Clustering: K-means and Kernel K-means

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Machine Learning (CS771A)

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- Given: N unlabeled examples $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$; no. of desired partitions K
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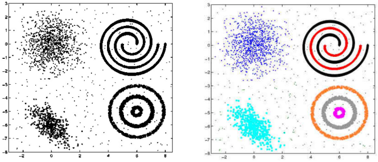

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Picture courtesy: "Data Clustering: 50 Years Beyond K-Means", A.K. Jain (2008)

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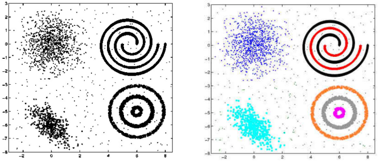

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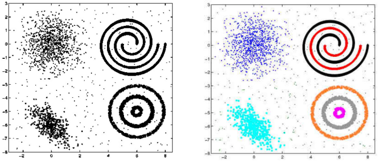

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- Loosely speaking, it is classification without ground truth labels
- A good clustering is one that achieves:
  - High within-cluster similarity
  - Low inter-cluster similarity

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Picture courtesy: `http://www.guy-sports.com/humor/videos/powerpoint_presentation_dogs.htm`

Clustering: Some Examples

- Document/Image/Webpage Clustering
- Image Segmentation (clustering pixels)

- Clustering web-search results
- Clustering (people) nodes in (social) networks/graphs
- .. and many more..

Picture courtesy: `http://people.cs.uchicago.edu/~pff/segment/`

Types of Clustering

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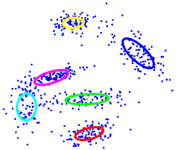
   - Partitions are independent of each other



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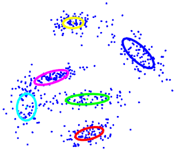

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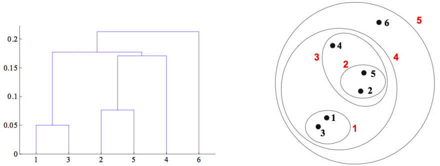
   - Partitions can be visualized using a tree structure (a dendrogram)



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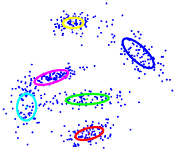

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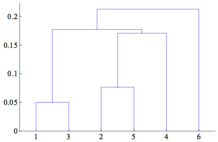

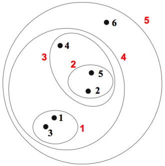

   - Possible to view partitions at different levels of granularities (i.e., can refine/coarsen clusters) using different K

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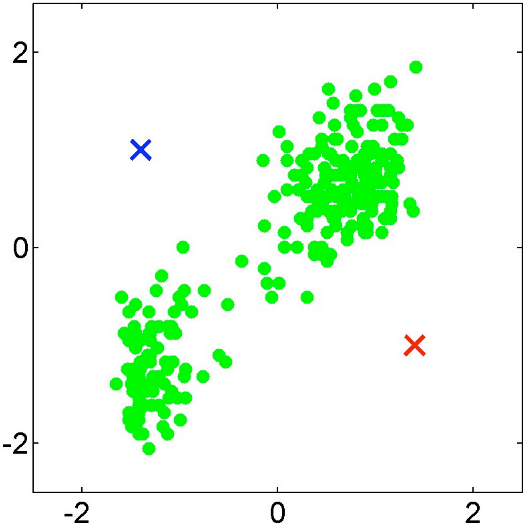
- Stop when cluster means or the "loss" does not change by much

K-means: Initialization (assume $K = 2$)



