Data Science - Exercise 3 - Clustering

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Data Sets

Toy Data Set

Data taken from:
https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html

Big Data Set: Census Income

Data taken from:
https://archive.ics.uci.edu/ml/datasets/Census-Income+%28KDD%29

Data Original Owner:
U.S. Census Bureau
http://www.census.gov/
United States Department of Commerce

Donor:
Terran Lane and Ronny Kohavi
Data Mining and Visualization
Silicon Graphics.
terran '@' ecn.purdue.edu, ronnyk '@' sgi.com

Small Data Set: Heart Disease

Data taken from:
https://archive.ics.uci.edu/ml/datasets/Heart+Disease

Data Creators:

1. Hungarian Institute of Cardiology. Budapest: Andras Janosi, M.D.
2. University Hospital, Zurich, Switzerland: William Steinbrunn, M.D.
3. University Hospital, Basel, Switzerland: Matthias Pfisterer, M.D.
4. V.A. MediMcal Center, Long Beach and Cleveland Clinic Foundation: Robert Detrano, M.D., Ph.D.

Algorithms

Three clustering algorithms were chosen based on the requirement to work with at least one partitive and one hierarchical algorithm and the fact that those algorithms seemed to be good based on the overview that can be found at the scikit learn platform https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html :

- Mini-Batch k-Means (partitive)
- Agglomerative Clustering (hierarchical)
- DBSCAN (density based)

Mini-Batch k-Means

For the required category of partitive clustering algorithms the Mini-Batch k-Means was selected because it is a variation of the k-Means that is suitable for large data sets. Small, randomly chosen batches are processed in each iteration instead of working on the whole data set at once.

Agglomerative Clustering

For the required category of hierarchical clustering algorithms an agglomerative algorithm was chosen. It follows a bottom-up approach, meaning that all individual data points are assigned to an individual cluster, which are then conntected to one another in hierarchical manner to form a new cluster until only the desired amount of clusters remains.

DBSCAN

The 'density-based spatial clustering of applications with noise' (DBSCAN) algorithm groups together data points that are closely located to one another. Points with no close neighbour points are detected and marked as outliers. This algorithm was chosen for this exercise because the density based approach seems to have the potential to find structures that the two previously mentioned algorithms do not. A density based alternative would have been the 'ordering points to identify the clustering structure' (OPTICS) algorithm. The DBSCAN was favored for this assignment because it is significantly faster due to the scikit learn overview referenced above.

Clustering Results

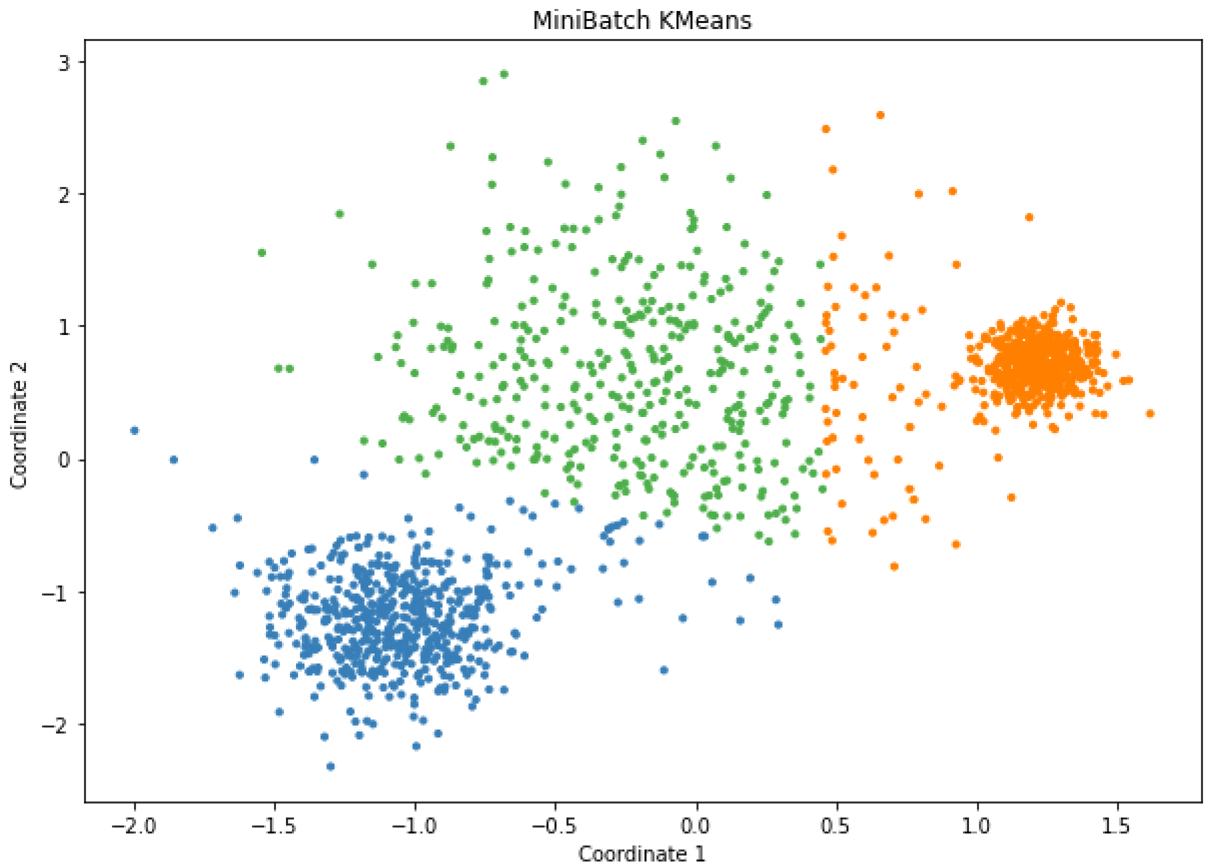
Because the data projection exercise did not indicate a suitable number of clusters, various target numbers of clusters were tried. For the two algorithms requiring a number of clusters beforehand an amount of three clusters was chosen. Two clusters seemed to be to coarse-grained but four and five clusters seemed to make it even harder to deduce a meaningful interpretation of the clustering calculated that three target clusters already do. E.g. with more than three target clusters the agglomerative algorithm on the big data set made it harder to distinguish visually between points belonging to one or another cluster.

