Data Clustering: K-means and Hierarchical Clustering

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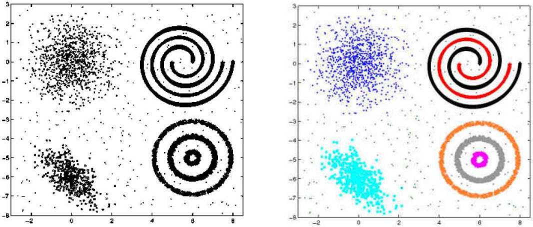
What is Data Clustering?

- Data Clustering is an unsupervised learning problem
- Given: N unlabeled examples $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$; the number of partitions K
- Goal: Group the examples into K partitions



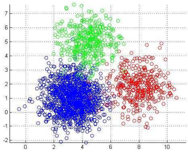
(a) Input data (b) Desired clustering

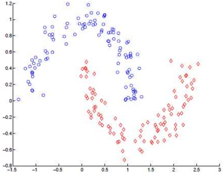
- The only information clustering uses is the similarity between examples
- Clustering groups examples based of their mutual similarities
- A good clustering is one that achieves:
  - High within-cluster similarity
  - Low inter-cluster similarity

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

Notions of Similarity

- Choice of the **similarity measure** is very important for clustering
- Similarity is inversely related to distance
- Different ways exist to measure distances. Some examples:
  - Euclidean distance: $d(\mathbf{x}, \mathbf{z}) = ||\mathbf{x} - \mathbf{z}|| = \sqrt{\sum_{d=1}^{D}(x_d - z_d)^2}$
  - Manhattan distance: $d(\mathbf{x}, \mathbf{z}) = \sum_{d=1}^{D} |x_d - z_d|$
  - Kernelized (non-linear) distance: $d(\mathbf{x}, \mathbf{z}) = ||\phi(\mathbf{x}) - \phi(\mathbf{z})||$





  - For the left figure above, Euclidean distance may be reasonable
  - For the right figure above, kernelized distance seems more reasonable

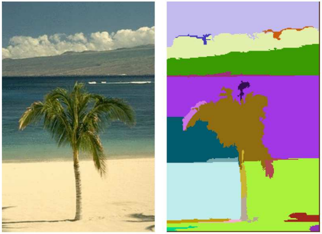
Similarity is Subjective

- Similarity is often hard to define

- Different similarity criteria can lead to different clusterings

Data Clustering: Some Real-World Examples

- Clustering images based on their perceptual similarities
- Image segmentation (clustering pixels)

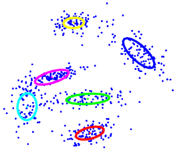


- Clustering webpages based on their content
- Clustering web-search results
- Clustering people in social networks based on user properties/preferences
- .. and many more..

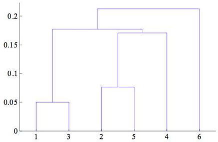
Picture courtesy: `http://people.cs.uchicago.edu/~pff/segment/`

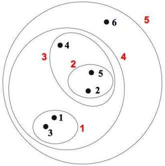
Types of Clustering

1. **Flat or Partitional clustering** (K-means, Gaussian mixture models, etc.)
   - Partitions are independent of each other



2. **Hierarchical clustering** (e.g., agglomerative clustering, divisive clustering)
   - Partitions can be visualized using a tree structure (a dendrogram)
   - Does not need the number of clusters as input
   - Possible to view partitions at different levels of granularities (i.e., can refine/coarsen clusters) using different K





Flat Clustering: K-means algorithm (Lloyd, 1957)

- **Input:** N examples $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ ($\mathbf{x}_n \in \mathbb{R}^D$); the number of partitions K
- **Initialize:** K cluster centers $\mu_1, \ldots, \mu_K$. Several initialization options:
  - Randomly initialized anywhere in $\mathbb{R}^D$
  - Choose any K examples as the cluster centers
- **Iterate:**
  - Assign each of example $\mathbf{x}_n$ to its closest cluster center

