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
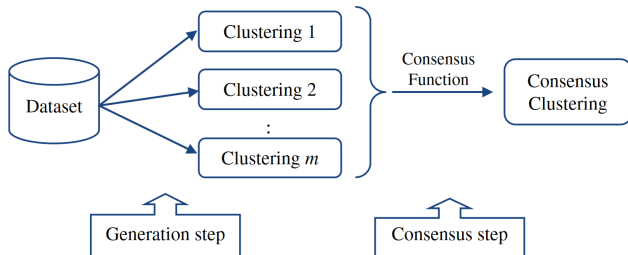
Combining clustering results may yield a better solution:

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
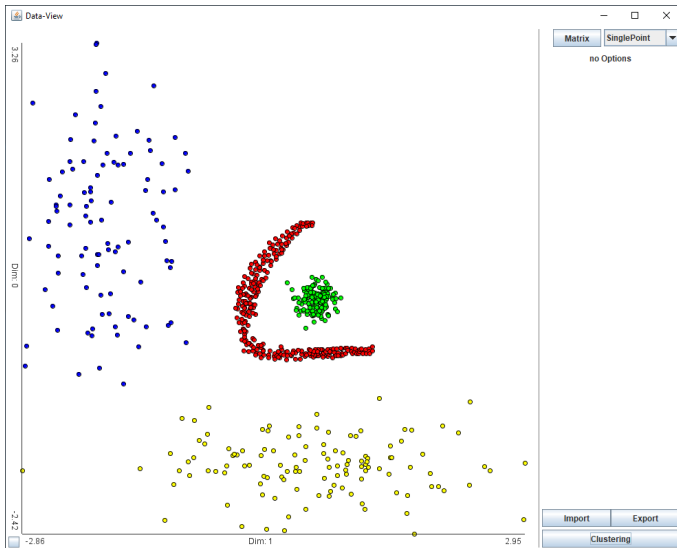
Figure 2: Data-View

The Tool: Data-View - Scatter Plot Matrix
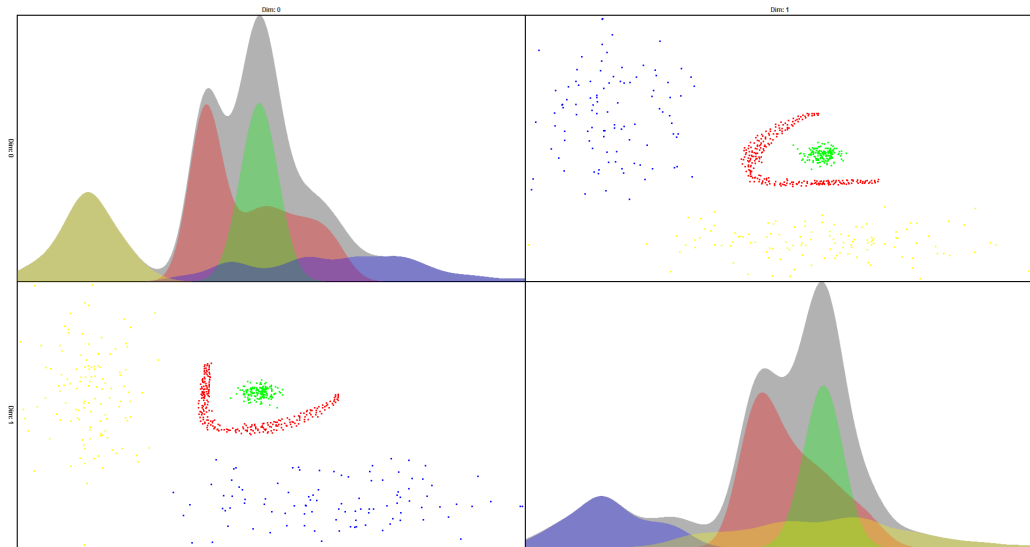
Figure 3: Scatter Plot Matrix