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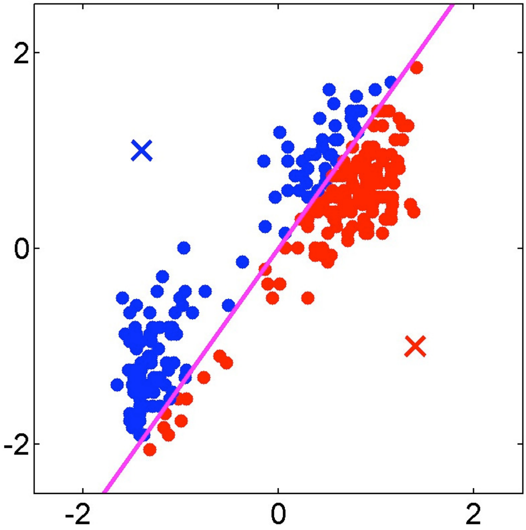
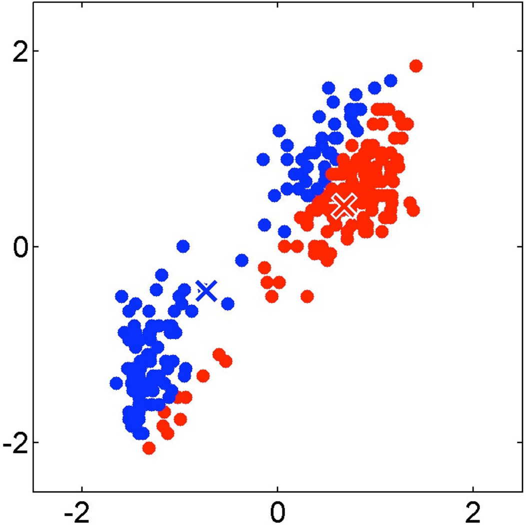
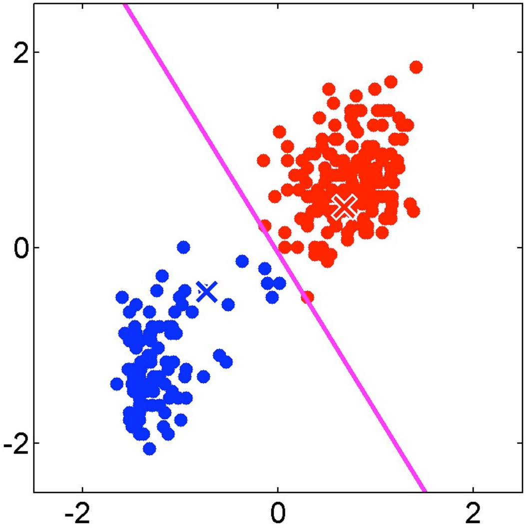


K-means iteration 1: Recomputing the centers



K-means iteration 2: Assigning points



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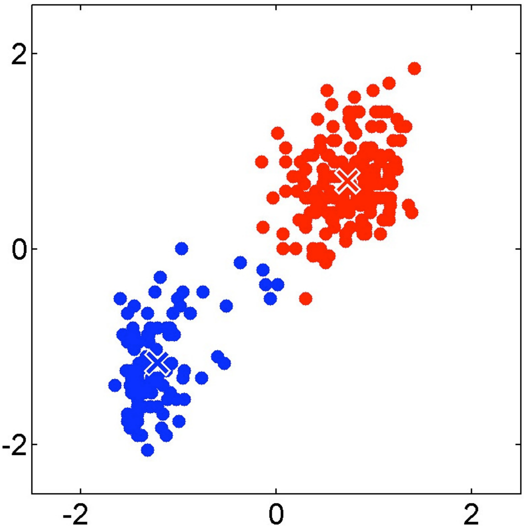
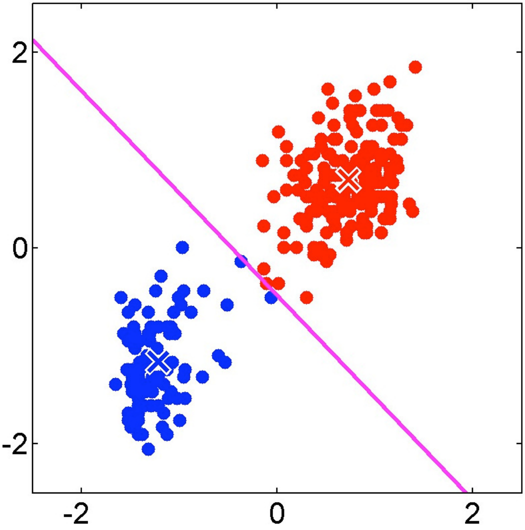


