Arbitrary Shaped Clustering Validation on the Test Bench

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Keywords: Machine Learning, Unsupervised Learning, Clustering, Clustering Validation, Arbitrary Shaped Clusters.

Abstract: Clustering is a highly important as well as highly subjective task in the field of data analytics. Selecting a suitable clustering method and a good clustering result is all but trivial and needs insight into not only the field of clustering, but also the application scenario, in which the clustering is utilized. Evaluating a single clustering is hard, especially as there exists a wide variety of indices to evaluate the quality of a clustering, both for simple convex and for arbitrary shaped clusterings. In this paper, we investigate the ability of 11 state-of-the-art Clustering Validation Indices (CVI) to evaluate arbitrary shaped clusterings. To this end, we provide a survey of the intuitive workings of these CVI and an extensive benchmark on newly generated datasets. Furthermore, we evaluate both the Euclidean distance and the density-based DC-distance to quantify the quality of arbitrary shaped clusters. We use the generation of novel datasets to evaluate the influence of a number of metafeatures on the CVI.

1 INTRODUCTION

Clustering is a well known field in machine learning with many application areas. The objective of clustering is to partition a collection of objects into multiple groups of somehow similar objects. However, as the notion of similarity differs across application settings, there exists a wide variety of algorithms complying with these different notions of similarity.

One way to view clusters is by defining a centroid of each cluster and assigning each object to the most similar centroid, which leads to convex clusters and is a very popular choice with algorithms like k*Means* (McQueen, 1967) or k*Center* (Lim et al., 2005). Another view of clusters is to view them as an area with a high density of objects, where this area can have a varying shape. This so-called density-connectivity view considers objects which are connected over dense areas as part of the same cluster. This view lead to algorithms like DBSCAN (Ester et al., 1996), Optics (Ankerst et al., 1999) and HDBSCAN (Campello et al., 2015). Multiple other views of clusterings exist, including hierarchical (Ward Jr, 1963) or fuzzy (Ruspini et al., 2019) clusterings, which will not be part of this paper. As these different notions are hard to compare, it is challenging (i) to find a singular "best" clustering (von Luxburg et al., 2012) and (ii) to evaluate the "goodness" of a clustering, even under clear assumptions.

A plethora of Clustering Validation Indices (CVIs) has been engineered to value the goodness of a density-connectivity based clustering. However, many of these works lack in a comparison with other CVIs following the same notion (Bayá and Granitto, 2013; Liu et al., 2013; Moulavi et al., 2014; Hu and Zhong, 2019; Rojas Thomas and Santos Peñas, 2021) or with a very limited selection (Xie et al., 2020; Guan and Loew, 2022; Şenol, 2022). Even in recent works, which aim at a comparative evaluation of CVIs (Schlake and Beecks, 2024b), the lack of controlled high-dimensional datasets makes it difficult to find meaningful qualitative findings on the existing CVIs. These findings might facilitate to identify weak spots in state-of-the-art CVIs, enabling the design and engineering of customized CVIs and also the selection of a suitable CVI for a given dataset, yielding to potentially better clustering results. By making use of a novel dataset generator like the recently proposed *Densired* (Jahn et al., 2024), it is possible to specifically design datasets with different metafeatures and to evaluate the impact of these datasets on the different CVIs. In this paper, we will thus investigate 11 different CVIs, 8 of which are specifically designed for density based clusterings, and elucidate how these CVIs react to a change in different metafeatures like the number of clusters, dimensions, the ratio of out-

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Schlake, G. S., Beecks and C.
Arbitrary Shaped Clustering Validation on the Test Bench.
DOI: 10.5220/0013495500003967
In *Proceedings of the 14th International Conference on Data Science, Technology and Applications (DATA 2025)*, pages 363-373
ISBN: 978-989-758-758-0; ISSN: 2184-285X

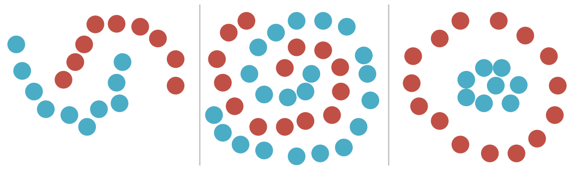


Figure 1: Three different datasets, which can be clearly split to two clusters, which are however not findable using convex algorithms.

liers or overlaps between clusters. To this end, we focus on simple interpretability and comparability of the individual CVIs and abstract from many implementation details so as to provide a guide for data scientists and practitioners alike.

2 RELATED WORK

Clustering is a very prominent field of unsupervised learning. A dataset of multiple objects is split into different groups, which contain similar objects. Both the notion of similarity and the idea, how to split the dataset are highly subjective and depend on the desired clustering and the use case (von Luxburg et al., 2012). For this reason, apart from a wide variety of distance or similarity functions, there exists a plethora of clustering algorithms. These clustering algorithms are designed to find vastly different clusterings. If we focus just on the shapes of the resulting clusterings (and ignore other areas of clustering like hierarchical structures (Ward Jr, 1963), fuzzy clusterings (Ruspini et al., 2019) or different subspaces (Parsons et al., 2004)), we can see two different groups of clustering algorithms.

