Unsupervised Learning: Clustering

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Based on the slides of Vibhav Gogate
Announcements

• Midterm (next Wednesday in class)

  • Closed book, closed notes, etc. (just you and a pencil)

  • Try to arrive as early as possible so as to maximize your exam taking time

  • Covers everything up to the end of boosting

  • Be prepared for theoretical questions! A practice exam will be made available on eLearning.

  • The exam is worth a significant percentage of the grade, talk to other students and use Piazza to make sure that you are prepared!
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
Goal of Segmentation is to partition an image into regions each of which has reasonably homogenous visual appearance.
$k$-Means for Segmentation

$k = 2$

$k = 3$

Original
$k$-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
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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

\[
j \in \arg \min_i \|x^{(j)} - \mu_i\|^2
\]

- 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?
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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
$k$-Means Summary

- Guaranteed to converge
  - But not to a global optimum
- Choice of $k$ and initialization can greatly affect the outcome
- Runtime: $O(kM)$ 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]