###################################### Todo: Describe the results, and what information you can obtain. Specifically, compare the outcomes of the different methods. ######################################

Toy Data Set

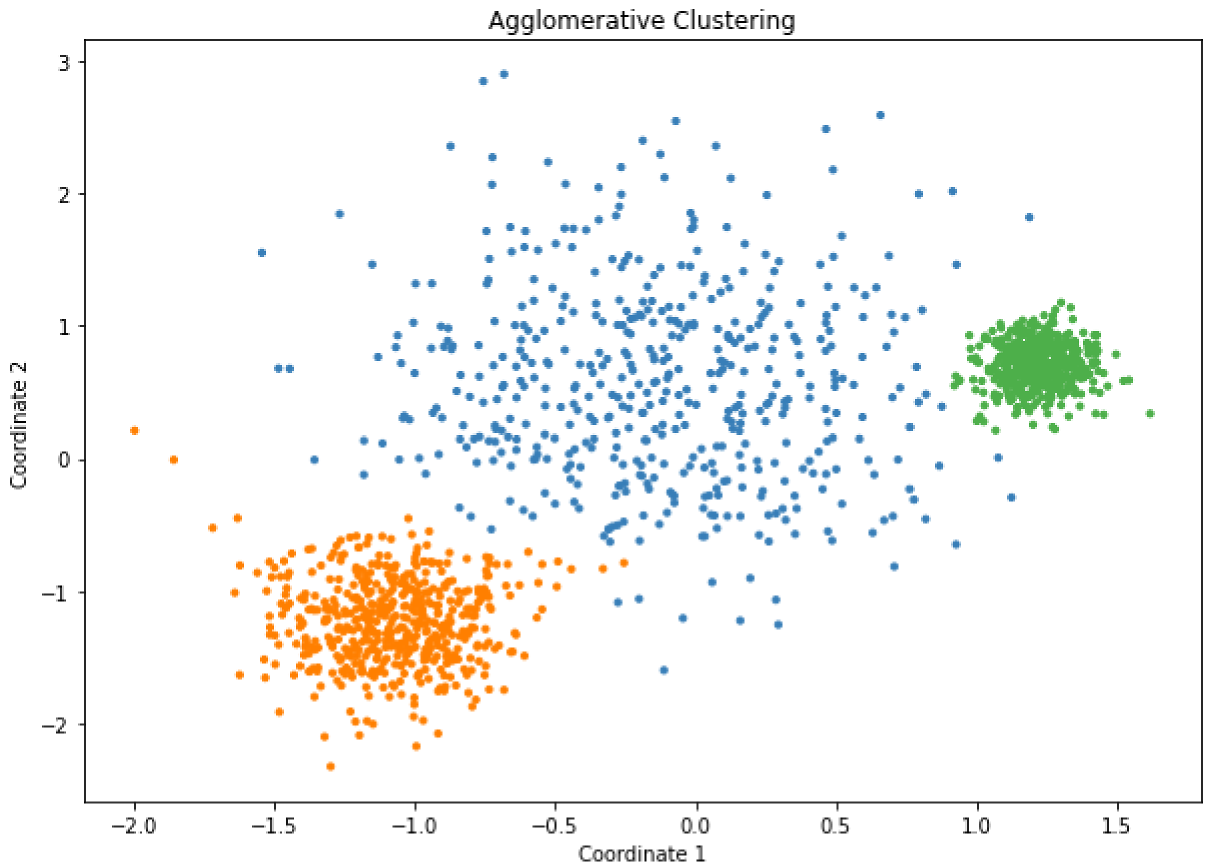
Algorithm 1: Mini-Batch k-Means

Subjectively, I would say, that the toy data set can be best described with three clusters. One compact one on the left side, one compact one an the right side an a loosely coupled, big one in the middle. When setting three clusters as target, the Mini-Batch k-Means algorithm produced a result reflecting these expectations. All tightly connected points on the left side are fully captured by the blue cluster and all tightly connected points on the right side are fully captured by the orange cluster. For an ideal result, I would have expected that only the dense, ball-shaped structures are captured for the outer clusters. Not only but especially regarding the orange cluster it seems that many points that are very loosely connected to the orange main accumulation are still marked orange although they visually seem to be more suitable in the green middle cluster of generally looser connected points.



