Tool for Visual Cluster Analysis and Consensus Clustering

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Introduction

Clustering:

- Grouping data-points such that their underlying relationships are reflected
- Gaining knowledge through this grouping

The process of clustering is not done when a solution is computed,
but when the researcher involved:
"... **evaluated**, **understood** and **accepted** the patterns." (Chen and Liu [2])

Challenges:

- Many possibilities for clustering:
  - Algorithms/Parameters/Assumptions
- Choice and interpretation of solution is difficult

Related Work: Clustering

There is a vast amount of clustering techniques, including:

- Partition-based methods (KMeans-like algorithms)
- Hierarchy-based methods (e.g. Joining of Sets/Linking)
- Density-based methods (e.g. DBSCAN/OPTICS)
  - Many more...

Related Work: Visual Frameworks

- ClusterVision
  - Ranking solutions according to a combination of quality metrics
  - Choosing from the highest ranked ones
- VISTA
  - In-depth analysis of individual solutions
  - Possibilities for relabeling of points (ClusterMap)
- Simple Visualizations
  - Included in most data-analysis tools
  - Scatter plots, bar charts, etc.

Related Work: Consensus Clustering

Combining clustering results may yield a better solution:

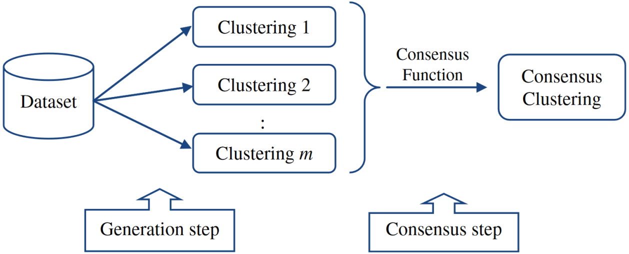


Figure 1: Workflow for generating consensus clusterings [5, p. 340]

Idea of our Tool: Facilitating clustering exploration

How can we assist users in exploring clustering results?

- Visualizing individual results
  - Scatter plot (matrices)/kernel density estimation
  - Dimensionality reduction
- Visualizing similarities between results
  - OPTICS meta-clustering
  - Heat maps
  - Multi-Dimensional-Scaling to approximate solution space

Idea of our Tool: Gathering more Information

Can we gain additional knowledge from multiple computed solutions?

- Previous frameworks only try to select the best one
  - Additional information lost
  - Difficult to objectively identify best one
- Consensus clustering
  - Can combine solutions or groups of solutions

Idea:

- Combine group of robust solutions into one

The Tool

Three main parts:

- Data-View
  - Loading/Saving/Creating data
  - Cleaning up data
  - Visualizing data
- Workflow-View
  - Creating clustering workflows
  - Defining parameters
- Meta-View
  - Visualizing clusterings and meta-clusterings
  - Selecting or creating final results (& consensus clustering)