The first group consists of algorithms creating convex datasets, mostly by defining cluster medoids and assigning objects to the cluster of the closest medoid. This group contains important and widely used algorithms like k*Means* (McQueen, 1967), k*Medoids* (Kaufman and Rousseeuw, 1990) or k*Center* (Lim et al., 2005). These algorithms are mostly fast and generate easily interpretable clusterings, where each cluster is a convex region and can be seen as a voronoi cell in the space of the used distance metric. However, these algorithms struggle in finding the correct clustering, if the clusters are not arranged in convex forms like the datasets depicted in Figure 1.

This is the reason, a second group of clustering algorithms exists, the density-connectivity based algorithms like *DBSCAN* (Ester et al., 1996), *OPTICS* (Ankerst et al., 1999) and *HDBSCAN* (Campello et al., 2015). These algorithms have no fixed idea of the shape of the dataset, but are based on a constant minimal density in the clusters. This means, that every object in a cluster has at least a minimum amount of other elements of the same cluster in the proximity. This way, these algorithms can generate clusters based on the dense regions and adapt to their shape.

As different clustering algorithms and different notions of clusterings exist, it is hard to compare the "goodness" of two clustering solutions. However, evaluating clusterings can be important in scenarios like Automated Clustering (Schlake and Beecks, 2023; Schlake and Beecks, 2024a; Schlake et al., 2024) or in different pipelines (von Luxburg et al., 2012). For this reason, a number of *Clustering Validation Indices* (CVIs) exists. Like the clustering algorithms, these CVI have different notions of a good clustering, so there cannot be one objectively best CVI for any situation. While there exists a number of surveys, these are either dated (Halkidi et al., 2001; Deborah et al., 2010), done on a small set of datasets and without in depth evaluation (Hassan et al., 2024) or lack qualitative insight into different metafeatures of datasets (Schlake and Beecks, 2024b).

This lack of qualitative studies might be connected to the problem of generating non-convex high dimensional datasets. While high-dimensional dataset generators are known and easily available (e.g. multiple in scikit-learn (Pedregosa et al., 2011)), these generating arbitrary shaped clusters is seldom. While a few generators can generate such datasets (Gan and Tao, 2015; Li and Zhou, 2023), none of them can guarantee that the datasets are not linearly separable. For this reason, we make use of the dataset generator *Densired* (Jahn et al., 2024), which complies with the aforementioned properties.

Earlier in this section, we reckoned the similarity or distance between objects to be of importance when generating a clustering solution. While the distance between objects like the points in Figure 1 can easily be represented by the Euclidean distance or other Minkowski distances, more complex objects required more intricate distances like the Signature Quadratic Form Distances (Beecks et al., 2010) for signatures or Dynamic Time Warping (Berndt and Clifford, 1994) for time series. While these distances enable the (dis)similarity quantification of complex objects, there also exist distances to change the overall notion of a distance, like the DC-distance (Beer et al., 2023). This distance is designed to incorporate the density-connectivity concept in the distance computation, enabling different algorithms or CVI to work with the notion of density-connectivity, even if this is not part of their original design.

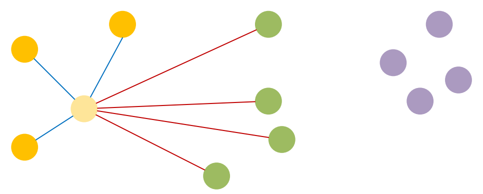


Figure 2: Exemplary Silhouette computation of the light yellow element. The (blue) distances between the light yellow element and the other yellow elements are used to compute the Compactness, while the (red) distances to the elements of the green cluster are used for the Separation. The elements of the purple cluster are not used for this Silhouette.

3 METHODS

As we aim for an intuitive overview, we will describe and (mostly) illustrate the intuition for the different CVI. For mathematical details, we refer the reader to the original papers or to our previous paper (Schlake and Beecks, 2024b) for a survey of all these CVI with consistent mathematical formulations and information on the complexity of the approaches.

3.1 Reference CVI

We do not only investigate CVI for arbitrary shaped clusters, but also a few "classical" CVIs as baseline models. These are not designed for arbitrary shaped clusters and will likely deliver worse results than specialised measures.

3.1.1 Silhouette Coefficient

A well known measure for clustering validation is the *Silhouette Coefficient* or *Silhouette Width Criterion* (SWC) (Rousseeuw, 1987). In this criterion, a *Silhouette* is computed for every object. These silhouettes are averaged to get a result for the complete dataset. To get the silhouette of an object, the average distance of said object to other objects of the same cluster is used as *Compactness*, while the *Separation* is the average distance to objects in the next different cluster. The difference between these values, normalized by the bigger of both, is used as Silhouette. The values for the SWC can range between -1 and 1, where a high value means a good clustering, as the Separation is much higher than the Compactness. An example of the computation of the SWC can be seen in Figure 2.