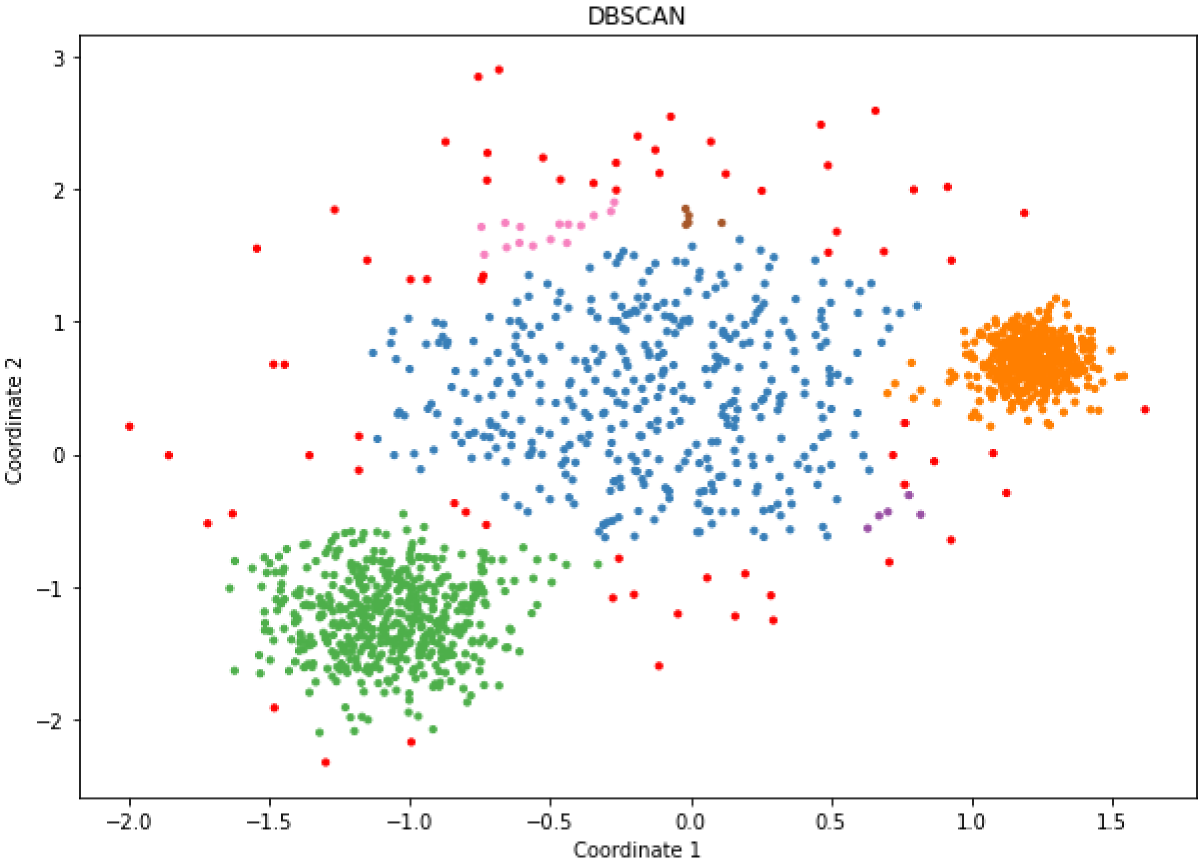
Algorithm 2: Agglomerative Clustering

The agglomerative algorithm with ward linkage and euclidean metric produces pretty exactly the expected output. In comparison to the Mini-Batch k-Means algorithm nearly all loosely connected points are not part of the two outer clusters but of the blue cluster in the middle. Subjectively I would argue that this algorithm fits the data better than the first one.



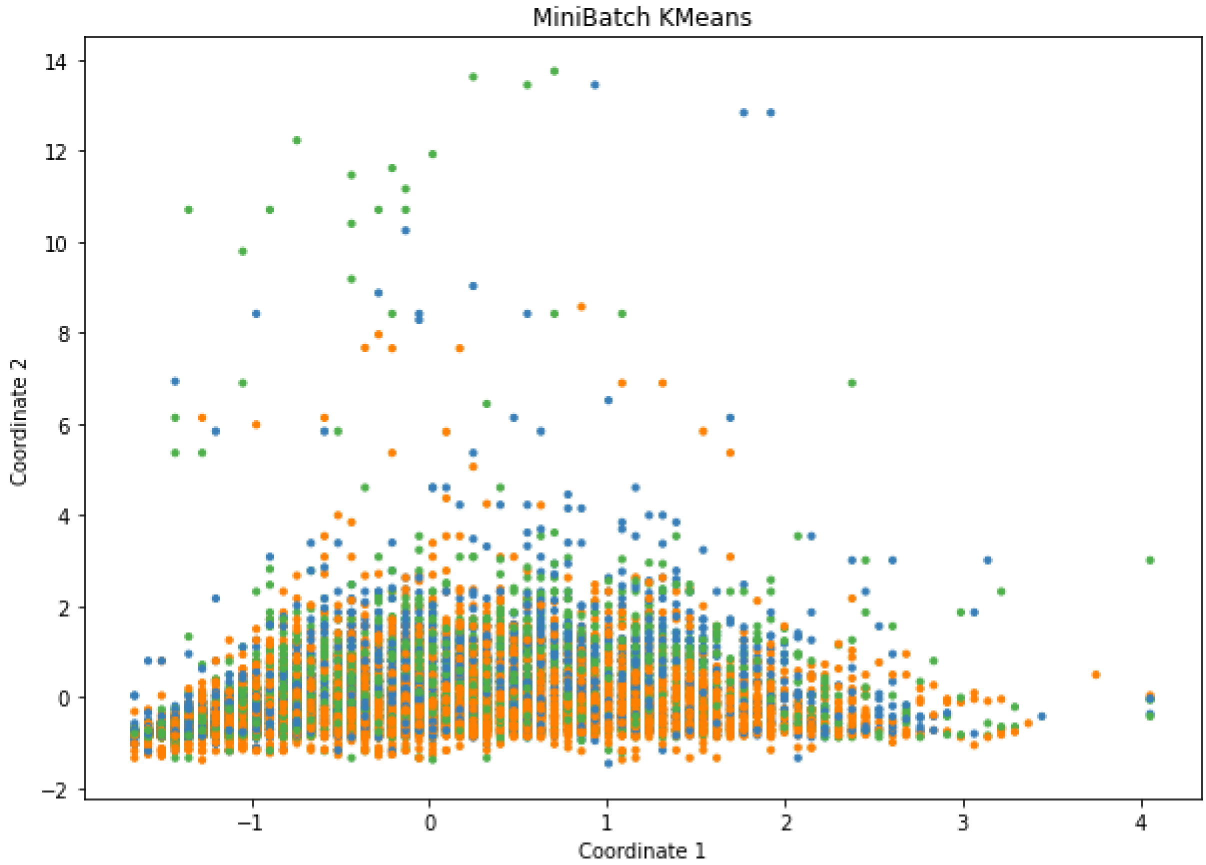
Algorithm 3: DBSCAN

The DBSCAN algorithm produces a result similar to the agglomerative clustering algorithm. The two main outer clusters are clearly seperated to the less dense blue cluster in the middle. In contrast to the agglomerative algorithm, where the number of clusters is fixed, three additional clusters are detected. They are all very small compared to the three main clusters and can be seen in the top middle (pink and brown) and in the bottom right (purple). Furthermore, outliners that are far away from the main clusters are detected and marked in red. Overall I would argue that the DBSCAN performs best in discovering the structure of the toy data set. The three main clusters are clearly captured and outliners are identified as such. If all data points should be assigned to one of the clusters, I would argue that the agglomerative clustering algorithm is the next best choice.