Aim: Facilitating use through clear separation

The Tool: Data-View

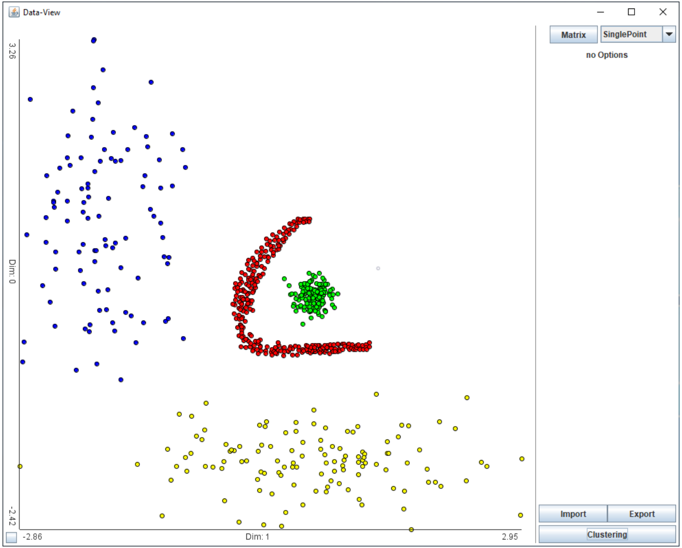


Figure 2: Data-View

The Tool: Data-View - Scatter Plot Matrix

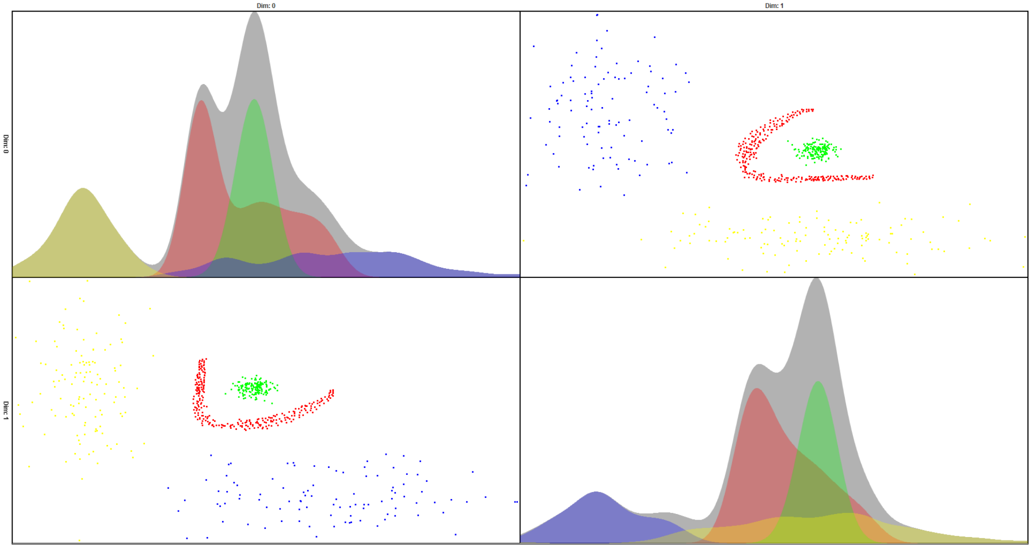


Figure 3: Scatter Plot Matrix

The Tool: Workflow-View

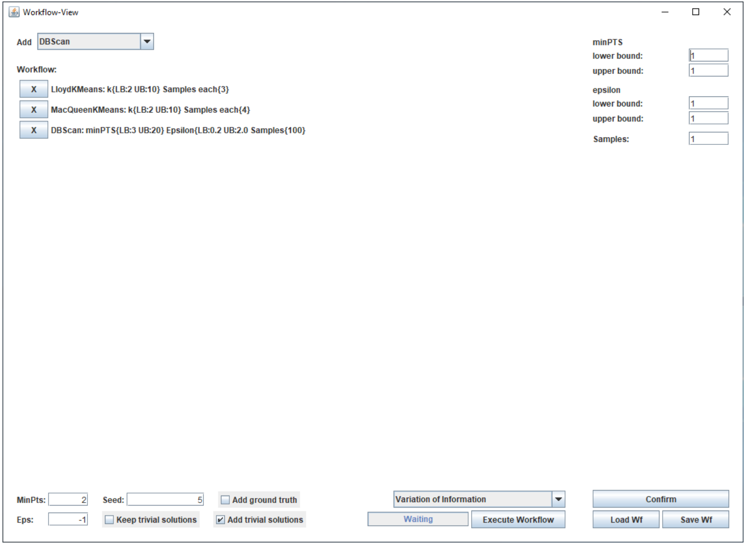


Figure 4: Workflow-View

The Tool: Meta-View

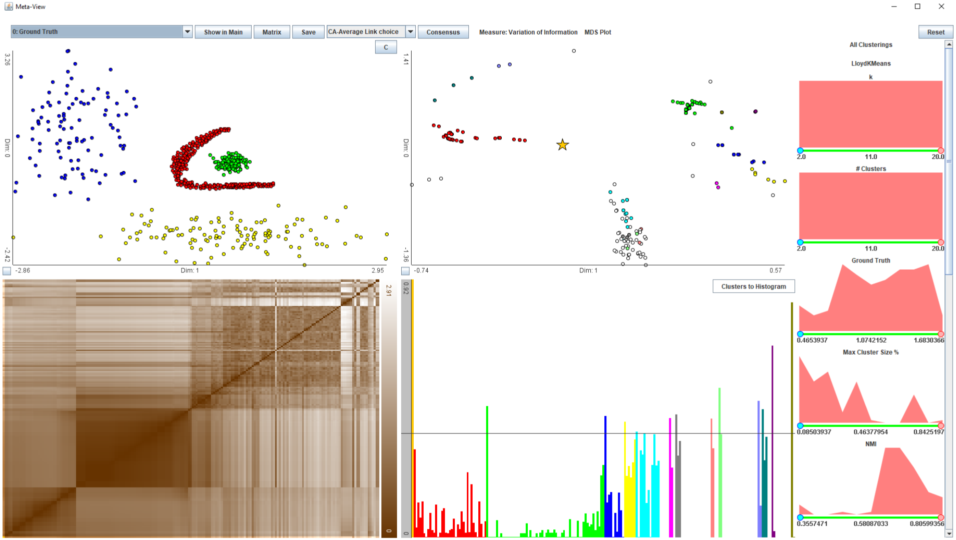


Figure 5: Meta-View

Recoloring Clusterings for Comparison

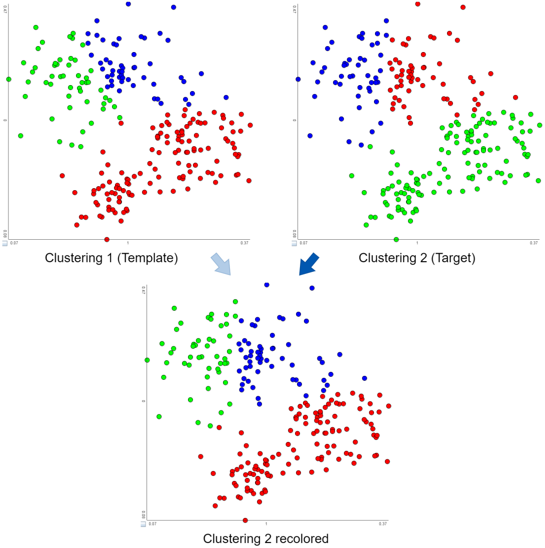


Figure 6: Depiction of Hungarian's Method

Implementation

Used tools:

- Java 1.8, utilizing Streams for parallelization
- Libraries:
  - ELKI [1] - Clustering
  - WEKA [3] - IO
  - Java Smile [4] - Additional Methods
- Swing's JComponents and overriding the *draw()* method

Ease of extension:

- All selectable methods provide simple interfaces

Tests: Introduction

We want to show that with our tool we can:

- Produce solutions better than any individual clustering result
- Obtain solutions unobtainable by single methods
- Find multiple alternative solutions which can be analyzed to find a fitting choice

And do so in a straightforward and useful way:

