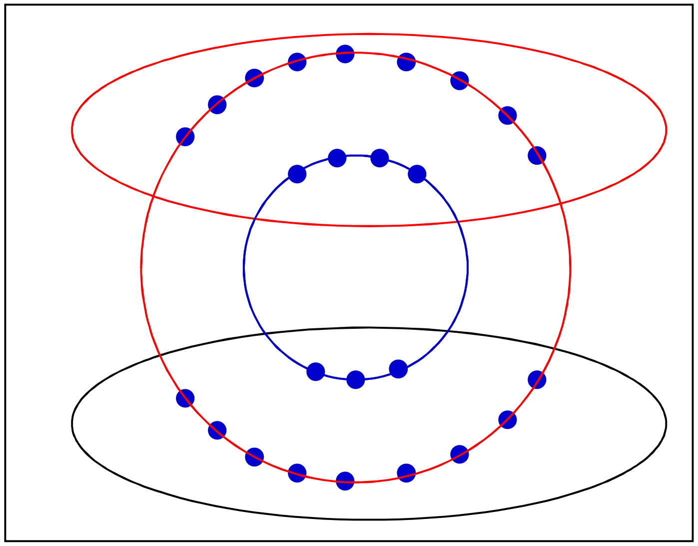
Representation: Each number is the #frames assigned to the codeword



- 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

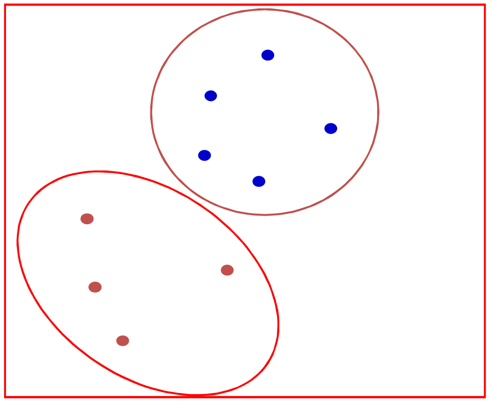
- The "Clustering criterion" actually has two aspects

- 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

“Compactness” criteria for clustering

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



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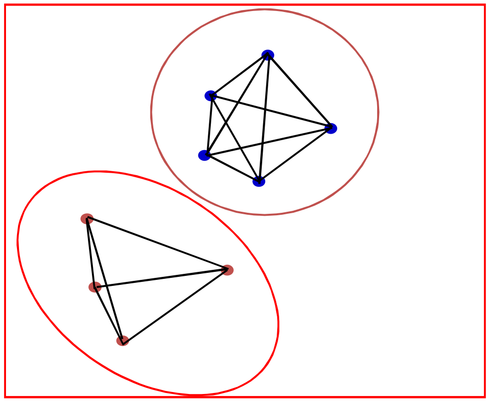

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  - Total distance between each element in the cluster and every other element in the cluster
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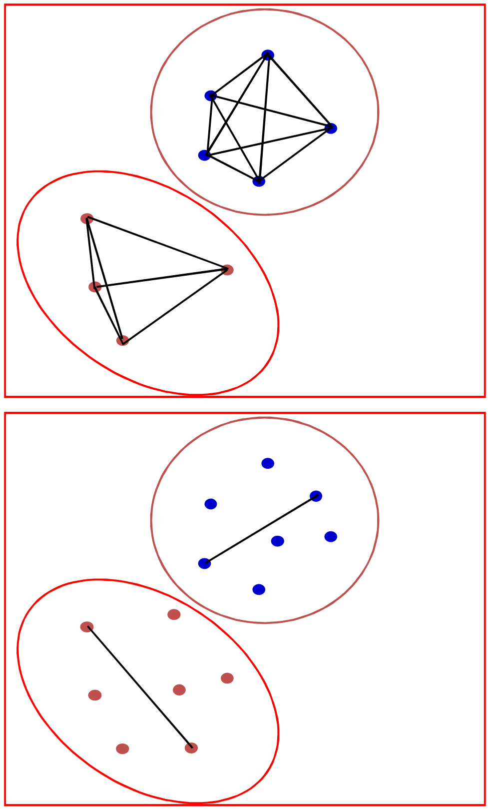

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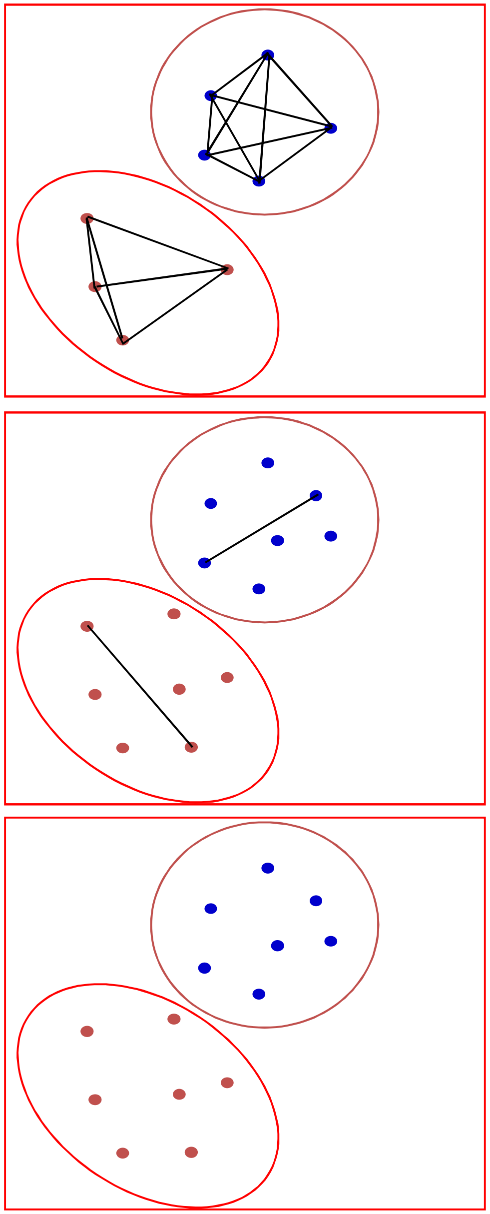
  - Total distance of every element in the cluster from the centroid of the cluster



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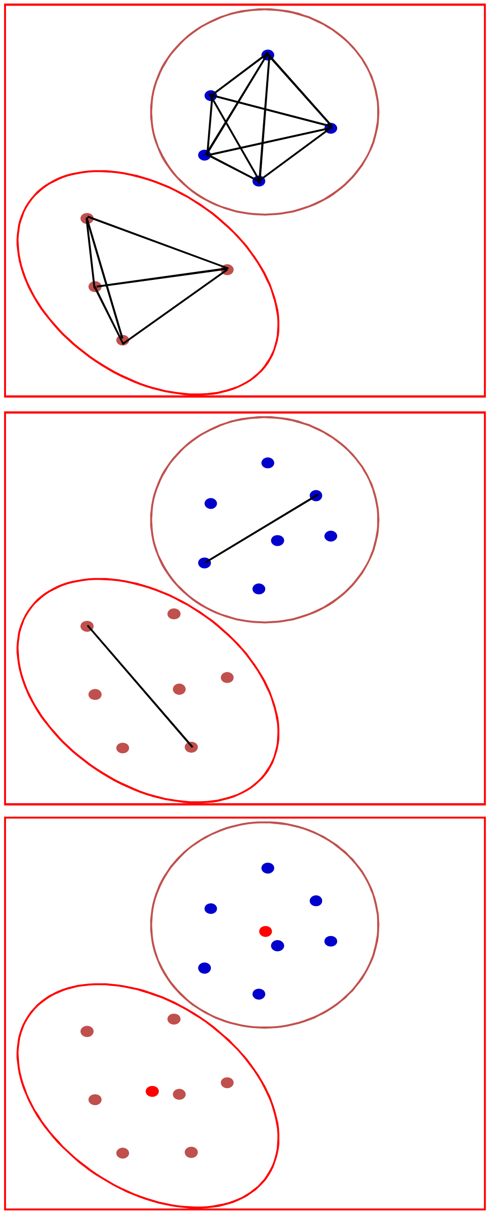

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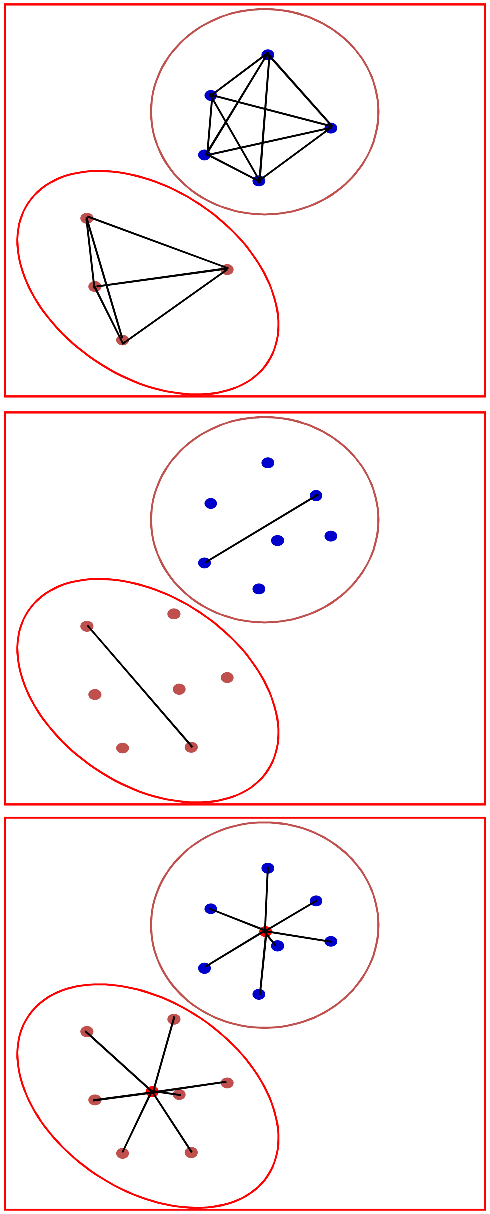
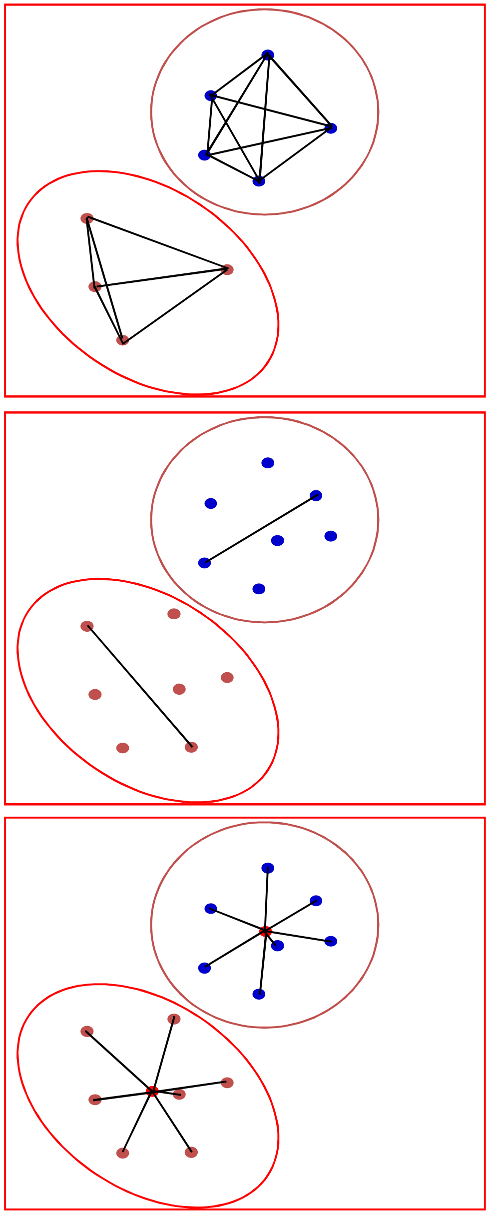