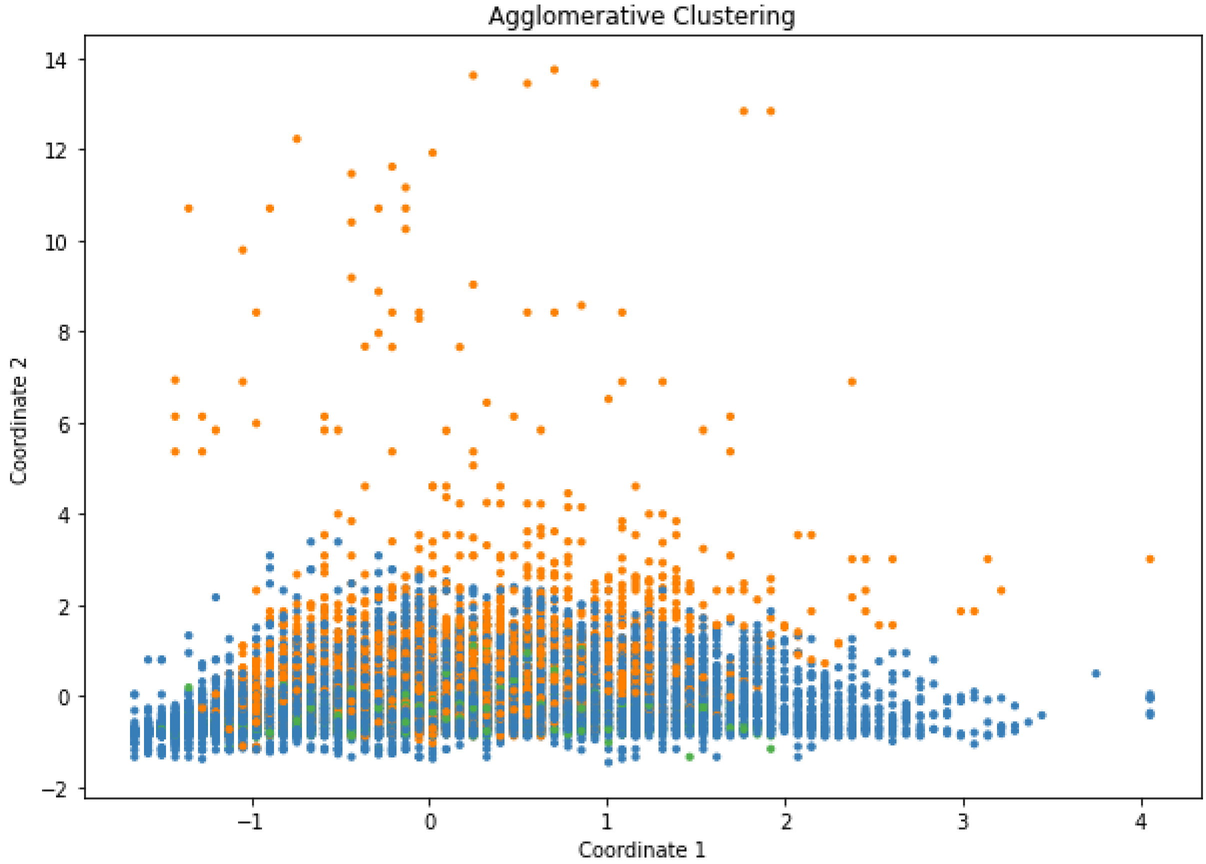

DBSCAN
Coordinate 1
Coordinate 2
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
3
2
1
0
−1
−2

