Improved Time-Series Clustering with UMAP dimension reduction method

Clément Péalat, Guillaume Bouleux, Vincent Cheutet
INSA Lyon, DISP EA4570

Time series clustering

Clustering is a classic unsupervised machine learning methods. The goal is to create clusters with elements of the datasets with similar behavior. The goal is then to maximize the similarities inside a cluster and to minimize it for elements outside this cluster.
Here, we are particularly interested by clustering of one-dimensional time series. It is a classic datatype that exists in various fields (financial, industrial, weather,...).

The main objective of this work is to determine the efficiency of UMAP as a pre-processing step for clustering algorithm.

UMAP : Uniform Manifold Approximation and Projection

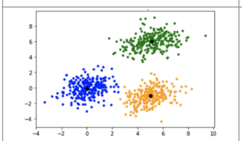
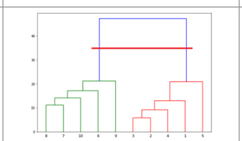
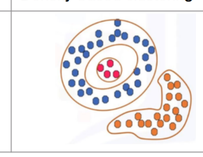
UMAP [2] is a recent reduction of dimension method. It was made mainly for visualisation of high dimensional data.

From a dataset, it starts by construct a graph G where each vertex is an element of the dataset. Then, the edges are degrees of membership. For an element Y, the m-th closest neighbor have an edge $\in [0, 1]$, with respect to the distance. Then, a Laplacian eigenmaps is used to create a graph G' of smaller dimension. From the cross-entropy between G and G', attractive and repulsive force are determined and a forced directed graph layout is computed. So, each vertex acts as a physical point under those two forces until a physical equilibrium is obtained. The cross-entropy is now minimized between the two graphs G and G'.
So, there is a few parameters for UMAP (as the number of neighbour). We decided to follow the advice on their website, to keep generic parameters for all databases.

As a reduction of dimension, UMAP can be used beforehand to clarify the data for clustering algorithm. However, there is still some theoretical controversies with UMAP. Indeed, by keeping the local structure, it can create pseudo groups that disturb clustering algorithm. In practice, we propose to apply UMAP with real data.

Clustering algorithms

To validate the efficiency of UMAP, we use three clustering algorithms. They are of three distinct types.

K-means : Centroid-based clustering	Hierarchic : Connectivity-based clustering	HDBSCAN : Density-based clustering
		

HDBSCAN [1] is a prolongation of DBSCAN. For both K-means and Hierachic, we need to know beforehand the number of clusters. To do so, we use the silhouette score. It calculates a score that gives the quality of the clustering. Small distance intra-clusters and high distance inter-clusters gives a small score. So, we apply those two clustering algorithms for multiple value of k and kept the number of clusters that minimzes the silhouette score.

Benchmark creation

For our benchmark, we used the databases available at UCR Time Series Classification Archive `www.cs.ucr.edu/~eamonn/time_series_data/`. 85 databases with labelled time series of same length were available. So, we applied the three clustering algorithms on those databases with and without UMAP beforehand. To compare the clustering results with the true labels, we use the v-measure score [3]. It is a similarity measure between two clustering results based on entropy. In the figure below, a summary of the construction of the benchmark is proposed.

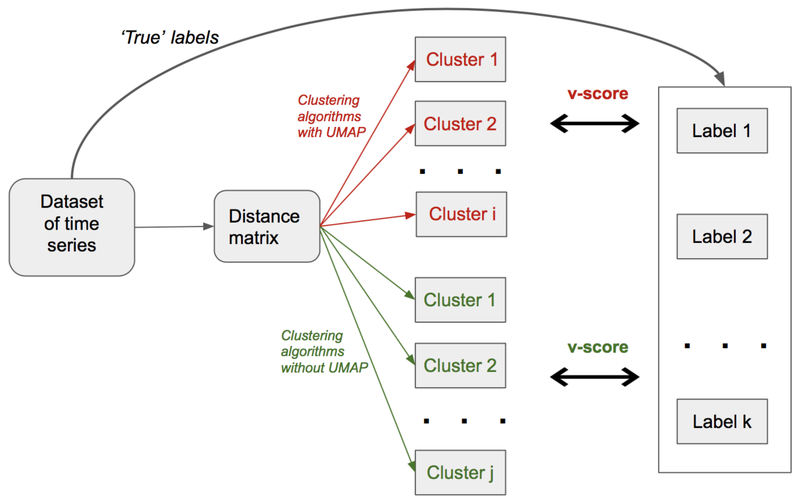


Fig. 1: Summary of the construction of our benchmark.

We used the euclidean distance on all databases. So, we had 6 clustering results with this distance for 85 databases.

We add also an other distance to complete the benchmark. For a given database, the time series are transformed in a trajectory matrix through a delay coordinate embedding (see figure below).

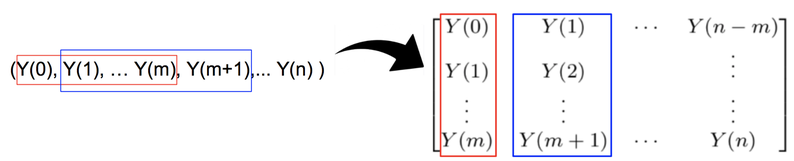


Fig. 2: Construction of the trajectory matrix.

Then, with a reduction of dimension and orthogonalization, the time series are seen as element of the Stiefel manifold : $V_{n,p} = \{A \in \mathbb{R}^{n\times p} : A^T A = Id\}$. The measure of similarity between two time series is then the geodesic (Principal angle) on this manifold. It is sufficient to apply the HDBSCAN and Hierarchic algorithms. However, for K-means, we need also the definition of a mean with respect to the geodesic : the Karcher mean.

Since the computation of the Karcher mean can be a bit long, we limitate this part of the benchmark on 6 databases of the UCR Time Series Classification Archive.

Results

We computed the average v-measure score obtained across the databases for all methods. The graph below represent the results on the 85 databases with the Euclidean distance.

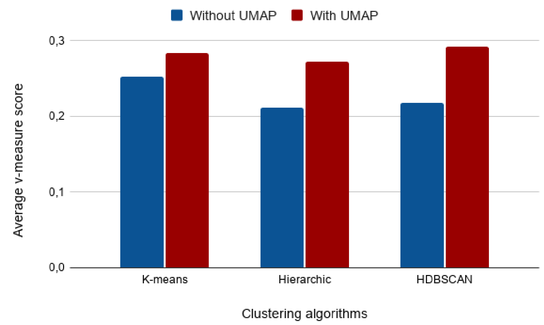


Fig. 3: Results with the Euclidean distance.

For all clustering algorithms, UMAP realizes an improvement : +11% for K-means, +29% for Hierarchic and +34% for HDBSCAN. Moreover, for 61% of the databases, K-means with UMAP is more accurate than K-means alone. It is 66% for Hierarchic and even 75% for HDBSCAN.
We find similar results with the geodesic on the Stiefel manifold. The three clustering algorithms are improved by UMAP, in particular HDBSCAN.

Discussion

Those results validate the use of UMAP for clustering even with the theoritical limits. Indeed, for all algorithms and distances, UMAP offers an improvement.
This is particuliarly true for HDBSCAN. It was expected since those two algorithms (UMAP and HDBSCAN) are based on the data density. UMAP+HDBSCAN is also the method with the best mean compared to the other clustering algorithms (with or without UMAP).
Moreover, we use generic parameters for UMAP. Indeed, it was not possible to optimize those parameters for each databases. So, there is still room for improvement according to the user's knowledge of the database.

Acknowledgements

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References

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