Clustering
Part 2

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Partitional Clustering

Original Points

A Partitional Clustering
Hierarchical Clustering

Traditional Hierarchical Clustering

Traditional Dendrogram

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Characteristics of Clustering Algorithms

• Type of clustering the algorithm produces:
  – Partitional versus hierarchical
  – Overlapping versus non-overlapping
  – Fuzzy versus non-fuzzy
  – Complete versus partial
Characteristics of Clustering Algorithms

• Type of clusters the algorithm seeks:
  – Well-separated, center-based, density-based or contiguity-based
  – Are the clusters found in the entire space or in a subspace
  – Are the clusters relatively similar to one another, or are they of differing sizes, shapes and densities
Characteristics of Clustering Algorithms

• Type of data the algorithm can handle:
  - Some clustering algorithms need a data matrix
    • The K-means algorithm assumes that it is meaningful to take the mean (average) of a set of data objects.
    • This makes sense for data that has continuous attributes and for document data, but not for record data that has categorical attributes.
  - Some clustering algorithms start from a proximity matrix
    • Typically assume symmetry
  - Does the data have noise and outliers?
  - Is the data high dimensional?
Characteristics of Clustering Algorithms

• How the algorithm operates:
  – Minimizing or maximizing a global objective function.
    • Enumerate all possible ways of dividing the points into clusters and evaluate the ‘goodness’ of each potential set of clusters by using the given objective function. (NP Hard)
  • Can have global or local objectives.
    – Hierarchical clustering algorithms typically have local objectives
    – Partitional algorithms typically have global objectives
  – A variation of the global objective function approach is to fit the data to a parameterized model.
    • Parameters for the model are determined from the data.
    • Mixture models assume that the data is a ‘mixture’ of a number of statistical distributions.
Characteristics of Clustering Algorithms

• How the algorithm operates …
  – Map the clustering problem to a different domain and solve a related problem in that domain.
  • Proximity matrix defines a weighted graph, where the nodes are the points being clustered, and the weighted edges represent the proximities between points.
  • Clustering is equivalent to breaking the graph into connected components, one for each cluster.
K-means Clustering

- Partitional clustering approach
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid.
- Number of clusters, K, must be specified.
- The basic algorithm is very simple.

1: Select $K$ points as the initial centroids.
2: repeat
3: Form $K$ clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: until The centroids don’t change
K-means Clustering – Details

• Initial centroids are often chosen randomly.
  – Clusters produced vary from one run to another.
• The centroid is (typically) the mean of the points in the cluster.
• ‘Closeness’ is measured by Euclidean distance, cosine similarity, correlation, etc.
• K-means will converge for common similarity measures mentioned above.
• Most of the convergence happens in the first few iterations.
  – Often the stopping condition is changed to ‘Until relatively few points change clusters’
• Complexity is $O( n \times K \times I \times d )$
  – $n =$ number of points, $K =$ number of clusters,
    $I =$ number of iterations, $d =$ number of attributes
Evaluating K-means Clusters

• Most common measure is the *Sum of the Squared Error* (SSE)
  – For each point, the error is the distance to the nearest cluster.
  – To get SSE, we square these errors and sum them.
  – Given two clusters, we can choose the one with the smallest error.
  – One easy way to reduce SSE is to increase K, the number of clusters.
    • A good clustering with smaller K can have a lower SSE than a poor clustering with higher K.
Two different K-means Clusterings

Original Points

Optimal Clustering

Sub-optimal Clustering
Importance of Choosing Initial Centroids

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Importance of Choosing Initial Centroids

Iteration 1

Iteration 2

Iteration 3

Iteration 4

Iteration 5

Iteration 6
Importance of Choosing Initial Centroids …
Importance of Choosing Initial Centroids …
Problems with Selecting Initial Points

- If there are K ‘real’ clusters then the chance of selecting one centroid from each cluster is small.
  - Chance is relatively small when K is large
  - If clusters are the same size, n, then

\[
P = \frac{\text{number of ways to select one centroid from each cluster}}{\text{number of ways to select } K \text{ centroids}} = \frac{K!n^K}{(Kn)^K} = \frac{K!}{K^K}
\]

- For example, if K = 10, then probability = 10!/1010 = 0.00036
- Sometimes the initial centroids will readjust themselves in ‘right’ way, and sometimes they don’t
- Consider an example of five pairs of clusters
10 Clusters Example

Iteration 4

Starting with two initial centroids in one cluster of each pair of clusters
10 Clusters Example

Starting with two initial centroids in one cluster of each pair of clusters

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10 Clusters Example

Starting with some pairs of clusters having three initial centroids, while other have only one.

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10 Clusters Example

Starting with some pairs of clusters having three initial centroids, while other have only one.
Solutions to Initial Centroids Problem

• Multiple runs
  – Helps, but probability is not on your side

• Bisecting K-means
  – Not as susceptible to initialization issues

• Sample and use hierarchical clustering to determine initial Centroids

• Select more than K initial centroids and then select among these initial centroids
  – Select most widely separated

• Post-processing
Handling Empty Clusters

- Basic K-means algorithm can yield empty clusters
- Several strategies
  - Choose the point that contributes most to SSE
  - Choose a point from the cluster with the highest SSE
  - If there are several empty clusters, the above can be repeated several times.
Updating Centers Incrementally

• In the basic K-means algorithm, centroids are updated after all points are assigned to a centroid.

• An alternative is to update the centroids after each assignment.
  – May need to update two centroids
  – More expensive
  – Introduces an order dependency
  – Never get an empty cluster
  – Can use “weights” to change the impact
Pre-processing and Post-processing

• Pre-processing
  – Normalize data so distance computations are fast.
  – Eliminate outliers

• Post-processing
  – Eliminate small clusters that may represent outliers
  – Split ‘loose’ clusters, i.e., clusters with relatively high SSE
  – Merge clusters that are ‘close’ and that have relatively low SSE
  – Can use these steps during the clustering process
    • ISODATA
Bisecting K-means

• Bisecting K-means algorithm
  – Variant of K-means that can produce a partitional or a hierarchical clustering

1: Initialize the list of clusters to contain the cluster containing all points.
2: repeat
3:   Select a cluster from the list of clusters
4:   for $i = 1$ to number_of_iterations do
5:     Bisect the selected cluster using basic K-means
6:   end for
7:   Add the two clusters from the bisection with the lowest SSE to the list of clusters.
8: until Until the list of clusters contains $K$ clusters
Bisecting K-means Example
Limitations of K-means

• K-means has problems when clusters are of differing
  – Sizes
  – Densities
  – Non-globular shapes

• K-means has problems when the data contains outliers.

• One solution is to use many clusters.
  – Find parts of clusters, but need to put together.
Limitations of K-means: Differing Sizes

Original Points

K-means Clusters
Limitations of K-means: Differing Density

Original Points

K-means Clusters
Limitations of K-means: Non-globular Shapes

Original Points

K-means Clusters

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Overcoming K-means Limitations

Original Points

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K-means Clusters