Visual Exploration Tools for Ensemble Clustering Analysis

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Abstract: Uncertainty Analysis is essential to support decisions, and it has been gaining attention in both visualization and machine learning communities —in the latter case, mainly because ensemble methods are becoming a robust approach in several applications. In particular, for unsupervised learning, there are several ensemble clustering methods that generate a *co-association matrix*, *i.e.*, a matrix whose element (i, j) represents the estimated probability that the given sample pair is on the same cluster. This work studies the following decision problem: “Given a similarity function, which groups of elements of a set form robust clusters?” *Robust* here means that all elements of each cluster are connected with a probability within a given interval. Our main contribution is a prototype that helps decision makers, through visual exploration, to have insights to solve this task. To do so, we provide visual tools for ensemble clustering analysis. Such tools are grounded in the co-association matrix generated by the ensemble. With these tools we are better equipped to recommend the group of elements that form each cluster, considering the uncertainty generated by ensemble clustering methods.

1 INTRODUCTION

Uncertainty Analysis is an active area of research: it helps decision makers through the quantification of uncertainties in relevant variables (Ghanem et al., 2017). One way to perform this quantification is to randomly generate an ensemble of possible outcomes of the given decision problem. Nowadays, the large amount of computer resources available makes such ensemble generation possible (Cunha Jr et al., 2014). The visual analysis of the generated ensembles emerges as an important visualization challenge (Obermaier et al., 2014). This paper deals with uncertainty visualization in the context of ensemble clustering analysis.

It is now common to have *ensemble classifiers* in supervised learning. They combine the outputs of multiple classifiers with the purpose of improving the classification accuracy (Dietterich, 2000). Likewise, *ensemble clustering* methods in unsupervised learning combine multiple partitions to provide better clustering of the data set (Vega-Pons and Ruiz-Shulcloper, 2011). Several ensemble clustering methods generate a *co-association matrix*, which is a matrix where each (i, j) element represents the estimated probability that the given sample pair is on the same cluster (Fred and Jain, 2005). These methods can also generate a standard deviation for each pair, which also represents an estimated uncertainty.

Objective and Contributions. This work aims to help decision makers to obtain insights to answer the following question: “Given a similarity function, which groups of elements of a dataset form robust clusters?” By *robust* we mean that all elements of each cluster are connected with a probability in a given interval.

To achieve our goal, we provide a visual tool for ensemble clustering analysis. Grounded in the co-association matrix generated by the ensemble, such tool supports us in recommending the group of elements that form each cluster, considering the uncertainty generated by ensemble clustering methods. The tool includes: variations over heatmaps to visualize the co-association matrices, violin plots of the silhouette of each group in the final partition, network and edge bundling to visualize the relationships between datapoints, a scatter plot of a 2D projection, and a map, when the data is georeferenced.

Paper Outline. The paper is structured as follows: Section 2 briefly describes related works on ensemble clustering visualization; Section 3 presents the characteristics of the visual exploration tool of ensemble

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results; Section 4 describes some analyses of a real-world use case with the tool and conclusions are given in Section 5.

2 RELATED WORK

Ensemble Clustering. Ensemble clustering combines multiple clustering results from the same dataset into a final partition (Vega-Pons and Ruiz-Shulcloper, 2011; Xu and Tian, 2015; Huang et al., 2015). It is considered a difficult task because cluster labels are symbolic, so it is also necessary to solve a correspondence problem.

Among the most popular clustering ensemble techniques we find methods based on co-association matrices. Iam-On et al. present two new similarity matrices, which are empirically evaluated and compared against the standard co-association matrix on six datasets using four different combination methods and six clustering validity criteria (Iam-On et al., 2008). The Evidence Accumulation matrix (EAC) method (Fred and Jain, 2005) is based on a co-association technique for extracting a consensus clustering from a clustering ensemble. An extension of EAC is the Weighted Evidence Accumulation matrix (WEAC) (Huang et al., 2015), which includes weights to penalize low quality clustering and agglomerative methods to obtain the consensus partition. Another option is the Probability Accumulation (PA) method (Wang et al., 2009), a clustering aggregation scheme that uses a correlation matrix based on cluster size. The Ensemble Clustering Matrix Completion (ECMC) method, proposed by (Yi et al., 2012), is robust to uncertainties in the data. The Robust Spectral Ensemble Clustering (RSEC) learns a robust representation for the co-association matrix through low-rank constraint, which reveals the cluster structure of a co-association matrix and captures various noises in it (Tao et al., 2016).

