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A novel committee - based clustering method

Dissertação de Mestrado

Dissertation presented to the Programa de Pós-Graduação em Informática of the Departamento de Informática, PUC-Rio as partial fulfillment of the requirements for the degree of Mestre em Informática

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Abstract

González, Sonia; Lopes, Hélio (advisor). **A novel committee - based clustering method**. Rio de Janeiro, 2016. 70p. Dissertação de Mestrado — Departamento de Informática, Pontifícia Universidade Católica do Rio de Janeiro.

In data analysis, in the process of quantitative modeling and in the construction of decision support models, clustering, classification and information retrieval algorithms are very useful. For these algorithms it is crucial to determine the relevant features in the original dataset. To deal with this problem, techniques for feature selection play an important role. Moreover, it is recognized that in unsupervised learning tasks it is also difficult to define the correct number of clusters. This research proposes a method based on ensemble methods using all features from a dataset and varying the number of clusters to calculate the similarity matrix between any two instances of the dataset. Each element in this matrix stores the probability of the corresponding instances to be in the same cluster in these multiple scenarios. Notice that the similarity matrix might be transformed to a distance matrix to be used in other clustering methods. The experiments were made with a real-world dataset of the crimes in Rio de Janeiro Capital showing the effectiveness of the proposed technique.

Keywords

Feature selection; Clustering methods; Similarity matrix; Unsupervised learning;

Resumo

González, Sonia; Lopes, Hélio. **Um novo método de agrupamento baseado em comitê**. Rio de Janeiro, 2016. 70p. Dissertação de Mestrado — Departamento de Informática, Pontifícia Universidade Católica do Rio de Janeiro.

Na análise de dados, no processo de modelagem quantitativa e na construção de modelos para suporte a decisões, os algoritmos de agrupamento, classificação e recuperação de informação são muito úteis. Para estes algoritmos é crucial determinar quais atributos são relevantes no dataset. Para lidar com esses problemas, técnicas de seleção de atributos possuem um papel importante. Além disso, é sabido que na tarefa de aprendizagem não supervisionada é difícil definir o número ideal de agrupamentos. Este trabalho propõe um método baseado em um conjunto de métodos usando todos os atributos do dataset e variando o número de agrupamentos para calcular uma matriz de similaridade entre as instâncias do dataset. Cada elemento desta matriz representa a probabilidade das instâncias associadas estarem no mesmo agrupamento nos múltiplos cenários. Esta matriz de similaridade pode ser transformada numa matriz de distância e aplicada em métodos de agrupamentos. O experimento foi feito com um dataset real dos dados de crimes na capital do Rio de Janeiro, que por sua natureza mostra a necessidade do uso do método proposto.

Palavras-chave

Seleção de atributos; Métodos de agrupamento; Matriz de similaridade; Aprendizagem não supervisionada;

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1
Introduction

Nowadays, biomedicine, bioinformatics, sociology, economy, marketing, pattern recognition and computer vision are examples of research areas that use Machine Learning to generalize behaviours. In this context, machine learning techniques come to reveal the natural structure of the data in such areas. A specific kind of problem within machine learning is to group the elements of a dataset according to their similarities. This is typically called a *clustering* problem, which is classified as an *unsupervised learning* problem. In unsupervised learning there is no known association of a value (discrete/continuous) to each element in the dataset. In particular, clustering is a challenging problem due to the lack of generalized algorithms. Instead, there are specific domain solutions using particular key details according to the application area [58].

On one hand, feature selection has become an important tool for decision support systems that use thousands of features [11]. The importance of this technique is not only in the reduction of execution time, but also in the improvement of the clustering quality. There are two different classifications: attribute selection [9, 27] and attribute transformation [15, 28]. These techniques are being widely used to remove related or irrelevant attributes in machine learning algorithms: in supervised learning [8, 13] as well as in unsupervised learning [21].

On the other hand, another technique that has been accepted by the scientific community is the use of *committees* in machine learning [62]. This is because it has proven to be effective and versatile solving real life problems combined with machine learning techniques [45, 16].

The objective of this work is to improve clustering results by combining multiple clustering and feature selection algorithms. To do so, we propose a committee-based technique using feature selection algorithms and different clustering methods to generate a matrix where the position *i, j* contains the probability of the element *i* and the element *j* to be in the same cluster. In addition, this work explores the resulting matrix not only as a distance matrix for clustering generation [24], but also as an adjacency matrix with weights where statistical network analysis [37] can be applied. Finally we developed a web application with visual tools to explore and analyze the results.

In summary, the main contributions of this work are:

- A method to obtain a consensus method in unsupervised learning.
- A web application with visual tools to explore the relations between the elements of the dataset.

This dissertation is organized as follows. Section 2 presents the theoretical background. Section 3 explains in details the proposed method. Section 4 describes the visual exploration tool. Section 5 presents the experiments and the results in seven known datasets and explores two complex real-world datasets. Finally, Section 6 presents the conclusions and suggests future work.

2
Theoretical Background

This chapter presents a literature review with some of the most relevant methods about clustering (Section 2.1), feature selection (Section 2.2), and clustering ensemble in unsupervised learning (Section 2.3). Finally, Section 2.4 presents some conclusions of the chapter.

2.1
Clustering Algorithms

Cluster analysis is one of the most important strategies for dealing with the unsupervised learning problem. It divides the dataset into meaningful or useful groups called *clusters*. Clustering algorithms analyze the data searching for a partition in which the elements of each cluster are more similar to each other than to the elements in other clusters. If meaningful clusters are the goal, then the resulting clusters should capture the natural structure of the data [52].

As the goal of clustering is to group similar objects together, so it is necessary to define what similarity is, in order to measure how similar two elements are. The similarity is defined in terms of a metric or probability density model, which are both dependent on the features selected to represent the data [41].

Generally, good data analysis requires a certain expertise in the domain in question to select the correct number of clusters, or to determine which features are important and which ones can be ignored. In addition, most clustering algorithms involve some kind of randomness, so even selecting the method to find the groups can be a challenge to obtain a valuable solution.

According to [20] a similarity measure indicates the strength of the relationship between two data points. The selection of similarity or dissimilarity measures depends on the data type as well as the range of variables. In this research, the Euclidian Distance has been adopted because it the most widely used one, but one can find in the literature other distances, such as Manhattan or Minkowski [26].

There are multiple classifications of clustering methods [35, 26, 60], according to the strategies they follow. Two frequently cited methods are partitioning clustering and hierarchical clustering.

The basic idea of clustering algorithms based on partitions is to regard the center of objects as the center of their corresponding cluster [60]. A partitioning method requires the definition of a fixed number of clusters k, and one must vary this parameter to obtain the results that better fit the natural structure of the dataset. Using the parameter k, the partitioning method classifies the data in k clusters, which together satisfy the requirements of a partition: each group must contain at least one object and each object must belong to exactly one group [35]. These conditions imply that there are at most as many groups as there are objects.

The most widely used partitioning clustering methods are K-Means [43] and K-Medoids [49, 57]. This research used the K-Means method and a version of K-Medoids proposed in [35], named Partitioning Around Medoids (PAM). The K-Means is a famous and widely used clustering algorithm. First it creates random centroids given an initial number of clusters. Then it assigns to each element to the cloest cluster and recomputes the centroids taking the mean of all the objects in each cluster. It repeats this process until there are no changes minimizing the square error function (see Equation 2-1). The K-Medoids is an improvement of K-Means because the centroids are elements of the dataset called medoids. This implies it is less sensible to outliers and noise in the data, but it increases the execution time. Taking into account the dimensions of the dataset (several thousand observations), algorithms such as CLARA [35] or CLARANS [48] can be more appropriate. Partitioning methods can have a reasonably low time complexity and a high computing efficiency, but they are not suitable for non-convex data, relatively sensitive to outliers and easily drawn to local optima.

$$E = \sum_{i=1}^{k} \sum_{x \in C_i} |x - m_i|^2 \tag{2-1}$$

where x is the point in space representing the given object and m_i is the mean of the cluster C_i.

Hierarchical clustering techniques produce a nested sequence of partitions, with a single, all-inclusive cluster at the top and singleton clusters of individual points at the bottom. Each intermediate level can be viewed as combining (splitting) two clusters from the next lower (next higher) level. Hierarchical clustering techniques that start with one large cluster and split it are termed divisive, while approaches that start with clusters containing a single point, and then merge them are called agglomerative [52]. There are some different ways to calculate distances between the clusters in hierarchical clustering like Single Link (SL), Complete Link (CL) and Average Link (AL).

SL uses the closest pair of elements to calculate the distances between the clusters. CL uses the farthest elements to calculate the distances between the clusters. AL uses a mean distance between elements of each cluster. In this work we used the Average Link Hierarchical Agglomerative Method.

There are other clustering methods, such as Density-Based Spatial Clustering of Application with Noise (DBSCAN) [19] and Divisive Analysis (DIANA) [35].

Since unsupervised learning do not have the labeled data, to evaluate the quality of the resulting clusters an internal measure like the silhouette coefficient [51] is widely used. For each element i in the cluster, the silhouette coefficient is calculated using formula 2-2, and the silhouette of a group is calculated as the mean of its internal silhouettes (see 2-3).

$$s(i) = \frac{b(i) - a(i)}{max\{a(i), b(i)\}} \tag{2-2}$$

where, $a(i)$ is the average distance between i and all other data point within the same cluster and $b(i)$ is the average distance between i and the closest cluster, of which i is not a member.

The coefficient value for $s(i)$ is $-1 \leq s(i) \leq 1$.

$$S = \frac{1}{n} \sum_{i=1}^{n} s(i) \tag{2-3}$$

The silhouette measure is independent of the clustering algorithm applied to the dataset and only depends on the clustering result. Taking this into consideration, it is a good candidate to compare the outputs of different clustering methods [51].

Other clustering measures such as cohesion and separation [35, 38] are also commonly used. Moreover, in the literature we find other measures, such as Davies-Bouldin (DB) index, Dunn's index and Calinsky-Harabasz (CH) index [26], which are used to infer the cohesion separation of the clusters. A lower (DB) index indicates compact clusters and with well separated centroids. So, the minimum possible DB index is taken as optimal. On the other hand, the Dunn index aims to identify clusters with small variance among their members and as distant as possible from member of other clusters. A high value of the Dunn index implies a high quality clustering. The CH uses a sum of the squares of the distances between and within the clusters to evaluate the quality of the results.

