Data Mining Programming Assignment 1: Subspace Clustering

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1 ORCLUS

We decided to implement the ORCLUS algorithm. ORCLUS is a spin on k-means which utilizes eigensystems to adapt the distance measure to non axis parallel correlation clusters.

We picked this algorithm because the paper is easy to read and contains good pseudocode which is of utmost importance when trying to actually implement the described algorithm.

Furthermore, since k-means was the first clustering algorithm we studied, it will forever have a special Gaussian-shaped spot in our heart—which makes ORCLUS, as a spiritual successor, a natural choice.

1.1 Description and Pseudocode

The algorithm proceeds in rounds in which the dimensionality of the clusters and the number of clusters is gradually reduced. The rate at which this happens should not be too quickly, to which end the authors propose two parameters α and β and a relation between these two, by which one can be calculated from the other. They suggest an α of 0.5, which we've also adopted.

In each round, the algorithm undertakes an assignment step which is the same as in k-means. Every point is assigned to the closest centroid. However, as a next step, the eigenvectors

associated with the smallest spread are computed on a per cluster basis—the rationale behind this is that those vectors define a subspace in which the points cluster well, i.e. have a low contribution to the overall cluster energy. The cardinality of this vector set dictates the dimensionality of the subspace to which the points are projected.

To reduce the amounts of clusters—the algorithm starts with more seeds than requested by the user, we've chosen to start with 5 times as many as the authors offer no suggestions—a merging step is performed next. Although quite lengthy, this operation is pretty simple. The objective is to find pairs of clusters which can be merged such that the overall cluster energy stays low. For this, all pairs of clusters are examined, their centroid and energy computed and then the cluster-pairs with the lowest energy are picked to be merged, being careful to update all relevant data structures after each merge.

These three steps are repeated until the desired dimensionality and number of clusters are reached. After a final assignment step the clustering is returned.

1.2 Implementation

We chose to implement the algorithm in Python 3. The implementation is rather straight forward and only depends on NumPy and some functionality from Python's standard library.

Notably we use numpy.linalg.eigh to decompose the cluster matrices into eigenvalues and eigenvectors. We know PCA could also be used but online literature¹ suggests that the LAPACK routines utilized in NumPy's implementation of eigh perform a tiny sliver better than SVD, which we expect to be used in sklearn.decomposition.PCA. However, this probably would make no practical difference whatsoever.

The initial seeds are distributed using the kmeans++ initialization strategy.

2 Evaluation

 $^{^1}$ https://stackoverflow.com/questions/50358310/how-does-numpy-linalg-eigh-vs-numpy-linalg-svd