The recent Locally Weighted Ensemble Clustering method is an ensemble clustering approach based on ensemble-driven cluster uncertainty estimation and local weighting co-association matrix strategy; it applies two novel consensus functions to construct the final partitions (Huang et al., 2018). Another example is a novel committee-based clustering method composed of three stages (Fiol-Gonzalez et al., 2018): (i) generating the clustering ensemble by combining feature selection strategies and clustering methods varying the number of clusters to generate multiple scenarios; (ii) combining the results of the multiple clustering scenarios generated to produce a co-association matrix; and (iii) creating sets of partitions using the co-association matrix and then selecting the *final* partition based on the best performance using the silhouette coefficient.

Visual Analysis of Ensembles. Due to their complexity and size, ensembles provide challenges in data management, analysis, and visualization (Potter et al., 2009). Wang et al. reported a survey on visualization techniques and analytic tasks involving ensemble data (Wang et al., 2018). They organize ensemble visualization techniques research into a pipeline, where ensemble data go to through a statistical aggregation step before visualization, a visual composition step after visualization, or a combination of both. In other words, these visualization techniques can be applied to get an overview of the entire ensemble or to compare the relationships between a small number of scenarios.

There are some tools to help visualize ensemble data. Ensemble-Vis links views built from means and standard deviations, using color and overlaid contours to view the complete ensemble dataset (Potter et al., 2009). IPFViewer combines small multiples views at multiple hierarchical levels to analyze hierarchical ensemble data (Thurau et al., 2014). Hao et al. apply ensemble visualization techniques in a network security analysis environment to produce a network ensemble visualization system (Hao et al., 2015). These techniques can cluster traffic with similar behavior and identify traffic with unusual patterns, facilitating the analysis of relationships between alerts and traffic flow.

Inspired by the related work and by the fact that it is possible to combine clustering results to improve the final partition, we want to visualize this final partition to understand its internal structure. We therefore address the following research questions:

- **RQ1:** How to visualize the final partition of a combination of clustering results?
- **RQ2:** Given a final partition, how to visualize its internal structure?
- **RQ3:** How to visualize the co-association matrix and uncertainty matrix from which the final partition was generated?
- **RQ4:** How to visually identify whether the patterns detected in the co-association matrix conform to the groups in the final partition?
- **RQ5:** How is it possible to identify the probability of obtaining connected components that agree with the final partition groups?
- **RQ6:** How to compare the final partition with other possible solutions (clusterings)?

3 VISUAL EXPLORATION TOOL OF ENSEMBLE RESULTS

This section proposes some visual exploration tools of the co-association matrix, to facilitate the understanding of the ensemble clustering result. There are several ensemble methods to construct the co-association matrix (Berikov, 2016; Lin et al., 2017; Fiol-Gonzalez et al., 2018). Among these, we selected Fiol et al.'s committee-based clustering method to generate the ensemble, because their algorithm generates as output the following matrices (see Section 2):

- Co-association matrix (CM), where the position (i,j) contains the probability that elements i and j are in the same cluster.
- Partitions Silhouette matrix (PSM), where the position (i,j) contains a tuple with the silhouette value and the cluster id ($< sil, cl\_id >$) for element i in partition j. The final partition is identified by an index f, where $0 \leq f \leq ncol(PSM)$.

The algorithm also generates a third matrix based on the CM to complement the uncertainty information in the overview task:

- Standard Deviation matrix (STD CM), where the position (i,j) contains the uncertainty (std) associated to the same element in the co-association matrix.

We propose to use some visualization techniques to assist in analytic tasks involving ensemble clustering data. Wang et al. reported six visual analytic tasks that cover most of the ensemble visualization literature, from which we chose three, as follows:

1. Overview: visual summary of ensemble data and overall uncertainty information.
2. Comparison: visual identification of the difference between two members.
3. Clustering: grouping of members or ensemble objects by similarity.

Based on these analytic tasks we defined three design goals for our visual exploration tool. We had to extrapolate the tasks from ensemble data members or object dimensions to ensemble clustering dimensions. The three main design goals are:

G1: Provide a visual representation of ensemble clustering (clustering task).