K-means iteration 3: Assigning points



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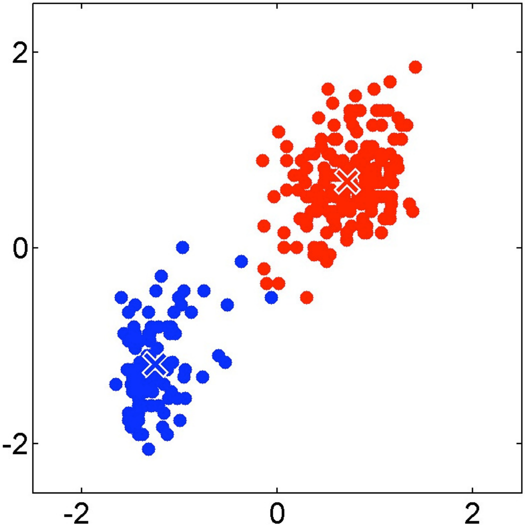

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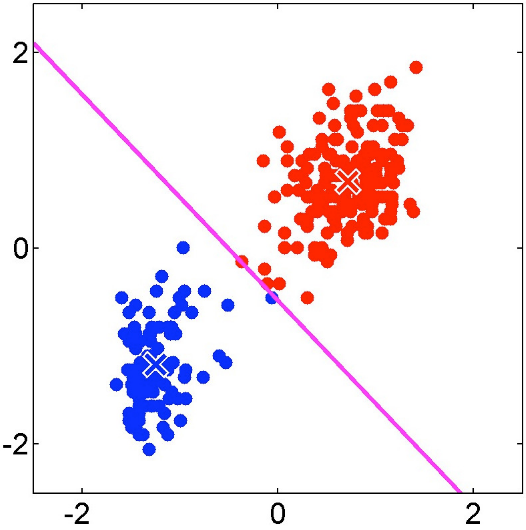

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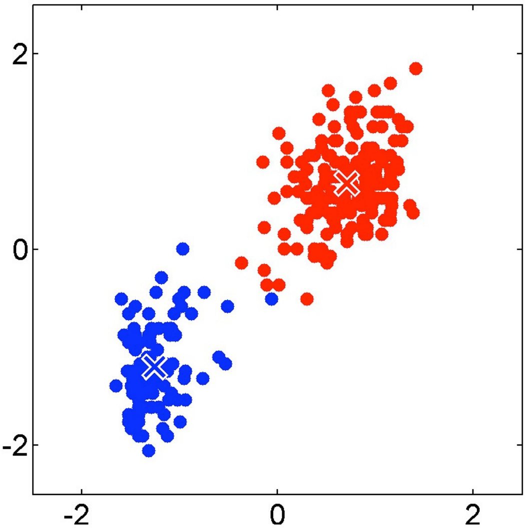

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  - Note that the objective only minimizes within-cluster distortions

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- Note: The algorithm usually converges to a local minima (though may not always, and it may just convergence "somewhere"). Multiple runs with different initializations can be tried to find a good solution.

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- Each step (updating $\mathbf{Z}$ or $\boldsymbol{\mu}$) can never increase the objective
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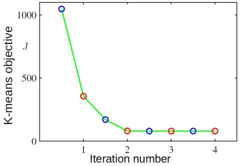
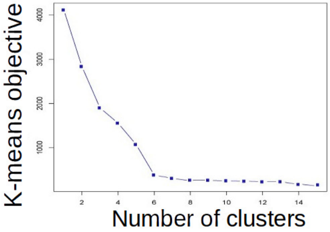
- Thus the K-means algorithm monotonically decreases the objective



(blue: after Z updated, red: after μ updated)

K-means: Choosing K

- One way to select K for the K-means algorithm is to try different values of K, plot the K-means objective versus K, and look at the "elbow-point"



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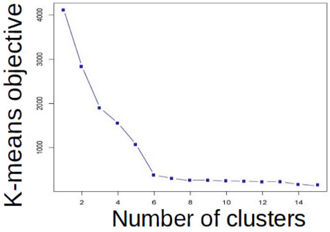

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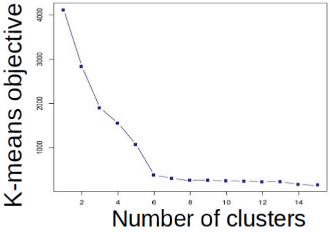