- Letting a user test our tool
- Also showing real world test data-sets

Tests: Better than individual Solutions

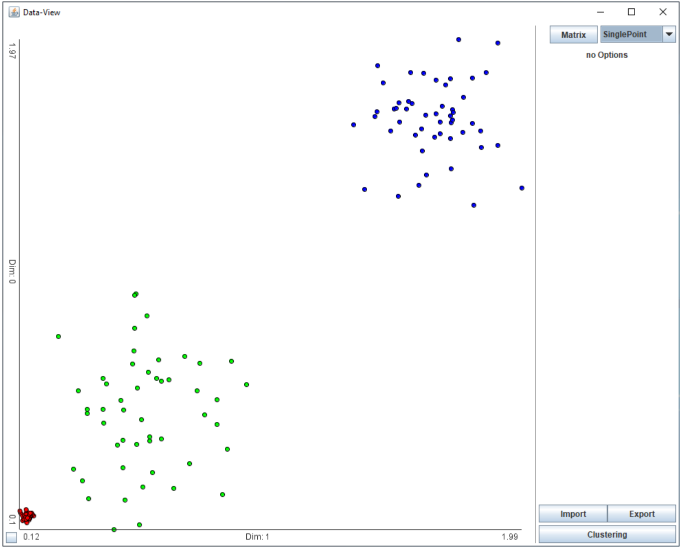


Figure 7: Synthetic Data with Ground Truth

Tests: Better than individual Solutions

Best individual result when sampling Lloyd's k-Means algorithm with $k = 2...20$ and 6 samples per k:

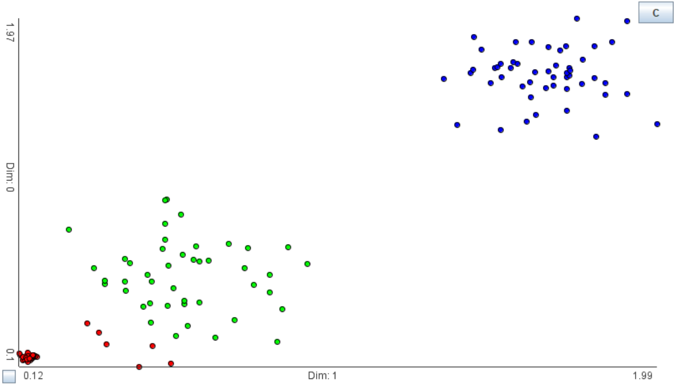


Figure 8: Result of best k-Means run for example Data-Set

Combining all solutions finds the ground truth exactly (without defining k)

Tests: Unobtainable Solutions

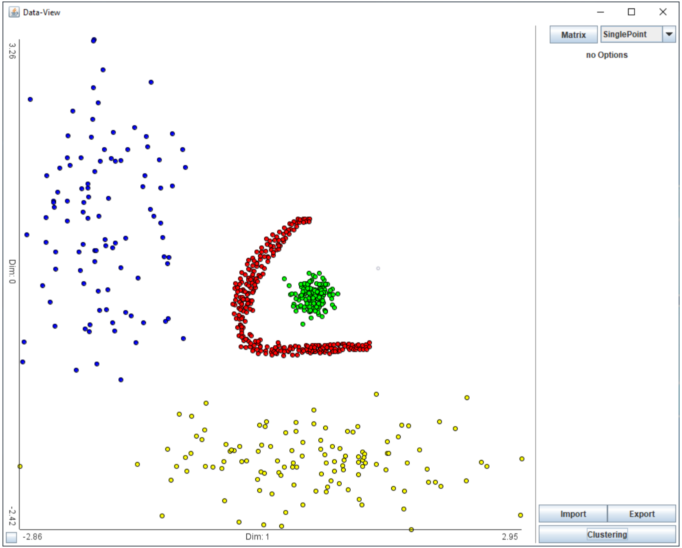


Figure 9: Synthetic Data with Ground Truth

Tests: Unobtainable Solutions

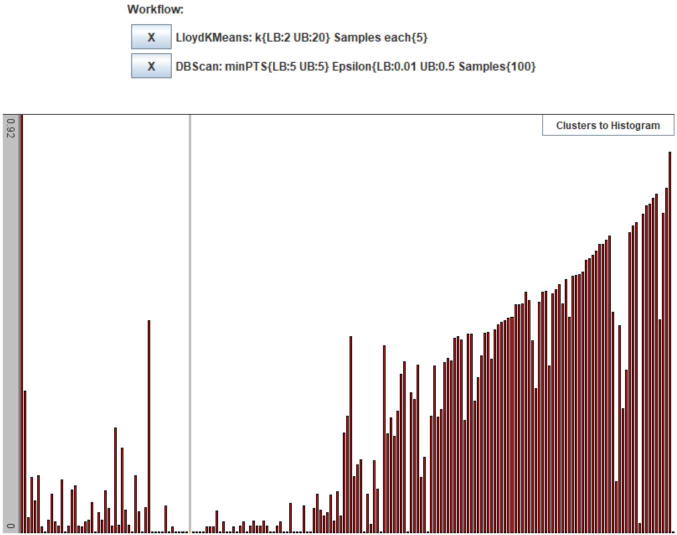
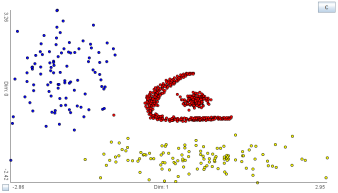
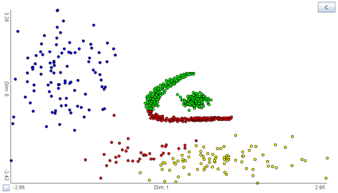


