Unsupervised Learning: Clustering

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Based on the slides of Vibhav Gogate
Clustering systems:

- Unsupervised learning
- Requires data, but no labels
- Detect patterns, e.g., in
  - Group emails or search results
  - Customer shopping patterns
- Useful when don’t know what you’re looking for...
  - But often get gibberish
Clustering

• Want to group together parts of a dataset that are close together in some metric

• Useful for finding the important parameters/features of a dataset
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Clustering

• Input: a collection of points $x^{(1)}, \ldots, x^{(m)} \in \mathbb{R}^n$, an integer $k$

• Output: A partitioning of the input points into $k$ sets that minimizes some metric of closeness
$k$-means Clustering

• Pick an initial set of $k$ means (usually at random)

• Repeat until the clusters do not change:
  • Partition the data points, assigning each data point to a cluster based on the mean that is closest to it
  • Update the cluster means so that the $i^{th}$ mean is equal to the average of all data points assigned to cluster $i$
$k$-means clustering: Example

Pick $k$ random points as cluster centers (means)
Iterative Step 1:
Assign data instances to closest cluster center
Iterative Step 2:
Change the cluster center to the average of the assigned points
$k$-means clustering: Example

Repeat until convergence
$k$-means clustering: Example
$k$-means clustering: Example
$k$-means clustering: Example

(i)
Goal of segmentation is to partition an image into regions, each of which has reasonably homogenous visual appearance.

$k = 2$

Original
$k$-Means for Segmentation

$k = 2$  
$k = 3$  
Original

$k = 10$
$k$-Means for Segmentation

$k = 2$

$k = 3$

$k = 10$

Original
$k$-means Clustering as Optimization

- Minimize the distance of each input point to the mean of the cluster/partition that contains it

$$\min_{S_1, \ldots, S_k} \sum_{i=1}^{k} \sum_{j \in S_i} \|x^{(j)} - \mu_i\|^2$$

where

- $S_i \subseteq \{1, \ldots, M\}$ is the $i^{th}$ cluster
- $S_i \cap S_j = \emptyset$ for $i \neq j$, $\cup_i S_i = \{1, \ldots, n\}$
- $\mu_i$ is the centroid of the $i^{th}$ cluster
$k$-means Clustering as Optimization

- Minimize the distance of each input point to the mean of the cluster/partition that contains it

$$\min_{S_1, \ldots, S_k} \sum_{i=1}^{k} \sum_{j \in S_i} \| x(j) - \mu_i \|^2$$

where

- $S_i \subseteq \{1, \ldots, M\}$ is the $i^{th}$ cluster
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Exactly minimizing this function is NP-hard (even for $k = 2$)
$k$-means Clustering

• The $k$-means clustering algorithm performs a block coordinate descent on the objective function

$$
\sum_{i=1}^{k} \sum_{j \in S_i} \|x^{(j)} - \mu_i\|^2
$$

• This is not a convex function: could get stuck in local minima
**k-Means as Optimization**

- **Consider the** $k$-means objective function

$$\phi(x, S, \mu) = \sum_{i=1}^{k} \sum_{j \in S_i} \|x^{(j)} - \mu_i\|^2$$

- **Two stages each iteration**
  - Update cluster assignments: fix means $\mu$, change assignments $S$
  - Update means: fix assignments $S$, change means $\mu$
Phase I: Update Assignments

- For each point, re-assign to closest mean, $x^{(j)} \in S_i$ if

$$j \in \text{arg min}_i \|x^{(j)} - \mu_i\|^2$$

- Can only decrease $\phi$ as the sum of the distances of all points to their respective means must decrease

$$\phi(x, S, \mu) = \sum_{i=1}^{k} \sum_{j \in S_i} \|x^{(j)} - \mu_i\|^2$$
Phase II: Update Means

• Move each mean to the average of its assigned points

\[ \mu_i = \sum_{j \in S_i} \frac{x^{(j)}}{|S_i|} \]

• Also can only decrease total distance...
  • Why?
Phase II: Update Means

• Move each mean to the average of its assigned points

\[ \mu_i = \sum_{j \in S_i} \frac{x^{(j)}}{|S_i|} \]

• Also can only decrease total distance...

• The point \( y \) with minimum squared Euclidean distance to a set of points is their mean
Initialization

• K-means is sensitive to initialization
  • It does matter what you pick!
  • What can go wrong?
Initialization

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Initialization

• K-means is sensitive to initialization
  • It does matter what you pick!
  • What can go wrong?
    • Various schemes to help alleviate this problem: initialization heuristics
\(k\)-means Clustering

- Not clear how to figure out the "best" \(k\) in advance
- Want to choose \(k\) to pick out the interesting clusters, but not to overfit the data points
  - Large \(k\) doesn't necessarily pick out interesting clusters
  - Small \(k\) can result in large clusters than can be broken down further
Local Optima
$k$-Means Summary

- Guaranteed to converge
  - But not to a global optimum
- Choice of $k$ and initialization can greatly affect the outcome
- Runtime: $O(kMn)$ per iteration
- Popular because it is fast, though there are other clustering methods that may be more suitable depending on your data
Hierarchical Clustering

- Agglomerative clustering
  - Incrementally build larger clusters out of smaller clusters

- Algorithm:
  - Maintain a set of clusters
  - Initially, each instance in its own cluster
  - Repeat:
    - Pick the two closest clusters
    - Merge them into a new cluster
    - Stop when there is only one cluster left

- Produces not one clustering, but a family of clusterings represented by a dendrogram
Agglomerative Clustering

• How should we define “closest” for clusters with multiple elements?

  Closest / farthest pair

  Average of all pairs

• Many more choices, each produces a different clustering...
Clustering Behavior

Average

Farthest

Nearest

Mouse tumor data from [Hastie]