To compare the results we obtained, which will be presented in Section 5.1, measures such as Proportion of correct classifications (P) [Agreement proportion in classification vectors], Adjusted Rand index (AR), Variation in Information (VI) [Variation in information of classification vectors] [44] and

Normalized Mutual Information (NMI) [53] will be used.

Mutual Information is a measure that, given any two random variables, quantifies the information that one variable shares with the other, that is, how much information they share [12]. As shown in [53], the normalized mutual information between 0 and 1 is calculated using equation 2-4.

$$NMI(X,Y) = \frac{I(X,Y)}{\sqrt{H(X)H(Y)}} = \frac{H(X)+H(Y)-H(X,Y)}{\sqrt{H(X)H(Y)}}, \tag{2-4}$$

where X and Y are two random variables and H(X), H(Y), H(X,Y) the entropy of X, Y and X join Y, respectively.

So the whole process of clustering can be defined by the following steps [6]:

1. Feature Selection: Extract and select the most representative features from the original dataset.

2. Similarity (or Proximity) Measure: Define the measure of similarity or dissimilarity, calculated over the selected features.

3. Clustering Criterion: Define how distance patterns determine cluster likelihood, preferring circular to elongated clusters.

4. Clustering Algorithm: The search method used with the clustering criterion to identify clusters.

5. Validation of Results: Using appropriate tests, usually statistical in nature.

6. Interpretation of Results: Domain experts interpret the resulting clusters and give a practical explanation of the results.

The feature selection problem will be reviewed in the next section (2.2).

2.2 Feature Selection Algorithms

In machine learning and in statistics, feature selection is a strategy for selecting a subset of relevant features to build robust learning models [50]. It is also known as variable selection, feature reduction, attribute selection or variable subset selection. Selecting the most relevant feature subset based on certain evaluation criteria is essentially a combinatorial optimization problem, which is computationally expensive [10].

Feature selection methods are largely studied separately according to the type of learning: supervised or unsupervised [63]. In supervised learning, the feature selection algorithms maximize some function of predictive accuracy. When using the class labels as prediction, it is natural to keep only the features related to the classification. But in unsupervised learning, the classes are not given. Therefore, some important questions arise, such as: How many features should be kept? and Why not use them all? The point is that not all features are relevant, some of them may be redundant, and some others can misguide the clustering results. Examples of the first case are correlated variables because they provide no additional information. In the latter case, the classifiers such as gender can turn the direction of the search into wrong paths. So, reducing the number of features facilitates unsupervised learning and prevents some algorithms from breaking down when dealing with high dimensional data [41]. According to [18], ”The goal of feature selection for unsupervised learning is to find the smallest feature subset that best uncovers ”interesting natural” groupings (clusters) from data according to the chosen criterion.”

The feature selection methods can be classified in a number of ways. The most common ones are: filter, wrapper, embedded and hybrid methods [36, 27, 34]. In the wrapper approach [18], the clustering algorithm is used as a black box and the basic idea is to search through a feature subset space, evaluating each candidate subset, F_t, by first running the clustering algorithm in space F_t and then evaluating the resulting clusters and feature subset using our chosen feature selection criterion. This process is repeated until the best feature subset with its corresponding clusters is found.

A search algorithm is needed to guide the feature selection process as it explores the space of all possible combinations of features. A search procedure usually examines a small portion of the search space, since this space can be enormous. When determining which state to evaluate next, a search algorithm makes use of the values of previously visited states in order to guide the feature selection engine into those regions of the search space where individual states have low error rates and few included features [17].

The most common search strategies used with multivariate filters can be categorized into exponential, sequential and randomized algorithms. The exponential algorithms evaluate a number of subsets that grows exponentially with the feature space size. The sequential algorithms add or remove features sequentially (one or few at a time), which may lead to local minima. The random algorithms incorporate randomness into their search procedure, which avoids local minima [17, 34].

Making an exhaustive search is impractical because the number of operations is exponential: the number of possible subsets is 2^f, where f is the number of features. For each subset the selection criterion should be maximized or minimized. On the other hand, it is very common to use greedy methods to avoid exhaustive search. The sequential search strategy usually employs the greedy hill-climbing method to generate the feature subset. Two possible methods for unsupervised feature selection in this context are Sequential Forward Selection (SFS) and Sequential Backward Elimination or Selection (SBS).

The algorithm for SFS [17] begins by adding the individual feature which obtains the best performance to the empty set of best features. Next, all the remaining features are tested together with this single feature to see which combination performs the best. The pair of features providing the best result is assigned to the best set of features. Continue adding features to the set in this way until the result of the evaluation function reaches some pre-determined threshold amount. The search stops at this point. Finally, the optimal set of features returned by this heuristic are those features contained in the best set.

The SBS algorithm works in the opposite manner when compared to SFS, since it removes features instead of adding them start with a set of all features. At each step in the algorithm, the feature whose removal turns in the smallest decrease of the value of the evaluation function is removed. In some cases, removing a feature may actually increase the value of the evaluation function, and so it should be removed as well. The algorithm halts when it is impossible to remove any single remaining feature given a predefined threshold [17].

Both methods visit only a small fraction of the space. The disadvantage in SFS is called "nesting effect" since, once selected, features cannot be later discarded. In the case of SFS, once discarded, a feature cannot be re-selected [47].

In conclusion, both forward and backward selection procedures give simple search techniques which avoid exhaustive enumeration [25]. However, the selection of the optimal subset is not guaranteed.

Other methods proposed in [17] like Bi-Directional Search, (p, q) Sequential Selection (PQSS), Simulated Annealing (SA) and Principal Features Analysis (PFA) [42] could be used. PQSS is a generalization of the SFS and SBS methods. The idea is to add p features and remove q features in each step. Bi-Directional Search uses SFS and SBS method at same time and the search ends when it converges in the middle of the search space. SA is a local search metaheuristic to obtain a subset of features with the best possible quality. It has a mechanism to avoid local optima by accepting worse solutions. The PFA method is based on Principal Component Analysis [33] and on reducing the original set of features to the ones that contain the essential information.

2.3 Ensemble Clustering

Different clustering methods applied to the same dataset produce different results. There is no silver bullet. Moreover, each method has both advantages and disadvantages. So, the idea of combining multiple clustering results seems reasonable. The clustering ensemble technique aims to combine multiple clustering results from the same dataset into a final clustering. Several papers make references to this problem [53, 22, 55, 24, 58, 56, 61, 30]. They all agree that it is a difficult problem.

There are several approaches to generate cluster ensemble, but in general they can be split in two main directions. The first one is to use different data representations and structures, such as graphs, vectors or strings, as well as to reduce the dimensionality of the problem by selecting some of the features to create different feature spaces. The second approach is to use different clustering algorithms and parameters, i.e., to apply multiple methods, the same method with different parameters, or even to use distinct dissimilarity measures to generate the desired partition [24].

The problem of combining the partitions into the final clusters has been addressed by several works. Among the most popular clustering ensemble techniques we find methods based in Co-association Matrix, Grap and Hypergraph Partitioning and Finite Mixture Models. There are other techniques available in [56]. [53] presented three effective and efficient techniques based on hypergraph representation for obtaining high quality combiners. The first is Cluster-based Similarity Partitioning Algorithm (CSPA); this technique uses the relation between the elements to build a co-association matrix and then reclusters the objects. The second one is HyperGraph Partitioning Algorithm (HGPA); this technique build clusters by removing edges from the hypergraph. The third one is Meta-Clustering Algorithm (MCLA). This method is based on the analysis of the similarity between clusters, treating them as nodes in the hypergraph and finally creating a meta-cluster using this hypergraph. [30] presented an algorithm based on bipartite graphs called Graph Partitioning with Multi-Granularity Link Analysis (GP-MGLA). They define levels of granularity, namely: instances, ensemble, and final clustering, then build a bipartite graph using instances and clusters to extract the consensus clustering. Another approach based on the finite mixture model, offered in [55] as a probabilistic model using the Expectation Maximization (EM) algorithm

[14] in order to assign labels to elements in the partitions. In addition, [24] explored the evidence accumulation (EAC) matrix and presented a framework based on the co-association technique for extracting a consensus clustering from the clustering ensemble, applying Average Link (EAC-AL) and Single Link (EAC-SL). Based on this work, [58] proposed to incorporate probability theory into the evidence accumulation matrix to create a probability accumulation. [61] proposed a solution to overcome uncertainty in the data by looking in the ensemble the different clusterings and selecting the ones that agreed the most, called Ensemble Clustering Matrix Completion (ECMC). Another approach to the EAC presented in [30] was the Weighted Evidence Accumulation Clustering (WEAC) method. This method include weights to penalize low quality clusterings and agglomerative methods (WEAC+SL, WEAC+AL, WEAC+CL) to obtain the consensus partition.

2.4 Discussion

Clustering ensemble has become a modern approach and a cutting edge technique when solving clustering problems with unconventional structures, due to its learning capabilities. It is a flexible technique because, according to the number of partitions, co-relation criteria and the number of iterations can be adjusted to solve a range of widely diverse problems. Even when the focus of the ensemble methods is to generate a consensus result which best fits the natural structure of the dataset, they all try different approaches and present diverse techniques to solve the problem. In general, there is no single way of dealing with ensemble clustering but a method with fixed and variable spots to fill in.

To explore the relationship between objects, given a subspace of the features, this work made a modification in both methods of feature selection. In case of the SFS, the method stops when the final set of features contains all features. In the SBS case, the method stops when the final set of features is empty. Even when the exploration goes beyond the threshold parameter, the relevant features keep this value as a limit to decide their importance.

Inspired on the similarity matrix [61], co-association or evidence accumulation matrix [24], probability accumulation matrix [58] and using the silhouette coeffiecient as in [38] to measure the association between two elements, this work proposes a new method to create a similarity matrix, which is presented in Chapter 3.