3.1.2 VRC

The *Variance Ratio Criterion* or *Calinski Harabasz Index* (Caliński and Harabasz, 1974) is also a well known baseline index, where the dispersion between groups and within groups is measured. The VRC cannot be adapted to use any distance functions, so it is only usable on a limited set of problems.

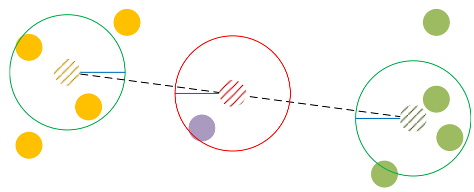


Figure 3: Exemplary computation of the D_bw for S_Dbw. The hatched yellow and green elements represent the medoids of their corresponding clusters, while the red hatched elements marks the mid between these points. The circles around these elements have the radius of *stdev*.

3.1.3 S_Dbw

The last baseline CVI investigated in this paper is *Scattering-Density between* (S_Dbw) (Halkidi and Vazirgiannis, 2001). In this approach, the *density between clusters* (D_bw) and the *Scattering* for the whole clustering are added to generate a value, where both values should be small. The Scattering is measured as the average standard deviation of all clusters divided by the standard deviation of the complete dataset, whereas the density between clusters is measured by dividing the density of objects in the midpoint between two clusters by the higher density of both clusters midpoints. The density of objects is in this CVI the number of objects closer than *stdev*, the average standard deviation of all clusters. An example for this can be seen in Figure 3.

3.2 MST Based

Multiple CVI are generated using a *Minimum Spanning Tree* (MST) of the data. This MST is a graph connecting all objects in the dataset while minimizing the total weight of the edges, where the weight of an edge between two objects corresponds to their similarity. An MST should - in case of a good clustering - connect elements of the same cluster and should have only very limited edges between objects of different clusters (in the optimal case the number of clusters, as all clusters need to be connected, but no edge between two clusters should be shorter than the shortest edge in a cluster). An MST automatically adapts to the shape of the dataset and hence is apt to help measuring arbitrary shaped clusterings.

3.2.1 DBCV

The density-connectivity based method of this paper is the *Density Based Clustering Validation* (DBCV) (Moulavi et al., 2014). The first important

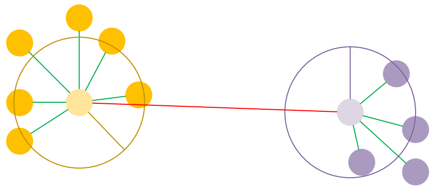


Figure 4: An example for the MRD between the light yellow and the light purple object. The circles around the object represent the core distance of each object based on the (green) similarity to objects in the same cluster. As the (red) distance between both objects is bigger, this distance is dominating the MRD.

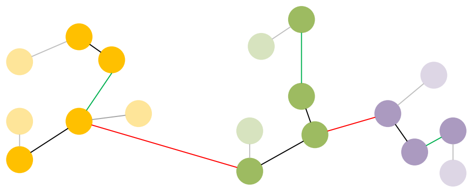


Figure 5: An example of the computation of the DBCV. The Sparsity per cluster is depicted as the green edge in each cluster. The light gray edges are not part of this computation, as they connect to border objects. The red edges represent the Separation between two clusters as the minimum distance between objects of these. The lighter coloured objects are excluded as those are border objects.

step of this algorithm is to adjust the distance between two objects by first assigning a core distance to each object based on the density of other objects of the same cluster and secondly replacing the "normal" distance between two objects by the maximum of each objects core distance and the "normal" distance between those objects as Mutual Reachability Distance (MRD). As the core distance will be high for an object in a sparse region, this will raise the distance between objects in sparse regions, whereas it will have little effect in dense regions or for objects far apart. An example of this computation can be seen in Figure 4.

Using this MRD, an MST is build in each cluster, which is then pruned of its border object, which are only connected by a single edge. Now, the DBCV for each cluster is based on the *Sparsity*, the maximum edge of these MSTs and the *Separation*, which is the minimum distance of a non-border object to any non-border object of a different cluster. An example of this can be seen in Figure 5. To combine these, the Sparsity is deducted from the Separation and the result is normalized by the bigger of these numbers. The result for the complete clustering is the weighted average of each cluster.

3.2.2 IC-av

Intracluster average gap (IC-av) (Bayá and Granitto, 2013) is an approach penalizing clusterings with long distances on the shortest path on an MST between

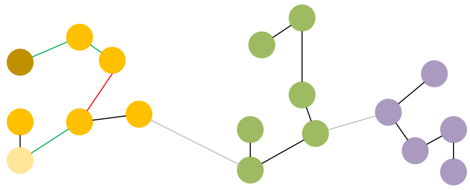


Figure 6: An example for the calculation for the path distance for IC-av of the light yellow and the dark yellow point. The green and red edges comprise the path between those objects. The red edge is used as distance between the objects, as it is the longest edge on the path. The weight of the green edges is shorter, so those are not taken into account for this distance.

two objects in the same cluster. The distance between two objects is measured as the longest distance on the shortest path between them. These distances are averaged to get the IC-av.