Figure 10: OPTICS reachability plot

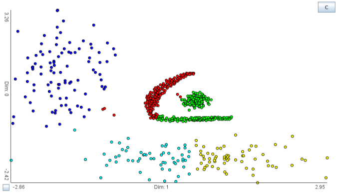
Tests: Unobtainable Solutions



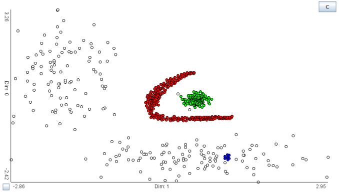
(a) K-Means with $k = 3$



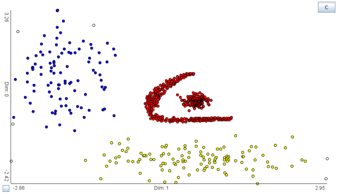
(b) K-Means with $k = 4$



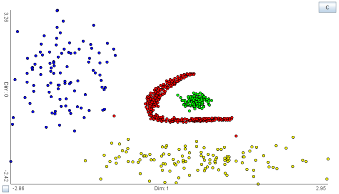
(c) K-Means with $k = 5$



(d) DBSCAN, best single Result



(e) Selected robust Clustering



(f) Consensus Result

Figure 11: Single Clustering results for Data-Set

Tests: Multiple Solutions

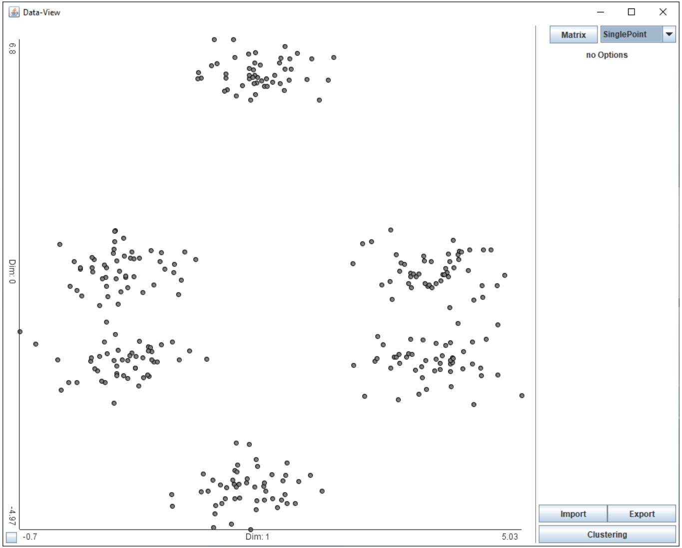


Figure 12: Example Data-Set with unknown Labels

Tests: Multiple Solutions

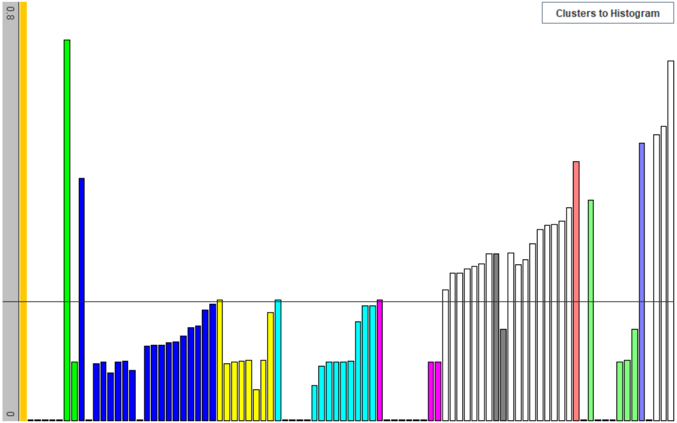
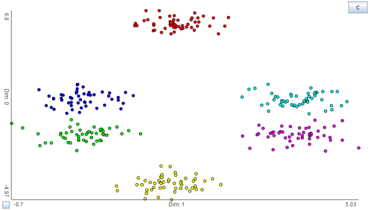
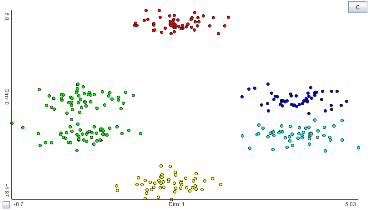


Figure 13: OPTICS Plot

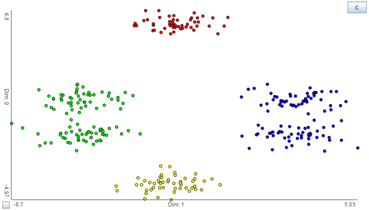
Tests: Multiple Solutions



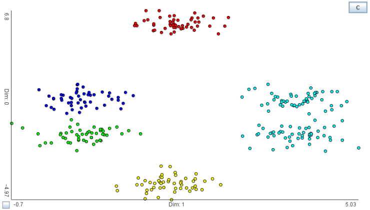
(a) Blue Cluster (19 base clu.)



(b) Light-blue Cluster (14 base clu.)



(c) Pink Cluster (9 base clu.)



(d) Yellow Cluster (8 base clu.)