“Compactness” criteria for clustering

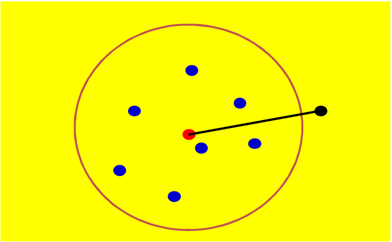
- Distance based measures
  - Total distance between each element in the cluster and every other element in the cluster
  - Distance between the two farthest points in the cluster
  - Total distance of every element in the cluster from the centroid of the cluster
  - Distance measures are often weighted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

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



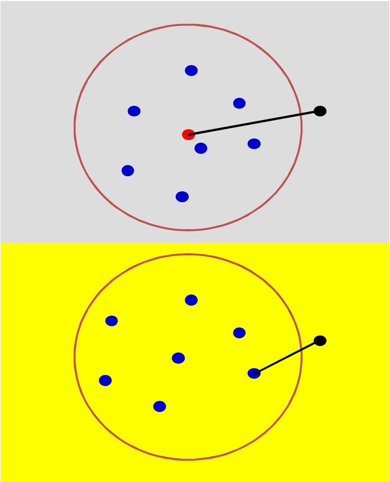
Clustering: Distance from cluster

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



Clustering: Distance from cluster

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



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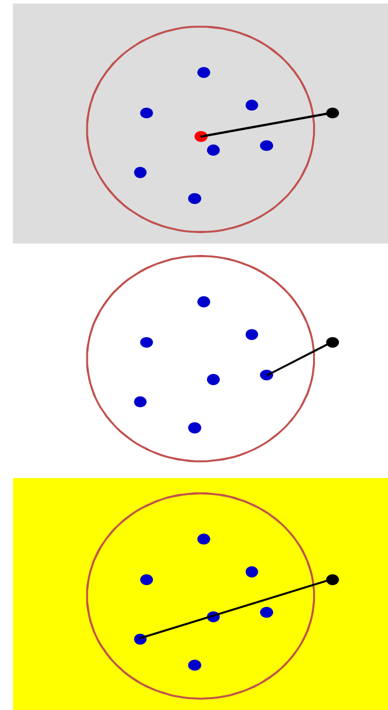

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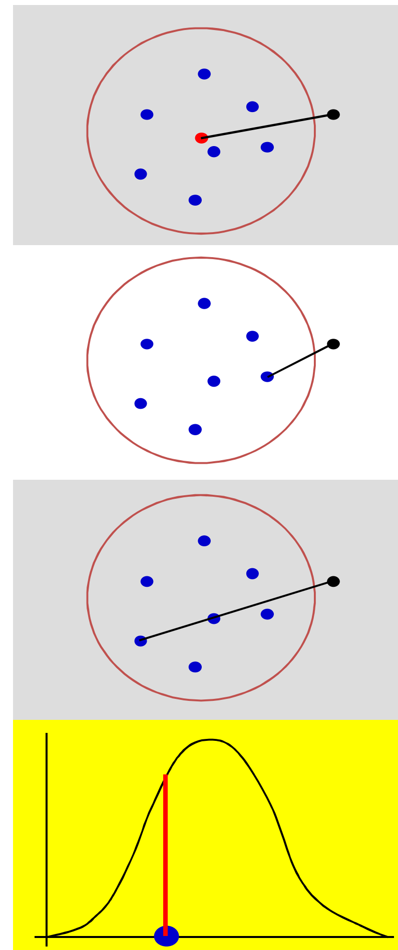
  - Probability of data measured on cluster distribution



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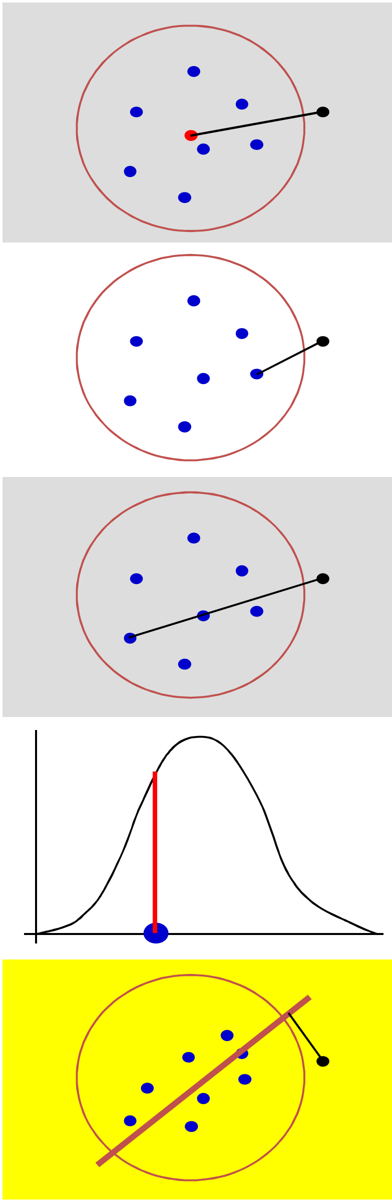
  - Probability of data measured on cluster distribution
  - Fit of data to cluster-based regression



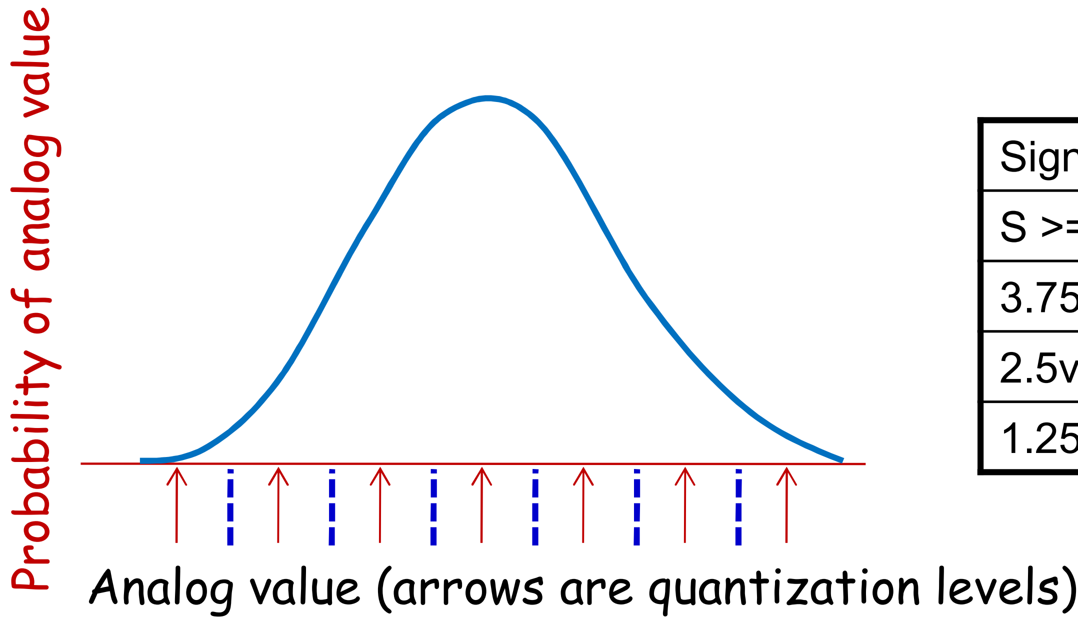
Optimal clustering: Exhaustive enumeration

