A simple iterative grid- and density-based Clustering Algorithm

Uwe Stöhr

Soloof EOOD, Sofia, Bulgaria
Email: research @ soloof.com
Project Page: https://codeberg.org/Soloof/Iteridense

Abstract

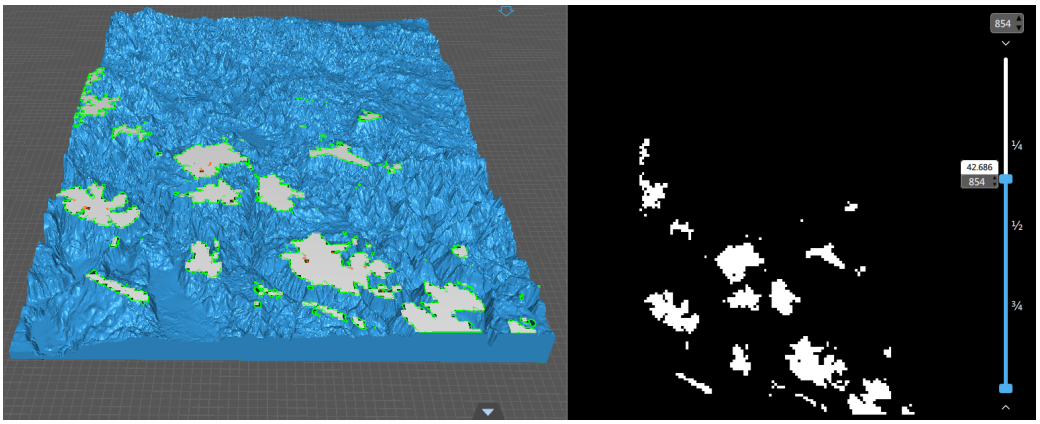
We introduce ITERIDENSE, an iterative clustering algorithm combining grid-based and density-based methods. It provides two possibilities to perform the clustering and for both it provides a clear path on how to change the algorithm's input parameters to achieve suitable results. We show that ITERIDENSE is applicable for data sets with any dimensionality. ITERIDENSE provides shorter computation times than pure density-based algorithms and that it performs clustering at least as good as the DBSCAN algorithm. We provide a reference implementation of ITERIDENSE as well as a stand-alone program with a graphical user interface.

1 Introduction

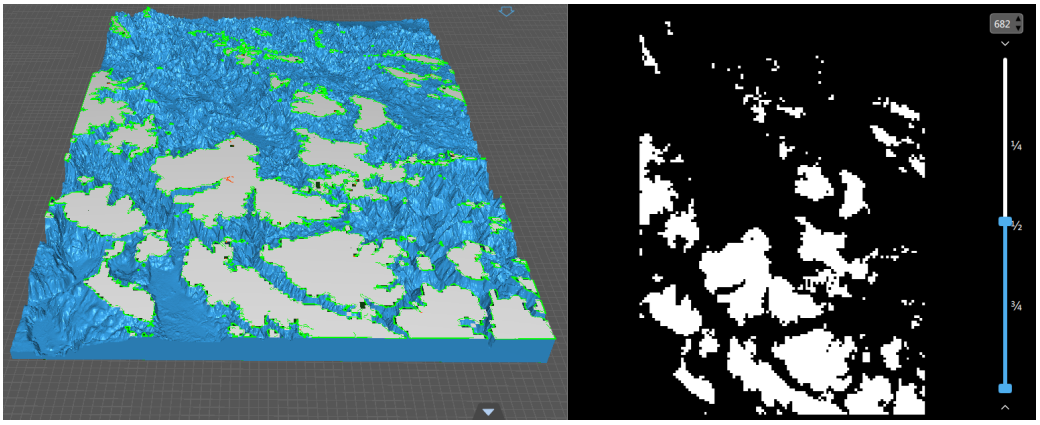
Density-based clustering algorithms have been proven useful for many practical applications. There exists a wide variety of algorithms, some optimized for particular use cases [1]. However, these algorithms have a major drawback – one needs to evaluate neighboring points for every data point in the data set to determine if it is part of a cluster. This is the case for most density-based clustering algorithms like PreDeCon [2] or HDBSCAN [3]. Other algorithms that combine grid-based with density-based methods like DENCLUE [4] or CLIQUE [5] don't have this drawback but make assumptions about the shape of the probability distribution of the data (what is the probability to find a data point inside the range of available data).

Another issue of many clustering algorithms is that as user there is no clear path on how to change the algorithm's input parameters to achieve a suitable clustering result. Taking for example the algorithm DBSCAN [6], it requires to specify the parameter ϵ, the maximum distance to another core point of a cluster. For many use cases there is no clear path on how to change ϵ to get a suitable result as we will also discuss in this paper.

The algorithm presented in this paper uses both, density-based and grid-based methods. Its main idea is to work with different probability-density functions of the data set and analyzing them in a grid. This approach makes it possible that even for small data sets in 2 dimensions the computation can be 10 times faster than a pure density-based algorithm like DBSCAN. Our algorithm follows an iterative approach to calculate the probability-density function and makes no assumptions about the shape of that function. Therefore it provides a clear path on how to set a start value of the algorithm's main parameter and how to change it to achieve a certain result.



(a) Cut at 2/3 of its maximal height.



(b) Cut at half of its maximal height.

Figure 1: Relief of a random geographic area cut at different heights.

2 Derivation of the Algorithm

The basic idea of the algorithm is how mountain peak areas are separated from each other in a geographical relief. Take for example the relief shown at the left in Fig. 1. To identify areas around a peak one cuts the relief at a desired height. The cut-off areas are then the mountain peak areas. For example in Fig. 1 (a) the relief was cut at about 2/3 of the maximal height leading to more than a dozen peak areas. In Fig. 1 (b) the relief was cut at about half the maximal size leading to larger areas. By decreasing the cutting height, the number of areas will become fewer unless at a zero height the whole relief area is part of a single mountain area.

Translating the relief height to the density of data points ρ, the cut is made at a certain ρ through the probability-density function of the data set. See also the section *Background and Motivation* of [1] for a similar visualization than in Fig. 1.

Detecting clusters by making a cut through the probability-distribution is state-of-the-art [1]. The novelty is how to generate the distribution and how to cut it. Instead of calculating a single probability-density function, we calculate different probability-density functions in an iterative process with increasing resolutions. Resolution means hereby into how many cells every dimension of the data set is divided to calculate the probability-density function. For every resolution a clustering of the cells is performed and one gets two results: the amount of clusters and the density of every cluster. Depending on the results, the algorithm is stopped, or it continues and calculates another probability-density function at a higher resolution.

We call our algorithm Iteridense (ITERative grID- and dENSity-based clustering). Based on our approach the key features of Iteridense are:

- The clustering works without the need to test neighbors of every data point, making the clustering more computation-efficient. The clusters are derived by counting the numbers of data points within a certain data area.
- One has two choices to stop the algorithm. Either one specifies ρ, the minimal density every found cluster must have to stop the algorithm, or **MinClusters**, the number of how many clusters should at least be detected (in that case the specification of ρ is not necessary). The possibility to specify **MinClusters** is a big advantage compared to pure density-based algorithms that by design cannot have this feature.
- For Iteridense ρ is defined being normalized so that the whole data set has $\rho = 1$. Because of the iteration with increasing resolutions our algorithm provides a clear path on how to set and change ρ: Start with a low $\rho > 1$ and increase ρ until you get a suitable result. The algorithm stops at a resolution that fulfills the specification of ρ. We will demonstrate this feature with an example in Sec. 4.2.

