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PyCVI: A Python package for internal Cluster Validity Indices, compatible with time-series data

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Summary

PyCVI is a Python package specialized in internal Clustering Validity Indices (CVIs) compatible with both time-series and non time-series data.

Clustering is a task that aims at finding groups within a given dataset. CVIs are used to select the best clustering among a pre-computed set of clusterings. In other words, CVIs select the division of the dataset into groups that best ensures that similar datapoints belong to the same group and non-related datapoints are in different groups.

PyCVI implements 12 state-of-the-art *internal* CVIs to improve clustering pipelines as well as the Variation of Information (Meilă, 2003), a measure between clusterings that can be used as an *external* CVI. The *internal* qualifier here refers to the general case in practice where no *external* information is available about the dataset such as the true association of the datapoints with groups, as opposed to *classification* tasks.

Statement of need

There exist many mature libraries in python for machine learning and in particular clustering scikit-learn (Pedregosa et al., 2011), TensorFlow (Abadi et al., 2015), PyTorch (Paszke et al., 2019), scikit-learn-extra (*Scikit-learn Extra*, n.d.), and even several specifically for time series data: aeon (*Aeon*, n.d.), sktime (Löning et al., 2019), tslearn (Tavenard et al., 2020).

However, although being fundamental to clustering tasks and being an active research topic, very few internal CVIs are implemented in standard python libraries (only 3 in scikit-learn, more were available in R but few were maintained and kept in CRAN (Charrad et al., 2014)). This is despite the well-known limitations of all existing CVIs (Arbelaitz et al., 2013), (Gagolewski et al., 2021), (Gurrutxaga et al., 2011), (Theodoridis & Koutroumbas, 2009) and the need to use the right one(s) according to the specific dataset at hand, similarly to matching the right clustering method with the given problem. A crucial step towards developing better CVIs would be an easy access to an implementation of existing CVIs in order to facilitate larger comparative studies.

In addition, all CVIs rely on the definition of a distance between datapoints and most of them on the notion of cluster center.

For non-time-series data, the distance between datapoints is usually the euclidean distance and the cluster center is defined as the usual average. Libraries such as scipy, numpy, scikit-learn, etc. offer a large selection of distance measures that are compatible with their main functions.

For time-series data however, the common distance used is Dynamic Time Warping (DTW) (Berndt & Clifford, 1994) and the barycenter of a group of time series is then not defined as the usual mean, but as the DTW Barycentric Average (DBA) (Petitjean et al., 2011). Unfortunately, DTW and DBA are not compatible with the libraries mentioned above.

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PyCVI then tries to fill that gap by implementing 12 state-of-the-art internal CVIs: Hartigan (Strauss & Hartigan, 1975), Calinski-Harabasz (Calinski & Harabasz, 1974), GapStatistic (Tibshirani et al., 2001), Silhouette (Rousseeuw, 1987), ScoreFunction (Saitta et al., 2007), Maulik-Bandyopadhyay (Maulik & Bandyopadhyay, 2002), SD (Halkidi et al., 2000), SDbw (Halkidi & Vazirgiannis, 2001), Dunn (Dunn, 1974), Xie-Beni (Xie & Beni, 1991), XB* (Kim & Ramakrishna, 2005) and Davies-Bouldin (Davies & Bouldin, 1979). Then, in PyCVI their definition is extended in order to make them compatible with DTW and DBA in addition to non time-series data. PyCVI is entirely compatible with scikit-learn, scikit-learn-extra, aeon and sktime, in order to be easily integrated into any clustering pipeline in python. To ensure a fast a reliable computation of DTW and DBA, PyCVI relies on the aeon library.

Example

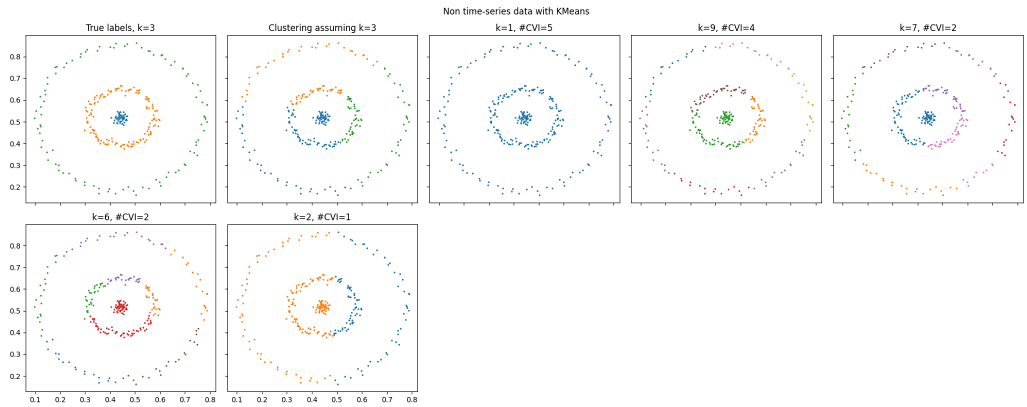

Figure 1: KMeans clustering on non time-series data, all implemented CVIs.