The Tool: Workflow-View

Figure 4: Workflow-View

The Tool: Meta-View
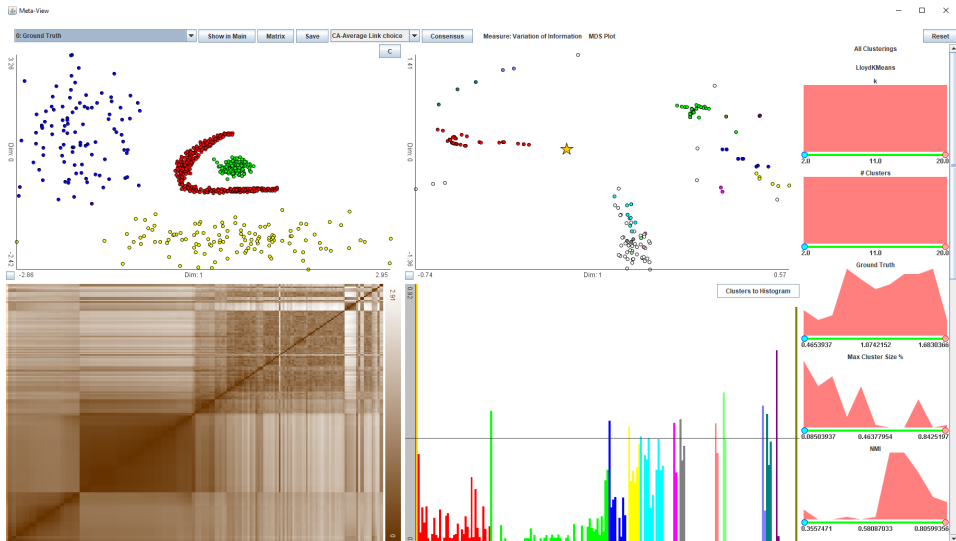
Figure 5: Meta-View

Recoloring Clusterings for Comparison
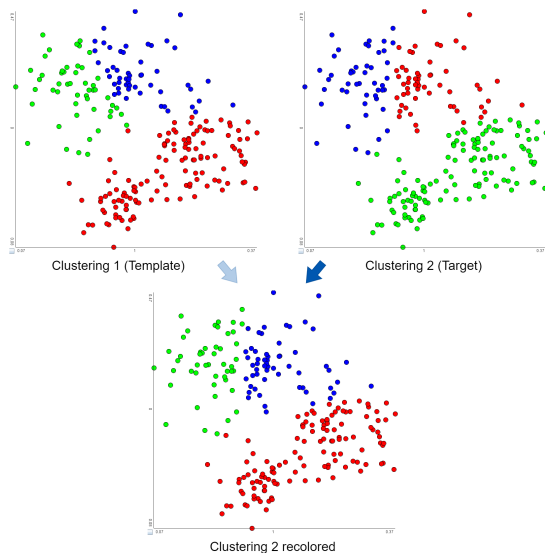

Clustering 1 (Template)

Clustering 2 (Target)

Clustering 2 recolored

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
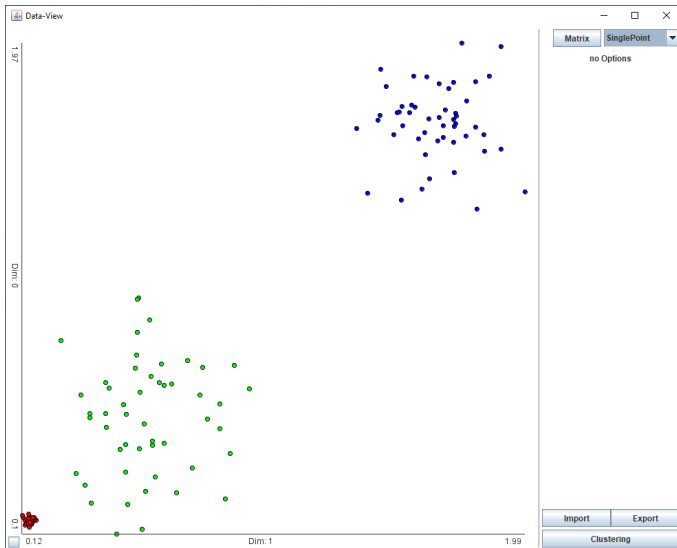
Tests: Better than individual Solutions

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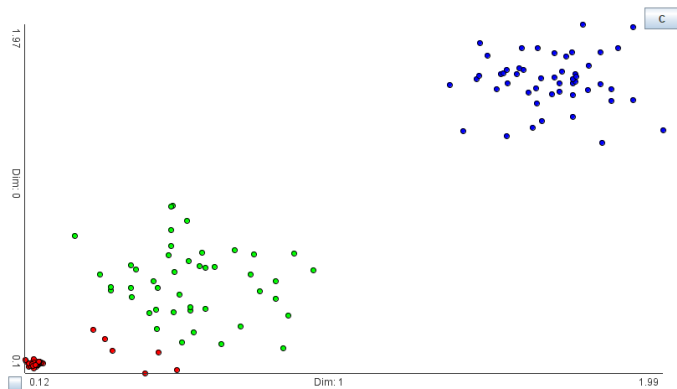
Figure 8: Result of best k-Means run for example Data-Set