G2: Provide a visual summary of the final partition and uncertainty information (overview task).

G3: Support a visual identification of the differences between groups (comparison task).

In the next subsections we explain in detail the solutions proposed for each design goal.

The tool was developed using the `R` script language (R Core Team, 2018) and the `shiny` (Chang et al., 2018), `plotly` (Sievert, 2018), `leaflet` (Cheng et al., 2018), `visNetwork` (Almende B.V. et al., 2018), `edgebundleR` (Tarr et al., 2016) packages. We chose `R` because we wanted to test quickly and easily different possibilities of visualizations and different datasets. We are already working on the development of the solutions presented here in a more robust tool using `Python` (Van Rossum and Drake, 2003).

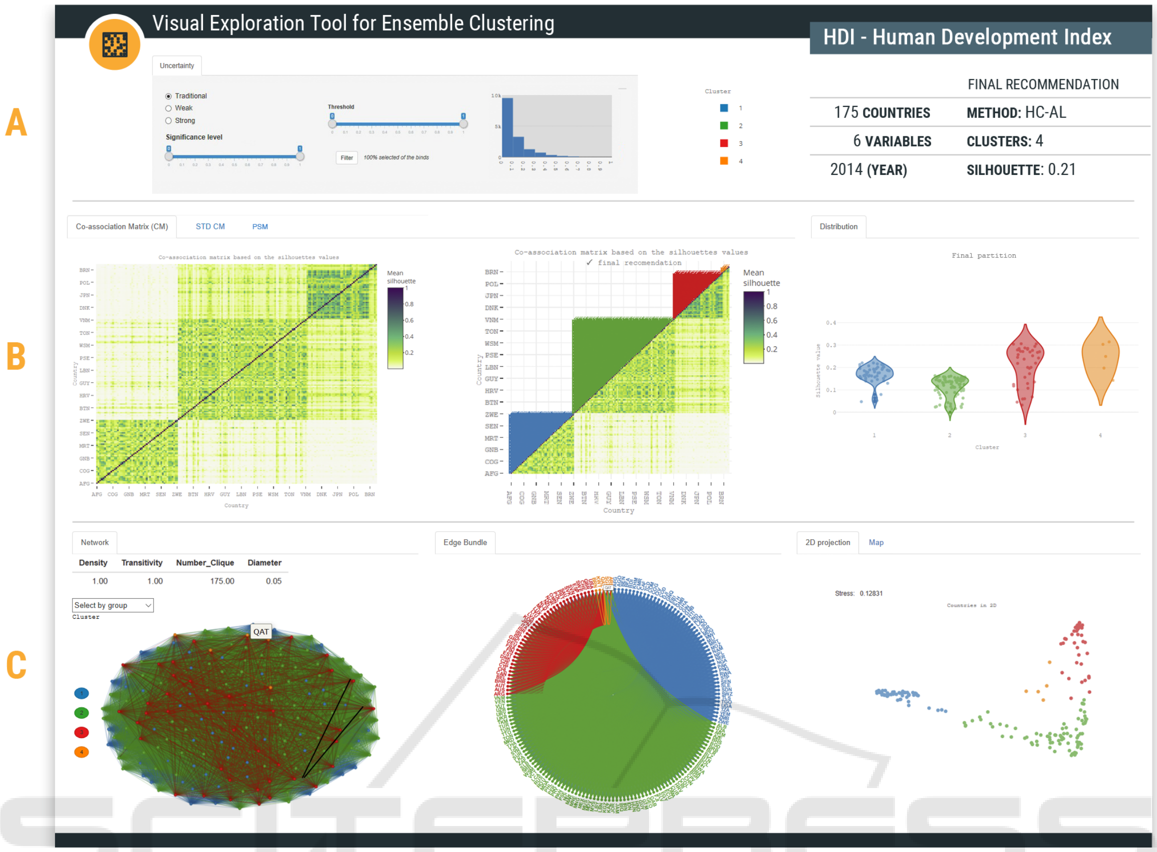
Our design consists of coordinated multiple views (Scherr, 2008), where views are displayed side-by-side and changes in one view affect the others. In fact, this solution is preferable when compared to single view because it can display different facets of the clustering ensemble information while avoiding visual clutter. Basically, the interaction area of the tool consists of three linked parts (Figure 1): A) confidence filtering; B) CM and related information; and C) group relationship, connections, 2D data points representation, and geospatial information.