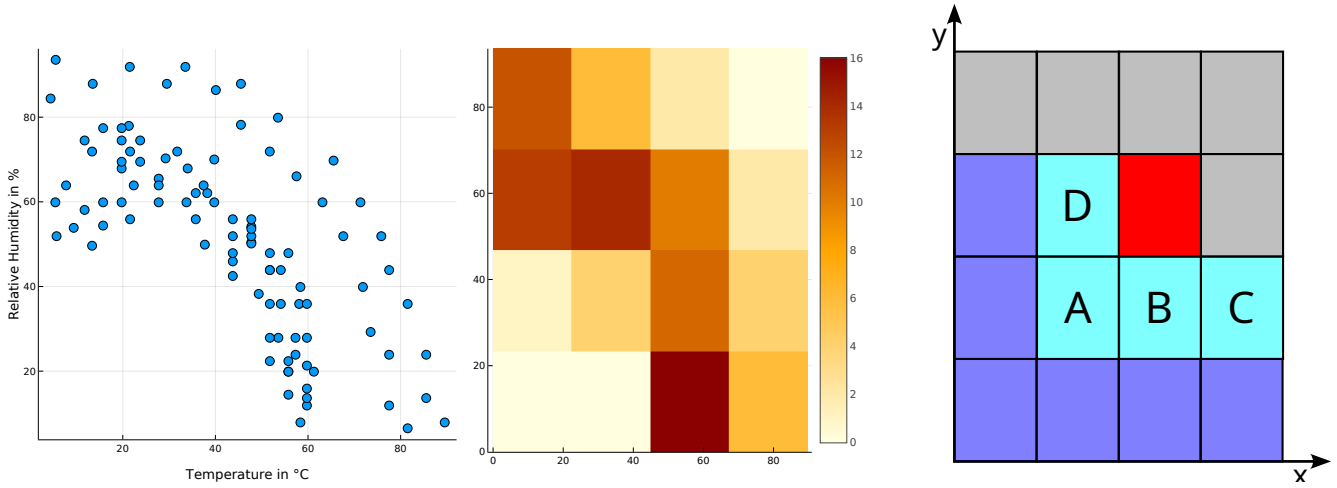
3 Description of the Iteridense Clustering Algorithm

3.1 Basic Algorithm

There are two possible input parameters to the algorithm, either to specify how many clusters should at least be detected (**MinClusters**) or the minimal data point density ρ to form a cluster. ρ is treated as a dimensionless number since the dimension of the data point space can be anything, depending on the source of the data points.

Fig. 2 (a) shows as example a 2-dimensional data set which represents the relative humidity and temperature of air inside a thermo-box after a certain chemical process. It looks like there might be a cluster of points inside an area in form of a quarter circle. To find that potential cluster Iteridense works on this data set the following way:

1) The space of the data set is divided into a grid of 4×4 cells. In our example the data range in dimension 1 "temperature" is $4 - 89\,°C$ and the range in dimension 2 "humidity" is $6 - 93\,\%$. These ranges define the space of the data set. As we divide into 4×4 cells, cell 1 covers the space of temperature range $4 - 25.25\,°C$ and humidity range $6 - 27.75\,\%$.
   A division into 4×4 cells is defined as a resolution of 4. A division into 5×5 cells would be a resolution of 5 and so on.
2) The number of data points in the cells are counted. The result is a count map as shown in Fig. 2 (b).
3) Now the actual clustering is performed. The evaluating scheme is depicted in Fig. 2 (c). Every cell is evaluated one after another first in x- then in y-direction. The most basic definition of a cluster is that a cluster consists of at least one cell that has at least 2 data points. Therefore, if a cell has more than 1 data point it could either be a sole cluster or part of a cluster. To decide this, its neighboring cells are evaluated. Thereby only those neighbors are evaluated that have already been evaluated (blue and light-blue in Fig. 2 (c)) because for them it is already known to which cluster they belong to.
   If none of the neighbor cells A – D are in a cluster, the current cell will start a new cluster. If any neighbor is in a cluster, the current cell will become part of that cluster. If neighbor cells are in different clusters, these clusters are merged and the current cell becomes part of that merged cluster. For example cell A and cell C could be in different clusters and the current cell unites both clusters.



(a) Data to be clustered.

(b) Count map generated in algorithm step 3.

(c) Clustering scheme of the count map.

Figure 2: Clustering process of ITERIDENSE. (a) Data to be clustered; (b) Count map generated in algorithm step 3 for resolution 4: 16 cells with the info how many data points are in.; (c) Clustering scheme of the count map. The red cell is the currently evaluated cell, the blue cells have already be evaluated, cells A – D are neighboring cells determining the clustering for the red cell.

4) The density of every cluster ρ_{cluster} is calculated as the number of points in the cluster divided by the number of cells in the cluster.

$$\rho_{\text{cluster}} = \frac{\text{num points in cluster}}{\text{num cells of cluster}} \tag{1}$$

To make ρ_{cluster} independent of the resolution, it has to be the normalized:

$$\rho_{\text{cluster norm}} = \frac{\text{num points in cluster}}{\text{num cells of cluster}} \cdot \frac{\text{total num of points}}{\text{total num of cells}} \cdot \frac{\text{dimension}}{2\,\text{resolution}^{\text{dimension}-2}} \tag{2}$$

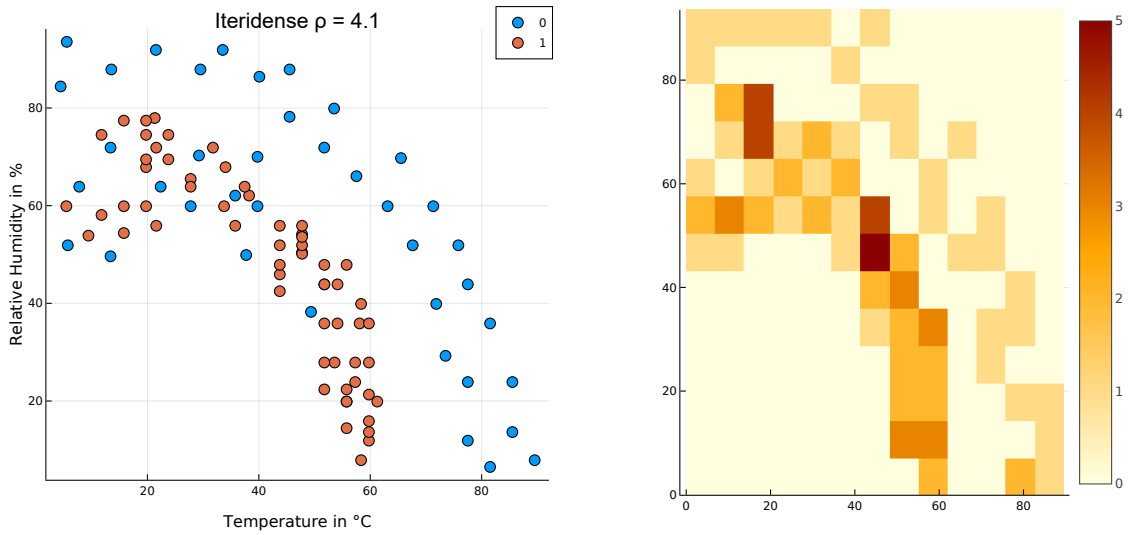
The normalization is derived in Sec. 3.3. For 2 dimensions the last term vanishes and $\rho_{\text{cluster norm}}$ describes by what factor the cluster is more dense than the whole data set.
The final density ρ_{final} is the minimum of all $\rho_{\text{cluster norm}}$.
(In the following ρ_{cluster} means $\rho_{\text{cluster norm}}$.)

5) All clusters are evaluated. Optionally clusters with ρ_{cluster} lower than a specified value will be deleted. If they contain fewer data points than a specified value, they are deleted as well. See the next section for a description of these optional settings. The result of this algorithm step is a set of clusters that are subsequently numbered.