3 Method for calculating the similarity matrix

The new method proposed in this chapter for calculating the similarity matrix is part of the idea of clustering ensemble in unsupervised learning. The method is comprised of three stages: the first generates the clustering ensemble, the second combines the results of the multiple scenarios generated and the last one creates a new partition using the combined data. Figure 3.1 illustrates an outline of the method as an activity diagram.

The two important characteristics of the method concern the resulting relevant features and the number of times two objects are assigned to the same cluster. Our method is independent of the clustering method and feature selection algorithms. The feature selection methods used are the sequential SFS and SBS. Each one of theme adopted clustering methods such as K-Means, K-Medoids (PAM) and Hierarchical Clustering with Average Link.

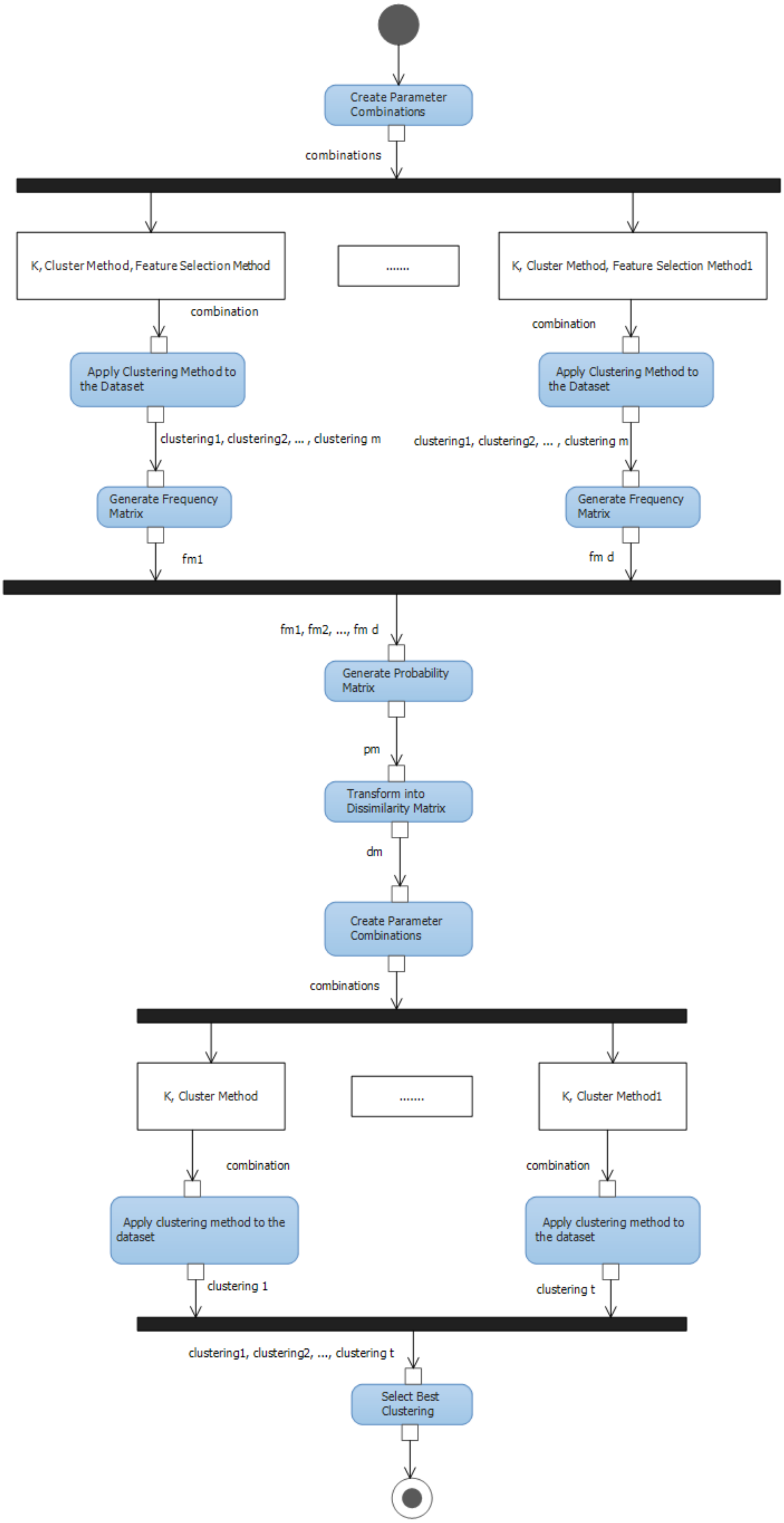

Create Parameter Combinations
combinations
K, Cluster Method, Feature Selection Method
....
K, Cluster Method, Feature Selection Method1
combination
combination
Apply Clustering Method to the Dataset
Apply Clustering Method to the Dataset
clustering1, clustering2, ... , clustering m
clustering1, clustering2, ... , clustering m
Generate Frequency Matrix
Generate Frequency Matrix
fm1
fm d
fm1, fm2, ..., fm d
Generate Probability Matrix
pm
Transform into Dissimilarity Matrix
dm
Create Parameter Combinations
combinations
K, Cluster Method
....
K, Cluster Method1
combination
combination
Apply clustering method to the dataset
Apply clustering method to the dataset
clustering 1
clustering t
clustering1, clustering2, ..., clustering t
Select Best Clustering

Figure 3.1: Outline of the method.

In the first stage, the ensemble is generated by combining the feature selection methods varying the clustering methods and the number of clusters k, where k varies from 2 to an input parameter l (by default $l = N/2$ where N is the total number of elements). Each possible combination is called a scenario. A solution belongs to a single scenario and can be defined as a tuple $< k, clm, fsm, rf, silh, fm >$, where:

- k is the number of clusters
- clm corresponds to the clustering method used
- fsm is the method of feature selection employed
- rf are the relevant features in the resulting clustering
- $silh$ is the value of the silhouette coefficient
- fm corresponding to the resulting frequency matrix

The frequency matrix (fm) contains in the position (i, j) the mean silhouette coefficient of the elements i and j, normalized between 0 and 1 (see Algorithm 2). The silhouette coefficient can be affected by outlier elements in the cluster. So, to avoid this issue the median was used instead of the mean. In the second stage, the similarity matrix sim is generated from the multiple scenarios as shown in Algorithm 1.

Algorithm 1 Algorithm to Generate and Combine the Multiple Scenarios

```
procedure GenerateScenarios($data, K, CMethods, FSMethods, threshold$)
    $sol\_scen \leftarrow list()$
    for each $k$ in $K$ do
        for each $cm$ in $CMethods$ do
            for each $fsm$ in $FSMethods$ do
                [rf, clMatrix, sMatrix, silh] ← CreateClustering(data, k, cm,
fsm, threshold)
                fm ← CreateFrequencyMatrix(clMatrix, sMatrix)
                $scenario$ ← [k, clm, fsm, rf, silh, fm]
                add $scenario$ to $sol\_scen$
    $sum\_fm \leftarrow$ add the $fm$ from multiple scenarios
    return $sim \leftarrow sum\_fm/|sol\_scen|$
```

To quantify the strength of the bind between two objects, the frequency matrices are filled and finally divided by the number of scenarios, creating the similarity matrix sim as shown in Algorithm 1, allowing further exploration of objects and their relationships. The bind between two objects i and j is defined as the element $sim_{i,j}$ and its value ranges from zero to one. So, it can be interpreted as a probability of element i being in the same cluster as element j. The relation between elements i and j is strong if it is greater than 0.50. This means that they are in the same group in more than half of the clusterings. The relation is weak when it is lower than 0.20. This means that they are in the same cluster in less than 20% of the clusterings.

Algorithm 2 Algorithm to Create a Frequency Matrix

```
procedure CreateFrequencyMatrix($clusteringMatrix, silhouettesMatrix$)
    $fm \leftarrow$ initialized with 0
    $n \leftarrow$ number of rows of $clusteringMatrix$
    $m \leftarrow$ number of columns of $clusteringMatrix$
    for $d = 1$ to $m$ do
        $s \leftarrow silhouettesMatrix_d$
        for each $i, j = (1, 1)$ to $(n, n)$ do
            $sm_{i,j} = \frac{\frac{s_i+s_j}{2}+1}{2} = \frac{1}{2} * (\frac{s_i+s_j}{2} + 1) = \frac{s_i+s_j+2}{4}$
            if $clusteringMatrix_d[i] == clusteringMatrix_d[j]$ then
                $fm_{i,j} \leftarrow fm_{i,j} + sm_{i,j}$
    return $\frac{fm}{m}$
```

In the result of a classical clustering algorithm, any two objects can either be in the same cluster or in different clusters, regardless of their bond. In other words, an element can have a strong bind with an element outside his cluster and a weak bind with elements inside it. For instance, when an element is in the boundaries between a group of clusters, it can be in any one of them, or when the clustering method has a random component like K-Means.

The main objective of this method is to obtain the similarity matrix *sim* and use it to verify the strength of the binds. As part of the third stage, each element $sim_{i,j}$ of this matrix can be transformed using Equation 3-1 or using Equation 3-2 to be used as the distance matrix *dm* in other clustering processes.

$$dm_{i,j} = 1 - sim_{i,j} \tag{3-1}$$

$$dm_{i,j} = 1 - \sqrt{sim_{i,j}} \tag{3-2}$$

Varying the number of clusters and the clustering methods, a new set of partitions is generated using the dissimilarity matrix *dm* as distances between the elements. Notice that here the features are not used to calculate distances like in the first stage of the method, only the relationships between the elements. Finally, the partition with the best silhouette coefficient is used to generate a recommendation of the final clustering and the number of clusters.

Having this in mind, this final recommendation is defined as a tuple $< sim, rfs, fcl, k >$ where *sim* is the similarity matrix, *rfs* are the relevant features, *fcl* is the final clustering and k is the number of clusters in *fcl*. This recommendation is given the initial parameters, namely: a set of cluster numbers, a set of clustering methods, and a set of feature selection methods.