The *threshold* in region A is a pair $< min, max >$ ($0 \leq min \leq max \leq 1$) of parameters the user can define. This filtering acts directly on the other parts (B and C), producing a clearer representation of the desired data and a better definition of patterns in the CM. The histogram next to the threshold represents the distribution of the CM. By manipulating the threshold, it is possible to identify the percentage of binds ($< i, j >$ pairs) that would remain after filtering.

By using the ensemble method results, we can use the confidence interval of the probability of each bind to propose three new approaches for filtering connections, as follows:

- **Traditional Interval Filter:** Takes into account the estimated probability of the bind. We accept the connection of the pair as true if the probability that the pair is on the same cluster is within the interval threshold.
- **Weak Interval Filter:** Verifies whether the confidence interval intersects the given threshold interval.
- **Strong Interval Filter:** Only accepts a pair as connected if the entire confidence interval of the bind is included in the threshold interval.

The confidence interval was constructed using the Gaussian probability distribution with significance level α ($CM_{i,j} \pm z_{\frac{\alpha}{2}} STD_{i,j}/\sqrt{n}$, where n is the number of scenarios in the ensemble). These intervals are related to uncertainty and they represent the range of potential values of the true connection probability. Using the strong filter, we only select binds with con-



HDI - Human Development Index

FINAL RECOMMENDATION

175 COUNTRIES	METHOD: HC-AL
6 VARIABLES	CLUSTERS: 4
2014 (YEAR)	SILHOUETTE: 0.21

Density	Transitivity	Number_Clique	Diameter
1.00	1.00	175.00	0.05

Stress: 0.12831

Figure 1: Visualization components of the tool.

fidence intervals within thresholds. In other words, there is a very small chance that the threshold does not contain the actual bind value. In the weak case, it is sufficient that the chance that the threshold containing the actual bind value is greater than zero.

We use colors to represent clusters. They serve as a visual aid to relate the different views, except for the heat map visualizations, which have their own color scale. The right-hand side of region A displays some information about the dataset and the final partition.

Region B is divided into two parts. The left-hand side groups in tabs the four co-association matrices and the silhouette value of all possible recommendations. The right-hand side shows the probability density of the silhouette of each group.

Region C includes four views: (i) a network component to visualize how each data point connects with the others; (ii) an edge bundling component that allows to view each network connection separately; (iii) the 2D spatial projection of each data point; and (iv) the map component to identify how each group is organized geographically (if applicable).

To achieve G1 (visual representation of an ensemble clustering), we chose three ways to visually represent clusters: cluster colors across all groups, a 2D projection through scatter plots, and a map.

2D Projection. To represent the similarity degree of the data points and the final partition, we use a Multidimensional Scaling (MDS) projection technique (Kruskal and Wish, 1978). We project each data point in two dimensions using scatter plots. To evaluate the quality of the projection, we inform the measure of the stress (see Figure 1, region C).

Each point of the 2D projection represents a member of the final partition and can be recognized by the color corresponding to its cluster. In this way, we can visualize a representation of the dispersion of the points inside and between clusters, allowing to evaluate the quality of the final partition.

Map. Georeferenced objects, such as neighborhoods, cities, and countries, are visualized in a map to easily analyze whether adjacent elements belong to the same cluster. When one clicks on a region, it shows a pop-up with the region name and the cluster number. This allows domain experts to recognize whether the final partition is in line with their experience.

Together, the 2D projection and map representations answer RQ1 (*How to visualize the final partition of a combination of clustering results?*).

To achieve G2 (visual summary of the final partition and overall uncertainty information), we chose heat maps, because they convey an overview of the behavior of datapoints. We represent four types of matrices in heat maps. Associated with them, the graph and the edge bundling provide an overview of the relationship between the datapoints.

Heat Map. We used the heat map to represent the CM in its traditional form (Wilkinson and Friendly, 2009), and the uncertainty matrix, adapted with scatter plots. This visualization compacts large amounts of information into a small space to bring out coherent patterns in the data. Each matrix has its symmetric and lower triangular variation. The data are sorted using the cluster numbers from the final partition in order to form the patterns corresponding with the clusters in the heat map.