Big Data Set: Census Income

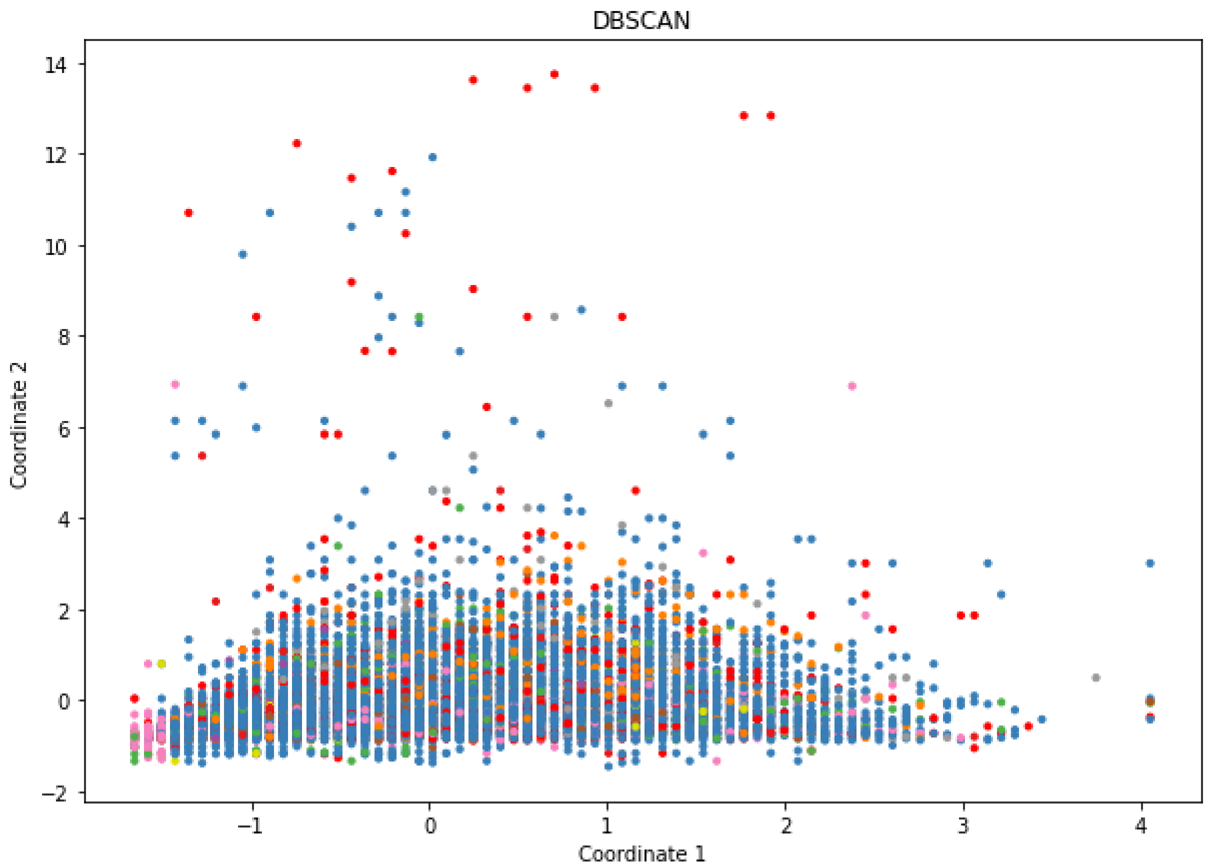
Algorithm 1: Mini-Batch k-Means



Algorithm 2: Agglomerative Clustering

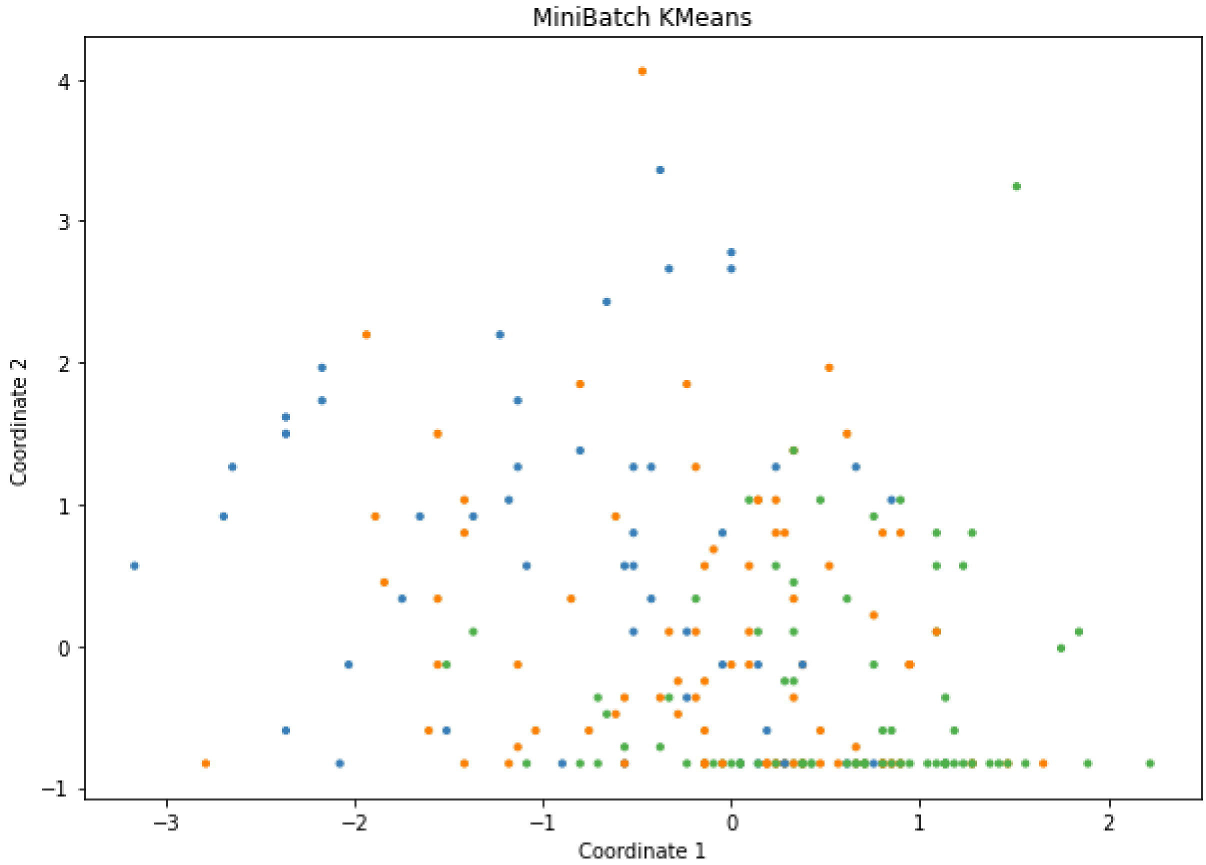


Algorithm 3: DBSCAN