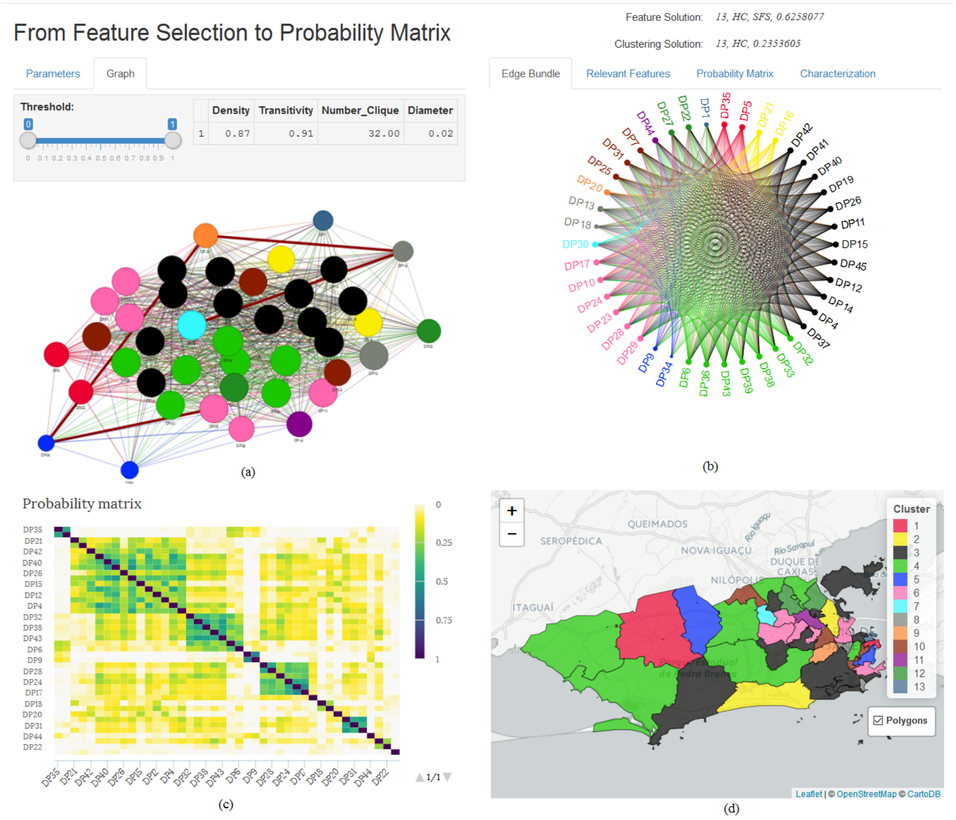
4
Visual Exploration Tools based on the Similarity Matrix

This chapter proposes some visual exploration tools of the similarity matrix, constructed according to the method proposed in the previous chapter, to facilitate the understanding of the internal structure of the final clustering.

At the user interface, the user sets a pair $< min, max >$ as a parameter, named *interval threshold* or simply *threshold*, with the following property: $0 \leq min \leq max \leq 1$.

The visual tool uses this interval to filter the data in the similarity matrix, removing all the values lower than *min* and all the values greater than *max*. The visualizations are then focused on analysing the sensibility of the threshold on the similarity matrix. Filtering the matrix also produces a clearer representation of the desired data and a better definition of patterns in the matrix.

In the proposed interface, the screen is composed of four sections (see Figure 4.1), three of them related to the similarity matrix from different points of view (heat map, graph and edge bundle) and a fourth section dedicated to the spatial visualization of the elements (map), in the case of georeferenced data. Even when showing different points of view, all the sections are related to allowing users to explore the one which they deem more useful for their current purposes. In addition, the colors used to represent each cluster serve as a visual aid to relate the different sections, with the exception of the heat map, which has its own color scale.



From Feature Selection to Probability Matrix

Feature Solution: 13, HC, SFS, 0.6258077

Clustering Solution: 13, HC, 0.2353605

Threshold: 0 – 1

	Density	Transitivity	Number_Clique	Diameter
1	0.87	0.91	32.00	0.02

Figure 4.1: Visualization components of the application.

4.1 Similarity Matrix as a Heat Map

The heat map is a graphical representation of data where the individual values contained in a matrix are represented as colors. This visualization allows to compact large amounts of information into a small space to bring out coherent patterns in the data [59].

The data is sorted using the cluster numbers from the recommended solution in order to form the patterns corresponding with the clusters in the heat map. There are specific patterns in the heat map formed around the main diagonal with rectangular shape containing the elements belonging to the same cluster. Let us call this patterns blocks. Visualizing the data (see Figure 4.1c) in this way allows the users to find darker regions, have an idea of the cohesion of groups, identify and count the blocks in the result. In Figure 4.1c one can see around eleven blocks.

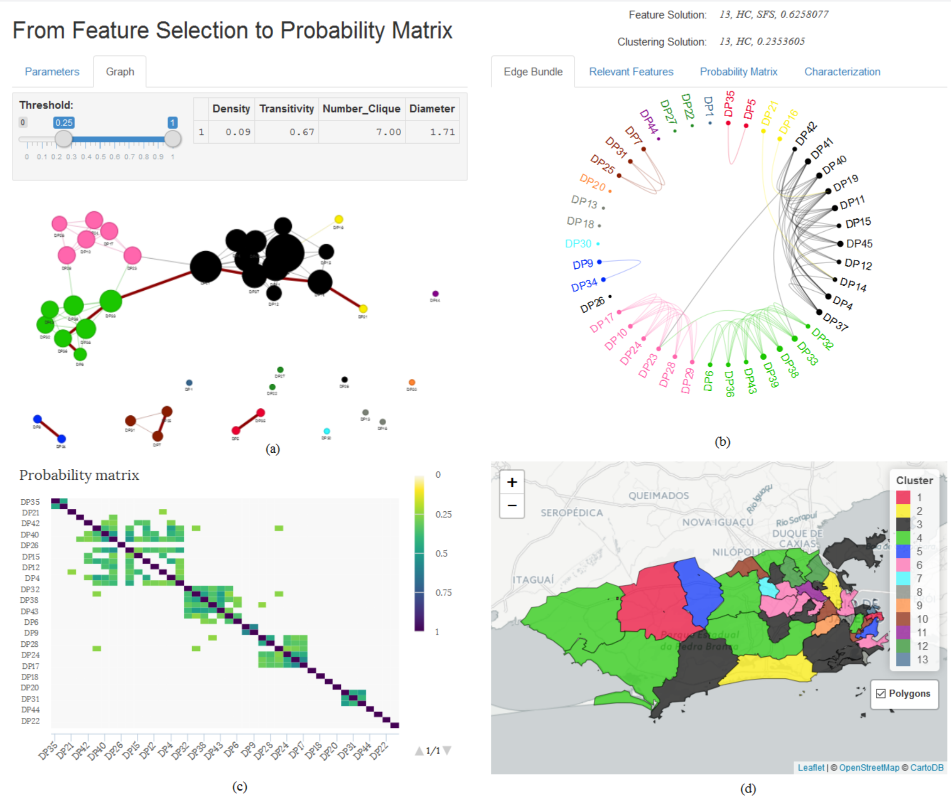
In the representation of the Similarity matrix as a heat map it is possible to notice that the main diagonal is one (dark color). In other words, it represents the probability of the element and itself to be in the same cluster. There are pairs with zero (light color) meaning that these two elements have no binds. A continuous color palette going from light to dark has been adopted to represent the probability of the two elements being on the same cluster.

4.2 Similarity Matrix as a Hierarchical Edge Bundling

Hierarchical edge bundling is a flexible and generic method that can be used in conjunction with existing tree visualization techniques to enable users to choose the tree visualization that they prefer and to facilitate integration into existing tools. It reduces visual clutter when dealing with large numbers of adjacency edges and provides an intuitive and continuous way to control the strength of bundling. Low bundling strength mainly provides low-level, node-to-node connectivity information, whereas high bundling strength provides high-level information as well by implicit visualization of adjacency edges between parent nodes that are the result of explicit adjacency edges between their respective child nodes [29].

At first glance, it lets you know the number of items per group. If an item is selected, users 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 with which it is linked are in the same group (and thus represented in the same color, in our approach), they reinforce the idea that this group is very cohesive.

The edges are filtered using the threshold parameter. Notice here that in the edge bundling one can turn the threshold into a percentage filter, allowing users to answer questions like: Which elements are connected in over 25% of the scenarios (see Figure 4.2b)? This section focuses on the objects and their relations, rather than on the clusters. Given the threshold, one may notice the connection between the elements in different clusters (e.g., elements DP23 with DP41 and DP33, DP21 with DP14 and DP16 with DP19 in Figure 4.2b); groups without any connections (e.g., DP22 and DP27, DP13 and DP18 in Figure 4.2b); and isolated elements (e.g., DP1, DP20, DP44 in Figure 4.2b).



From Feature Selection to Probability Matrix

Feature Solution: *13, HC, SFS, 0.6258077*

Clustering Solution: *13, HC, 0.2353605*

Parameters | Graph

Edge Bundle | Relevant Features | Probability Matrix | Characterization

Threshold: 0.25 – 1

	Density	Transitivity	Number_Clique	Diameter
1	0.09	0.67	7.00	1.71

Figure 4.2: Visualization of the similarity matrix in the edge bundling with threshold range 0.25 to 1.

4.3 Similarity Matrix as a Graph

To visualize the similarity matrix in a graph, one can define a complete undirected weighted graph as $G¡V, E¿$ where V are the elements of the dataset. The edges E have a weight value equal to the probability with which the two elements are together, given 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 in the interface, it shows the probability associated with its pair of nodes.

This section (see Figure 4.2a) shares the threshold of the previous sections, so setting a threshold value 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, particularity, edge in red color.

4.4 Clustering Solution in Map

Georeferenced objects, such as schools, police stations, neighborhoods, cities and countries, are visualized in a map to easily analyze whether adjacent elements belong to the same cluster; to compare regions; to uncover a geographic pattern of the data; to locate which regions should be further analyzed by domain experts (see Figure 4.1d); and to investigate why some regions have unexpected behaviours. When one clicks on a region, a pop-up with some data as region name about it appears.