When representing the CM as a heat map it is possible to notice that all the values in the main diagonal are 1 (dark color), *i.e.*, representing the probability of the element being in the same cluster as itself. Conversely, pairs with value 0 (light color) mean that the two elements have no binds, i.e., they never appear in the same cluster. By hovering over each cell of the matrix, a tooltip with information about the pair of binds appears: the pair's name, relationship value, group, and standard deviation (in the case of the uncertainty matrix).

Symmetric Co-association Matrix: There are specific patterns with rectangular shape (henceforth *blocks*) formed around the main diagonal in the heat map, containing the elements belonging to the same cluster. Visualizing the data in this way (see Figure 1-B) allows users to find darker regions, have an idea of the cohesion of groups, identify and count the blocks in the result. In Figure 1-B one can see three blocks. We can see the same pattern in all four representations of the matrix, but it is more evident here.

Lower Triangular Co-association Matrix: The lower part of this matrix represents the same information as the previous one. At the upper part, we map the clusters according to the final partition (see Figure 1-B). It is helpful when we cannot find well-defined patterns in the symmetric matrix (e.g., the red cluster in Figure 1-B). This feature helps us answer RQ4 (*How to visually identify whether the patterns detected in the co-association matrix conform to the groups in the final partition?*).

STD CMs: In this view, instead of painting the entire matrix cell, we use circles whose size is proportional to the standard deviation value. The smaller the circle size, the lower the uncertainty associated with the pair of binds. The color remains the same as in the other heatmaps.

The set of matrices provides an overview of the aggregate ensemble, allowing to analyze the probability of two data points falling in the same cluster in the multiple combinations and to know the uncertainty associated with that probability. This allows us to answer RQ3 (*How to visualize the co-association matrix and uncertainty matrix from which the final partition was generated?*).

Graph. To visualize the CM in a graph, one can define a complete undirected weighted graph as $G < V, E >$ where V are the elements of the dataset and E are the edges connecting each two elements. The weight of an edge is equal to the probability with which the two elements are together in the explored scenarios. Visually, the size of each node corresponds to its degree (number of nodes with which it is connected). When an edge is selected, the tool shows the probability associated with its pair of nodes.

This third section (see Figure 1-C) shares the threshold of the previous sections: setting a threshold range disables the edges with weights outside of the range, allowing to decompose the fully connected graph in separate connected components. This visualization enhances the study of components containing elements of different clusters, allowing users to notice the nodes which tend to be isolated even with low thresholds, to analyze the articulation points (represented with a thicker border) of the graph in depth; and to obtain an overview of some graph statistics, such as diameter, density, transitivity, and the number of cliques. In addition, the edges of the diameter in each connected component are presented in a different way, *e.g.*, edge in red color (see Figure 1-C).

Hierarchical Edge Bundling. Hierarchical edge bundling is a flexible and generic method that can be used in conjunction with existing tree visualization techniques. Low bundling strength mainly provides low-level, node-to-node connectivity information, whereas high bundling strength provides high-level information (Holten, 2006).

At first glance, it allows identifying the number of items per group. If an item is selected, we may quickly see the related items (*i.e.*, items that share an edge with the selected one) and whether they are in the same group or not. If all the elements linked to it are in the same group (*i.e.*, represented in the same color), the group is very cohesive.

As we modify the threshold, we can see the connections increasing or decreasing (both in the graph and in the edge bundling), which allows us to identify values in which related components are formed. This way we can answer RQ5 (*How is it possible to identify the probability of obtaining connected components that agree with the final partition groups?*).

Finally, to achieve G3 (visual identification of differences between groups), we use violin plots superimposed by a dot chart for each group, placed side by side. **Violin plots** summarize density shapes into a single plot of the data within each group, allowing comparison between groups (Hintze and Nelson, 1998). Inside each violin it is possible to identify the amount of data points per group. Hovering over each violin shows a tooltip with the interquartile information. This way we can answer RQ2 (*Given a final partition, how to visualize its internal structure?*)

Scatter Plot for PSM shows the silhouette values for each possible partition, as well as the final partition. The triangle markings shows the silhouette value in the final partition: an upward triangle indicating that the silhouette value is above the average for that data point, and the downward triangle otherwise. This allows us to answer RQ6 (*How to compare final partition with other possible solutions (clusterings)?*).