6) The resolution is incremented by one and the steps 1 – 5 are repeated until either $\rho_{\text{final}} > \rho$ or until as many clusters were detected as specified as **MinClusters**. To assure that the steps are not repeated forever, the loop is stopped if the resolution reaches the total number of points in the data set. The resolution reached at the end of this step is the final resolution.

7) All data points are assigned according to the found clusters. Points in cluster "0" are hereby not part of a cluster.

8) Due to the grid generated in step 1, single points might appear in the corner of a cell and are thus not detected as part of a cluster. Therefore steps 1 – 5 are repeated with the final resolution plus 1.



(a) Resulting data point assignment.

(b) Final count map (resolution 13).

Figure 3: Result of ITERIDENSE for the data shown in Fig. 2 (a) for $\rho = 4.1$.

9) Points that were before step 8 not part of a cluster but now are, are finally assigned to that cluster. This will only be done if the number of clusters did not change in step 8 and if no data point belongs now to another cluster than before step 8.

Fig. 3 shows the result for $\rho = 4.1$. In that case the final resolution is 13 and there is one cluster with $\rho_{\text{cluster}} = 4.3$. Note that this case is just an example for the algorithm. A suitable clustering result for this data set would probably be one with 2 clusters and we will discuss what "suitable" means later.

3.2 Optional Settings

The algorithm can optionally be modified this way:

1) Specification of the start resolution for step 1 (**StartResolution**). The default and minimum is 2, the maximum is the total number of points in the data set.
2) In step 3 don't take cells into account that are diagonally connected to the current cell (**NoDiagonals**). In Fig. 2 (b) cells A and C would then not be evaluated.
3) Specification of the minimal number of data points in a cluster (**MinClusterSize**). Clusters with less points will be erased. The default is 3, the minimum is 2, the maximum is the total number of points in the data set minus 1.
4) Specification of the minimal ρ_{cluster} of a cluster (**MinClusterDensity**). Clusters with lower ρ_{cluster} will be erased. The minimum and default is 1.0.
5) Specification of a resolution at which the loop step 1 – 5 is stopped (**StopResolution**).

Option 1 can speed up the computation significantly.

Option 2 can be useful for a low ρ (and thus low resolutions)[1] while for higher ρ and also high dimensions it might lead to bad results. Therefore this option should only be used if really desired.

1. For example with **NoDiagonals** in Fig. 3 with $\rho = 2.2$ the cluster would contain more points.

Option 3 is useful to exclude unsuitably small clusters. It is recommended to set **MinClusterSize** $\geq D+1$ where D is the dimensionality of the data set.

Option 4 has only an effect if **MinClusters** is used. It helps to sort out clusters with a density too low to be sensible for the use case.

Option 5 prevents undesired many loops. For example if ρ was set to a high value and no cluster will be found.

A reference implementation of ITERIDENSE in the programming language JULIA is online available [7]. Its outputs are the assignments of the points to clusters, the size of clusters, density of clusters, final resolution, number of clusters, the count map as tensor in the final resolution (the actual probability-density function) and a tensor like the count map but with information about what cluster a grid cell belongs to. There is also a stand-alone program available with a graphical user interface (GUI) that uses the reference implementation [8].

3.3 Density Normalization

To be able to use the cluster density in a useful way, it has to be normalized. The point is that without it, the density will increase with the increase of the resolution. We define ρ_{cluster} as:

$$\rho_{\text{cluster}} = \frac{\text{num points in cluster}}{\text{num cells of cluster}} \tag{3}$$

When the resolution doubles, ρ_{cluster} will increase because the cluster will keep its number of points but will have more cells. The ITERIDENSE algorithm requires ρ_{cluster} to be independent of the resolution. One approach would be to normalize ρ_{cluster} with the density of the whole data set

$$\rho_{\text{data set}} = \frac{\text{total num of points}}{\text{total num of cells}} \tag{4}$$

and we would then have

$$\rho_{\text{cluster norm}} = \frac{\rho_{\text{cluster}}}{\rho_{\text{data set}}}$$

This density is independent of the resolution but not on the dimension. In practice is is often a tricky question if more or less dimensions are applicable for the effect one wants to evaluate. By taking another dimension into account, the density would increase, even if the new dimension does not influence the cluster at all.

Take for example this case: $D = 1$, resolution $R = 8$, number of cells of cluster $C = R/4$ (C depends on R), number of points in cluster $P = 8$, total number of points $N = 16$. We get then $\rho_{\text{cluster}} = \frac{P}{C} = 4$, $\rho_{\text{data set 1D}} = \frac{N}{R} = 2$, $\rho_{\text{cluster norm 1D}} = \frac{PR}{CN} = 2$, so the cluster is in 1D 2 times more dense than the data set.

Now another dimension is added. Here we have to make assumptions how the number of data points change by this addition:

- we assume that for the 1D case we have 2 equal clusters that contain together all data points, so $N = 2P$
- we assume that every dimension adds 2 more of these clusters (like a hypercube gets 2 more facets with every dimension)

With this we have for 2D:

$$\rho_{\text{cluster}} = \frac{P}{C},\ \rho_{\text{data set 2D}} = \frac{2 \cdot 2 \cdot P}{R^2},\ \rho_{\text{cluster norm 2D}} = \frac{P \cdot R^2}{C \cdot 2 \cdot 2 \cdot P} = 8,$$

so the cluster is 8 times more dense than the data set and $\rho_{\text{cluster norm}}$ is 4 times the one for the 1D case. This is a problem because the idea of ITERIDENSE is that you can increase ρ to find clusters. The addition of a dimension would lead to the fact that one has to increase ρ drastically to find the same cluster. This makes the usage of ρ hard.

The solution is to preserve the $\rho_{\text{cluster norm}}$ of the 1D case to all greater dimensions using the assumptions we made for adding a dimension. That means we have to multiply $\rho_{\text{cluster norm}}$ with a correction factor γ that depends on the dimension. In our example γ would be 1/4.

ρ_{cluster} is independent of D, therefore γ only depends on $\rho_{\text{data set}}$. With our assumptions we have

$$\rho_{\text{data set}} = \frac{2D \cdot P}{R^D} \tag{5}$$

and

$$\gamma_{1D} = \frac{\rho_{\text{data set D}}}{\rho_{\text{data set 1D}}} = \frac{R \cdot 2D \cdot P}{2 \cdot PR^D} = \frac{D}{R^{D-1}} \tag{6}$$

and

$$\rho_{\text{cluster norm 1D}} = \rho_{\text{cluster norm}} \cdot \gamma_{1D} = \frac{P}{C} \cdot \frac{R^D}{2D \cdot P} \cdot \frac{D}{R^{D-1}} = \frac{R}{2C} \tag{7}$$

Since for $D = 1$ $C \propto R$, $\rho_{\text{cluster norm}}$ is independent of the dimension and the resolution.