3.2.3 DCVI

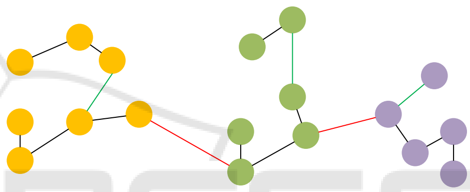


Figure 7: An example of the computation of the DCVI. The Compactness resembles the green edges, whilst the Separation resembles the red edges.

Density-core-based clustering validation index (DCVI) (Xie et al., 2020) is a similar measure to the DBCV, but without using a sophisticated reachability distance. The *Separation* of a cluster is measured as the minimal distance of an object in the cluster to an element in another cluster, whilst the *Compactness* is measured as the maximum edge weight in the MST of a cluster. The Compactness is divided by the Separation to gain each clusters value, which is averaged over all clusters.

3.2.4 CVDD

Another Approach is the *Cluster Validity index based on Density-involved Distance* (CVDD) (Hu and Zhong, 2019). Here, a density is generated based on the *k*-nearest Neighbors of an object and a density-connectivity distance is used. As this approach uses a wide variety of correcting factors deduced from the dataset, it is not possible for us to give more than the crudest intuition of this method in our given space, so we refer to the original paper for more information.

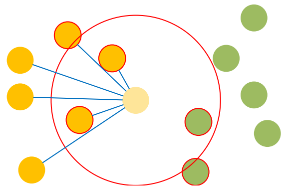


Figure 8: The Separation of the light yellow objects resembles the share of other clusters objects in its k nearest Neighbors, whilst for the compactness, every distances two objects in the same cluster (blue) are computed.

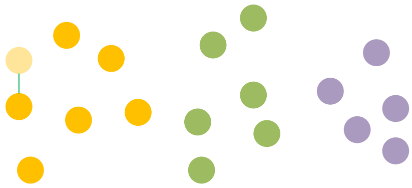


Figure 9: The local density of the light yellow objects for the CDR is its closest distance to another object of the same cluster, depicted by the green edge.

3.3 Other Methods

We use this umbrella subsection, to introduce a few other, unique CVI, which do not use MSTs to approximate the shape of the data.

3.3.1 CVNN

The *Clustering validation index based on nearest neighbours* (CVNN) (Liu et al., 2013) uses Nearest Neighbors for its notion of *Separation*, where the maximum Separation of a cluster is the average number of other clusters elements in the k-Nearest Neighbors of the clusters objects. The maximum Separation of any cluster is used as Separation for the clustering. The *Compactness* is measured as the average pairwise distance between two objects of the same cluster. An example for an object with $k := 5$ can be seen in Figure 8. In the end, Separation and Compactness of the clustering are added to retrieve the value. A slight variation of the weighting is found in (Halkidi et al., 2015), which we also investigate as *CVNN_hal*.

3.3.2 CDR

Another CVI is the *Contiguous Density Region* (CDR) index (Rojas Thomas and Santos Peñas, 2021). In this CVI, the local density is measured by the distance to the next object in the same cluster. The notion of the CDR is, that this local density should be very close the average density of the same cluster.

3.3.3 VIASCKDE

The *Validity Index for Arbitrary-Shaped Clusters Based on the Kernel Density Estimation* (VIASCKDE) (Şenol, 2022) is very similar to the SWC (see subsubsection 3.1.1). However, each object is valued by the weight of a *Kernel Density Estimation* of the dataset, meaning objects in more populated regions will have a higher weight.

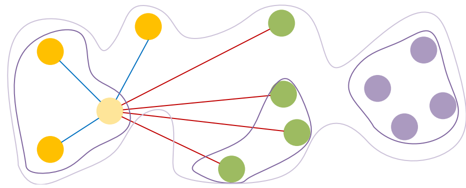


Figure 10: Exemplary VIASCKDE computation of the light yellow element. The (blue) distances between the light yellow element and the other yellow elements are used to compute the Compactness, while the (red) distances to the elements of the green cluster are used for the Separation. The elements of the purple cluster are not used for this Silhouette. The purple lines represent the isolines of the KDE, so that elements inside those lines will have a higher weight.

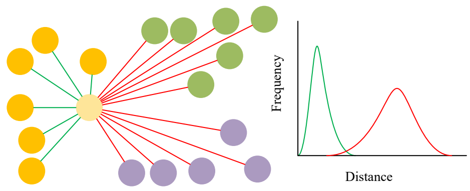


Figure 11: An illustration of the DSI computation. The (green) distances of the light yellow object to the other yellow objects are part of the inner cluster distances of the yellow cluster. The (red) distances to objects of the other clusters are part of the between cluster distances of the yellow cluster. The difference between these histograms (seen on the right) is used to calculate the DSI for the cluster.