4 USE CASE

The publicly available Human Development Index (HDI)[1] was createdas part of the United Nations program, among other objectives, to compare and characterize the countries according to their development level. The online data are organized by year, and for each year it contains a set of features to compute the index. The 175 countries are classified in four groups: *very high, high, medium, and low*, but we only use this information to verify our clustering. We used the following variables to build the dataset: Infant mortality rate (per 1,000 live births) - 2013, Gross national income (GNI) per capita (2011 PPP$) - 2014, Labour force participation rate (% ages 15 and older) - 2013, Mean years of schooling - 2014, Expected years of schooling - 2014 and Life expectancy at birth - 2014.

The goal is to obtain a final partition using the ensemble method. We use the following parameters: K varying from 2 to 28; Sequential Forward Selection and Sequential Backward Selection as feature selection methods; and K-means, K-medoids and Hierarchical Clustering with Average Link (HC-AL) as clustering methods to create the ensemble. To obtain the final partition we used the K-medoids and HC-AL methods. We used $\alpha = 0.05$ to create the confidence interval.

Results. The method proposed 4 clusters with a silhouette around 0.21 and using HC-AL. Figure 1 B-2 shows the CM generated from the aggregate ensemble and the final partition of the method.

The orange cluster contains the *very high* countries, such as QAT (Qatar), ARE (United Arab Emirates), KWT (Kuwait), SGP (Singapore), BRN (Brunei Darussalam), but with the highest GNI. The other *very high* countries are located in the red cluster. The *high* countries are in the green cluster and the poor countries are in the blue cluster. The countries with *medium* development are mixed in the green and blue clusters. We can see the clusters in the world map (Figure 1C-3).

In the symmetric representation of CM (Figure 1B-1), we have four well defined blocks. The fourth cluster (in orange) is the smallest one, with only 5 data points. We can see it most clearly in Figure 1B-2. These blocks are filled with green dots, while the connection with the elements in other blocks are mostly in yellow, so the connection within the cluster is stronger than outside it. In order to highlight this fact, the threshold was set to 0.30 with traditional filter. This configuration results in 8.2% of all connections.

In the final partition, the blue group and the green group have the smallest ranges of the silhouette values (see Figure 1 B-3), while the red group has the largest range, which matches the variation in the CM (see Figure 1 B-1).

With a 0.40 threshold and weak filter, the groups have more intra-connections, as well as some connections between the groups, mixing different groups in the same connected component (see Figure 2b, dotted outline). This configuration results in 5.0% of all connections. The selected connected component (in red, green and blue) has 103 countries represented on the map (see Figure 4a). The countries in blue are IND (India), NAM (Namibia), and STP (Sao Tome and Principe), and they have a medium HDI. This case is less restrictive, with more heterogeneous countries and a range of HDI from 0.51 to 0.94.

With a 0.40 threshold and traditional filter (figure omitted for brevity), the elements looks sparse, but the green and red dots are still joined by an articulation point (node POL-Poland in red). Most of the countries in the green subgroup (see Figure 4b) have a high HDI. This configuration results in 3.8% of all connections, *i.e.*, 1.2% fewer than when filtered with the weak filter. The selected connected component (in red and green) has 50 countries.

With a 0.40 threshold and strong filter, the graph looks more cohesive (see Figure 3). This configuration results in 3.0% of all connections, *i.e.*, 2.0% and 0.8% fewer than when filtered with the weak and traditional filters, respectively. The selected connected component (in red) has 33 countries, and all of them have very high HDI ranging from 0.82 to 0.94. Strong

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[1] Human Development Index: https://goo.gl/so6LpE last visited in September, 2018