However, this normalization will preserve the density from the 1D case. For most practical use cases, one starts with 2D. Therefore we normalize according to the 2D case:

$$\gamma_{2D} = \frac{\rho_{\text{data set D}}}{\rho_{\text{data set 2D}}} = \frac{R^2 \cdot 2D \cdot P}{4 \cdot PR^D} = \frac{D}{2R^{D-2}} \tag{8}$$

The final normalization is

$$\rho_{\text{cluster norm}} = \frac{\text{num points in cluster}}{\text{num cells of cluster}} \cdot \frac{\text{total num of points}}{\text{total num of cells}} \cdot \frac{\text{dimension}}{2\,\text{resolution}^{\text{dimension}-2}} \tag{9}$$

This normalization cannot cover all cases but keeps ρ_{cluster} stable enough for practical usage. To get a feeling about the stability we take the case $D = 2$, $R = 8$ and clusters with each $P = 8$ and $C = 2$, thus $\rho_{\text{cluster}} = 4$. We look at these 4 cases:

- 2 clusters, one at the upper right corner, the other one of the lower left corner of the data grid.
  - Now a new dimension is added which only adds a single new cluster of the same size. Then we have $\rho_{\text{data set 2D}} = \frac{2P}{R^2}$ and thus $\rho_{\text{cluster norm 2D}} = 16$. And for $D = 3$ we have $\rho_{\text{data set 3D}} = \frac{3P}{R^3}$ and thus $\rho_{\text{cluster norm 3D}} = 16$. So no change for $\rho_{\text{cluster norm}}$.
  - Now a new dimension is added which adds two new clusters of the same size. Then we have for $D = 3$ $\rho_{\text{data set 3D}} = \frac{4P}{R^3}$ and thus $\rho_{\text{cluster norm 3D}} = 12$. So $\rho_{\text{cluster norm}}$ increased by a factor 0.75. Without γ_{2D} it would have increased by a factor 4.

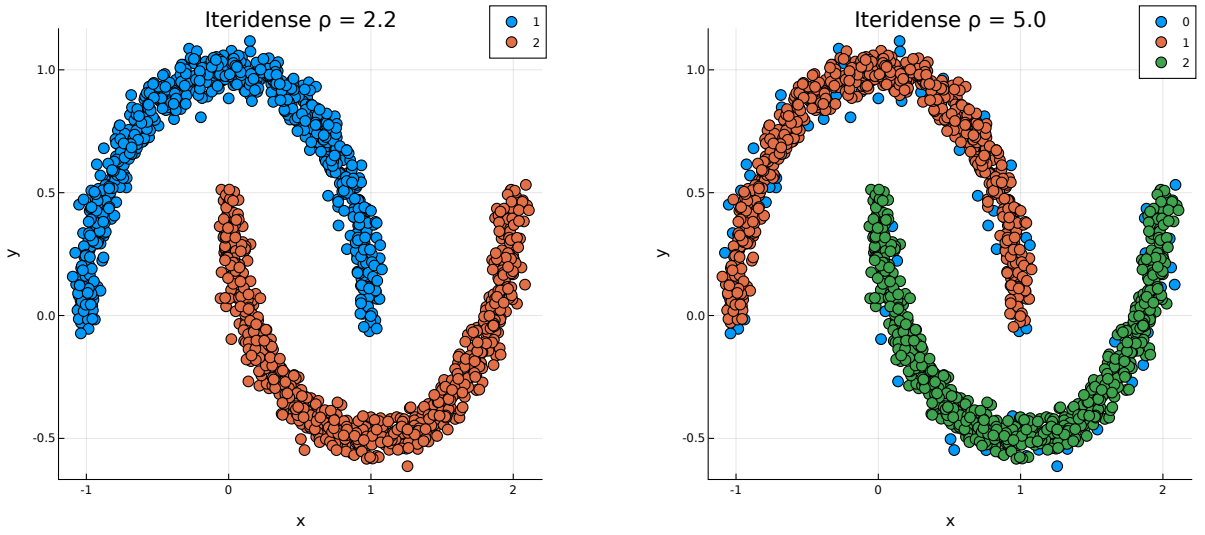
- 4 clusters at every corner of the data grid.
  - Now a new dimension is added which only adds a single new cluster of the same size. Then we have $\rho_{\text{data set 2D}} = \frac{4P}{R^2}$ and thus $\rho_{\text{cluster norm 2D}} = 8$. And for $D = 3$ we have $\rho_{\text{data set 3D}} = \frac{5P}{R^3}$ and thus $\rho_{\text{cluster norm 3D}} = 9.6$. So an increase of $\rho_{\text{cluster norm}}$ by a factor of 1.2. Without γ_{2D} it would have increased by a factor 6.4.
  - Now a new dimension is added which adds two new clusters of the same size. Then we have for $D = 3$ $\rho_{\text{data set 3D}} = \frac{6P}{R^3}$ and thus $\rho_{\text{cluster norm 3D}} = 8$. So no change for $\rho_{\text{cluster norm}}$.

4 Clustering Results

To show the clustering results artificial data was generated using the library *sklearn.datasets* from the scikit-learn project [9]. Real data were taken from the *Rdatasets* database [10]. The clustering results figures were created using the package *Plots* of the Julia programming language [11] and the GUI reference implementation for Iteridense that uses the component *TAChart* of the Lazarus Component Library [12].

4.1 Effect of the Density Parameter

The data shown in Fig. 4 and Fig. 5 was generated using the *make_moons* call to *sklearn.datasets*. Fig. 4 (a) shows the result for $\rho = 2.2$, Fig. 4 (b) shows the result for $\rho = 5.0$. As derived in Sec. 2, the greater the density, means (translated to the relief example) the area of the cluster gets smaller. Therefore less points are assigned to the clusters for $\rho = 5.0$.



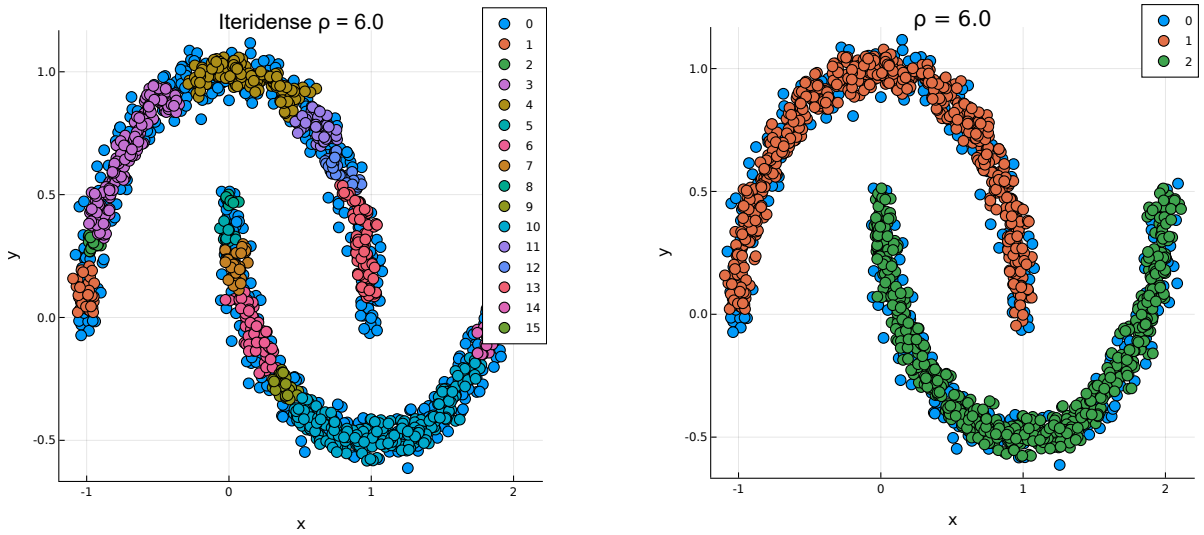
(a) $\rho = 2.2$, final resolution: 12

(b) $\rho = 5.0$, final resolution: 43

Figure 4: Result of Iteridense for intersected moon-like clusters using different ρ.

By increasing ρ one can for example define points as outliers: One could define that all data points that are not part of a cluster at density $\rho = 4.0$ are outliers. If the data points are the result of a measurement, one can repeat the measurement of an outlier point to verify if the result is still an outlier, check the measurement setup etc.