Combining all solutions finds the ground truth exactly (without defining k)
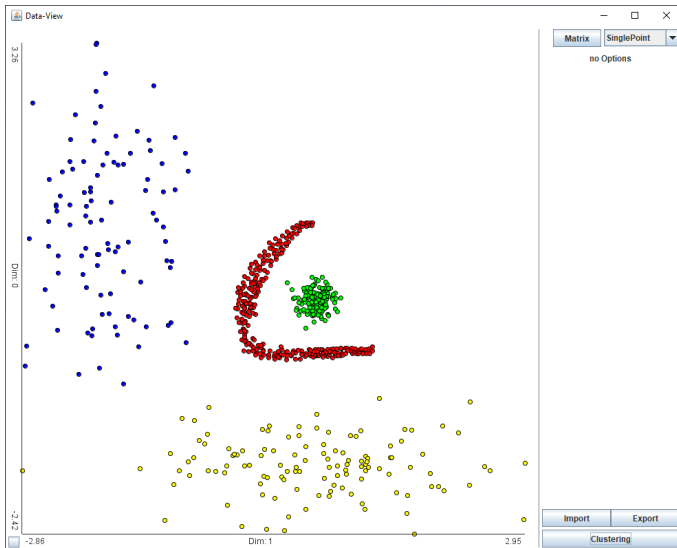
Tests: Unobtainable Solutions

Figure 9: Synthetic Data with Ground Truth

Tests: Unobtainable Solutions

Workflow:

X LloydKMeans: k{LB:2 UB:20} Samples each{5}

X DBScan: minPTS{LB:5 UB:5} Epsilon{LB:0.01 UB:0.5 Samples{100}
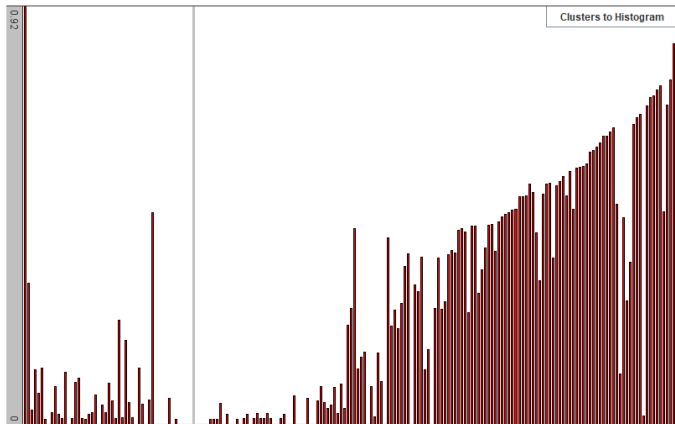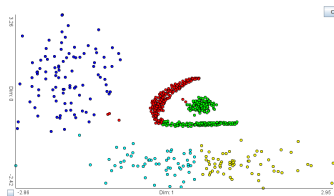

Figure 10: OPTICS reachability plot
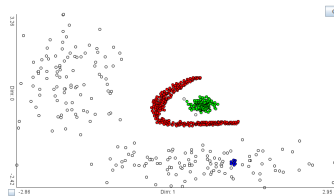
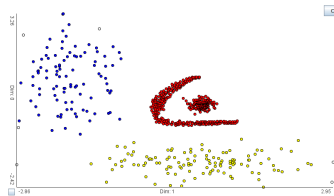# Tests: Unobtainable Solutions
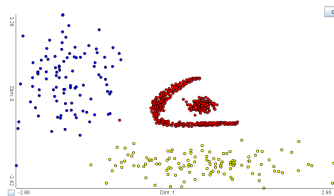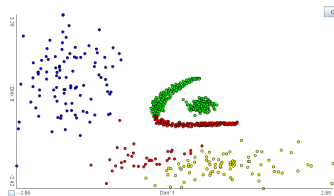
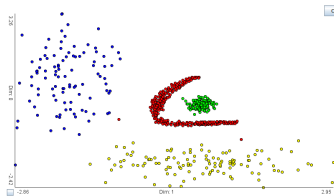(a) K-Means with $k = 3$ (b) K-Means with $k = 4$ (c) K-Means with $k = 5$