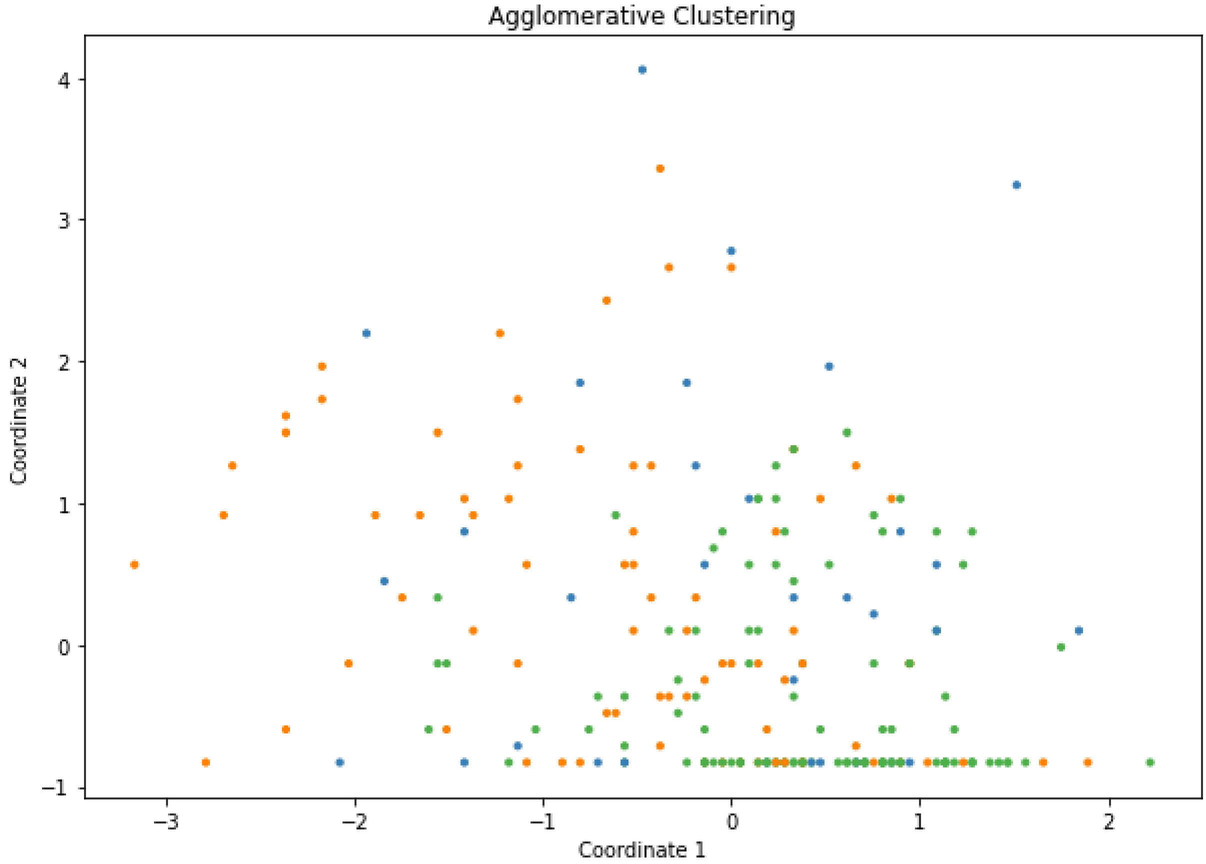


Small Data Set: Heart Disease

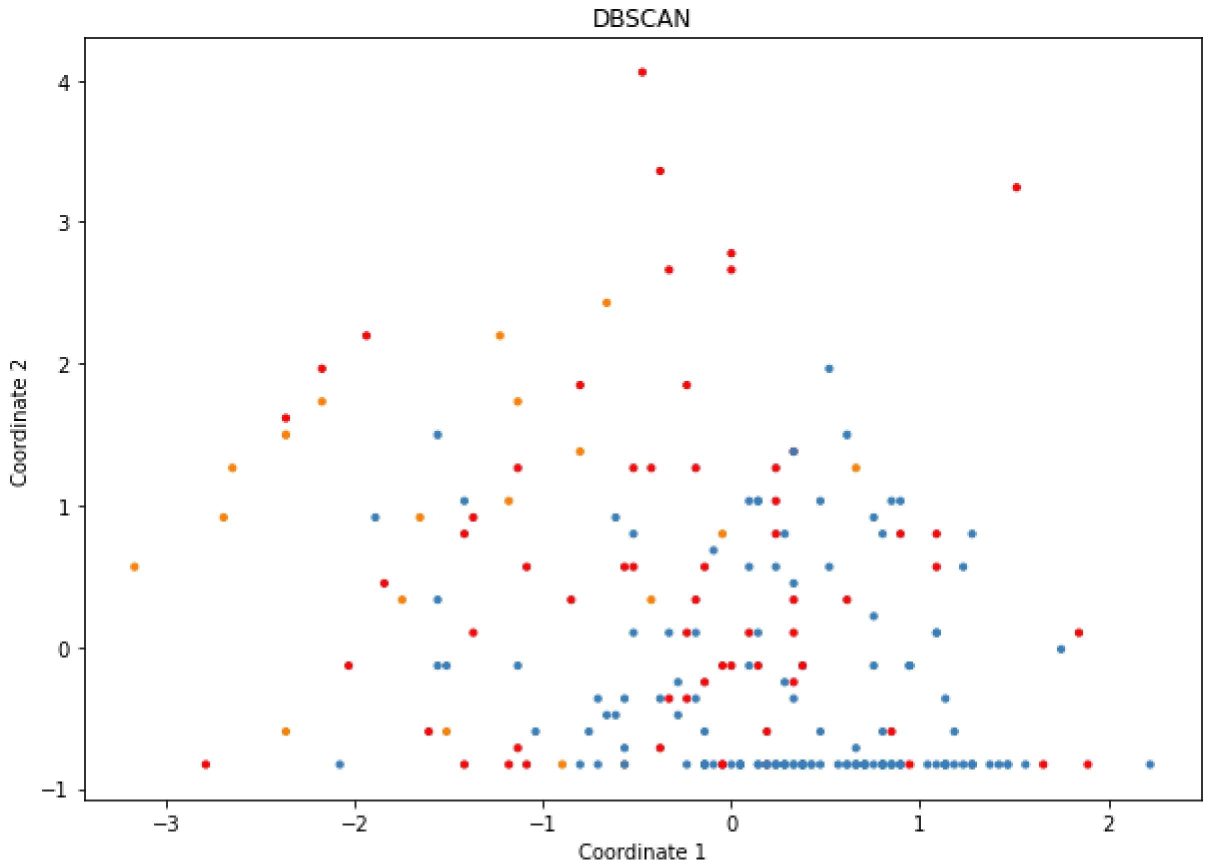
Algorithm 1: Mini-Batch k-Means



Algorithm 2: Agglomerative Clustering



Algorithm 3: DBSCAN



Todo: Quantitative Comparison

Todo: chose two evaluation criteria to compare the algorithms also quantitatively: illustrate the different characteristics of the clustering