Fig. 5 shows the result for $\rho = 6.0$. The density is now so high that the moon-like clusters break down into many small clusters if the option **NoDiagonals** is used for the clustering.



(a) $\rho = 6.0$, **MinClusterSize** = 10 with option **NoDiagonals**, final resolution: 60

(b) $\rho = 6.0$, final resolution: 52

Figure 5: Effect of a high ρ and the option to evaluate neighbor cells.

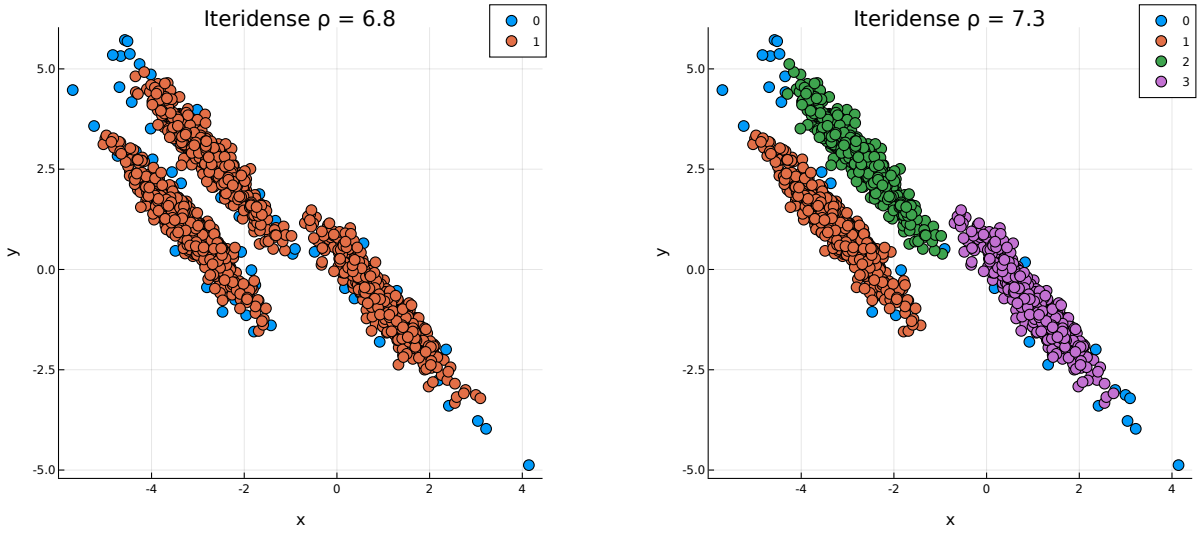
4.2 Clustering Performance

An advantage compared to other clustering algorithm is that ITERIDENSE treats all data points the same way. There is no separation between core points, border points or the like. Another major feature of ITERIDENSE is that it provides two ways to achieve results and a clear path for the user on how to change the input parameters to get a suitable result:

- Either start with a low ρ and increase it gradually to get a suitable result. If the result is not suitable, look at the resulting ρ_{cluster} and set for the next run ρ above their minimum.
- Or specify with **MinClusters** the desired number of clusters. If the result is not suitable, increase gradually either **MinClusterSize** or **MinClusterDensity**.

The second path is computationally the fastest, as discussed in the next section. However, it can only be taken if there is a physical or technical reason for the number of clusters. For the path to specify ρ Fig. 6 (a) – Fig. 7 (a) shows the results (with **MinClusterSize** = 6): Until $\rho \leq 6.8$ only one cluster is detected and starting at $\rho = 7.3$ there are 3 clusters. Increasing ρ leads to more and more clusters. This can be used to identify regions with higher density inside a "base" cluster. In the example there are 3 base clusters and every one has more dense regions that are unveiled with greater ρ.

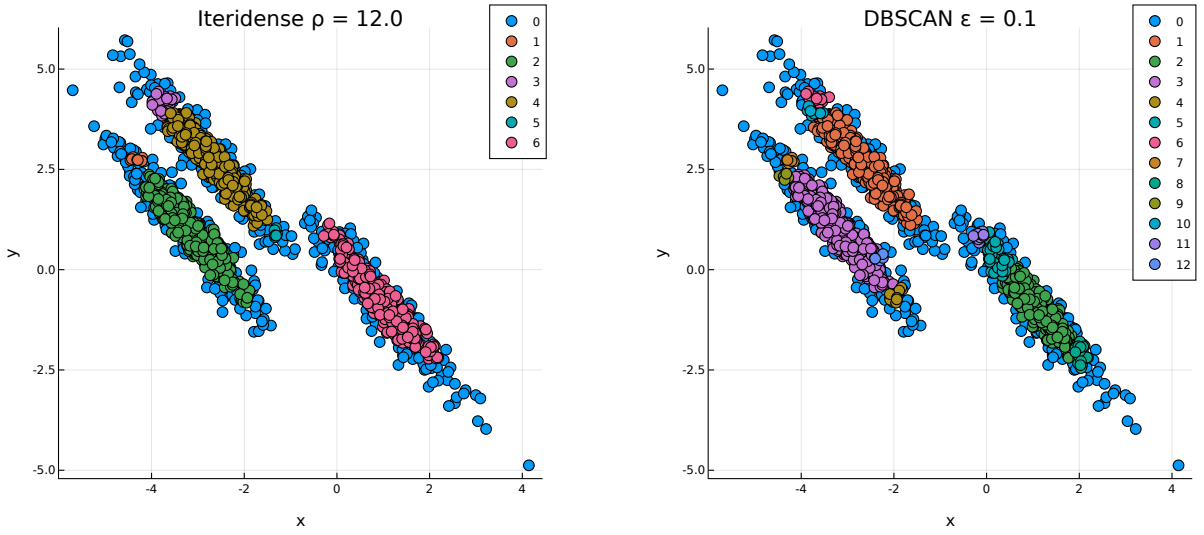
For comparison, the algorithm DBSCAN does not provide a clear path on how to change its input parameters. An example is the data shown in Fig. 7 (b). This data was generated using the *make_blobs* call to *sklearn.datasets* with a subsequent transformation. Like in the previous example, there are 1500 data points. $\epsilon = 0.1$ (the maximum distance to another core point of a cluster) seems to be a sensible start value for DBSCAN. The result is Fig. 8 (b). As the result is not a useful one might increase ϵ in small steps and gets with **MinPts** (minimal points to form a dense region) of 6 as results Fig. 8 – Fig. 9. For this data set a human would expect 3 base clusters but DBSCAN does not find exactly 3 clusters. One has to try different ϵ to get this result. For data in 2 or 3 dimensions one can plot the data to get a feeling for ϵ and for example increase **MinPts**. However, for data in higher dimensions this is hardly possible.