3.3.4 DSI

In the *Distance-based Separability Index* (DSI) (Guan and Loew, 2022), the distances inside one cluster are compared to the distances to objects of other clusters. Instead of directly using the distances in the computations, two sets of distances are generated, comprising the inner-cluster and the between-cluster distances of one cluster. Then the difference between those histograms is computed to gain a value for this cluster. These values get averaged to retrieve a value for the complete cluster.

3.4 Used Distances

The notion of similarity used to compute the distance between two objects plays an important role in the evaluation of a clustering. Almost all presented methods are able to cope with different distance metrics without any problem. The exception are the VRC, which directly works on the vector representation of the objects, the S_Dbw, which needs a

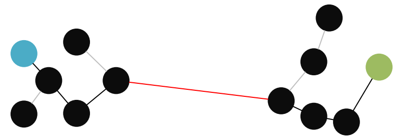


Figure 12: An illustration of the DC-distance computation between the blue and the green object. The edges depict the MST of the dataset. The gray edges are ignored, because they are not part of the path between both objects. The black edges are shorter than the red edge, which resembles the distance between both objects.

midpoint of clusters and between two objects and the VIASCKDE, which needs a KDE based on the distance between objects. We will investigate all other methods not only using the Euclidean distance, but also the *DC-distance* (Beer et al., 2023). The DC-distance measures the distance between two objects in a density-connectivity based fashion, so that using this distance function even classical CVI like the SWC should be able to find arbitrary shaped clusterings. Similar to the DBCV, every object is assigned a core distance, which is the distance to its μ nearest neighbor. It also uses a mutual reachability distance, where the MRD between two objects is the maximum of both objects core distance and their Euclidean distance. To find the DC-distance between two objects, an MST is build on the dataset using the MRDs. The distance is now the longest edge on the path between two points on this MST.

4 EXPERIMENTS

In this section, we will describe our experiments.[1] We will start with a description of the used datasets (subsection 4.1), before we will explain which algorithms were used to generate clusterings (subsection 4.2). To conclude this section, we will describe the setup used to generate our results (subsection 4.3).

4.1 Datasets

In order to generate valuable and qualitative results, we generate datasets using the *Densired* dataset generator (Jahn et al., 2024). This generator is capable of generating clusterings of arbitrary shapes, which are guaranteed to be density-connectivity separable and allows for a variety of parameters to be tuned. In addition to the parameters discussed in the following paragraphs, we set the parameters `safety` to False, which allows noise points to be generated next to or inside a cluster. For each parameterization, we created three datasets to prevent an influence of chance and to see the variance of the CVI in similar datasets. The actual values used for each test can be seen in Table 1.

Dimensionality. The first metafeature we tuned was the dimensionality. It is wide known, that real datasets can contain many dimensions. However, many arbitrary shaped, synthetical datasets are only two- or three-dimensional, so many evaluations of methods or even surveys like (Schlake and Beecks, 2024b) might be misled, if CVI perform especially well in the lower dimensional space. We used 5 dimensions as standard value in order to not prevent former mistakes of only investigating a low dimensional space, but also to not investigate too high dimensional spaces.

Number of Clusters. The number of clusters is another interesting metafeature of datasets. While some algorithms take information of all clusters into account, others only compare neighboring clusters. We change the number of clusters in the clustering to see, whether this leads to CVI scaling with the number of clusters. Our default will be 10 clusters.

Overlap Factor. Overlaps between clusters have been shown to be a problem for a number of density-connectivity based CVI (Schlake and Beecks, 2024b). In the generation of datasets, the separability between two clusters is guaranteed based on the Overlap factor. By lowering this value below 1, overlaps between two clusters can happen, which can lead to problems for some CVI. Our standard value will be 1.1, to ensure no overlaps for our standard tests.

Number of Connections. Another way to generate overlapping clusters is the existence of lower density bridges between two clusters. With this parameter, we can control, how many low linkage bridges exist between different clusterings. As standard, we will have no bridges between two clusters.

Noise Ration. Another very important factor is the ability to handle noise. While noise is occurring in almost all real world scenarios, many CVI are not able to handle it properly. For this reason, our standard noise ratio will be 0.

Number of Objects. Our last tests will be about the number of objects. As datasets tend to vary in size, we will use datasets in varying sizes. Our standard datasets will have the size of 5.000.

[1]Our implementation of the CVI can be found under https://github.com/g-schlake/ASCVI

Table 1: The different metafeatures, their respective parameters and the investigated values. The default value is printed in bold.

Metafeature	Parameter	Values
Dimensionality	`dim`	2, 3, **5**, 10, 20
Number of Clusters	`clunum`	2, 3, 5, **10**, 20
Overlap Factor	`min_dist`	0.5, 0.8, 0.9, 1, **1.1**, 1.2, 1.3
Number of Connections	`connections`	**0**, 1, 4, 8, 10
Noise Ration	`ratio_noise`	**0**, 0.05, 0.1, 0.2
Number of Objects	`data_num`	100, 500, 1.000, **5.000**, 10.000

4.2 Used Algorithms

To generate a number of clusterings, we use three different clustering algorithms, out of which one is partition-based and two are density-based.