Figure 14: Consensus Clustering results

Tests: User & Real world data

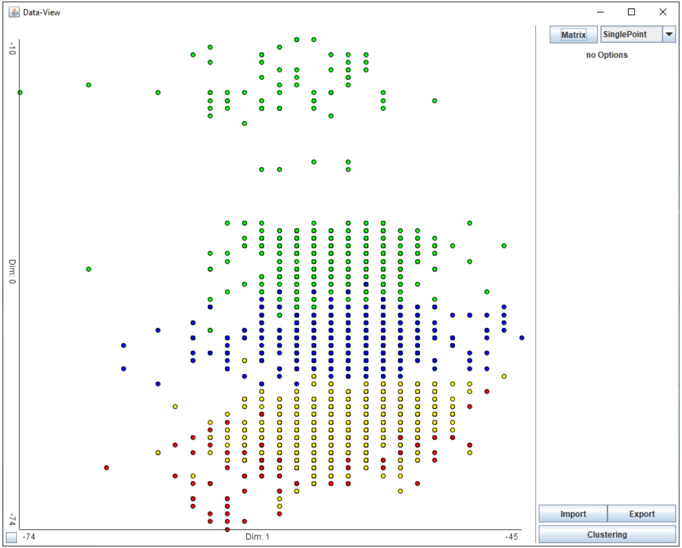


Figure 15: WiFi Localization Data-Set with first two Dimensions shown

Tests: User & Real world data

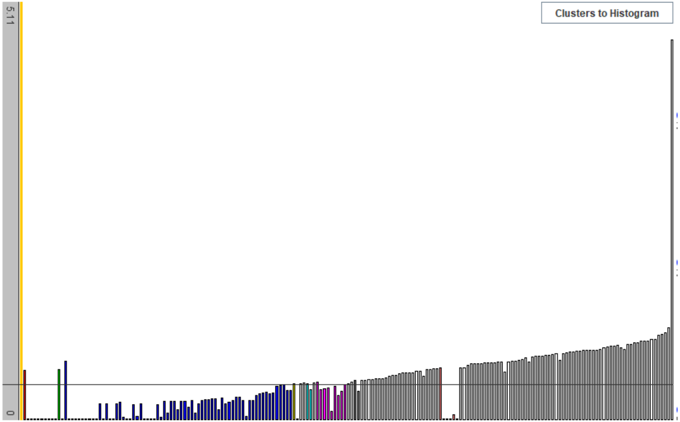
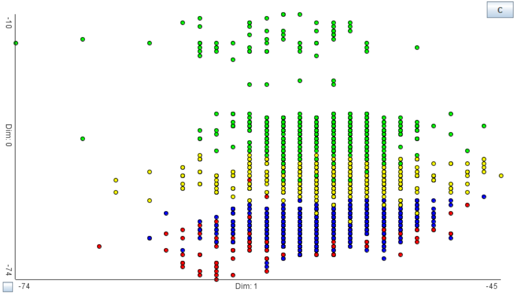
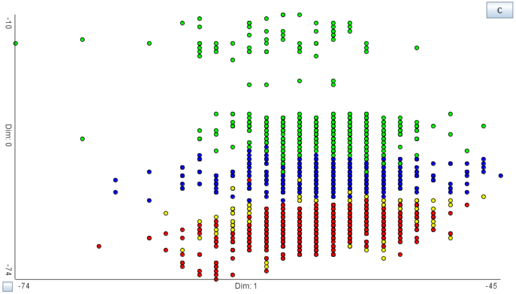


Figure 16: OPTICS Plot for WiFi Localization Data-Set

Tests: User & Real world data



(a) User Consensus Result:
NMI: 0.9142
blue (largest) Meta-Cluster

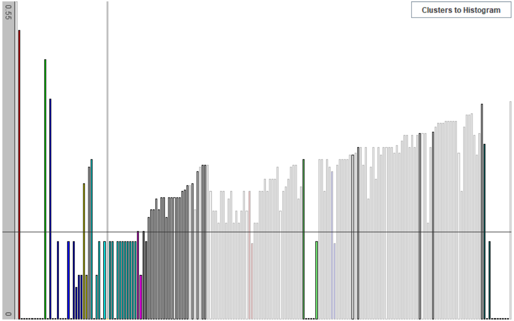


(b) Best Result of single Clustering Run
NMI: 0.8904

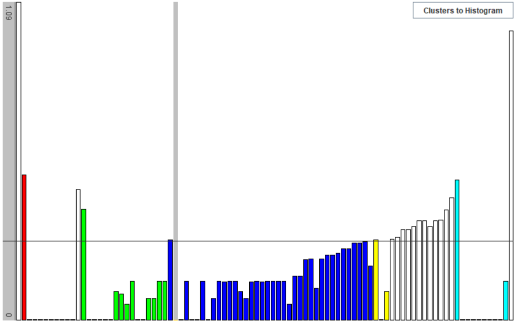
Figure 17: Clustering results for WiFi Localization Data-Set

Tests: Finding a good Sampling Range

- User testing on QCM3 data-set (different alcohols passed through sensors)
- Sampling with K-Means Algorithm, 10 samples per k



(a) K-Means results with: $k = 2..20$ ($k > 10$ grayed out)



(b) K-Means results with: $k = 2..10$

Figure 18: OPTICS Plots for different Sampling Ranges

Future Work

Further evaluating usability:

- Additional study on usability
- Gathering information on which parts are especially useful
- Evaluating alternative views and functionality

Research on consensus clustering:

- Analysis of generation/selection mechanisms
- Evaluation of selection criteria (is there a better choice than robustness)

Conclusion

- We created a new visual tool for cluster analysis:
  - Visualizing clusterings on a meta-level
  - Showing groups of robust clusterings
  - Allowing to find solutions using consensus clustering
- We showed:
  - Robust groups indicate good results
  - Combined results facilitate choice and can be better than any individual result
- Link to the tool:
  - `https://github.com/chris9182/Visual_Cluster_Exploration`

References I

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