(a) $\rho = 6.8$, final resolution: 30

(b) $\rho = 7.3$, final resolution: 35

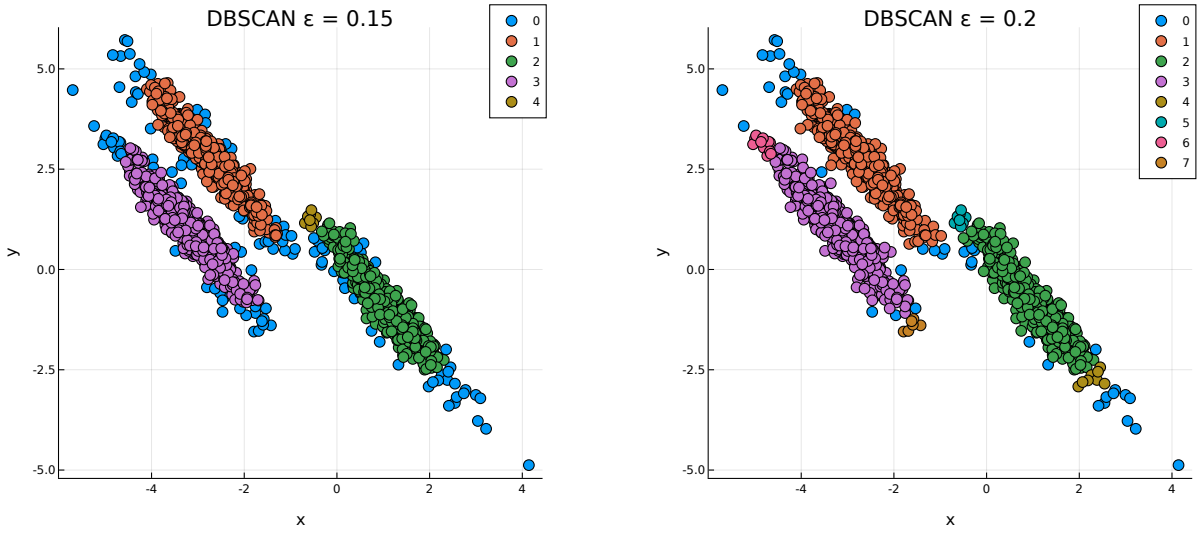
Figure 6: Result of ITERIDENSE for $\rho \geq 6.8$ at anistotope clusters.



(a) $\rho = 12.0$, final resolution: 68

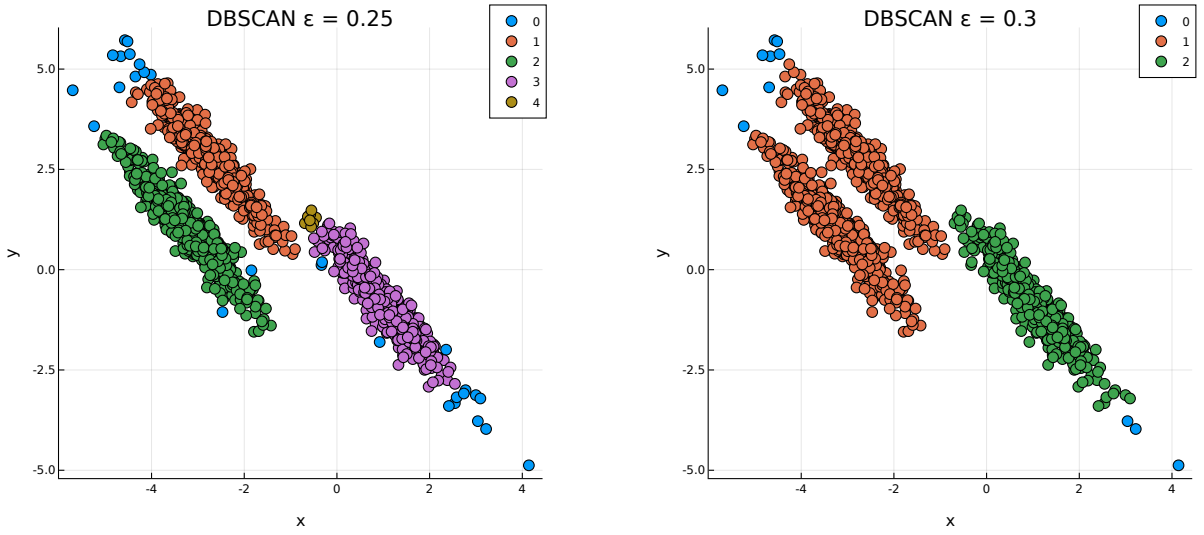
(b) $\epsilon = 0.1$

Figure 7: Result of ITERIDENSE for $\rho = 12.0$ and DBSCAN for $\epsilon = 0.1$ at anistotope clusters.



(a) $\epsilon = 0.15$ **(b)** $\epsilon = 0.2$

Figure 8: Result of DBSCAN at anistotope clusters with $\epsilon \leq 0.2$.



(a) $\epsilon = 0.25$ **(b)** $\epsilon = 0.3$

Figure 9: Result of DBSCAN at anistotope clusters with $\epsilon > 0.2$.

(a) MinClusters = 2 **(b) MinClusters** = 3 **(c)** $\rho = 4.0$, **MinClusterSize** = 50

Figure 10: Result of ITERIDENSE for clusters with different densities.

What is "suitable" depends on the application. For example the data shown in Fig. 10 consist also of 1500 data points. It was generated using the *make_blobs* call to *sklearn.datasets* with a subsequent transformation. One might see in the data 2 clusters and therefore set **MinClusters** to 2 and **MinClusterSize** to 20. As result one gets Fig. 10 (a). There cluster 1 has $\rho_{\text{cluster}} = 2.6$ and is a merge of a high- and a low-density region. This might not be suitable because one had the 2 dense regions in mind to form each a cluster. There are now two ways to change the result:

- Either set **MinClusters** to 3 to get two clusters with a high density and one with a lower density, see Fig. 10 (b).
- Or increase ρ and also increase **MinClusterSize** e.g. to 50 unless one gets only 2 high-density clusters, see Fig. 10 (c). Increasing **MinClusterSize** is hereby necessary to avoid small clusters in the low-density area.

The change of **MinClusterSize** might not be obvious when one cannot plot for example high-dimensional data. It is therefore a useful feature of the ITERIDENSE algorithm that for the case ρ_{cluster} is too low for a suitable result, one can increase **MinClusterSize** together with ρ.

4.3 Computation Performance

ITERIDENSE creates two tensors, the count tensor to could how many data points are in a cell and the cluster tensor that stores to what cluster a cell belongs to. Both tensors have the rank D whereas D are the dimensions of the data (or features). Each tensor has R^D entries (cells) whereas R denote the resolution. Therefore ITERIDENSE is memory-limited. This is an important point as this limits the practical usability.

To estimate the computational complexity $\mathcal{O}$ we look at the different steps:

Counting $\mathcal{O}(ND)$ because a computation is performed for every data point in every dimension

Clustering Every cell has B neighbor cells: $B = 3^D - 1$ (for the case that option **NoDiagonals** is used $B = 2D$). For the clustering we only evaluate $B/2$ of the neighbors. Therefore checking a neighbors has $\mathcal{O}\left(0.5BR^D\right) \approx \mathcal{O}\left(0.5\left(3R\right)^D\right)$.

Evaluation To evaluate how many clusters there are and now many cells they have, we need to step over all cluster tensor cells, therefore we have $\mathcal{O}\left(R^D\right)$ for this step

Assignment To assign the cluster number to every data point the complexity is $\mathcal{O}\left(N\right)$

Iteridense iteratively clusters with increasing $R = R_{\text{start}} \ldots R_{\text{final}} + 1$. Note that the assignment is only performed once for the final R. So we have these number of computes:

$$N + \sum_{R=R_{\text{start}}}^{R_{\text{final}}+1} \left(ND) + R^D \left(\frac{3^D}{2} + 1 \right) \right) \tag{10}$$

$$\approx N + \left(R_{\text{final}} + 1 - R_{\text{start}} + 1\right) ND + \frac{3^D}{2} \sum_{R=R_{\text{start}}}^{R_{\text{final}}+1} R^D \tag{11}$$

as approximation we can write

$$\sum_{R=R_{\text{start}}}^{R_{\text{final}}+1} R^D \approx \frac{\left(R_{\text{final}} + 1\right)^{D+1} - R_{\text{start}}^{D+1}}{D+1}$$

and we get

$$\mathcal{O} \rightarrow \mathcal{O}\left(N + \left(R_{\text{final}} - R_{\text{start}} + 2\right) ND + \frac{3^D \left(\left(R_{\text{final}} + 1\right)^{D+1} - R_{\text{start}}^{D+1} \right)}{2(D+1)} \right) \tag{12}$$

$$\mathcal{O} \approx \mathcal{O}\left(\left(R_{\text{final}} - R_{\text{start}} + 2\right) ND + 3^D \left(\left(R_{\text{final}} + 1\right)^{D+1} - R_{\text{start}}^{D+1} \right) \right) \tag{13}$$

In the naive approach, $R_{\text{start}} = 2$ as this is the lowest possible resolution we have

$$\mathcal{O}_{\text{worst case}} \approx \mathcal{O}\left(R_{\text{final}} ND + 3^D \left(R_{\text{final}} + 1\right)^{D+1} \right) \tag{14}$$

Table 1 lists $\mathcal{O}$ of different clustering algorithms.