4.5 Discussion

The visualizations adopted in this approach support the descriptive analysis of the results. Combining different points of view, users can achieve more sophisticated results and explore the data more efficiently. Some of the most interesting facts about the data can be in one articulation point or an outlier, and conventional exploration of the data can cause users to miss some of these key details, which are relevant qualitative information that can explain or help to understand a problem. Enhancing the user experience not only is a good practice, but it also reduces the time spent on the descriptive analysis of the dataset in a research project.

5 Experiments and Results

This chapter presents the experiments and the results obtained. To evaluate the performance of the method (Section 5.1), first it presents a comparison between several clustering methods like K-Means, PAM, HC with Average Link and the proposed method (subsection 5.1.1), and then it shows another comparison between clustering methods based on ensemble techniques and our method (subsection 5.1.2). The comparison measures the quality of the resulting clusters using normalized mutual information. Section 5.2 shows several experiments applying our method in two real life datasets. The first one is about the crime data in the State of Rio de Janeiro (subsection 5.2.1) and the second one is about the Human Development Index in the year 2014 (subsection 5.2.2). Section 5.3 concludes this chapter with a discussion about the results.

5.1 Performances of our Method

In this experiment were used seven well known datasets. All of them are available in the UCI Machine Learning Repository [40]. Table 5.1 gives details of these datasets.

	Dataset	Nb.Instances	Nb.Attributes	Nb.Classes
1	Iris	150	4	3
2	Wine	178	13	3
3	Seeds	210	7	3
5	Glass	214	9	6
4	Breast Cancer	683	10	2
6	Yeast	1484	8	10
7	Segmentation	2310	19	7

Table 5.1: Overview of datasets.

In order to compare the clustering methods, several quality measures were adopted Proportion of correct classifications (P), Adjusted Rand index (AR), Variation in Information (VI) [44]. In addition we also used the Silhouette coefficient (Sil) and the Normalized Mutual Information (NMI).

The clustering methods used are available in `R` [1], K-Means and HC-AL from the `stats package`, PAM from `cluster package`; the measures Silhouette from `cluster package`, P, AR and VI from `MixSim package` and, finally, NMI using the `infotheo package`.

The clustering methods used were divided in two groups: first, individual clustering algorithms and second a group based on ensemble clustering.

5.1.1
Comparison with individual clustering methods

The individual clustering method used in this experiment are K-Means, PAM and HC with Average Link and the results are given in Table 5.2. In bold are highlighted the better results of each method according to Proportion of correct classifications (P) and Normalized Mutual Information (NMI).

	Dataset	Method	P	AR	VI	Sil	NMI[a]
1	Iris	K-Means	0.580	0.433	0.818	0.550	0.593
2		PAM	0.847	0.642	0.713	0.406	0.675
3		HC-AL	0.687	0.562	0.524	0.696	0.728
4		Meth - PAM	**0.960**	0.886	0.298	0.362	**0.864**
5		Meth - HC-AL	**0.960**	0.886	0.298	0.362	**0.864**
6	Wine	K-Means	0.966	0.897	0.270	0.360	0.876
7		PAM	0.910	0.741	0.471	0.311	0.783
8		HC-AL	0.388	-0.005	1.184	0.178	0.031
9		Meth - PAM	**0.978**	0.933	0.192	0.371	**0.912**
10		Meth - HC-AL	**0.983**	0.949	0.156	0.370	**0.928**
11	Seeds	K-Means	**0.919**	0.773	0.598	0.453	**0.728**
12		PAM	**0.910**	0.747	0.626	0.468	**0.714**
13		HC-AL	**0.881**	0.686	0.770	0.494	0.649
14		Meth - PAM	0.867	0.653	0.796	0.407	0.637
15		Meth - HC-AL	**0.881**	0.690	0.681	0.401	**0.689**
16	Glass	K-Means	**0.453**	0.170	2.021	0.369	**0.315**
17		PAM	0.430	0.157	2.033	0.396	0.306
18		HC-AL	0.379	0.019	1.618	0.412	0.149
19		Meth - PAM	**0.439**	0.197	1.997	0.251	**0.348**
20		Meth - HC-AL	**0.472**	0.218	1.521	0.244	**0.354**
21	Breast Cancer	K-Means	**0.958**	0.836	0.343	0.511	**0.733**
22		PAM	**0.965**	0.863	0.299	0.509	**0.768**
23		HC-AL	0.647	-0.003	0.665	0.626	0.011
24		Meth - PAM	0.956	0.830	0.343	0.508	0.732
25		Meth - HC-AL	**0.947**	0.798	0.382	0.509	**0.699**

Table 5.2: Performance of the K-Means, PAM and HC-AL clustering methods and the proposed method in terms of NMI.

[a] An example of how NMI is calculated is shown in Figure A.1.

	Dataset	Method	P	AR	VI	Sil	NMI
1	Yeast	K-Means	**0.414**	0.163	2.704	0.154	**0.289**
2		PAM	**0.380**	0.156	2.747	0.182	**0.289**
3		HC-AL	**0.324**	0.019	1.813	0.533	**0.120**
4		Meth - PAM	0.291	0.095	3.078	0.100	0.207
5		Meth - HC-AL	0.312	-0.021	2.459	0.215	0.104
6	Segmentation	K-Means	0.532	0.413	1.625	0.258	0.575
7		PAM	**0.677**	0.507	1.528	0.271	0.606
8		HC-AL	0.435	0.238	1.192	0.361	0.624
9		Meth - PAM	0.646	0.507	1.349	0.282	**0.646**
10		Meth - HC-AL	**0.578**	0.442	1.115	0.474	**0.675**

Table 5.3: Performance of the K-Means, PAM and HC-AL clustering methods and the proposed method in terms of NMI.

In the first and the second dataset, our method correctly classifies almost all the elements, very different from the individual methods. In the other dataset the results are very similar. In the variation of the information we can see that the method has less information varying in the obtained results. The normalized mutual information is better in the first two datasets and similar in the remaining ones. It is important to notice here that the silhouette values are in most cases worse than the individual methods, proving that high values of the silhouette coefficient do not imply a clustering fitting the natural data structure.

5.1.2 Comparison with ensemble methods

In order to compare the result obtained from the method we used several algorithms previously mentioned in section 2.3, such as MCLA, CSPA, HPGA, EAC, GP-MGLA, WEAC and ECMC. In addition,we used another six methods. In [61] they compared their results against the Ensemble clustering based on Quadratic Mutual Information (QMI) [54]. This method uses the EM algorithm to maximize the mutual information measure between the final clustering and the ensemble. The Divisive Clustering Ensemble with Automatic Cluster Number (DiCLNES) [46] was another method used in the comparisons and computes the consensus partition based on minimum spanning trees. In [30], we find four more algorithms to compare with our approach. The first one is the Hybrid Bipartite Graph Formulation (HBGF), presented in [23]. In this method a graph is built containing the elements and the clusters together, the bipartite graph is created with edges between elements and clusters. The second is the Weighted Consensus Clustering (WCC) [39]. This method assigns weights to the ensemble clusterings to unbalance and adapt their influence in the final solution. The third is SimRank Similarity Based Method (SRS) [31], whith proposes an analysis of the neighborhood of the elements, following the principle that two elements are similar if their respective neighbors are similar too. The last one is the Weighted Connected Triple Method (WCT) [32]; this method builds a link network model from the ensemble in order to compute their similarity and finally refine the similarity to reach the consensus clustering. In the EAC, WEAC, ECMC, SRS and WCT there were used three variants of the agglomerative clustering (AL, CL, and SL).

The datasets used in the comparison are well known in the scientific community and several previous work shows the resulted measures on them. The other methods results are based on the values of the rows with NMI from Table III in [61] and the column True-k from Table 6 in [30]. These results are compared with our method in Tables 5.4 and 5.5 respectively. In bold are highlighted the better results of each method using the NMI measure.

Method	Breast-Cancer	Yeast	Segmentation
ECMC	0.519	**0.277**	0.540
MCLA	0.501	0.113	0.024
CSPA	0.489	0.161	0.502
HPGA	0.382	0.106	0.387
EAC_SL	0.442	0.092	0.415
EAC_AL	0.418	0.271	0.530
QMI	0.510	0.202	0.537
DiCLENS	0.512	0.089	0.349
Meth_PAM	**0.732**	0.207	**0.646**
Meth_HC_AL	**0.699**	0.104	**0.675**

Table 5.4: Performances of different ensemble clustering methods and the proposed method in terms of NMI.

Table 5.4 illustrates only the NMI measures for the three datasets. One can see that our method is better than all the other methods in the first and third dataset, and in the second dataset the results are similar. Notice that the ensemble clusters methods shown in Table 5.4 are not better than a simple K-Means (see final of Table 5.2 column NMI) while the results we present are better or similar.

	Method	Breast_Cancer	Iris	Seeds	Yeast	Wine	Segmentation
1	GP_MGLA	0.618	0.695	0.514	0.167	0.717	0.549
2	WEAC_AL	0.596	0.673	0.517	0.147	0.664	0.533
3	WEAC_CL	0.073	0.653	0.197	0.093	0.177	0.317
4	WEAC_SL	0.030	0.493	0.317	0.046	0.235	0.420
5	HBGF	0.648	0.640	0.493	0.181	0.647	0.491
6	WCC	0.459	0.539	0.493	**0.208**	0.581	0.527
7	EAC_AL	0.512	0.667	0.399	0.109	0.444	0.503
8	EAC_CL	0.058	0.497	0.206	0.065	0.168	0.323
9	EAC_SL	0.010	0.632	0.244	0.034	0.104	0.413
10	ECMC_AL	0.399	0.140	0.126	0.021	0.154	0.081
11	ECMC_CL	0.358	0.181	0.146	0.022	0.159	0.102
12	ECMC_SL	0.259	0.272	0.064	0.017	0.078	0.026
13	SRS_AL	0.519	0.676	0.438	0.122	0.254	0.513
14	SRS_CL	0.489	0.648	0.356	0.116	0.407	0.530
15	SRS_SL	0.029	0.661	0.344	0.034	0.001	0.411
16	WCT_AL	0.075	0.673	0.403	0.120	0.478	0.494
17	WCT_CL	0.110	0.644	0.326	0.095	0.396	0.492
18	WCT_SL	0.124	0.650	0.289	0.035	0.184	0.416
19	Meth_PAM	**0.732**	**0.864**	**0.637**	0.207	**0.912**	**0.646**
20	Meth_HC_AL	**0.699**	**0.864**	**0.689**	0.104	**0.928**	**0.675**

Table 5.5: Performances of different ensemble clustering methods and the proposed method in terms of NMI.