- 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

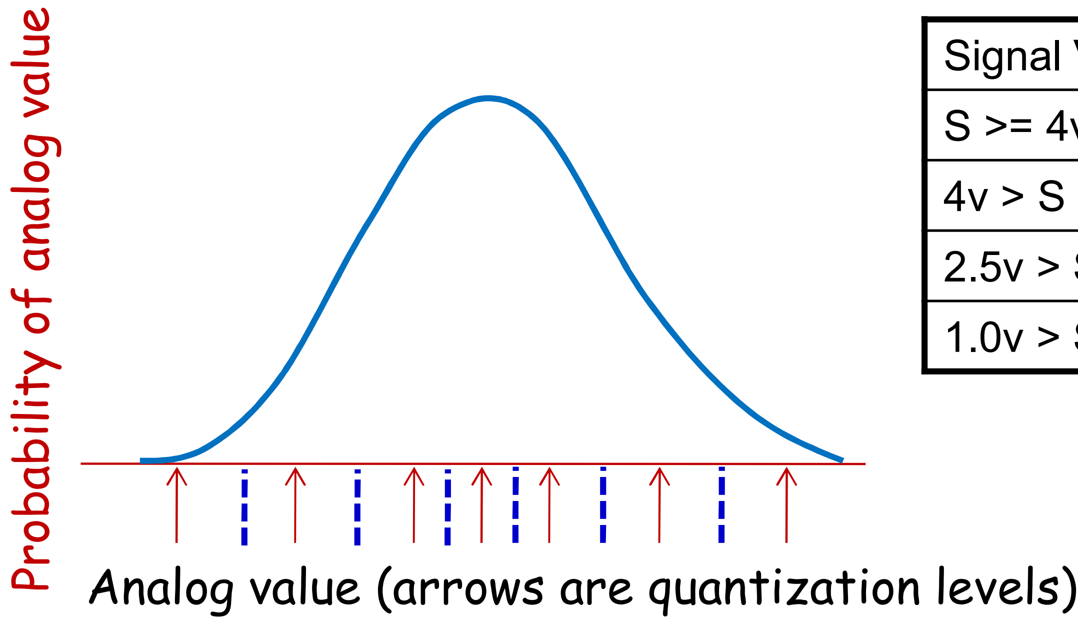
Not-quite non sequitur: Quantization



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	00	0

- 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

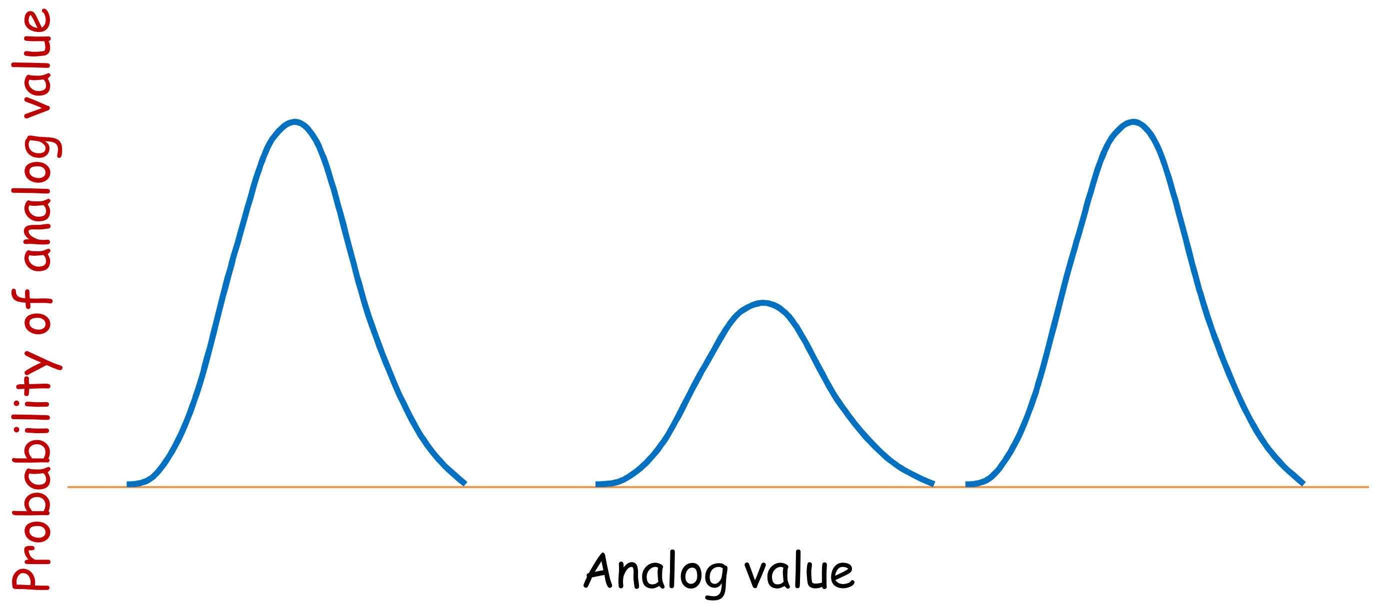
Not-quite non sequitur: Quantization



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	00	0.5

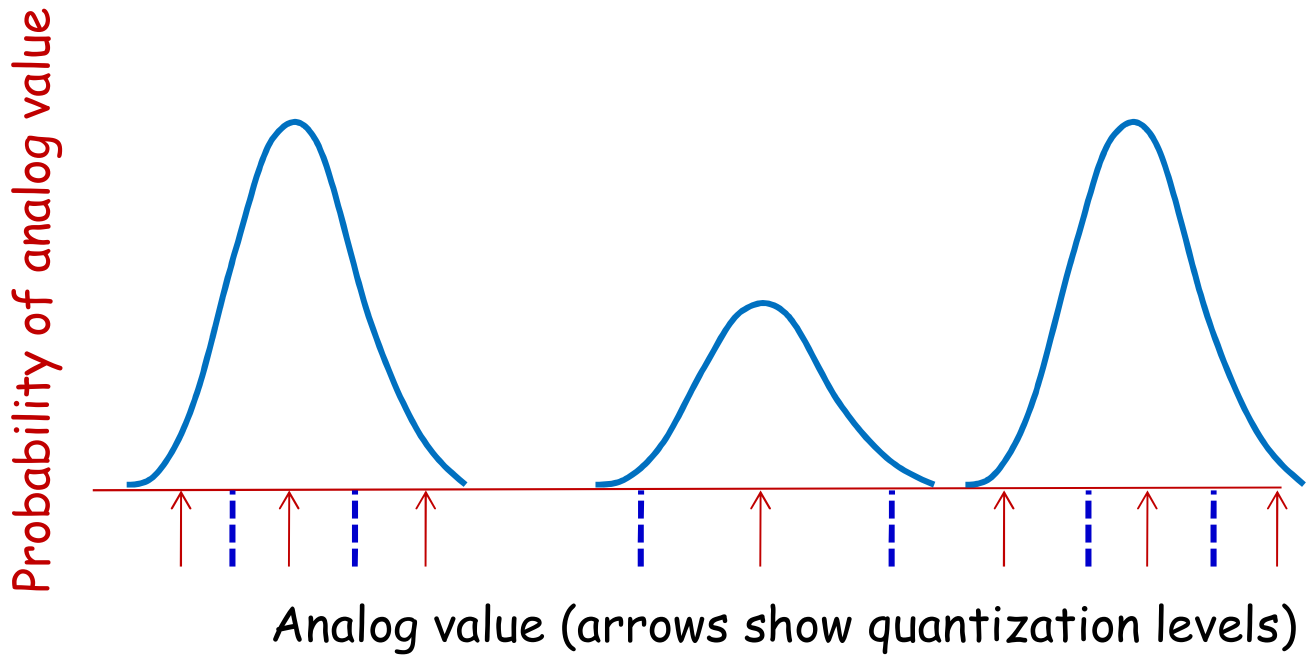
- Non-Linear quantization:
  - Each digital value represents a different range of analog values
    - Finer resolution in high-density areas
    - Mu-law / A-law assumes a Gaussian-like distribution of data
  - Digital-to-analog conversion represented by a “non-uniform” table

Non-uniform quantization



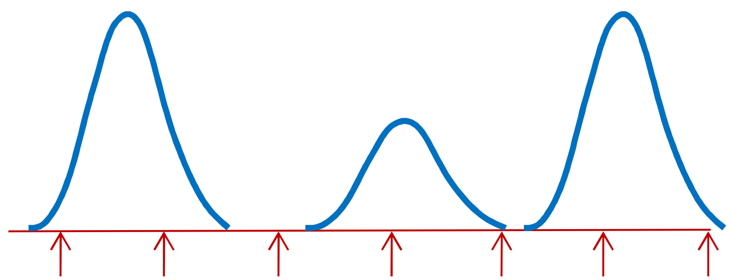
- If data distribution is not Gaussian-ish?
  - Mu-law / A-law are not optimal
  - How to compute the optimal ranges for quantization?
    - Or the optimal table

The Lloyd Quantizer



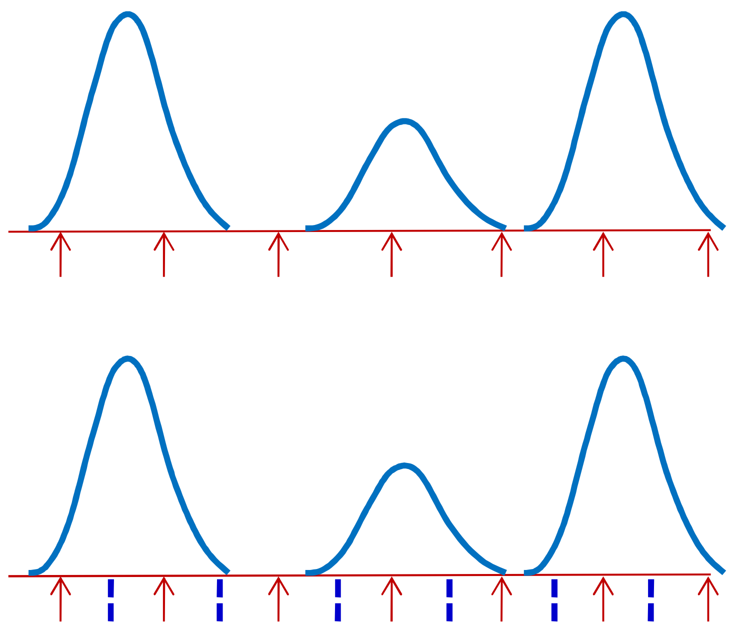
- Lloyd quantizer: An iterative algorithm for computing optimal quantization tables for non-uniformly distributed data
- **Learned from "training" data**