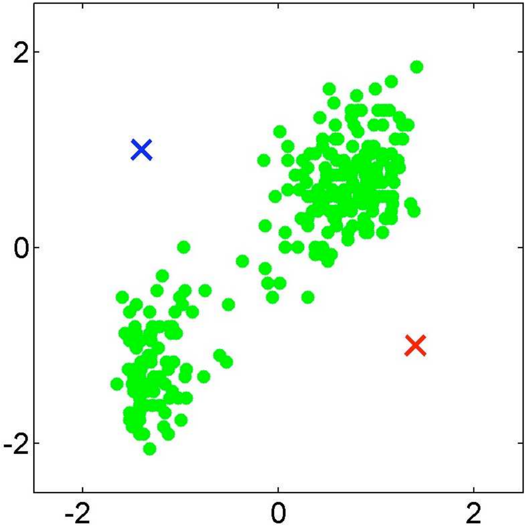
$$\mathcal{C}_k = \{n : \quad k = \arg\min_k ||\mathbf{x}_n - \mu_k||^2\}$$

  ($\mathcal{C}_k$ is the set of examples closest to μ_k)
  - Recompute the new cluster centers μ_k (mean/centroid of the set $\mathcal{C}_k$)

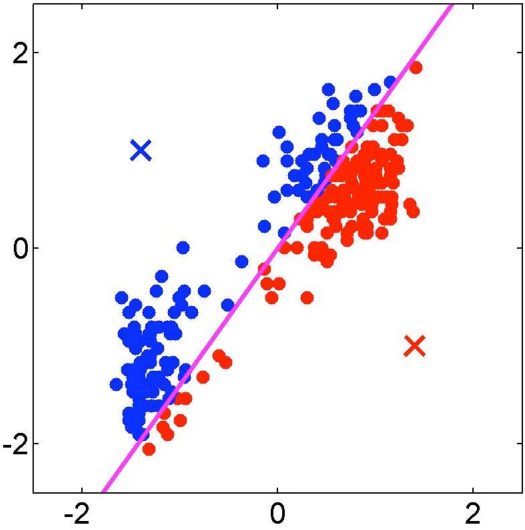
$$\mu_k = \frac{1}{|\mathcal{C}_k|} \sum_{n \in \mathcal{C}_k} \mathbf{x}_n$$

  - Repeat while not converged
- A possible convergence criteria: cluster centers do not change anymore

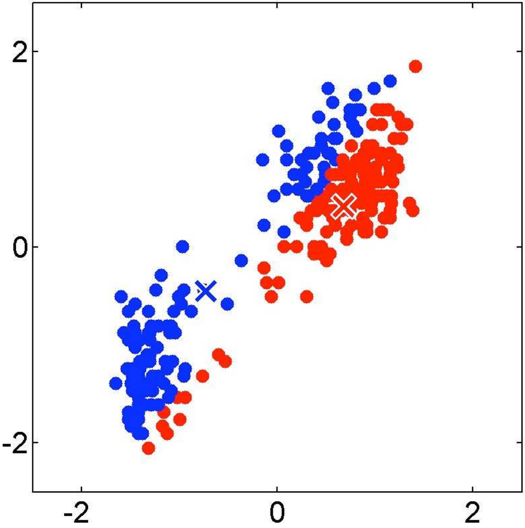
K-means: Initialization (assume $K = 2$)



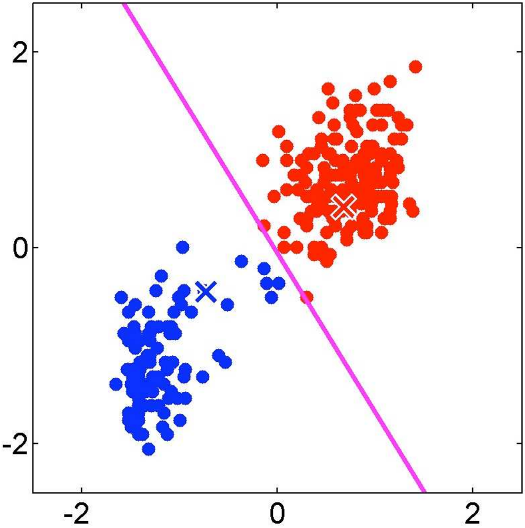
K-means iteration 1: Assigning points



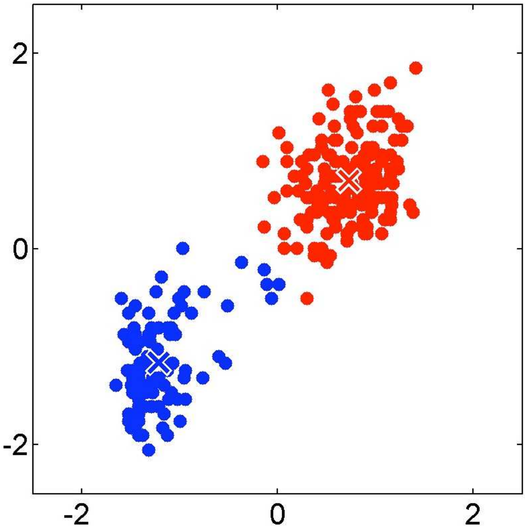
K-means iteration 1: Recomputing the cluster centers