In Table 5.5, the comparisons are only taking into account the NMI coefficient. The proposed method has a better result in five of the six datasets. In the other one the best results of our method is 0.207, only lower than WCC with 0.208. Notice here that in the Wine dataset the best result of the methods is 0.717 and the worst proposed in the method is 0.912.

5.2 Exploring Real World Datasets

Taking into consideration the performance of our method with the datasets of Table 5.1, it makes sense to apply our method in datasets where the classification is unknown, i.e. in a real unsupervised dataset.

5.2.1 Exploring the CrimesRJ Dataset

In Rio de Janeiro, the public access to data is not straightforward. The Public Safety Institute (ISP) publishes monthly spreadsheets since 2002, orginized by public safety area (Áreas de Segurança Pública – AISPs) [2]. An AISP is a territorial subdivision for administrative purposes. The state is divided in 41 AISPs, and each one is composed of a distinct number of DPs, where crime occurrences are recorded. Therefore, a monthly report is composed of 41 spreadsheets, and each spreadsheet includes the total number of occurrences for 39 kinds of crime for each DP that comprises the AISP.

To exemplify the difficulty in obtaining data, in a temporal analysis of a certain type of crime it would be necessary to download all the monthly files, almost 150 at the time of this study, to locate in each file the AISP, the DP, the type of crime, and only then collect the desired information. This way of publishing public data can satisfy a legal obligation, but it certainly does not serve the society in a convenient way.

The process of gathering data comprises several activities:

1. processing criminality data from ISP spreadsheets;
2. gathering spatial data from ISP and IBGE [3];
3. establishing the correspondence of the spatial data from each source; and
4. associating demographic data (IBGE) to the geographic areas.

The monthly spreadsheets were obtained from the ISP website, which does not have an area for direct access (e.g., FTP). We developed an algorithm that scrapes the ISP web page, identifies the name of the data files and downloads them to local storage. By executing this program we can obtain all the available spreadsheets. The data in all spreadsheets were interpreted, aggregated, and stored in a single file without losing information. This operation was not straightforward, because those monthly spreadsheets present variations in structure and in the identification of type of crime, which require a series of adjustments. For instance, to identify the type of crime we built a dictionary to relate a standard noun to its diverse aliases adopted over the years.

All contextualization of data on criminality depends on several social and economic factors, which interact and change according to their location, city, neighborhood, etc. Therefore the delimitation of the territory to which crimes are associated is fundamental to the analyses. In the data at hand, the most fine-grained territory delimitation is the DP, i.e., the most detailed information is the number of occurrences of each type of crime recorded at each DP. In

May 2015, ISP made available in its website the geographic boundaries of the DPs in digital format (as *shapefiles*). With these official digital maps one can truly recognize the boundaries of each DP. In theory, with that information it would be possible to relate those territories with the information about the population (associated to territories called census sectors by IBGE) and build a socioeconomic database to enrich the analyses. The apparently simple idea of aggregating the census sectors with the DP areas proved to be complicated. The digital DP maps did not coincide with the census sectors boundaries, making it impossible to automatically relate or aggregate the data. Figure 5.1 illustrates the problem. The figure on the left shows the boundaries of a DP (in red) over the boundaries of census sectors in the city of Rio de Janeiro in 2010, and figure on the right shows the boundaries of the census sectors over the DP boundaries. Notice that some red lines still appear in the right figure, indicating that on those locations the boundaries do not coincide. This generates a large number of small polygons (*slivers*) in the overlays. An even coarser error can be observed on the top of both figures, where a region of a DP in the capital region is outside the boundaries of the city itself. To solve this problem, we developed an algorithm to automatically correct distortions and associate the census data to each DP. This algorithm detects all sectors under the boundaries of a DP area and alters these boundaries according to the following criteria: If the sector belongs to the same city as the DP and if the area that exceeds the DP boundaries is smaller than the internal area, then the DP area is extended to include the sector; otherwise, the DP area is shrunk to exclude the entire sector. In these adjustments, the percentage of the included or excluded area was always less than 5%. The algorithm was executed for the entire state of Rio de Janeiro, in the $28,318$ census sectors, generating the correction of the polygons of the 138 DPs and a list of census sectors corresponding to each DP.

Adjusting the spatial regions for their boundaries to coincide enabled querying the IBGE databases and obtaining the populations of each DP area in 2000 and 2010. This in turn allowed us to estimate the population of each DP from 2003 to 2014. The estimated populations were considered as a reference and used as a constant for every month of the corresponding year. As there is no information of the DP boundaries for all years, the boundaries made available in 2015 were used for the entire period of study.

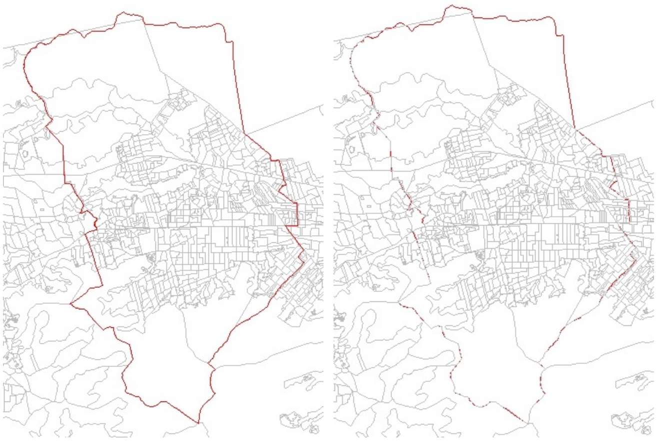


Figure 5.1: Overlaying the maps: evidence of the boundary differences (*slivers*): DP boundaries over census sectors boundaries (left); Census sectors boundaries over DP boundaries (right).

The last five paragraphs and Figure 5.1 were extracted from [7].

The final result is a dataset containing 138 entities (DP) and 38 features for the years between 2003 and 2014. In this work we used the data related to the year 2014. The features are related to the different types of crime for instance: *Homicídios dolosos*, *Lesão Corporal Seguida de Morte*, *Latrocínio* classified as violent deaths. A complete list of features is provided in the Appendix B.1.

Table B.2 presents a summary of the variables details. The dataset has two variables, *Atentado Violento ao Pudor* (*t_atv_pudor_*2014) and *Lesão Corporal Culposa* (*t_lcor_cul_*2014) containing unavailable values (NA). In addition, there are unused features such as *Policiais Civis Mortos em Serviço* (*t_civ_morto_*2014) which has zero for the 138 DP's. Other variables like *Extorsão Mediante Sequestro* (*t_e_seq_*2014) contains zero for 137 elements and only one entry different from zero discretizing the dataset.

In our analysis, the previously mentioned variables were not taken into account for the experiments and removed as part of a preprocessing of the data. Notice in Table B.2 that the features are in different scales, so the data was normalized to the same scale using the formula 5-1:

$$z = \frac{x - \bar{X}}{sd(X)} \tag{5-1}$$

where x is an element, X the column vector and $sd(\cdot)$ the standard deviation.

Crime in the Capital and the State has different behaviors, therefore the experiments will be concentrated in the capital. The data related to the capital was separated in a new dataset resulting in 42 DPs. Once the data was preprocessed, the correlation matrix is shown in Table B.5 and continues in Tables B.6, B.7 and B.8. For each variable, we identified the most correlated variable to create the Table 5.6. This table shows 23 variables correlated over 60 percent and there are three variables with a correlation of 0.99.

	v1	v2	corr
1	lcor_morte	r_caixa	0.99
2	r_caixa	esteli	0.99
3	esteli	r_caixa	0.99
4	r_tran	r_cel	0.98
5	r_banco	esteli	0.98
6	r_cel	r_tran	0.98
7	extor	esteli	0.98
8	r_comercial	r_tran	0.97
9	lcor_dol	ameaca	0.96
10	ameaca	lcor_dol	0.96
11	r_carg	r_tran	0.94
12	r_colet	r_tran	0.94
13	prisao	adol	0.88
14	adol	prisao	0.88
15	recup_veic	auto_resis	0.84
16	auto_resis	recup_veic	0.84
17	ossada	r_colet	0.82
18	f_veic	r_comercial	0.82
19	desap	r_colet	0.79
20	estup	ameaca	0.75
21	r_vei	recup_veic	0.72
22	drogas	lcor_dol	0.63
23	r_res	f_veic	0.61
24	m_susp	armas	0.59
25	armas	m_susp	0.59
26	latro	r_vei	0.56
27	mandado	adol	0.55
28	r_saque	seq_relam	0.54
29	seq_relam	r_saque	0.54
30	h_dol	armas	0.52
31	cadaver	prisao	0.39
32	tenh	drogas	0.35
33	h_culp	cadaver	0.32
34	milit_morto	recup_veic	0.30

Table 5.6: Maximum correlation by variable.

Capital

In order to have an idea of the dataset we are dealing with, we devised an experiment that selects a random subset with 3 to 12 features, the PAM is set as the clustering method and the silhouette as the quality measure. We run 100000 simulations with 4, 7 and 10 groups. Table 5.7 shows the results. In addition, for each number of clusters, we applied the SFS and the SBS methods. The results are summarized in Table 5.8.

Observing the column max(Sil) of Table 5.7, one can see that when the number of variables is increased, there is a tendency to reduce the silhouette coefficient. Also, the mean and median have similar values; therefore the silhouette distribution resulted from the simulations is symmetric. Notice that there are no values near to -1, so there are no extremely bad clusterings.