Lloyd Quantizer



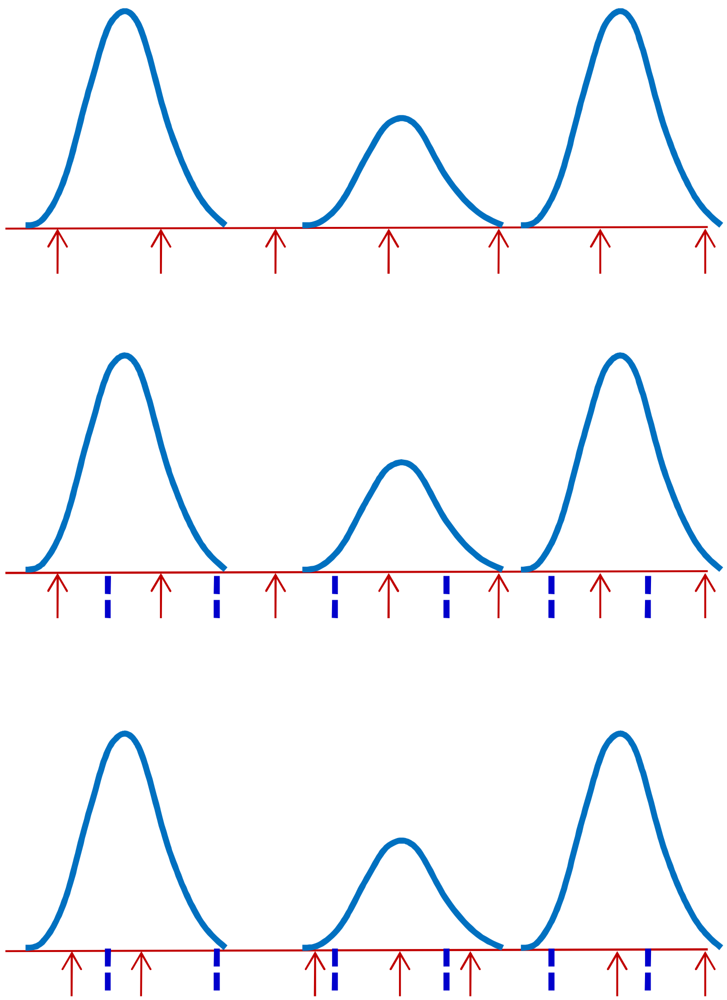
- Randomly initialize quantization points
  - Right column entries of quantization table

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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- Assign all training points to the nearest quantization point
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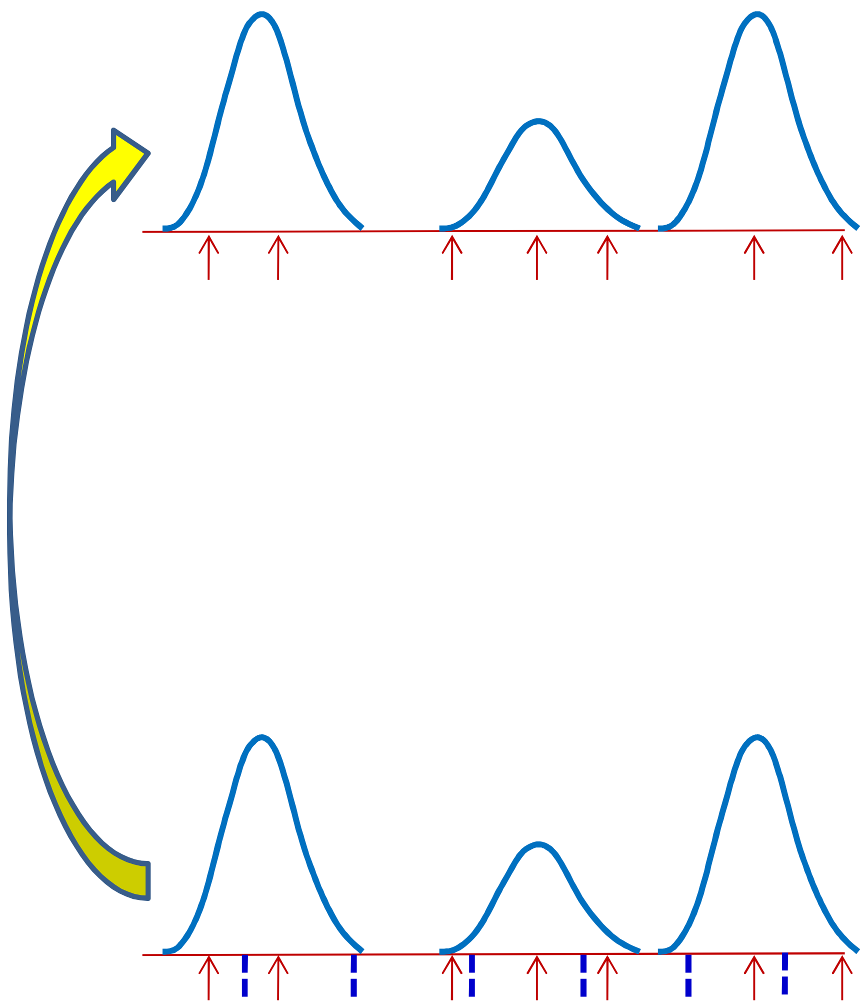
- Reestimate quantization points

Lloyd Quantizer



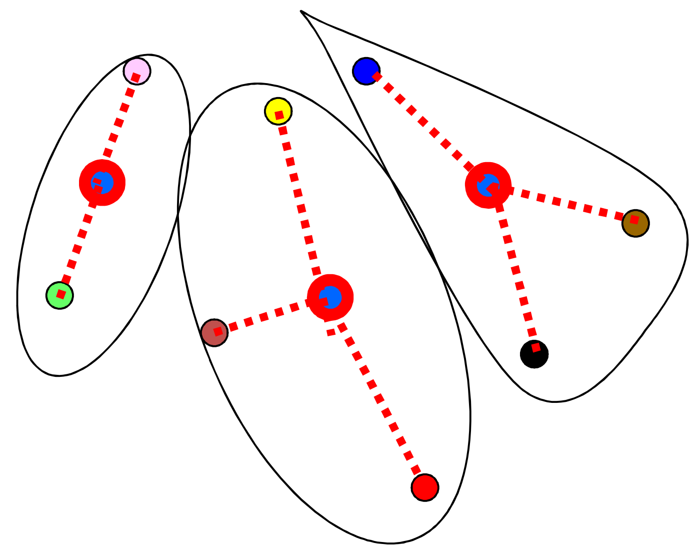
- Randomly initialize quantization points
  - Right column entries of quantization table
- Assign all training points to the nearest quantization point
  - Draw boundaries
- Reestimate quantization points
- Iterate until convergence

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

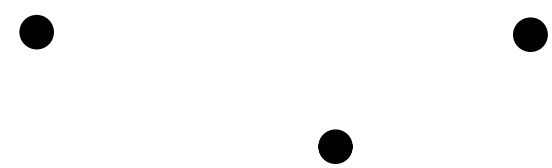
- Problem: Given a set of data vectors, find natural clusters
- Clustering criterion is **scatter**: distance from the centroid
  - Every cluster has a centroid
  - The centroid represents the cluster
- **Definition**: The **centroid** is the weighted mean of the cluster
  - Weight = 1 for basic scheme



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

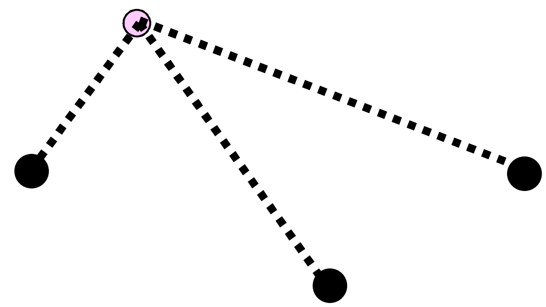
K–means

1. Initialize a set of centroids randomly



K–means

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



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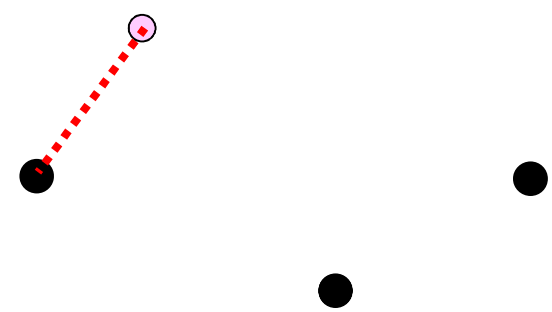
3. Put data point in the cluster of the closest centroid
   - Cluster for which $\boldsymbol{d}_{\text{cluster}}$ is minimum



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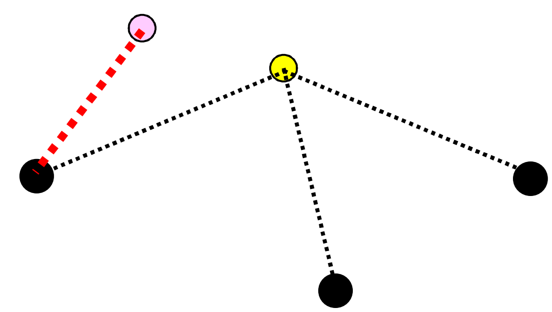

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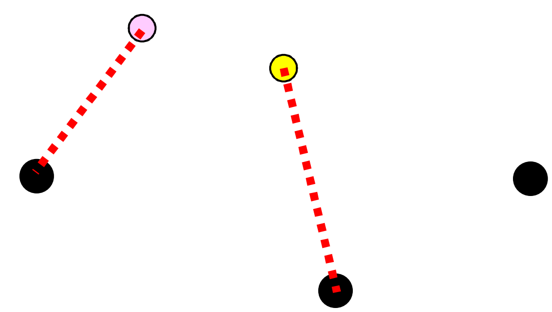

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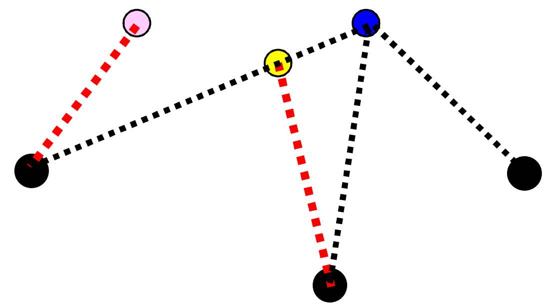

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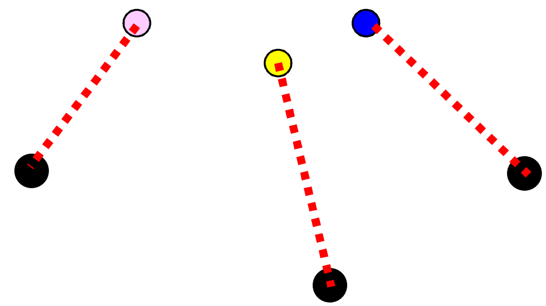

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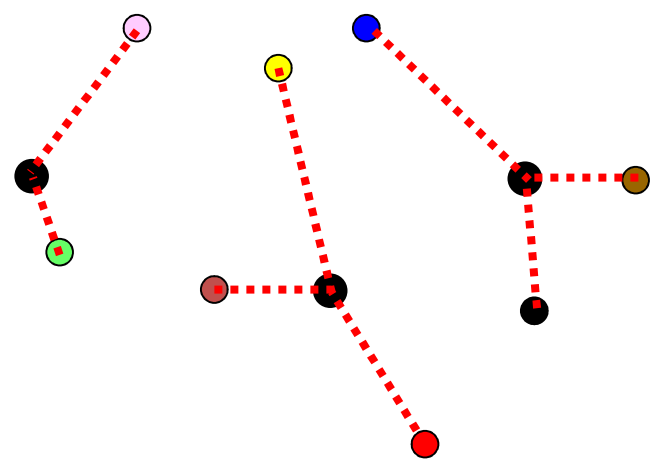