The k*Means* (McQueen, 1967) algorithm is a very wide known algorithm to assign clusters based on centroids. This algorithm is not capable of finding arbitrary shaped clusters, but it is important to also include a partition based algorithm, as otherwise a lack of partition based results might lead to CVI choosing density based results, because they lack higher valued partition based alternatives. For the k Parameter, we used the values ranging between $\frac{\texttt{clunum}}{3}$ and $3 \cdot \texttt{clunum}$ and the implementation from (Pedregosa et al., 2011), so we had (mostly) 27 different values.

DBSCAN (Ester et al., 1996) is a widely known algorithm for density-connectivity based clustering, which is still in wide use today (Schubert et al., 2017). In this algorithm, objects with enough other objects in close proximity are regarded as core objects of a cluster and objects, which are close to these are part of the same cluster. We used the implementation from (Pedregosa et al., 2011), where we set `MinPts` to the even values in $[4,20]$ and `eps` to 100 equidistant values in the distances between the minimum and the maximum distance between two objects, resulting in theoretically up to 900 clusterings. However, as most of these are identical due to the very minor changes, only the differing ones (maximum 102 per Dataset) are considered.

An updated approach is *HDBSCAN* (Campello et al., 2015), which uses hierarchical properties to make a decision for a data scientist easier. We used the implementation in (McInnes et al., 2017), where we only tuned the `MinPts` parameter, which we set to the even values in $[4,20]$, resulting in 8 clusterings per dataset.

4.3 Experimental Setup

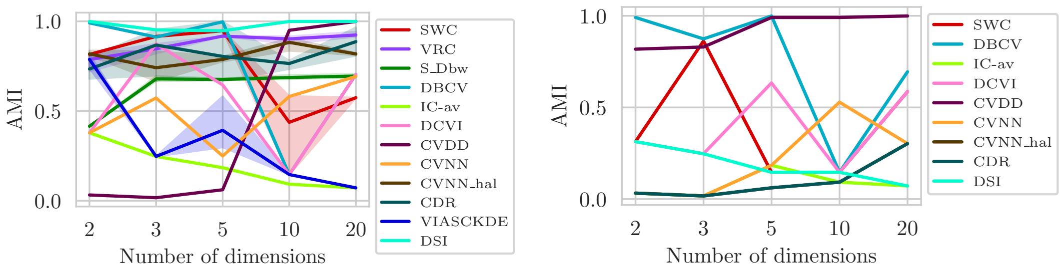
In order to evaluate our clusterings, we test how well they select a clustering resembling the ground truth of the dataset. Even though the clustering Problem in general is ambiguous (von Luxburg et al., 2012), we can assume that the ground truth of our generated datasets is what we are looking for, as it was generated and evaluated with the same notion of similarity and "good" clusterings. For every test, we have generated 3 datasets for each test value, which are then clustered using our three algorithms using the described parameters. Following this, we select the best cluster on each dataset for each CVI based on the value of the CVI. As not every CVI can process noise objects, we remove objects clustered as noise from the clustering and multiply the result of the clustering with a penalty term based on the share of noise in the dataset like described in (Schlake and Beecks, 2024b). Where possible, we also evaluated the clusterings using the DC-distance as distance function. As we have 3 datasets per test and value, we get 3 results per test, value and CVI, out of which we will mostly focus on the median. We will evaluate the quality of each clustering by measuring the *Adjusted Mutual Information* (AMI) (Nguyen et al., 2009) with the ground truth. As the AMI has no special considerations for noise, we will assign every noise object to its own, singleton cluster. This will prevent the AMI from confusing a cluster in one clustering with similar noise objects in the other clustering.

5 RESULTS

In the following section, we will present the results of our 6 tests. Every subsection will show the results of both used distances. We will start with the dimensionality (subsection 5.1) and number of clusters (subsection 5.2), before we will have a look at the overlap factor (subsection 5.3) and the number of connections (subsection 5.4). We will finish with the noise ratio (subsection 5.5) and the number of objects (subsection 5.6).

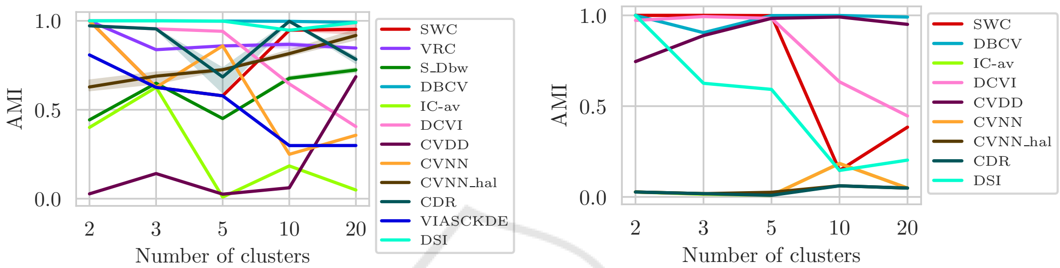
5.1 Dimensionality

When looking at the results at different dimensionalities, we see widely varying results in many datasets



(a) Euclidean. (b) DC-distance.