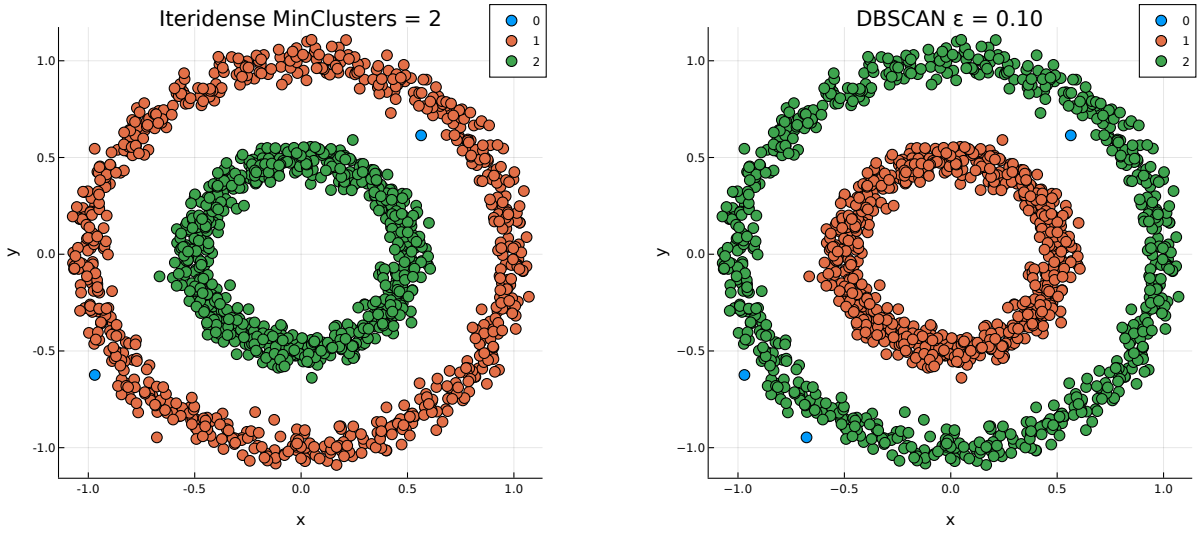
Table 1: Computational and memory complexity for different cluster algorithms.

Algorithm	Computational Complexity	note
Iteridense	$\mathcal{O}\left(DN\right)$	actually formula (13)
DBSCAN	$\mathcal{O}(DN \log N)$ to $\mathcal{O}\left(DN^2\right)$ [13]	$\mathcal{O}\left(DN^2\right)$ if brute force
DENCLUE	$\mathcal{O}(DN \log N)$ to $\mathcal{O}\left(DN^3\right)$ [14]	$\mathcal{O}\left(N^3\right)$ worst case for N iterations
K-Means	$\mathcal{O}(DN)$ [15]	

The data shown in Fig. 11 was generated using the *make_circles* call to *sklearn.datasets*.

In that case, there must be 2 clusters, therefore one can specify **MinClusters**. This will lead to a shorter computation as with the specification of ρ since the algorithm loop is stopped as soon as 2 clusters are detected, otherwise there might be further loops. For our example 10,000 cluster runs with **MinClusters** = 2 took $\approx 4.5\,\text{s}$[2] and the final resolution was 13. For $\rho = 2.0$ the final resolution was 25 and with $\approx 11.7\,\text{s}$ more time was needed. By starting the algorithm at a higher resolution, e. g.

2. The times were measured using the feature *@elapsed* of the Julia programming language.



(a) MinClusters = 2, final resolution: 16 **(b)** $\epsilon = 0.1$

Figure 11: Result of ITERIDENSE and DBSCAN for intersected circle-like clusters.

with **StartResolution** = 10 the time decreases from $\approx 4.5\,\text{s}$ to $\approx 3.7\,\text{s}$ and from $\approx 11.7\,\text{s}$ to $\approx 10.5\,\text{s}$, respectively. In effect the maximal calculated resolution determines the runtime.

Fig. 11 (a) shows the ITERIDENSE result. For comparison Fig. 11 (b) shows the result using the DBSCAN algorithm for $\epsilon = 0.1$ and **MinPts** $= 3$.

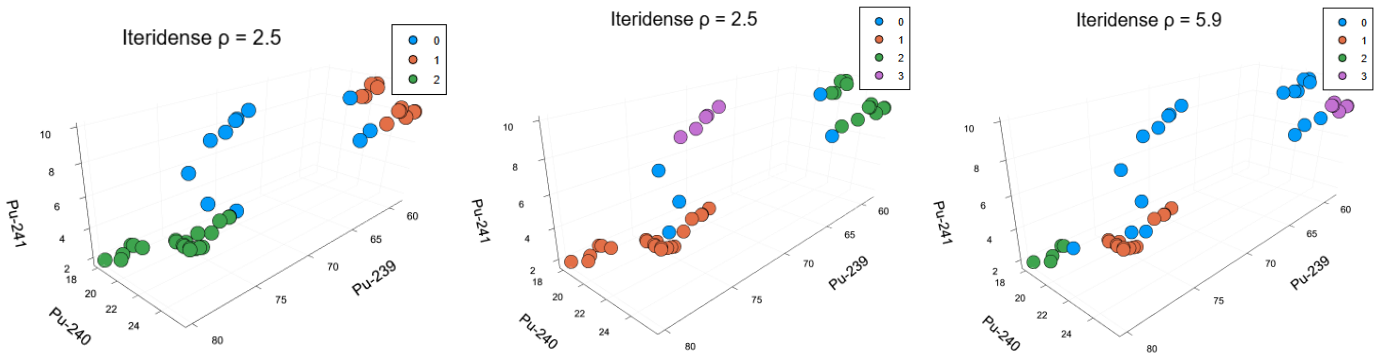
The benefit of ITERIDENSE compared to density-based algorithms is the computation time. In this example the data set has 1500 data points. To generate the count map in algorithm step 1, every data point has to be evaluated in form of generating its coordinate value for the current grid coordinate system. This is the most costly operation, especially for high-dimensional data. Afterwards, only the cells have to be evaluated, not the data points. For DBSCAN in comparison the coordinates for every data point are only read out once but the distances between every point and neighboring points have to be calculated. The larger ϵ or the greater the point density the more points are neighbors and have to be evaluated. This can become very computation-intensive. For the data of Fig. 11 with $\epsilon = 0.1$ and **MinPts** $= 3$ 10,000 cluster runs took $\approx 12.1\,\text{s}$ while the same with $\epsilon = 0.5$ took $\approx 49\,\text{s}$.[3] Therefore setting ϵ to a suitable value does not only affect the result a lot but also the computation time. Since there is no clear path on how to change ϵ to get a useful result, more cluster runs have to be performed than with ITERIDENSE.