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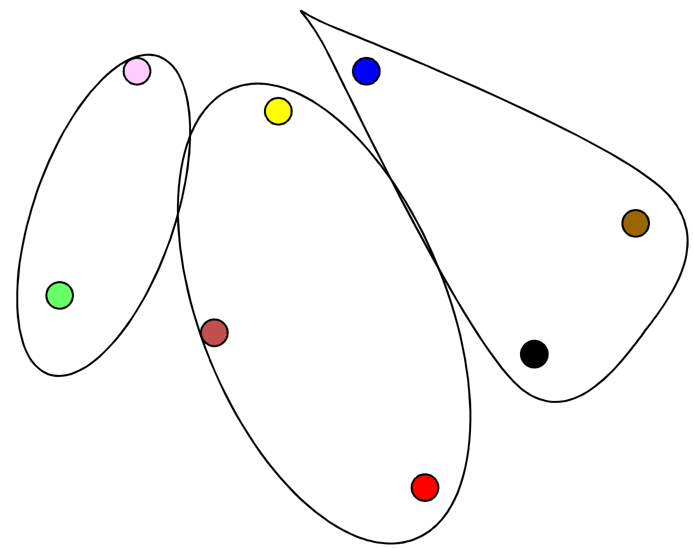

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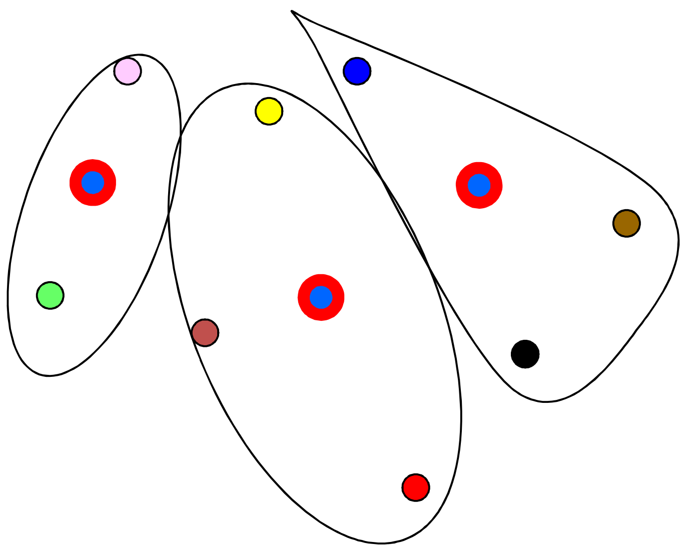
4. When all data points are clustered, recompute centroids

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



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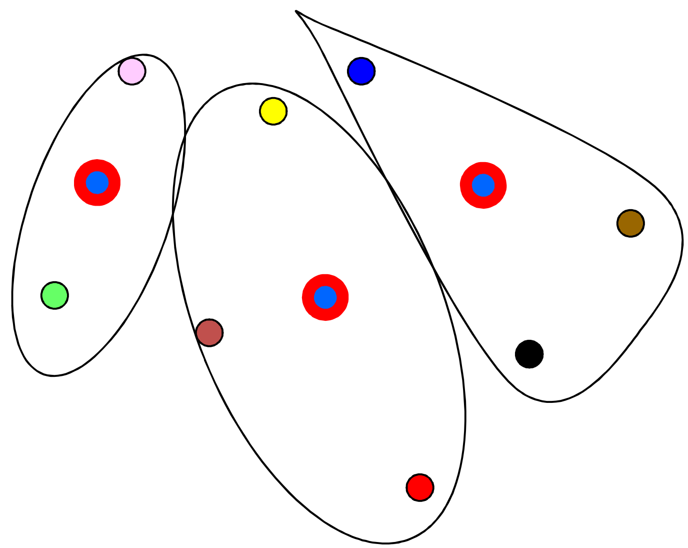
5. If not converged, go back to 2



K-Means comments

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

$$\textbf{distance}_{cluster}(x, m_{cluster}) = \| x - m_{cluster} \|_2$$

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

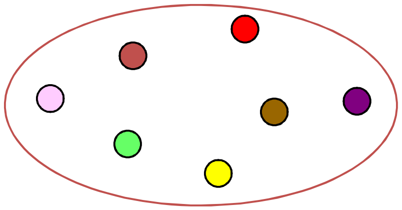
  - If we replace every x by $m_{cluster}(x)$, we get *Vector Quantization*
- K-means is an instance of *generalized* EM
- Not guaranteed to converge for all distance metrics

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

K-Means for Top–Down clustering

1. Start with one cluster



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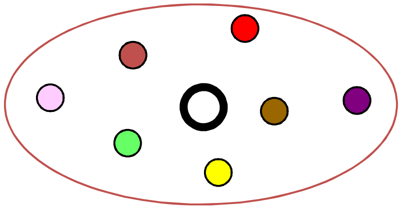

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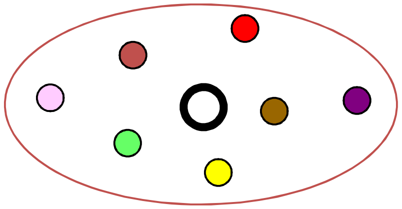

2. Split each cluster into two:
   - Perturb centroid of cluster slightly (by < 5%) to generate two centroids

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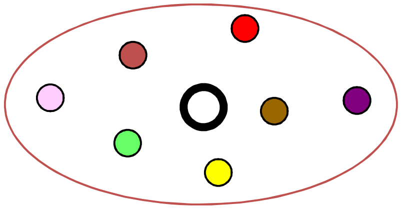

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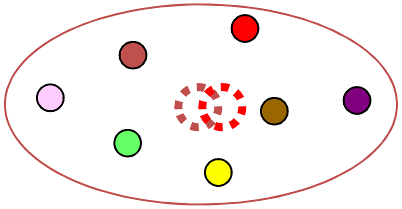

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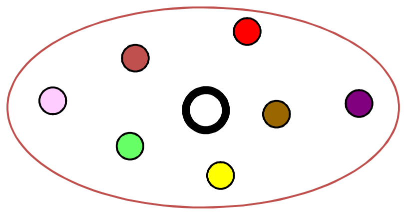

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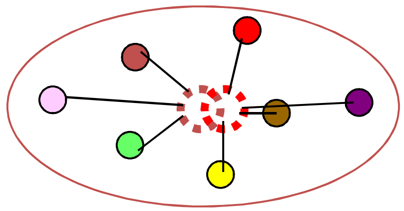

3. Initialize K means with new set of centroids

K-Means for Top–Down clustering

1. Start with one cluster

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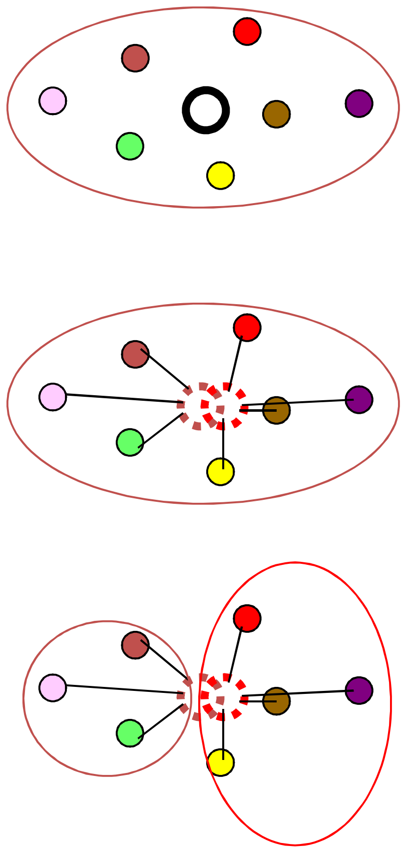
4. Iterate Kmeans until convergence



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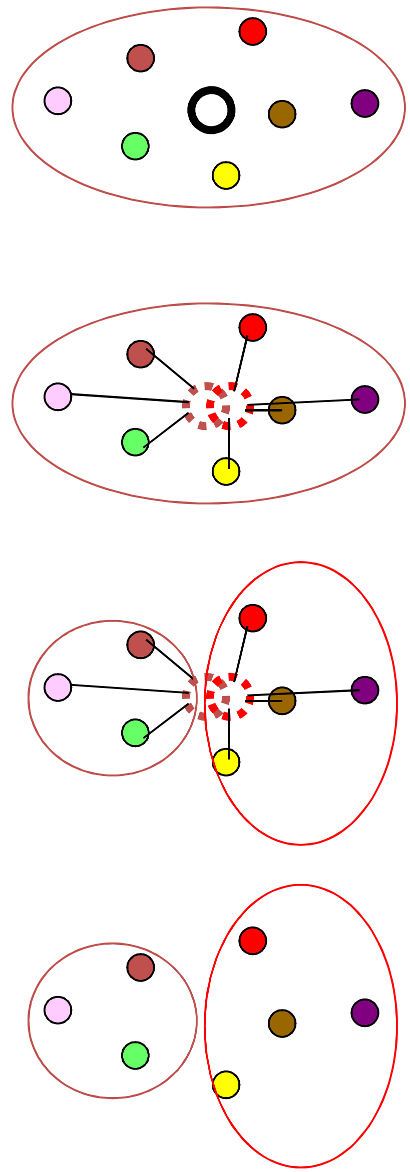