Figure 13: AMI per CVI using datasets of different dimensionalities. The thick line represents the median value on three datasets, while the shaded area is based on maximum and minimum value.



(a) Euclidean. (b) DC-distance.

Figure 14: AMI per CVI using datasets with a different number of clusters. The thick line represents the median value on three datasets, while the shaded area is based on maximum and minimum value.

(see Figure 13). When focusing on the Euclidean distance (Figure 13a), it can be seen that DSI, VRC, CVNN_hal and CDR seem to find good clusterings using all dimensionalities. IC-av and VIASCKDE struggle to evaluate the clusterings correctly in higher dimensional spaces. CVNN and DCVI have high variations between the different dimensionalities. The S_Dbw struggles in the two-dimensional case, but is constant in all the other dimensionalities. The SWC and the DBCV seem to deliver good results, but both have a negative outlier at 10 dimensions. It can be seen, that VIASCKDE, DCVI, SWC and CDR have different results for the different datasets and are quite sensitive to minimal changes.

When looking at the results using the DC-distance (Figure 13b), it can be seen that the CVDD delivers good results using all dimensionalities, whilst IC-av, CVNN, CVNN_hal, DSI and have struggles to find good clusterings. SWC, DBCV and DCVI have varying results.

5.2 Number of Clusters

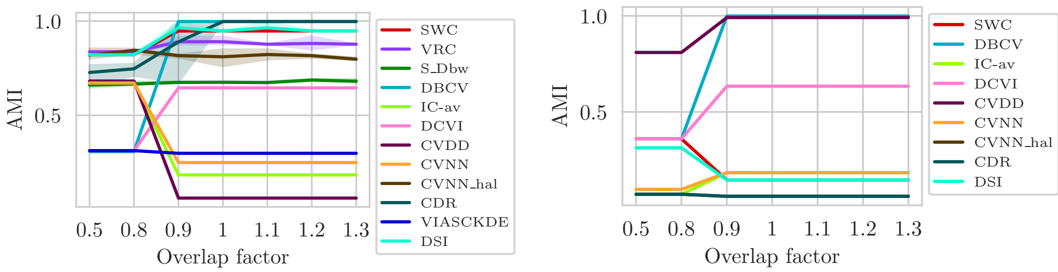
When looking at the varying number of clusters using the Euclidean distance (Figure 14a), it can be seen that DBCV, DSI and produce good clusterings regardless of the number of clusters. CVNN, VIASCKDE and IC-av work well for 2 and 3 clusters, but struggle to find good clusterings using more clusters. The SWC works well only for a high number of clusters. Similarly, the CVDD has low results on the most numbers of clusters but works well using 20 clusters. CVNN_hal seems to find better clusterings, the more clusters are in the ground truth.

Using the DC-dist, most algorithms seem to either find very good (SWC, DCVI, DBCV, CVDD) or very bad (CVNN, CVNN_hal, CDR, IC-av) clusterings with 5 or less clusters. The exception is DSI, which only fingds good clusterings with 2 clusters and struggles even from 3 on. The SWC and DCVI struggle, when there are more than 5 clusters present.

5.3 Overlap Factor

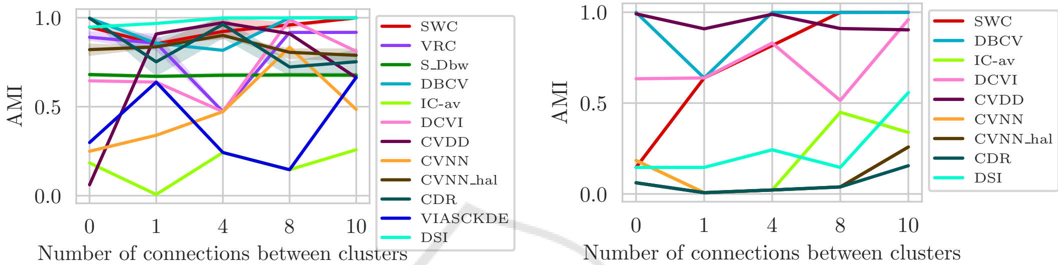
The only notable change in the CVI using the Overlap happens between 0.8 and 0.9. DBCV, DCVI, SWC and CDR produce much better results when there are no overlaps. CVDD, CVNN and IC-av produce their only good results if there are overlaps.

The trend is similar using the DC-distance. However, the SWC and CDR are producing better results with overlaps using this distance.



(a) Euclidean. (b) DC-distance.

Figure 15: AMI per CVI using datasets with different overlap factors. The thick line represents the median value on three datasets, while the shaded area is based on maximum and minimum value.



(a) Euclidean. (b) DC-distance.

Figure 16: AMI per CVI using datasets with a different number of connections. The thick line represents the median value on three datasets, while the shaded area is based on maximum and minimum value.