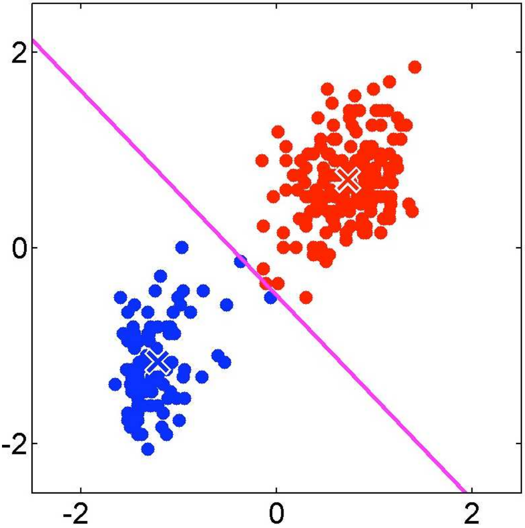
K-means iteration 2: Assigning points



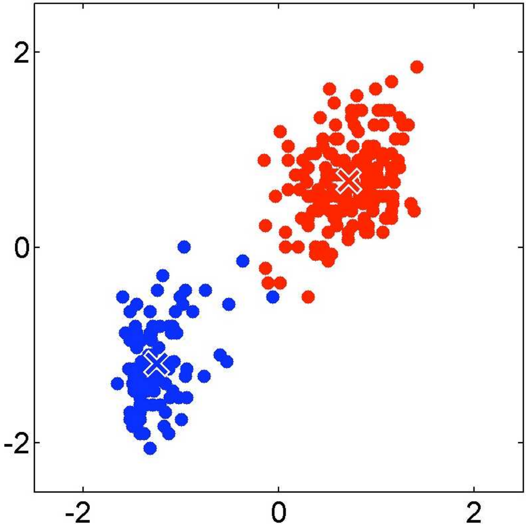
K-means iteration 2: Recomputing the cluster centers



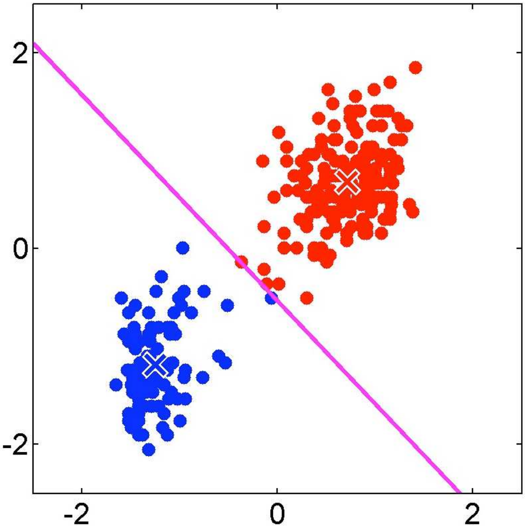
K-means iteration 3: Assigning points



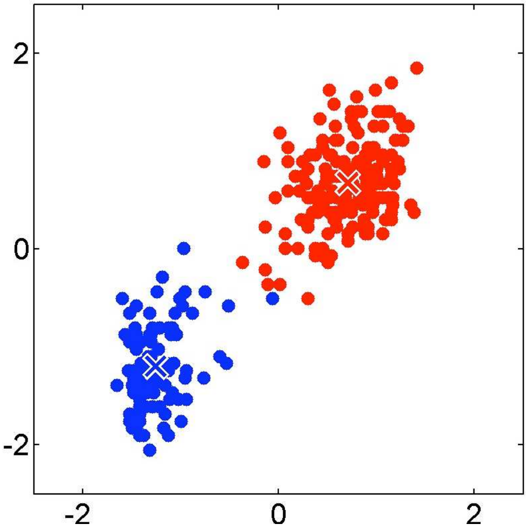
K-means iteration 3: Recomputing the cluster centers