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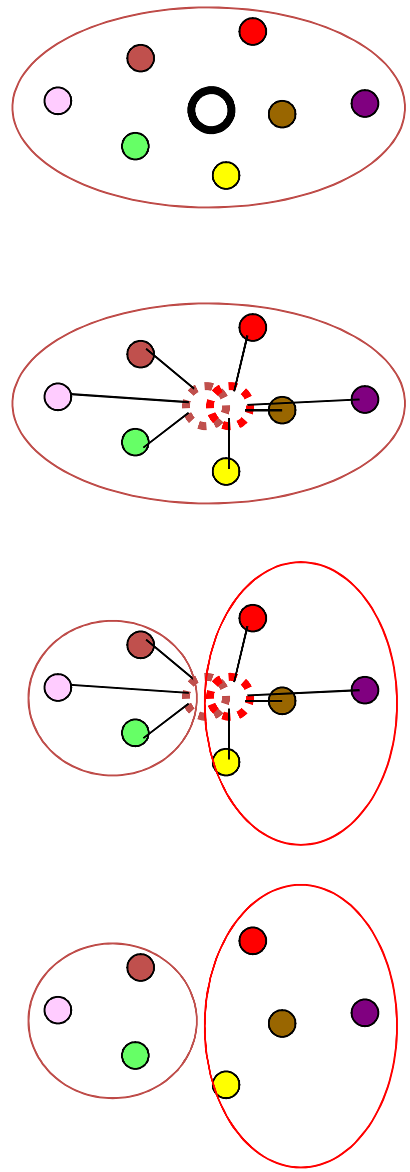
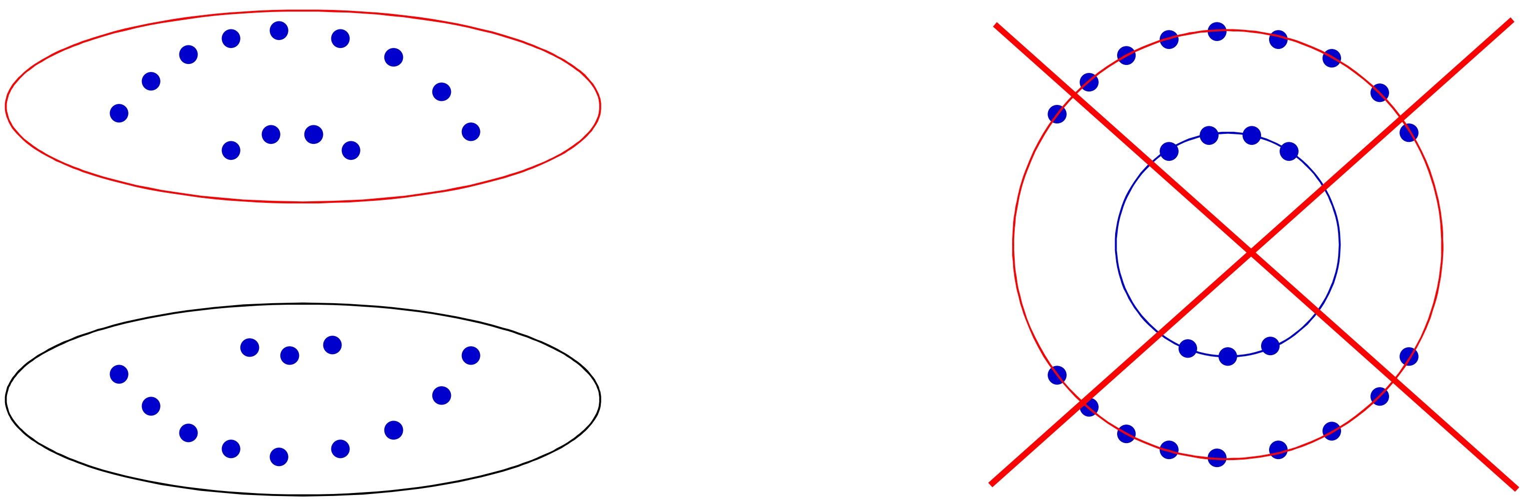
5. If the desired number of clusters is not obtained, return to 2

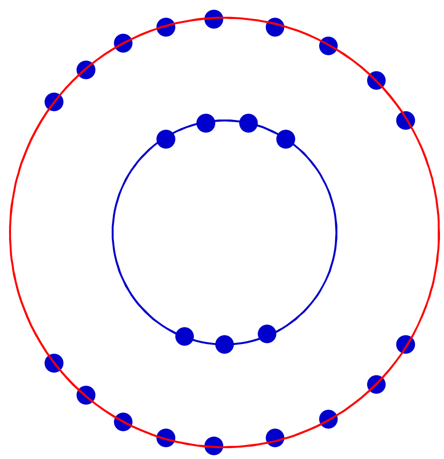


Non-Euclidean clusters

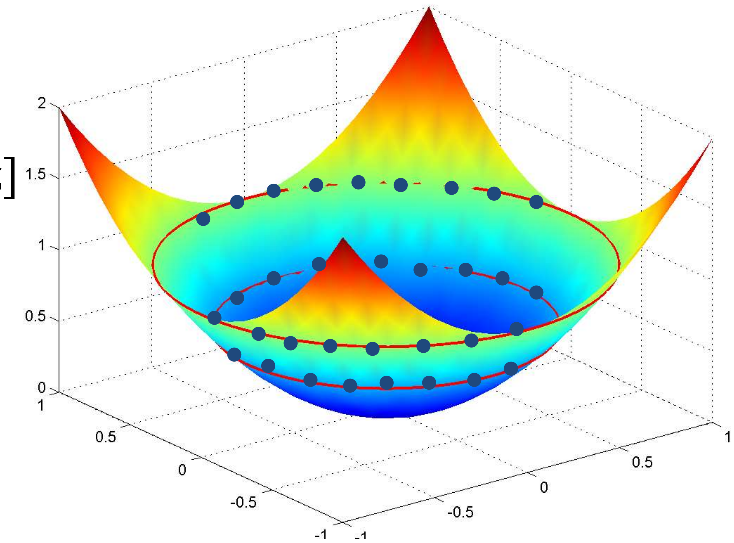


- Basic K-means results in good clusters in Euclidean spaces
  - Alternately stated, will only find clusters that are "good" in terms of Euclidean distances
- Will not find other types of clusters

Non-Euclidean clusters

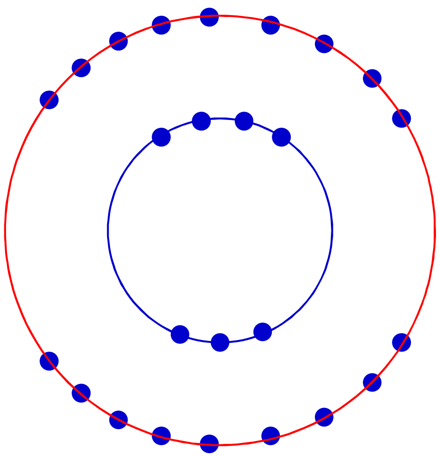


$f([x,y]) \rightarrow [x,y,z]$
$x = x$
$y = y$
$z = \alpha(x^2 + y^2)$



- 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 mechanisms:
  - Spectral clustering
    - Non-linear weighting of adjacency
  - Normalized cuts..

The Kernel Trick



f([x,y]) -> [x,y,z]
x = x
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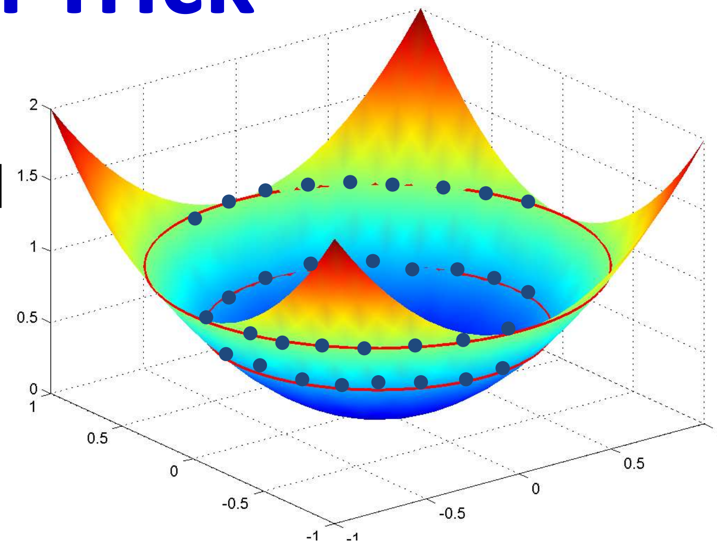


- Transform the data into a synthetic higher-dimensional space where the desired patterns become natural clusters based on *Euclidean* distance
  - E.g. the quadratic transform above

- 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

Distance in higher-dimensional space

- Transform data $\mathbf{x}$ through a *possibly unknown* function $\Phi(\mathbf{x})$ into a higher (potentially infinite) dimensional space
  - $\mathbf{z} = \Phi(\mathbf{x})$

- The distance between two points is computed in the higher-dimensional space
  - $d(\mathbf{x}_1, \mathbf{x}_2) = ||\mathbf{z}_1 - \mathbf{z}_2||^2 = ||\Phi(\mathbf{x}_1) - \Phi(\mathbf{x}_2)||^2$

- $d(\mathbf{x}_1, \mathbf{x}_2)$ can be computed without computing $\mathbf{z}$
  - Since it is a direct function of $\mathbf{x}_1$ and $\mathbf{x}_2$

Distance in higher-dimensional space

- Distance in lower-dimensional space: A combination of dot products
  - $||\mathbf{z}_1 - \mathbf{z}_2||^2 = (\mathbf{z}_1 - \mathbf{z}_2)^T(\mathbf{z}_1 - \mathbf{z}_2) = \mathbf{z}_1.\mathbf{z}_1 + \mathbf{z}_2.\mathbf{z}_2 - 2\,\mathbf{z}_1.\mathbf{z}_2$

- Distance in higher-dimensional space
  - $d(\mathbf{x}_1, \mathbf{x}_2) = ||\Phi(\mathbf{x}_1) - \Phi(\mathbf{x}_2)||^2$
    $= \Phi(\mathbf{x}_1).\,\Phi(\mathbf{x}_1) + \Phi(\mathbf{x}_2).\,\Phi(\mathbf{x}_2) - 2\,\Phi(\mathbf{x}_1).\,\Phi(\mathbf{x}_2)$

- $d(\mathbf{x}_1, \mathbf{x}_2)$ can be computed without knowing $\Phi(\mathbf{x})$ if:
  - $\Phi(\mathbf{x}_1).\,\Phi(\mathbf{x}_2)$ can be computed for any $\mathbf{x}_1$ and $\mathbf{x}_2$ without knowing $\Phi(.)$

The Kernel function

- A kernel function $K(\mathbf{x}_1,\mathbf{x}_2)$ is a function such that:
  - $K(\mathbf{x}_1,\mathbf{x}_2) = \Phi(\mathbf{x}_1).\ \Phi(\mathbf{x}_2)$
- 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 $\mathbf{v}$, $\mathbf{v}^T\mathbf{v} = ||\mathbf{v}||^2 >= 0$
  - This is just the length of $\mathbf{v}$ and is therefore non-negative