- For the above plot, $K = 6$ is the elbow point
- Can also information criterion such as AIC (Akaike Information Criterion)

$$AIC = 2L(\hat{\mu}, \mathbf{X}, \hat{\mathbf{Z}}) + K \log D$$

.. and choose the K that has the smallest AIC (discourages large K)

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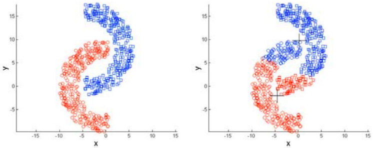

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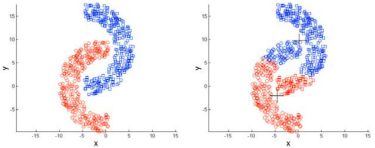

- Kernel K-means or Spectral clustering can handle non-convex

Kernel K-means

- Basic idea: Replace the Euclidean distance/similarity computations in K-means by the kernelized versions. E.g., $d(\boldsymbol{x}_n, \boldsymbol{\mu}_k) = ||\phi(\boldsymbol{x}_n) - \phi(\boldsymbol{\mu}_k)||$ by

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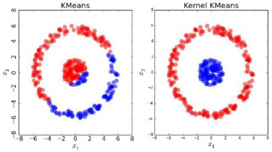
Kernel K-means vs. K-means



Pyclust: Open Source Data Clustering Pckage

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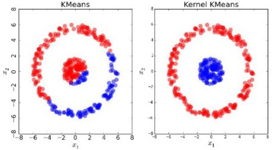

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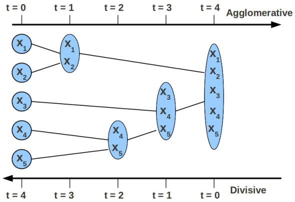
  - A small technical note: When computing $k(\boldsymbol{\mu}_k, \boldsymbol{\mu}_k)$ and $k(\boldsymbol{x}_n, \boldsymbol{\mu}_k)$, remember that $\phi(\boldsymbol{\mu}_k)$ is the average of ϕ's the data points assigned to cluster k

Extra Slides: Hierarchical Clustering

Hierarchical Clustering



- **Agglomerative (bottom-up) Clustering**
  1. Start with each example in its own singleton cluster
  2. At each time-step, greedily merge 2 most similar clusters
  3. Stop when there is a single cluster of all examples, else go to 2
- **Divisive (top-down) Clustering**
  1. Start with all examples in the same cluster
  2. At each time-step, remove the "outsiders" from the least cohesive cluster
  3. Stop when each example is in its own singleton cluster, else go to 2
- Agglomerative is more popular and simpler than divisive (but less accurarate)

(Dis)similarity between clusters

- We know how to compute the dissimilarity $d(\boldsymbol{x}_i, \boldsymbol{x}_j)$ between two examples
- How to compute the dissimilarity between two clusters R and S?
- **Min-link or single-link:** results in chaining (clusters can get very large)

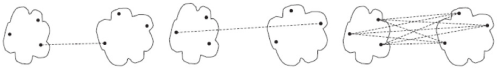
$$d(R,S) = \min_{\boldsymbol{x}_R \in R, \boldsymbol{x}_S \in S} d(\boldsymbol{x}_R, \boldsymbol{x}_S)$$

- **Max-link or complete-link:** results in small, round shaped clusters

$$d(R,S) = \max_{\boldsymbol{x}_R \in R, \boldsymbol{x}_S \in S} d(\boldsymbol{x}_R, \boldsymbol{x}_S)$$

- **Average-link:** compromise between single and complexte linkage

$$d(R,S) = \frac{1}{|R||S|} \sum_{\boldsymbol{x}_R \in R, \boldsymbol{x}_S \in S} d(\boldsymbol{x}_R, \boldsymbol{x}_S)$$



(a) MIN (single link.) (b) MAX (complete link.) (c) Group average.

Flat vs Hierarchical Clustering

- Flat clustering produces a single partitioning
- Hierarchical Clustering can give different partitionings depending on the level-of-resolution we are looking at
- Flat clustering is usually more efficient run-time wise
- Hierarchical clustering can be slow (has to make several merge/split decisions)