

Introduction to Symbolic and Statistical NLP in Scheme

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Optimization Clustering

- Given a clustering criterion
 - How to find a partition into n groups that optimizes the criterion?
- Find all possible partitions and calculate their value of the given criterion.
- Choose the partition with the optimal value.

Vector Space Modeling

- Contextual vectors (distributional model):

$$\mathcal{X} = \begin{bmatrix} \mathbf{x}_{1,1} & \mathbf{x}_{1,2} & \cdots & \mathbf{x}_{1,d} \\ \mathbf{x}_{2,1} & \mathbf{x}_{2,2} & \cdots & \mathbf{x}_{2,d} \\ \vdots & & & \\ \mathbf{x}_{k,1} & \mathbf{x}_{k,2} & \cdots & \mathbf{x}_{k,d} \end{bmatrix}$$

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Optimization Clustering

- K-means generates
 - k number of disjoint clusters (non-hierarchical)
 - globular clusters (spherical, elliptical, convex)
- properties:
 - numerical
 - unsupervised
 - iterative

Optimization Clustering

- K-means
 - k clusters
 - At least one element per cluster
 - No overlapping clusters
 - Non-hierarchical

Optimization Clustering

- K-means
 - Every member of a cluster is closer to its cluster than to any other cluster
 - Procedure

Optimization Clustering

- K-means
 - Initial partitioning of data set into k clusters
 - For each data point: calculate distance to each cluster
 - If one data point is closer to another cluster, relocate it
 - Repeat until no further relocations possible

Optimization Clustering

- K-means advantages
 - For large number of variables it is faster than hierarchical algorithms (for small k 's)
 - Tighter clusters than hierarchical clustering, if cluster are globular

Optimization Clustering

- K-means disadvantages
 - Initial set of k clusters can affect the result
 - Does not work well with non-globular clusters

Optimization Clustering

- K-means example

Individual	Variable 1	Variable 2
1	1.0	1.0
2	1.5	2.0
3	3.0	4.0
4	5.0	7.0
5	3.5	5.0
6	4.5	5.0
7	3.5	4.5

Optimization Clustering

- Initial 2 clusters on the basis of the most distant individuals:

	Individual	Mean Vector
Group 1	1	(1.0, 1.0)
Group 2	4	(5.0, 7.0)

Optimization Clustering

- Initial clustering of all remaining individuals:
 - For every other individual:
 - * Calculate Euclidean distance to the centroid of every cluster
 - * Assign individual to cluster
 - * Recalculate centroid for every cluster

Optimization Clustering

- Mean vector or centroid (with coordinates x_1 to x_n) with equal weight coordinates:

$$\bar{x} = \frac{\sum_{i=1}^n x_i}{n} \quad (1)$$

Optimization Clustering

- Mean vector or centroid example for $x = \{(3, 5), (7, 9)\}$, i. e. $n = |x| = 2$:

$$\begin{aligned} \bar{x} &= \frac{\sum_{i=1}^2 x_i}{2} = \frac{(3, 5) + (7, 9)}{2} = \\ &= \frac{(3 + 7, 5 + 9)}{2} = \left(\frac{10}{2}, \frac{14}{2}\right) = (5, 7) \end{aligned}$$

Optimization Clustering

- Initial clustering of all remaining individuals:

	Group 1		Group 2	
	Individual	Mean Vector	Individual	Mean Vector
Step 1	1	(1.0, 1.0)	4	(5.0, 7.0)
Step 2	1, 2	(1.3, 1.5)	4	(5.0, 7.0)
Step 3	1, 2, 3	(1.8, 2.3)	4	(5.0, 7.0)
Step 4	1, 2, 3	(1.8, 2.3)	4, 5	(4.3, 6.0)
Step 5	1, 2, 3	(1.8, 2.3)	4, 5, 6	(4.3, 5.7)
Step 6	1, 2, 3	(1.8, 2.3)	4, 5, 6, 7	(4.1, 5.4)

Optimization Clustering

- Initial partitions and clustering criterion:

	Individual	Mean Vector	Sum of SQR error
Group 1	1, 2, 3	(1.8, 2.3)	6.84
Group 2	4, 5, 6, 7	(4.1, 5.4)	5.38
total			12.22

Optimization Clustering

- Error = for every point distance to centroid
 - Criterion: the smaller the sum of square errors, the better the cluster
- Two dimensional Euclidean distance:

$$\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} \quad (2)$$

Optimization Clustering

- Error = for every point distance to centroid
- N -dimensional Euclidean distance, with p_i and q_i the coordinates for p and q in dimension i :

$$\sqrt{\sum_{i=1}^N (p_i - q_i)^2} \quad (3)$$

Optimization Clustering

- Optimization Iteration:
 - Compare each individual's distance to its own mean with distance to the opposite group mean.
 - If distance to the mean in opposite group is smaller, relocate the individual.
 - Calculate the sum of square errors, if smaller than before, this is an improvement.

Optimization Clustering

- Distance to means:

Individual	distance to mean 1	distance to mean 2
1	1.5	5.4
2	0.4	4.3
3	2.1	1.8
4	5.7	1.8
5	3.2	0.7
6	3.8	0.8
7	2.8	1.1

Optimization Clustering

- Subsequent partitions and new clustering criterion:

	Individual	Mean Vector	Sum of SQR error
Group 1	1, 2	(1.3, 1.5)	0.63
Group 2	3, 4, 5, 6, 7	(3.9, 5.1)	7.9
total			8.53

- Decrease of clustering criterion (from 12.22 to 8.53).

Optimization Clustering

- Remember:

- *k-means* or *k-nearest neighbors* is a fast and efficient algorithm.
- You have to know how many clusters you are looking for.
- Specific cluster shapes will not be discovered.