- For any vector $\mathbf{u} = \Sigma_i a_i \mathbf{v}_i$, $||\mathbf{u}||^2 >= 0$

  $\Rightarrow (\Sigma_i a_i \mathbf{v}_i)^T(\Sigma_i a_i \mathbf{v}_i) >= 0$

  $\Rightarrow \Sigma_i \Sigma_j a_i a_j \mathbf{v}_i . \mathbf{v}_j >= 0$

- This holds for ANY real $\{a_1, a_2, \ldots\}$

The Mercer Condition

- **If** $\mathbf{z} = \Phi(\mathbf{x})$ is a high-dimensional vector derived from $\mathbf{x}$ **then** for all real $\{a_1, a_2, \ldots\}$ and any set $\{\mathbf{z}_1, \mathbf{z}_2, \ldots\} = \{\Phi(\mathbf{x}_1), \Phi(\mathbf{x}_2), \ldots\}$
  - $\Sigma_i \Sigma_j a_i a_j \mathbf{z}_i . \mathbf{z}_j \;\; >= 0$
  - $\Sigma_i \Sigma_j a_i a_j \Phi(\mathbf{x}_i).\Phi(\mathbf{x}_j) \;\; >= 0$

- If $K(\mathbf{x}_1,\mathbf{x}_2) = \Phi(\mathbf{x}_1).\ \Phi(\mathbf{x}_2)$

  $=>$ $\mathbf{\Sigma_i \Sigma_j a_i a_j K(x_i,x_j) \;\; >= 0}$

- Any function K() that satisfies the above condition is a valid kernel function

The Mercer Condition

- $K(\mathbf{x}_1,\mathbf{x}_2) = \Phi(\mathbf{x}_1).\ \Phi(\mathbf{x}_2)$

  $\Rightarrow \Sigma_i \Sigma_j a_i a_j K(\mathbf{x}_i,\mathbf{x}_j) >= 0$

- **A corollary**: If any kernel $K(.)$ satisfies the Mercer condition

  $d(\mathbf{x}_1, \mathbf{x}_2) = K(\mathbf{x}_1,\mathbf{x}_1) + K(\mathbf{x}_2,\mathbf{x}_2) - 2K(\mathbf{x}_1,\mathbf{x}_2)$

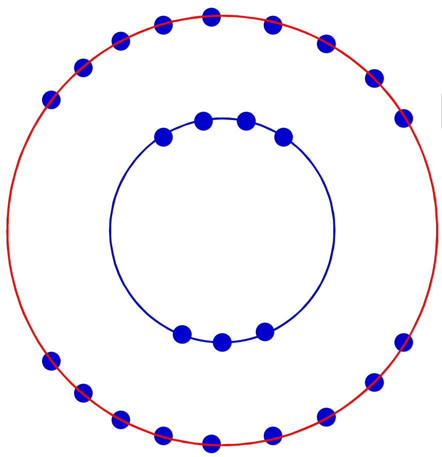
  satisfies the following requirements for a "distance"

  - $d(\mathbf{x},\mathbf{x}) = 0$
  - $d(\mathbf{x},\mathbf{y}) >= 0$
  - $d(\mathbf{x},\mathbf{w}) + d(\mathbf{w},\mathbf{y}) >= d(\mathbf{x},\mathbf{y})$

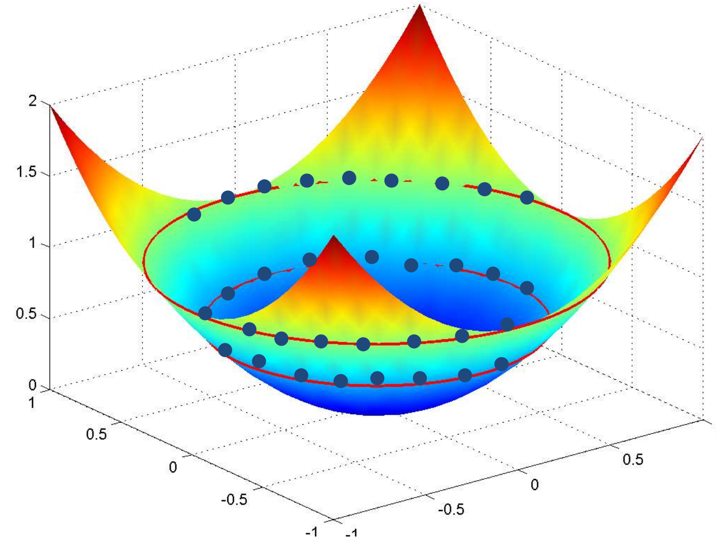
Typical Kernel Functions

- Linear: $K(\mathbf{x},\mathbf{y}) = \mathbf{x}^T\mathbf{y} + c$
- Polynomial $K(\mathbf{x},\mathbf{y}) = (a\mathbf{x}^T\mathbf{y} + c)^n$
- Gaussian: $K(\mathbf{x},\mathbf{y}) = \exp(-||\mathbf{x}-\mathbf{y}||^2/\sigma^2)$
- 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

Kernel K-means



$K(x,y) = (x^T y + c)^2$



- Perform the K-mean in the Kernel space
  - The space of $\mathbf{z} = \Phi(\mathbf{x})$

- 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

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

The mean of a cluster

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

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

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

- Alternately the weighted average

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

K–means

- Initialize the clusters with a random set of K points
  - $N_{cluster}$ is no. of points in cluster

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

- For each data point x, find the closest cluster

$$cluster(x) = \min_{cluster} d(x, cluster) = \min_{cluster} \| \Phi(x) - m_{cluster} \|^2$$

$$d(x, cluster) = \| \Phi(x) - m_{cluster} \|^2 = \left(\Phi(x) - \frac{1}{N_{cluster}} \sum_{i \in cluster} \Phi(x_i) \right)^T \left(\Phi(x) - \frac{1}{N_{cluster}} \sum_{i \in cluster} \Phi(x_i) \right)$$

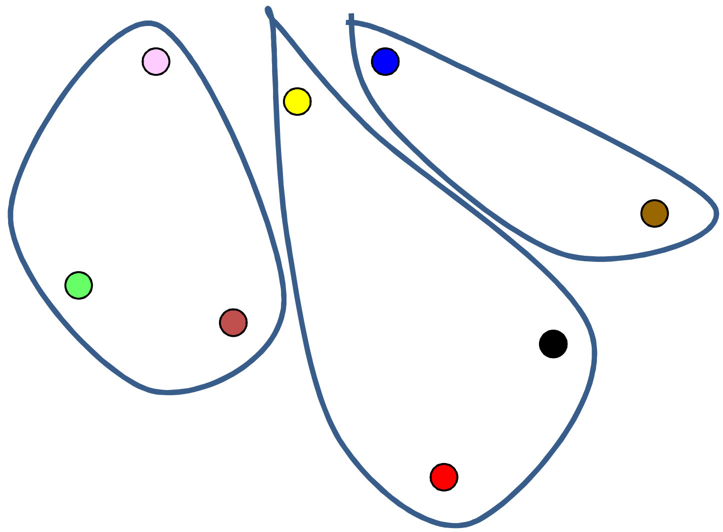
$$= \left(\Phi(x)^T \Phi(x) - \frac{2}{N_{cluster}} \sum_{i \in cluster} \Phi(x)^T \Phi(x_i) + \frac{1}{N_{cluster}^2} \sum_{i \in cluster} \sum_{j \in cluster} \Phi(x_i)^T \Phi(x_j) \right)$$

$$= K(x, x) - \frac{2}{N_{cluster}} \sum_{i \in cluster} K(x, x_i) + \frac{1}{N_{cluster}^2} \sum_{i \in cluster} \sum_{j \in cluster} K(x_i, x_j)$$

Computed entirely using only the kernel function!

K–means

1. Initialize a set of *clusters* randomly



K–means

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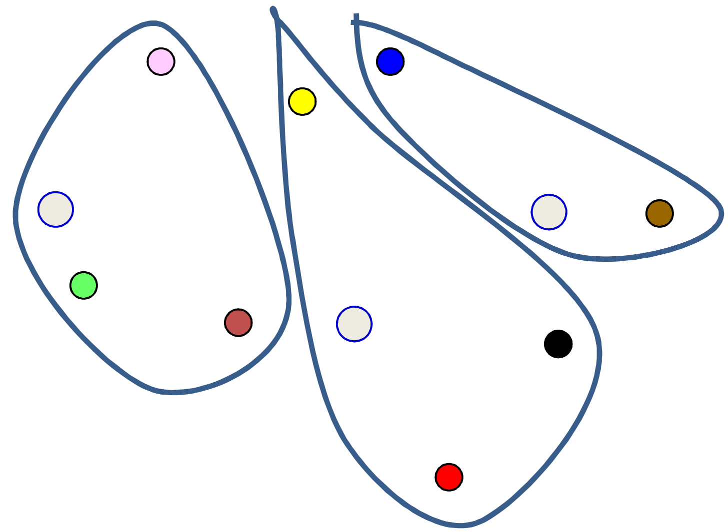
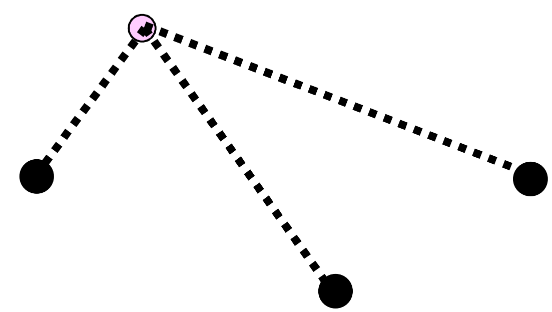


The centroids are *virtual*: we don't actually compute them explicitly!