(d) DBSCAN, best single Result (e) Selected robust Clustering (f) Consensus Result

Figure 11: Single Clustering results for Data-Set
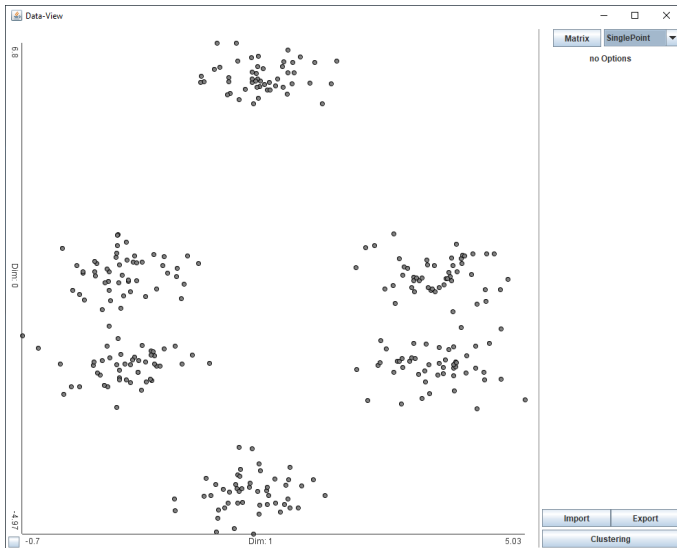
Tests: Multiple Solutions

Figure 12: Example Data-Set with unknown Labels
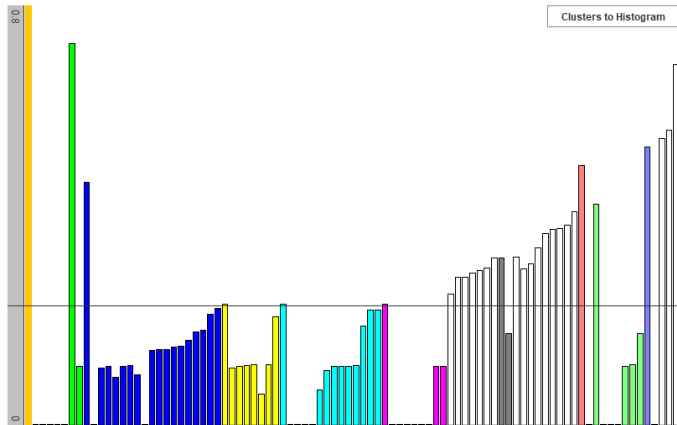
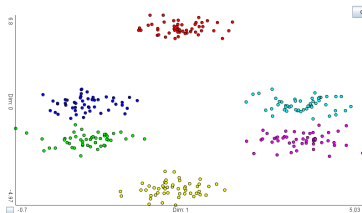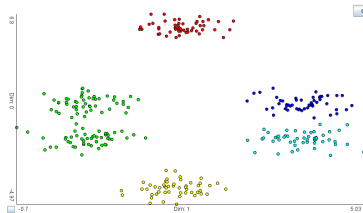# Tests: Multiple Solutions
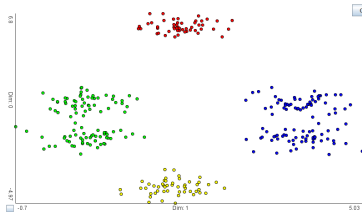

Figure 13: OPTICS Plot
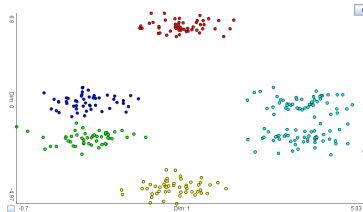
Tests: Multiple Solutions

(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.)