K-means iteration 4: Assigning points



K-means iteration 4: Recomputing the cluster centers



K-means: The Objective Function

The K-means objective function

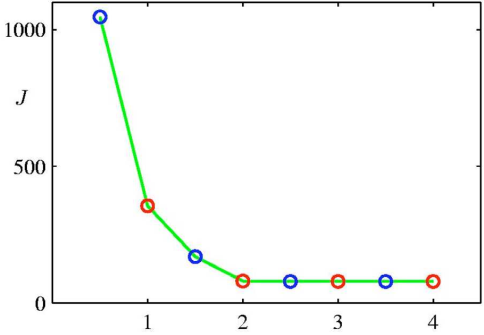
- Let $\mu_1, \ldots, \mu_K$ be the K cluster centroids (means)
- Let $r_{nk} \in \{0, 1\}$ be indicator denoting whether point $\mathbf{x}_n$ belongs to cluster k
- K-means objective minimizes the total distortion (sum of distances of points from their cluster centers)

$$J(\mu, r) = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} ||\mathbf{x}_n - \mu_k||^2$$

- Note: Exact optimization of the K-means objective is NP-hard
- The K-means algorithm is a heuristic that converges to a local optimum

K-means: Choosing the number of clusters 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" in the plot



- For the above plot, $K = 2$ is the elbow point

Picture courtesy: "Pattern Recognition and Machine Learning, Chris Bishop (2006)

K-means: Initialization issues

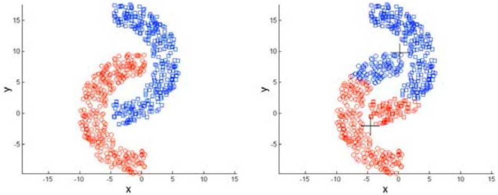
- K-means is extremely sensitive to cluster center initialization
- Bad initialization can lead to
  - Poor convergence speed
  - Bad overall clustering
- Safeguarding measures:
  - Choose first center as one of the examples, second which is the farthest from the first, third which is the farthest from both, and so on.
  - Try multiple initializations and choose the best result
  - Other smarter initialization schemes (e.g., look at the K-means++ algorithm by Arthur and Vassilvitskii)

K-means: Limitations

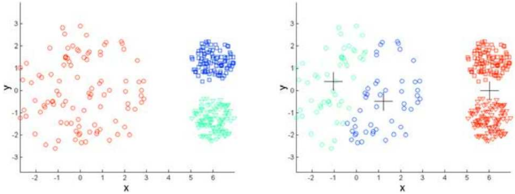
- Makes hard assignments of points to clusters
  - A point either completely belongs to a cluster or not belongs at all
  - No notion of a soft assignment (i.e., probability of being assigned to each cluster: say $K = 3$ and for some point $\mathbf{x}_n$, $p_1 = 0.7, p_2 = 0.2, p_3 = 0.1$)
  - Gaussian mixture models and Fuzzy K-means allow soft assignments
- Sensitive to outlier examples (such examples can affect the mean by a lot)
  - K-medians algorithm is a more robust alternative for data with outliers
  - Reason: Median is more robust than mean in presence of outliers
- Works well only for round shaped, and of roughly equal sizes/density clusters
- Does badly if the clusters have non-convex shapes
  - Spectral clustering or kernelized K-means can be an alternative

K-means Limitations Illustrated

Non-convex/non-round-shaped clusters: Standard K-means fails!

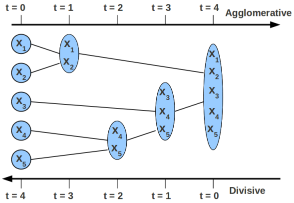


Clusters with different densities



Picture courtesy: Christof Monz (Queen Mary, Univ. of London)

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)

Hierarchical Clustering: (Dis)similarity between clusters

- We know how to compute the dissimilarity $d(\mathbf{x}_i, \mathbf{x}_j)$ 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)

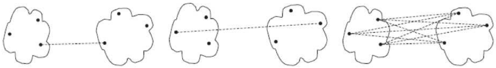
$$d(R, S) = \min_{\mathbf{x}_R \in R, \mathbf{x}_S \in S} d(\mathbf{x}_R, \mathbf{x}_S)$$

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

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

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

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



(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 needs the number of clusters to be specified
- Hierarchical clustering doesn't need the number of clusters to be specified
- Flat clustering is usually more efficient run-time wise
- Hierarchical clustering can be slow (has to make several merge/split decisions)
- No clear consensus on which of the two produces better clustering