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

K–means

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



$$d_{cluster} = K(x,x) - 2C \sum_{i \in cluster} w_i K(x, x_i) + C^2 \sum_{i \in cluster} \sum_{j \in cluster} w_i w_j K(x_i, x_j)$$

K–means

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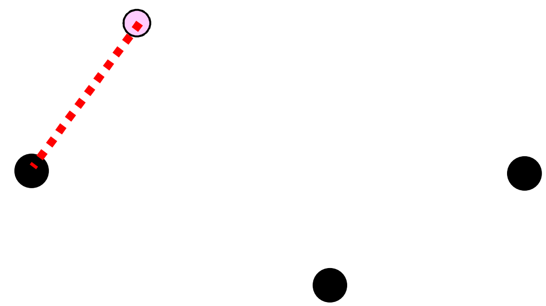
3. Put data point in the cluster of the closest centroid
   - Cluster for which $\boldsymbol{d}_{\text{cluster}}$ is minimum



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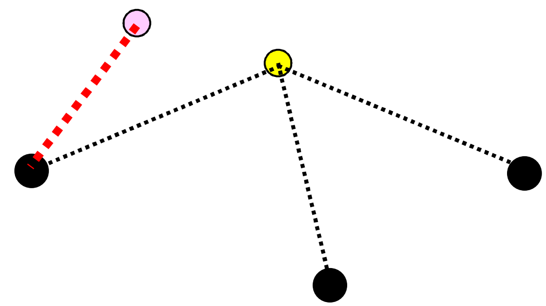

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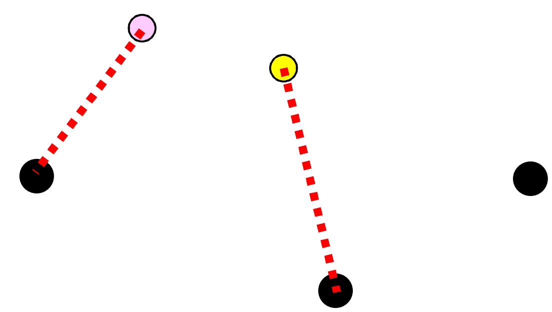

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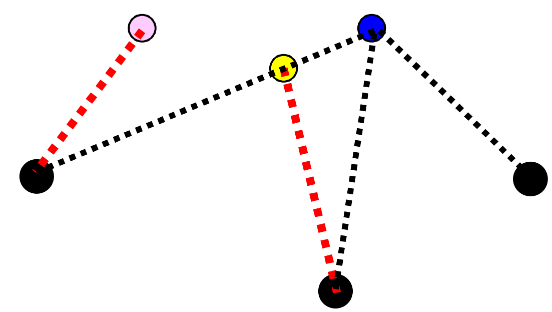

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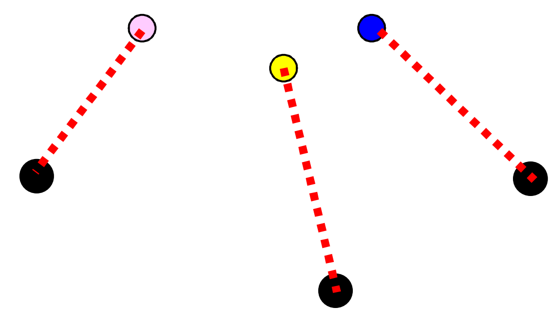

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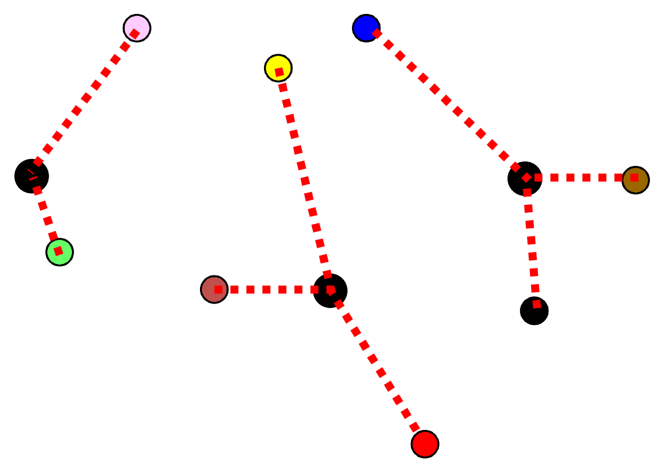

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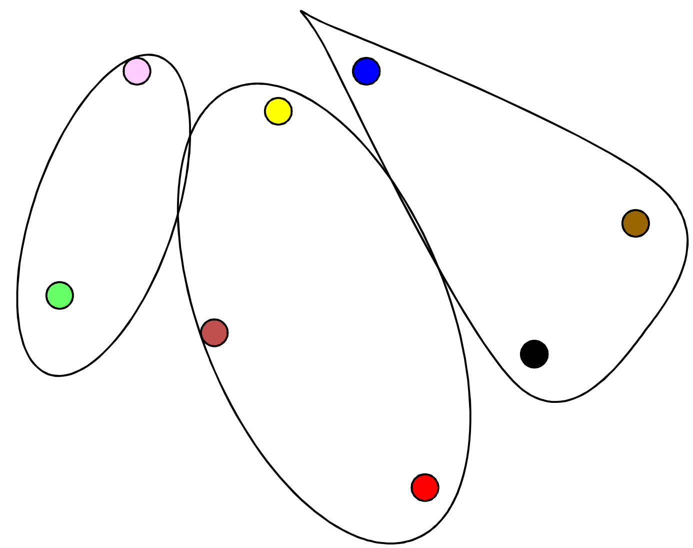

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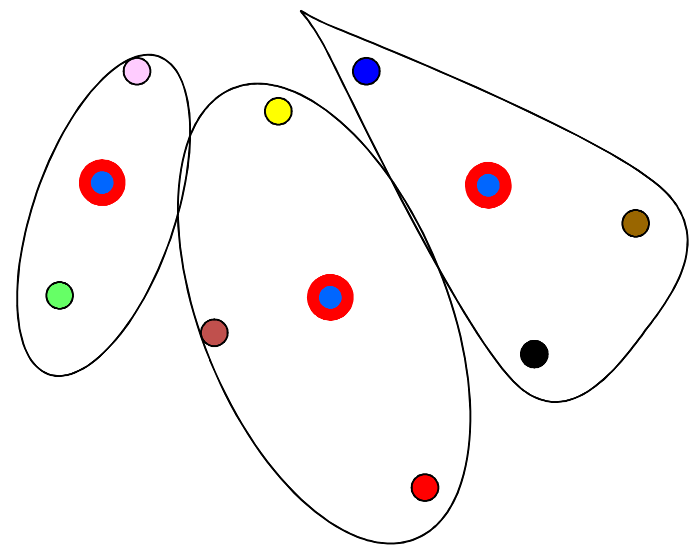
4. *When all data points are clustered, recompute centroids*

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



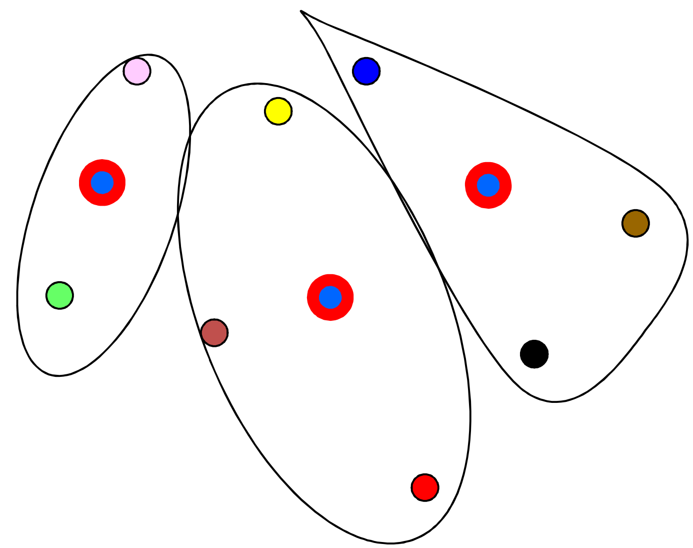
- We do not explicitly compute the means
- May be impossible – we do not know the high-dimensional space
- We only know how to compute inner products in it

Kernel K–means

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

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

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

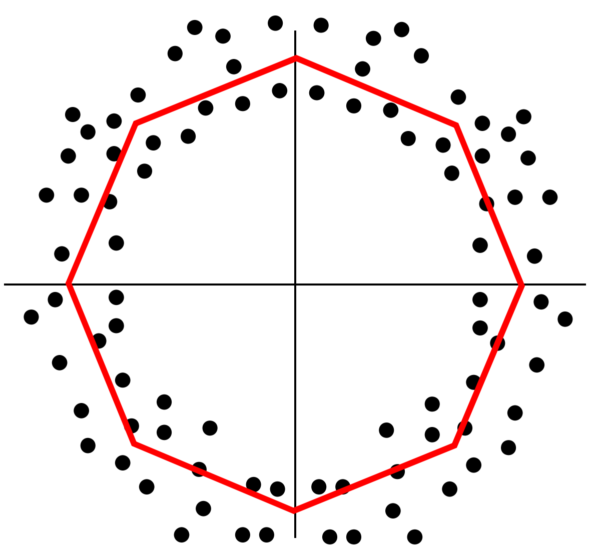
- Kernel correlation matrix $\mathbf{K}$
  - $\mathbf{K}_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$
- Find Eigen values Λ and Eigen vectors $\mathbf{e}$ of kernel matrix
  - No. of clusters = no. of dominant $\lambda_i (1^T\mathbf{e}_i)$ terms

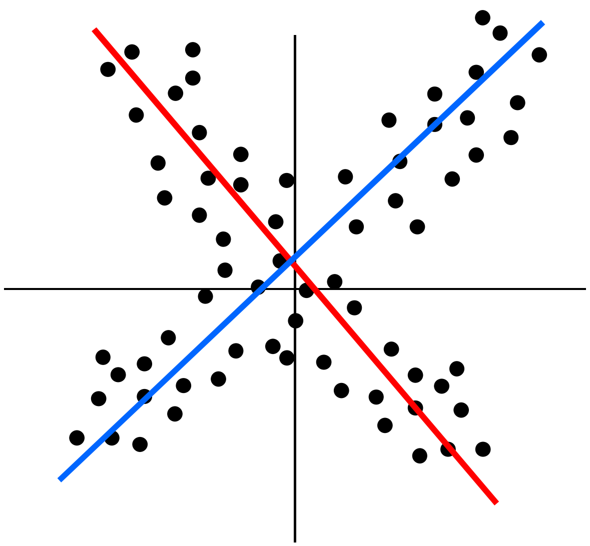
Spectral Methods

- "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 K-means

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..
- Key Features:
  - Identifies latent structure in the distribution of the data
  - Provides an L2-sense optimal quantized representation of the data
    - We will build on this in the next class