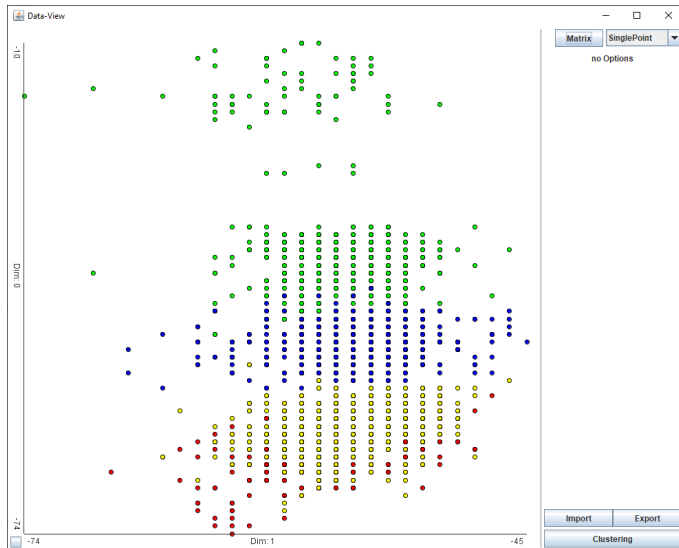Figure 14: Consensus Clustering results

Tests: User & Real world data

Figure 15: WiFi Localization Data-Set with first two Dimensions shown
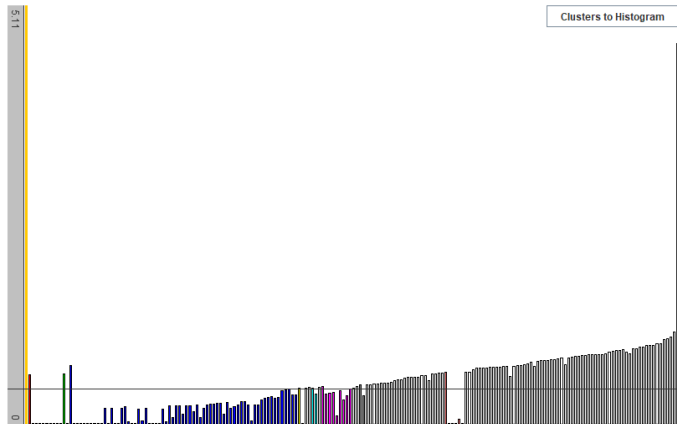
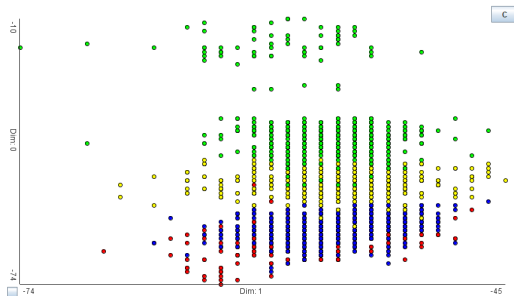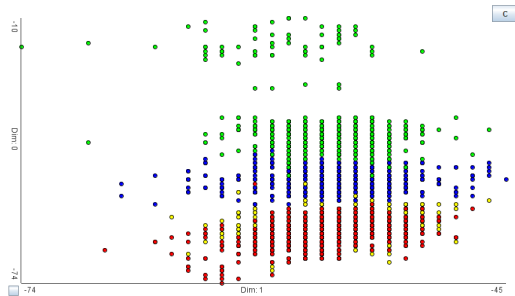# Tests: User & Real world data

Figure 16: OPTICS Plot for WiFi Localization Data-Set

Tests: User & Real world data

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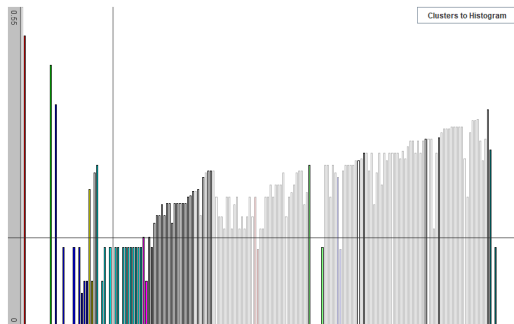NMI: 0.9142
blue (largest) Meta-Cluster

(b) Best Result of single Clustering Run
NMI: 0.8904
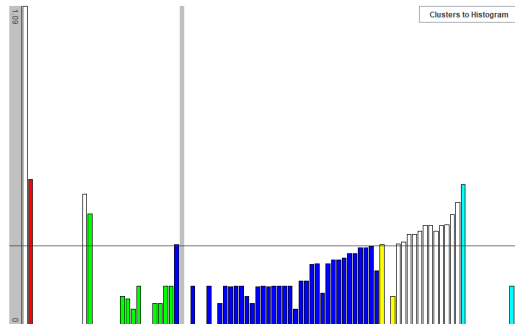
Figure 17: Clustering results for WiFi Localization Data-Set

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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