For ITERIDENSE the worst case in terms of computation is to set ρ so high that the algorithm runs 1500 loops as there are 1500 data points. A single run of this takes $\approx 13.4\,\text{s}$. So 1500 loops take longer than 10.000 times the 12 loops from the default **StartResolution** 2 to the final resolution 13. This is because the number of cells in the grid scales in 2 dimensions squarely with the resolution. To prevent that undesired many loops are run, the parameter **StopResolution** can be set.

4.4 Results in higher Dimensions

Data with higher dimensions are a main use case for clustering algorithms as no human could do the clustering according to plots. Fig. 12 is an example and also demonstrate the clustering performance

3. The computation time measurement of the DBSCAN algorithm was performed using its implementation in the package *Clustering* of the JULIA programming language [16].
With $\epsilon = 0.5$ both clusters were not detected.



(a) Clustering with only the shown dimensions taken into account.

(b) Clustering with all dimensions taken into account.

(c) like (b) but $\rho = 5.9$

Figure 12: Result of Iteridense for the *pluton* data set.

of Iteridense. The data are the publicly available *pluton* data set[17] containing concentrations of the different Plutonium isotopes in 45 ore samples. It has 4 dimensions.

By plotting 3 dimensions of the data set and performing Iteridense only on the plotted dimensions, the result would be Fig. 12 (a). Taking all dimensions into account, the result is Fig. 12 (b). The points of high Pu-241 concentrations are then identified as a cluster. Cluster 1 is so large because its density in all 4 dimensions matters. If one wants for some reason cluster 1 to be split into 2 clusters, one follows the Iteridense path and increases ρ above the lowest ρ_{cluster} and ends up with Fig. 12 (c).

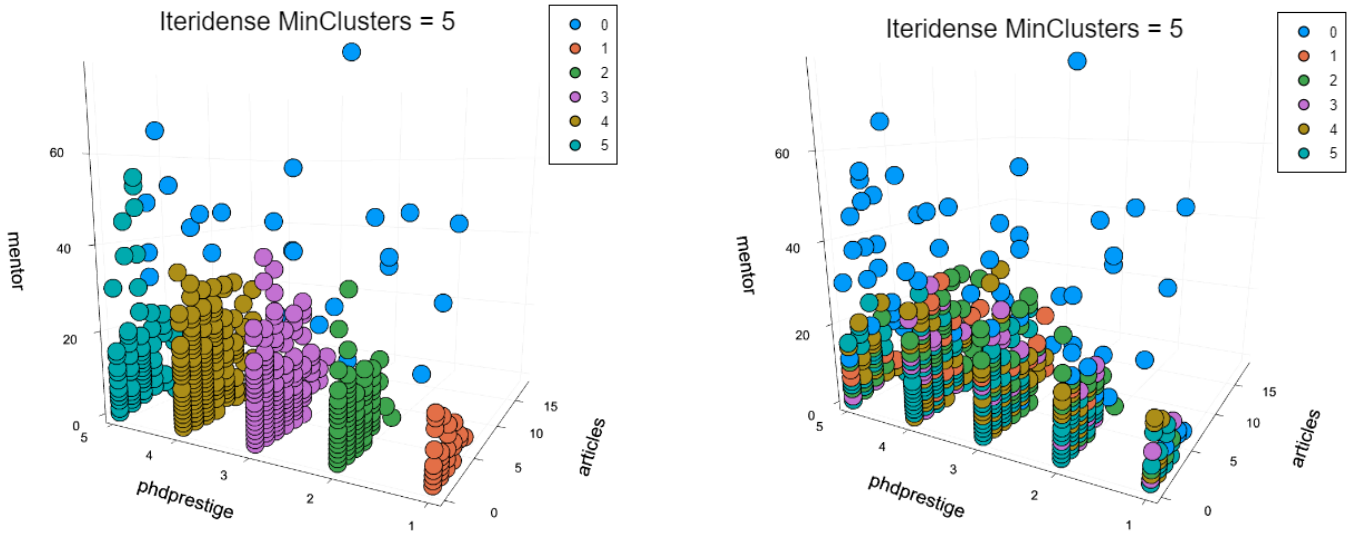
Fig. 13 shows a use case in which Iteridense shows its strengths. The data is the publicly available *PhDPublications* data set [18]. It has 6 dimensions and we selected 3 for the visualization. Since there are 5 classes in the set, **MinClusters** was set to 5. By evaluating only the 3 shown dimensions, one gets Fig. 13 (a). This shows that Iteridense's grid-based approach combined with its density analysis makes it possible to deal directly with classes inside data sets. Pure density-based algorithms cannot directly cluster the data set in the same way.

When evaluating all available dimensions the clusters run across the clusters, Fig. 13 (b). To find in this case clusters inside the classes, one has to extract the classes to different data sets and then run Iteridense on every class. This is requires more efforts but leads to sensible results when going the way to specify ρ.

5 Discussion

As shown in the previous sections, the Iteridense algorithm is applicable for general purposes. It is more computation-efficient than pure density-based algorithms that evaluate neighboring data points. But it shares with density-based algorithms the drawback that clusters overlapping each other cannot be detected. For example it will perform as poor as DBSCAN on Fisher's Iris data set [19].

Iteridense shows some similarities to the grid-based DENCLUE algorithm. However, the assignments of the data points to the clusters is different because DENCLUE assumes a Gaussian distribution function as shape of the density function. Another big difference to DENCLUE is that there is not only a single probability-density function created but iteratively several ones with increasing resolution. This increases the computation efforts but one does not have to make assumptions about the density in the data set. DENCLUE requires at least 2 input variables. ξ is similar to ρ in Iteridense. The parameter σ defines the width of the Gaussian that is used to assign the data points to the clusters. Its value has to be guessed and therefore introduces for some



(a) Evaluation of the 3 shown dimensions

(b) Evaluation of all 6 dimension

Figure 13: Result of Iteridense on the *PhDPublications* data set.

practical applications a trial and error process. There are approaches to improve the initial setting of the DENCLUE parameters, see [14], but in general this will remain as a practical challenge.

Compared to the grid-based algorithm CLIQUE, Iteridense does not require to specify the size of the cell (CLIQUE's parameter ξ) since the cell width is iteratively approached. There is also no need to specify the number of data points in a cell to treat the cell as being part of a cell (CLIQUE's parameter τ). The Iteridense algorithm treats every cell with at least 2 data points as part of a cluster. This is possible because at the end of every loop (steps 1 – 5) the clusters are evaluated and if their ρ_{cluster} is too low, the cluster is deleted. This is an advantage to CLIQUE because especially for high-dimensional data it is hard to estimate how many data points might end up in a cell.

Iteridense is a simple algorithm: The user does not need to estimate in advance a cell size, how many data points will be in a cell, the mean distance between data points in a cluster or the like. One can either specify **MinClusters** or ρ , sets **MinClusterSize** and gets in many cases directly a suitable result. If necessary, Iteridense's clear path on how to change the input parameters guides the user to more suitable or different results.

6 Conclusions

This paper introduced Iteridense, an iterative clustering algorithm combining grid-based and density-based methods. It is simple to use because it does not require to estimate settings in advance and because it provides two possibilities to run the clustering and for both a clear path on how to change the algorithm's input parameters to achieve suitable results. Iteridense is applicable for data sets with any dimensionality.

The Iteridense algorithm provides shorter computation times than pure density-based algorithms. Compared to pure grid-based algorithms it has the advantage that the user does not have to make assumptions on how the grid should be defined or about the shape of the probability-distribution.

It was demonstrated that Iteridense performs clustering as good to the DBSCAN algorithm and for cases of high-dimension data sets even better.

Iteridense provides different options to affect either the clustering result and to improve the computation time. We provide online a reference implementation together with an example worksheet, [7], demonstrating the clustering with Iteridense on the data sets shown in this paper.

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