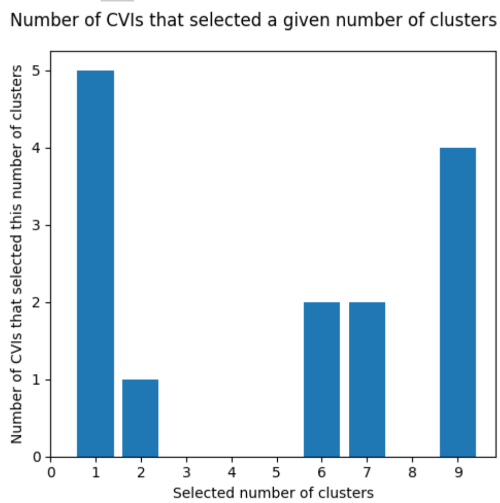

Figure 2: KMeans clustering on non time-series data, selected number of clusters according to all implemented CVIs.

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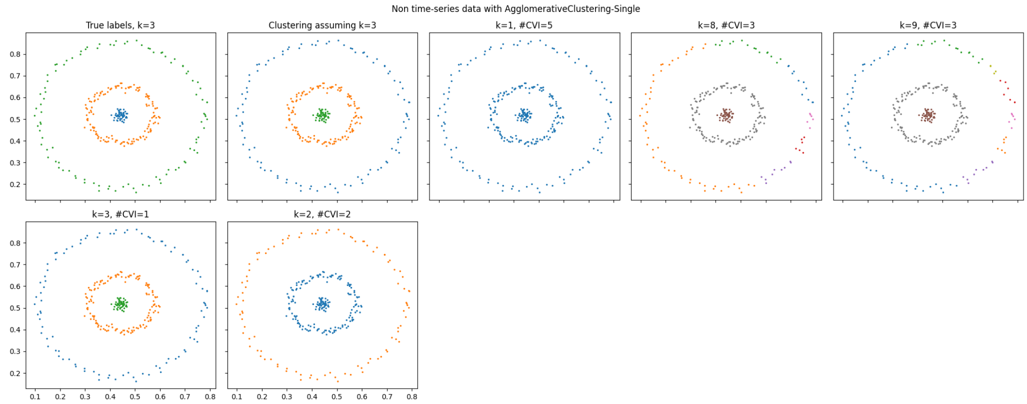

Figure 3: Agglomerative clustering on non time-series data, all implemented CVIs.

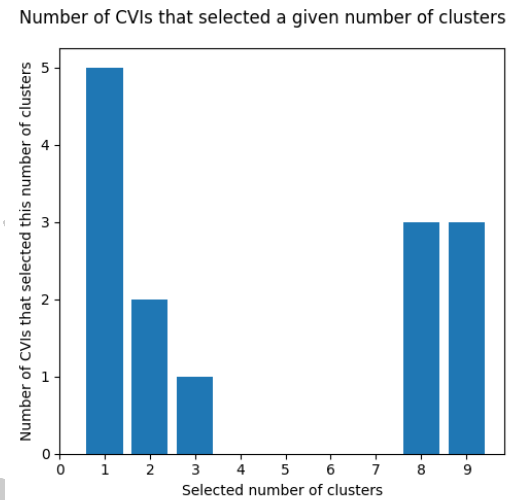

Figure 4: Agglomerative clustering on non time-series data, selected number of clusters according to all implemented CVIs.