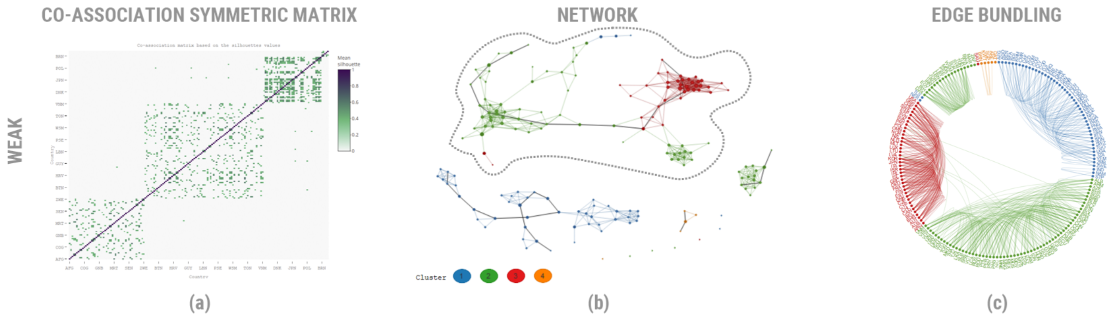

Figure 2: Visualization of the final partition for the HDI dataset with a threshold of [0.40;1] and weak filter.

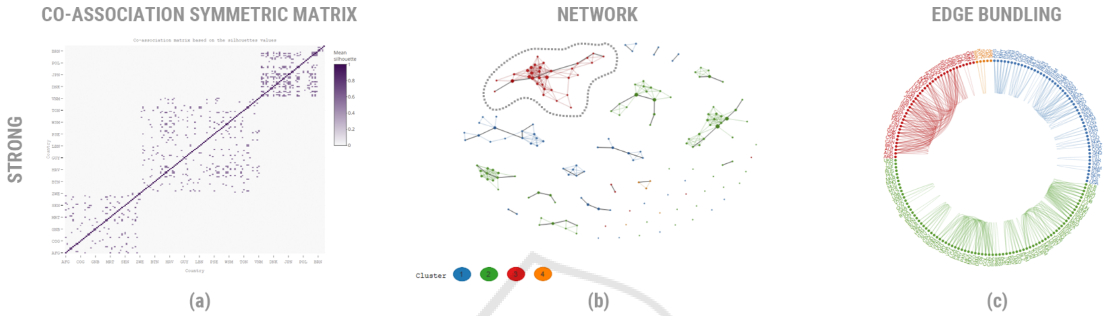

Figure 3: Visualization of the final partition for the HDI dataset with a threshold of [0.40;1] and strong filter.

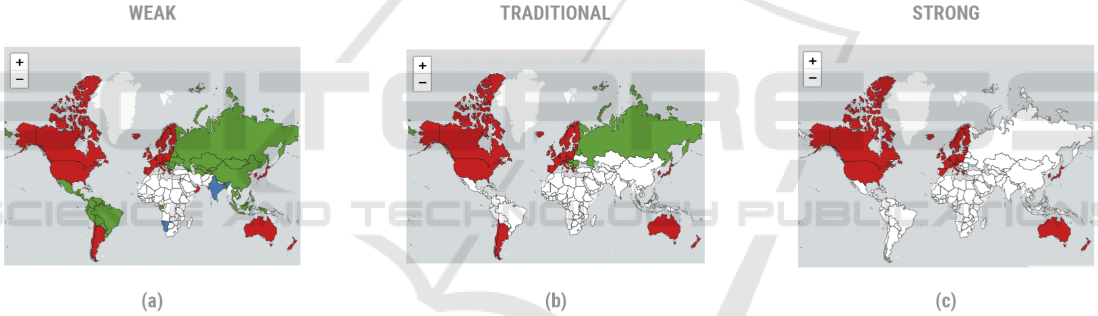

Figure 4: Visualization of the selected connected components for the HDI dataset with a threshold of [0.40;1].

filters are good to identify more cohesive groups.

5 CONCLUSIONS

This work proposed a visual tool prototype that supports the exploration of different aspects of a dataset. It is a useful tool to deeply analyze the connection between the elements, characterize the instances, and locate them on a map. This is an interesting approach for spatial analysis, where the number of elements is reduced. With all the results, the proposed research goals were accomplished. Although we tested the approach with different datasets, we could only present here one of them.

Our first step in this work was to explore different types of visualizations to assist in the analysis of the final partition. Our next step is to evaluate our tool in an empirical study to identify: (i) different insights that analysts gain when interacting with the visualizations; (ii) possible interaction design enhancements of the tool; and (iii) new features that could allow a deeper and more comprehensive analysis.

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