	Nb_Clust	Nb_Var	max(Sil)	mean(Sil)	median(Sil)	min(Sil)
1	4	3	0.949	0.350	0.351	0.000
2		4	0.697	0.286	0.282	-0.011
3		5	0.675	0.235	0.230	-0.061
4		6	0.609	0.200	0.192	-0.056
5		7	0.567	0.173	0.168	-0.079
6		8	0.492	0.153	0.149	-0.072
7		9	0.488	0.134	0.131	-0.084
8		10	0.420	0.119	0.117	-0.054
9		11	0.466	0.108	0.106	-0.067
10		12	0.366	0.099	0.097	-0.066
11	7	3	0.837	0.341	0.346	0.000
12		4	0.729	0.279	0.288	0.000
13		5	0.713	0.236	0.244	0.000
14		6	0.534	0.208	0.217	0.000
15		7	0.563	0.186	0.194	0.000
16		8	0.515	0.167	0.175	0.000
17		9	0.432	0.153	0.159	0.000
18		10	0.440	0.138	0.144	0.000
19		11	0.409	0.127	0.133	0.000
20		12	0.393	0.117	0.121	0.000
21	10	3	0.797	0.309	0.317	0.000
22		4	0.657	0.246	0.255	0.000
23		5	0.637	0.204	0.213	0.000
24		6	0.497	0.175	0.182	0.000
25		7	0.446	0.154	0.160	0.000
26		8	0.401	0.136	0.139	0.000
27		9	0.396	0.121	0.119	0.000
28		10	0.358	0.108	0.104	0.000
29		11	0.401	0.100	0.095	0.000
30		12	0.365	0.088	0.081	0.000

Table 5.7: Summary over 100000 simulation of PAM with 4,7 and 10 number of clusters in CrimesRJ dataset.

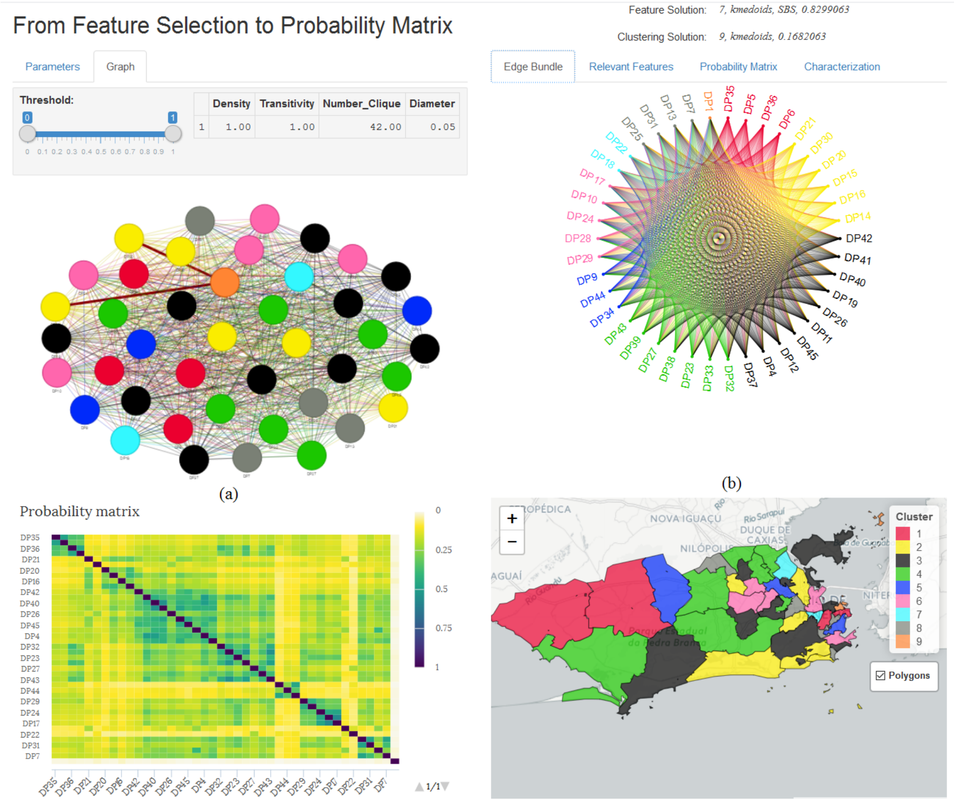
Next, the results for simulations is compared with those obtained by the methods of feature selection in terms of number of clusters and variables. Considering 4 clusters, the SFS (with 11 variables) and the SBS (with 3 variables) obtained similar silhouette values (0.509 and 0.544, respectively).

Considering 7 clusters, the simulation obtained better results with a silhouette of 0.713 for the SBS method and 0.589 for the SFS.

	FSM	Nb_Clust	Sil	Nb_Var	InfoVar
1		4	0.509	11	8, 22, 36, 2, 18, 25, 17, 27, 23, 19, 31
2	SFS	7	0.589	5	13, 22, 36, 2, 17
3		10	0.514	8	13, 22, 36, 24, 18, 25, 2, 23
4		4	0.544	3	24, 27, 34
5	SBS	7	0.830	1	13
6		10	0.525	2	13, 28

Table 5.8: Summary of SFS and SBS with PAM and 0.5 of threshold with 4, 7 and 10 number of clusters in the CrimesRJ dataset.

As the parameters used to apply the method the number of clusters vary from 2 to 21, the feature selection algorithms were SFS and SBS. The clustering methods used were K-Means, PAM and HC-AL. The final results are given in Figure 5.2.



From Feature Selection to Probability Matrix

Feature Solution: *7, kmedoids, SBS, 0.8299063*

Clustering Solution: *9, kmedoids, 0.1682063*

Threshold: 0 – 1

	Density	Transitivity	Number_Clique	Diameter
1	1.00	1.00	42.00	0.05

Parameters
Graph
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
Edge Bundle
Relevant Features
Probability Matrix
Characterization
DP35 DP5 DP36 DP6 DP21 DP30 DP20 DP15 DP16 DP14 DP42 DP41 DP40 DP19 DP26 DP11 DP45 DP12 DP4 DP37 DP32 DP33 DP23 DP38 DP27 DP39 DP43 DP34 DP44 DP9 DP29 DP28 DP24 DP10 DP17 DP18 DP22 DP25 DP31 DP13 DP7 DP1
Probability matrix
DP35 DP36 DP21 DP20 DP16 DP42 DP40 DP26 DP45 DP4 DP32 DP23 DP27 DP43 DP44 DP29 DP24 DP17 DP22 DP31 DP7
0
0.25
0.5
0.75
1
1/1
+
−
NOVA IGUAÇU
NILÓPOLIS
DUQUE DE CAXIAS
Cluster
1
2
3
4
5
6
7
8
9
☑ Polygons

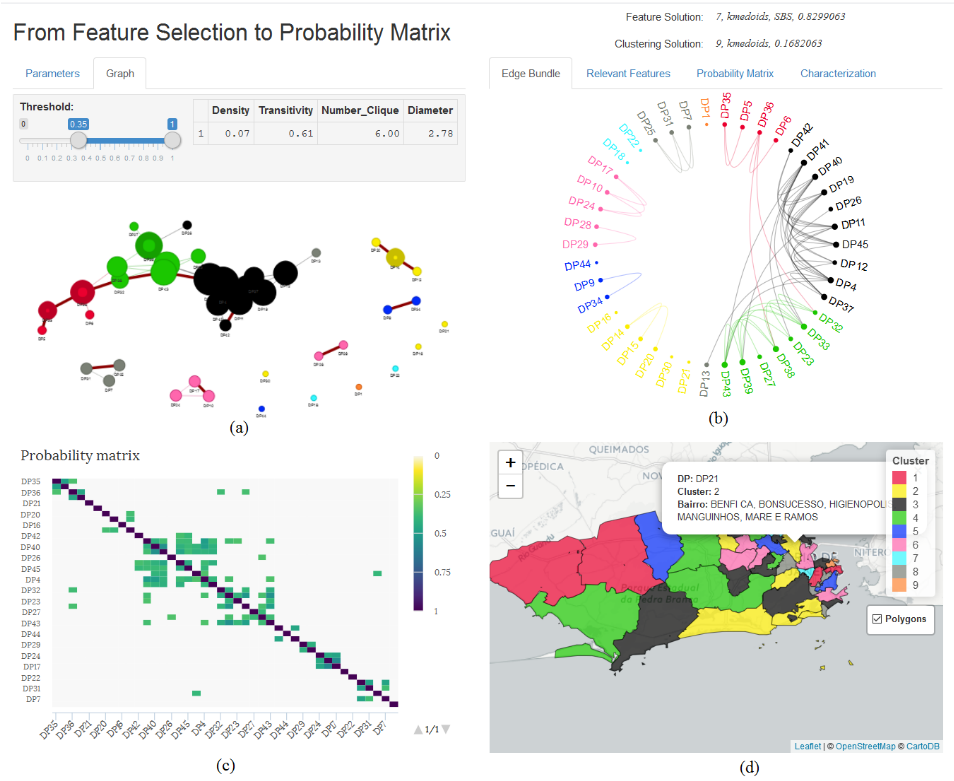
(a) (b) (c) (d)

Figure 5.2: Visualization of the suggested solution for the CrimesRJ dataset.

Analyzing the proposed clustering result, the most relevant feature was *Roubo de Veículo*, obtained from the tuple $< 7, SBS, PAM >$. This tuple obtained the highest silhouette value, around 0.8. Using the similarity matrix, our method proposed 9 clusters with a silhouette around 0.17 and using PAM.

In the map it is possible to identify a black cluster formed with Rocinha (DP11), Complexo Alamão (DP45), some districts of the Ilha do Governador (DP37), part of Copacabana, Leme (DP12), part of Centro (DP4), Pechincha (DP41), Alto de Boa Vista (DP19), Coelho Neto (DP40) and Recreio (DP42).

Isolated in orange is the DP1 in Centro. This DP is an outlier because to the variables in this area are affected by the large flow of people, and there is no way to calculate or estimate this flow.