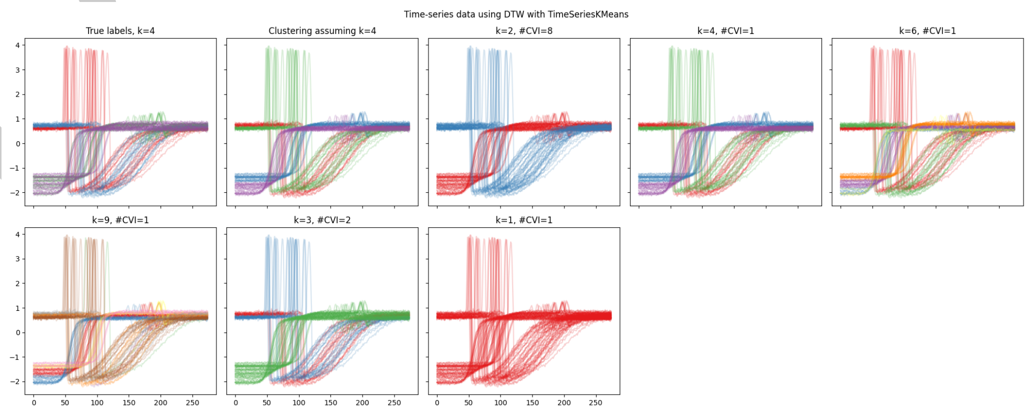

Figure 5: KMeans clustering on time-series data, with DTW, all implemented CVIs.

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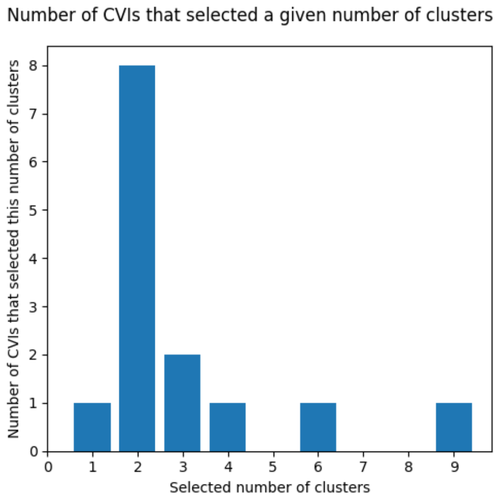

Figure 6: KMeans clustering on time-series data, with DTW, selected number of clusters according to all implemented CVIs.

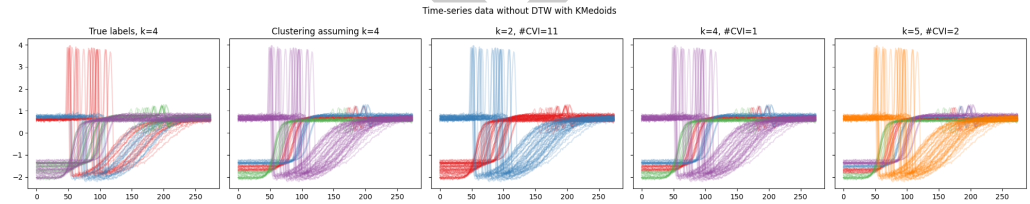

Figure 7: KMedoids clustering on time-series data, without DTW, all implemented CVIs.

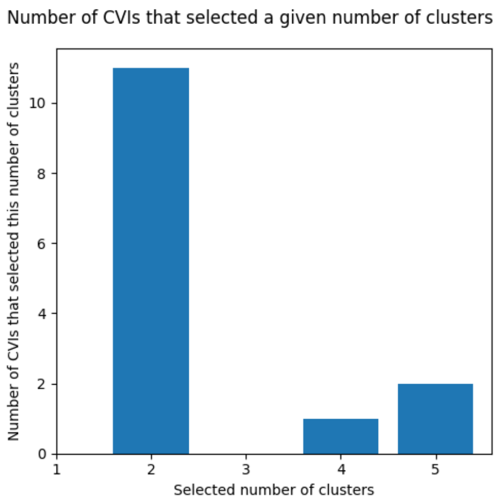

Figure 8: KMedoids clustering on time-series data, with DTW, selected number of clusters according to all implemented CVIs.

We experimented on 3 different cases: non time-series data (Barton, 2015), time-series data (Dau et al., 2018) with euclidean distance and time-series data with DTW and DBA as distance measure and center of clusters.

For each case, we used a different clustering method from a different library: KMeans (Lloyd, 1982) and AgglomerativeClustering (Ward, 1963) from scikit-learn, TimeSeriesKMeans from aeon and KMedoids ("Partitioning Around Medoids (Program PAM)," 1990) from scikit-learn-extra in order to give examples of integration with other clustering libraries. Then, for each case, we ran all the CVIs implemented in PyCVI, selected the best clustering according to each CVI and plotted the selected clustering.

Finally, we computed the variation of information (VI) between each selected clustering and the true clustering (second plot of all figures). A large variation of information there indicates a poor clustering quality due to the clustering method. In Figure 1 and Figure 3, we can see the difference of quality when assuming the correct number of clusters between the AgglomerativeClustering and the KMeans clustering method on the non time-series data. Therefore, when the quality of the clustering selected by the CVI is poor it can then either be due to the clustering method or the CVI, hence the necessity of robust evaluation pipeline for both clustering methods and CVIs.

The code of this example is available on the GitHub repository of the package, as well as on its documentation.

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