5.4 Number of Connections

When looking at the presence of connections between different clusters using the Euclidean distance (Figure 16b), it can be seen that this has little effect on S_Dbw, DBCV, DSI, SWC and CVNN_hal. However, more connections seem to lead to better results for CVDD, CVNN and VIASCKDE. VRC and DCVI have no general trend, but a relatively large drop at 4 connections.

Using the DC-distance (Figure 16a), you can see that the effect of the number of connections is much smaller. SWC, DCVI, DSI and IC-av have slight trend to find better clusterings with a higher number of connections between clusters. Apart from this, most CVI have a stable trend with little outliers.

5.5 Noise Ratio

When looking at the noise ratio using the Euclidean distance (Figure 17a), it can be seen that most algorithms (all apart from IC-av, S_Dbw, CVDD, VRC and CVNN_hal) have a massive drop in selecting the correct clustering when too many outliers are present. This drop happens earlier for the DSI than for the other methods.

Using the DC-distance (Figure 17b), the noise ratios chosen by us have little influence on the performance of the CVI.

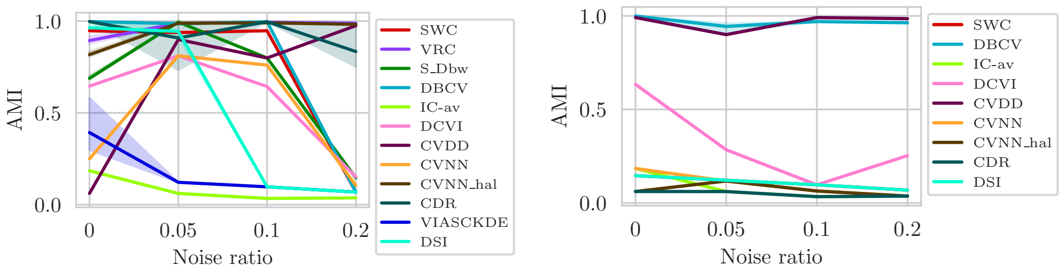
5.6 Number of Objects

When looking at the number of objects, you can see that most CVI stay constant using the Euclidean distance (Figure 18a), IC-av and CVNN show much better results using only a little number of object. The performance of CVDD has a general positive trend, but also has many negative outliers.

Using the DC-distance (Figure 14b), you can see that the SWC works better, the more objects are present.

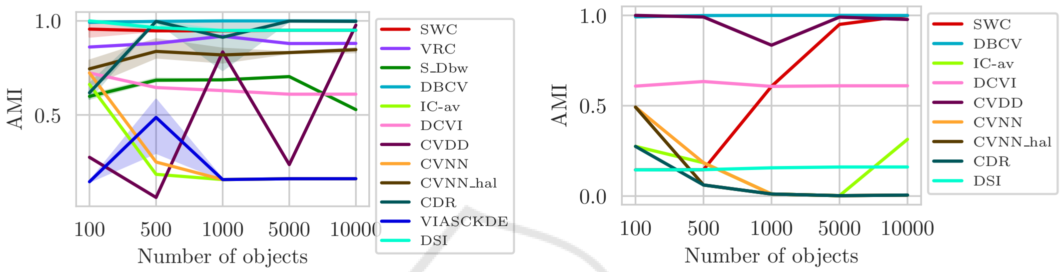
6 DISCUSSION

In this section, we will discuss our results and conclude our findings. We have seen that some CVI like CVDD work well in high dimensional cases or with many clusters and might have struggles in “easier” cases, which are similar to many well known benchmark datasets, explaining the poor results in previous surveys (Schlake and Beecks, 2024b). Of all CVI, the DBCV seems to work well in most scenarios, except for a high number of outliers, where CVNN_hal, CDR and CVDD perform better. Interestingly, CVNN, IC-av and CVDD perform better, when there are overlaps



(a) Euclidean. (b) DC-distance.

Figure 17: AMI per CVI using datasets with different noise ratios. The thick line represents the median value on three datasets, while the shaded area is based on maximum and minimum value.



(a) Euclidean. (b) DC-distance.

Figure 18: AMI per CVI using datasets of different sizes. The thick line represents the median value on three datasets, while the shaded area is based on maximum and minimum value.

between clusters. This might be interesting for further research. We also figured out that the combination of DC-distance and DBCV or CVDD will aptly find clusterings in all our scenarios.

However, our results have to be treated with some caveats. While we did investigate all these different factors in isolation, the combination of these factors might lead to completely different results. An investigation of all combinations of these properties is not possible due to their sheer numbers. The second big caveat is that the quality of these results is dependent on the quality of the Densired dataset generator. While many CVI have trends, which are expected or invariant and support the use of this dataset generator, some results are unexpected and unintuitive. Obviously, this might be due to an interesting behaviour of the corresponding CVI, but also some suboptimal generated datasets are possible. Another caveat is, that there is no possibility to measure the "arbitrary" of a clusterings shape. It is possible that some datasets actually contain partitioning based clusters, which would explain the good performance of the SWC. However, this unintuitively good performance matches the results of (Schlake and Beecks, 2024b), so that it could be, that there are some properties making the SWC better suited for arbitrary shaped data than known.

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