From Feature Selection to Probability Matrix

Feature Solution: *7, kmedoids, SBS, 0.8299063*

Clustering Solution: *9, kmedoids, 0.1682063*

Threshold: 0.35 – 1

	Density	Transitivity	Number_Clique	Diameter
1	0.07	0.61	6.00	2.78

DP: DP21
Cluster: 2
Bairro: BENFI CA, BONSUCESSO, HIGIENOPOL
MANGUINHOS, MARE E RAMOS

Parameters
Graph
Edge Bundle
Relevant Features
Probability Matrix
Characterization
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
DP25 DP31 DP7 DP1 DP35 DP5 DP36 DP6 DP42 DP41 DP40 DP19 DP26 DP11 DP45 DP12 DP4 DP37 DP32 DP33 DP23 DP38 DP27 DP39 DP43 DP13 DP21 DP30 DP20 DP15 DP14 DP16 DP34 DP9 DP44 DP29 DP28 DP24 DP10 DP17 DP18 DP22
Probability matrix
0
0.25
0.5
0.75
1
Cluster
1
2
3
4
5
6
7
8
9
☑ Polygons
QUEIMADOS
Leaflet | © OpenStreetMap © CartoDB

(a)

(b)

(c)

(d)

Figure 5.3: Visualization of the suggested solution for the CrimesRJ dataset with a threshold of 0.35.

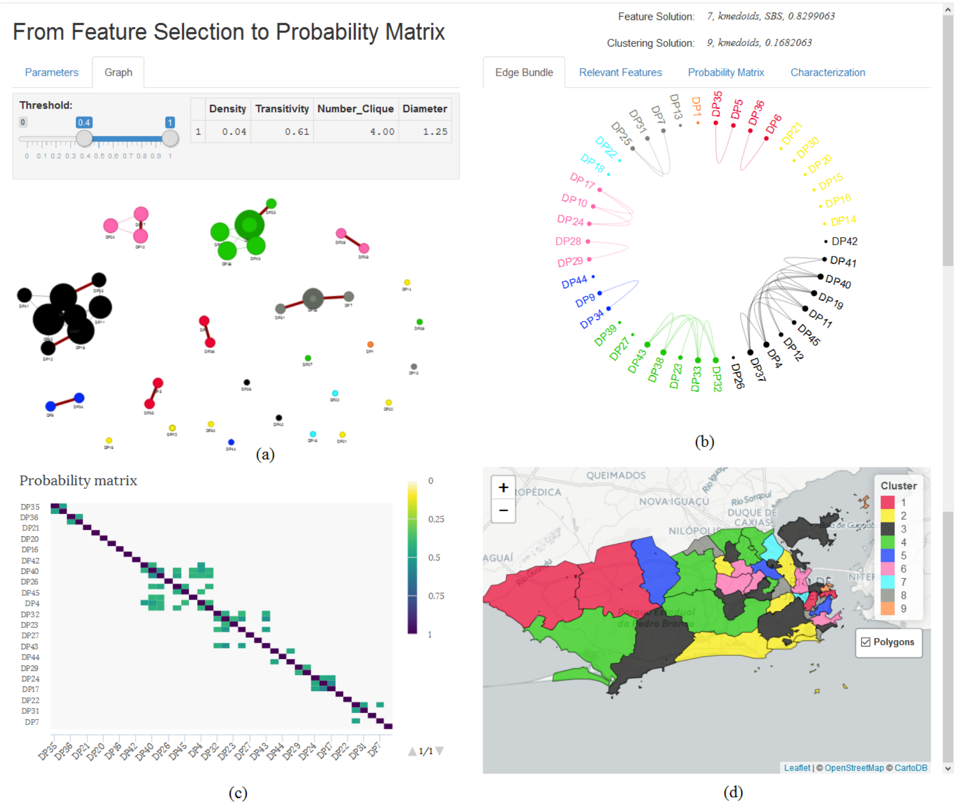
In Figure 5.3a, the largest connected component contains elements from four different groups (red, black, green and gray), but on the other hand the light blue cluster is internally disconnected, as well as the dark blue with a single connection. This proves that there are strongest binds between elements of the black and green clusters rather than internally in the dark blue cluster.

The connected component in pink has five elements, but it is possible to see that a threshold value of 0.35 disconnects it in two separated components, meaning that the probability that the five elements should in the same cluster is less than 0.35.

Another interesting fact is that a threshold value of 0.05 completely isolates DP1 from the rest of the elements. In fact, all the probabilities related to the DP1 are 0.01 or 0.02, highlighting its nature as an outlier. The other isolated nodes together with DP1 are the elements with weaker binds within the dataset. In addition to all of this, the number of cliques in the first image was 42, proving that the graph is fully connected, with a 0.35 threshold the number of clique decreases to 6 and with 0.55 it decreases to 2. With this threshold there is only one connection in the graph between Botafogo and Caju districts, with a value of 0.58.

In the heat map, one can see that there are few points in green and only the main diagonal in blue. Notice that all the yellow points were removed by the threshold, meaning that the highest values are around 0.5.

Barra de Tijuca (DP16), Gávea (DP15), Leblon e Ipanema (DP14) and Vila Isabel (DP20), are residential districts and are together in the same cluster with the suburbial neighborhood Maré (DP21). How is this possible? In fact, even when they are in the same cluster, a deeper analysis shows that the relationship between them is weak as shown in Figure 5.4.


From Feature Selection to Probability Matrix

Feature Solution: 7, kmedoids, SBS, 0.8299063

Clustering Solution: 9, kmedoids, 0.1682063

Threshold: 0 0.4 1

	Density	Transitivity	Number_Clique	Diameter
1	0.04	0.61	4.00	1.25

(a) (b) (c) (d)

Figure 5.4: Visualization of the suggested solution for the CrimesRJ dataset with a threshold of 0.40.

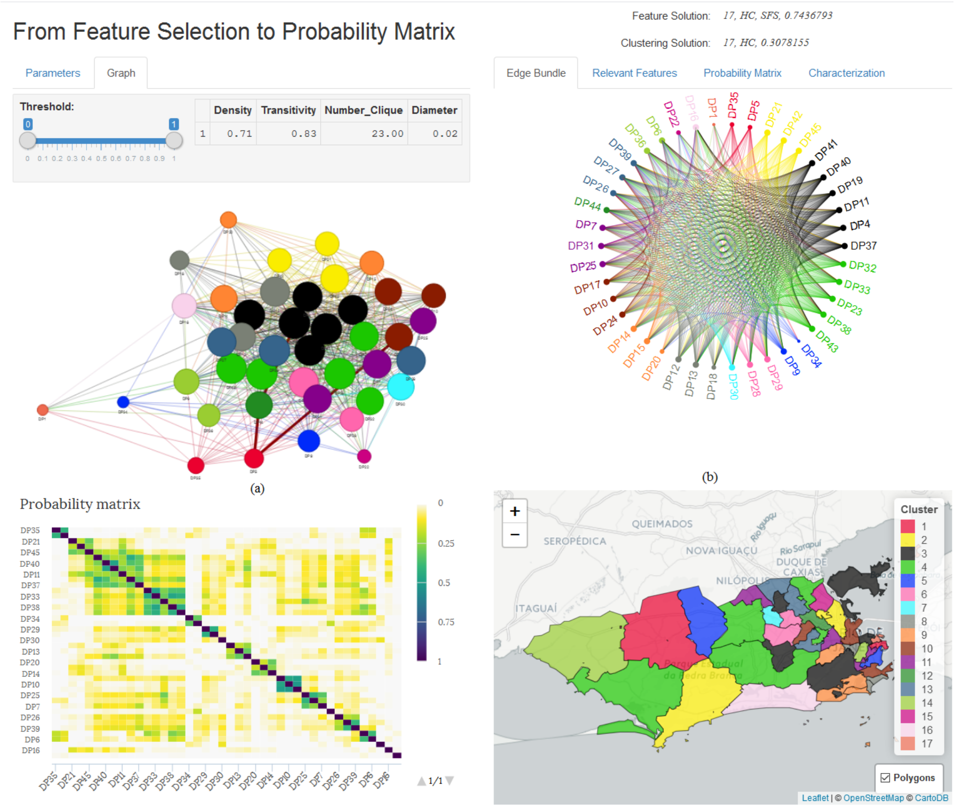
This group is particularly interesting due to socio-economic differences. The DP16 is the less connected while DP20 and DP21 are in the limits of the clustering. In *Barra da Tijuca* there are few street shops, long avenues and it is uncommon to see people walking on the streets. This DP has the lower records of the group, who knows if it is due to urban planning characteristics? *Mare*, even though it is a suburb, contains *UPP* (Pacifying Police Unit)[4] and has similar results with the rest of the cluster as shown, in Figure B.1.

The yellow cluster is fully disconnected, with a threshold of 0.4. Also with this threshold disappear all the connections between elements in different clusters and there is still a strong connectivity in the black and green clusters. The black cluster still has no articulation points and the green cluster has only one but has a clique number of 4, the biggest in the whole graph. On the other hand, the yellow, gray, dark blue and red have connections lower than the number on elements, so these are sparsely connected components.

Finally, it is important to say that the most important variable is the *Roubo de Veiculo* and there are subgroups with very similar characteristics that deserve a qualitative analysis and a more detailed study of the similarity reasons.

The other experiment is related to the location of the AISPs (Integrated Area of Public Security). The AISPs are administrative areas that fit with the areas in charge of the Battalions of Military Police, without taking into account the socio-economic or crime related characteristics of the region.

In the capital there are 17 AISPs, so it would be interesting to fix 17 as the number of clusters to verify whether there are similar behaviours inside these areas. The clustering proposed by the method has a silhouette of 0.31 and was obtained with HC-Al. The most significant variable was *Roubo a Establecimento Comercial*, with a silhouette around 0.74. Figure 5.5 shows the details.



From Feature Selection to Probability Matrix

Feature Solution: 17, HC, SFS, 0.7436793

Clustering Solution: 17, HC, 0.3078155

Parameters | Graph

Edge Bundle | Relevant Features | Probability Matrix | Characterization

Threshold: 0 – 1

	Density	Transitivity	Number_Clique	Diameter
1	0.71	0.83	23.00	0.02

(a)

(b)

(c)

(d)

Figure 5.5: Visualization of the suggested solution for 17 clusters in the CrimesRJ dataset.

We can see that there is no pattern corresponding with the AISP layout shown in Figure 5.6. The only two DPs in the same cluster and in the same AISP are DP14 (Ipanema and Leblon) and DP15 (Gávea , Jardim Botanico, Lagoa, São Conrado, and Vidigal).

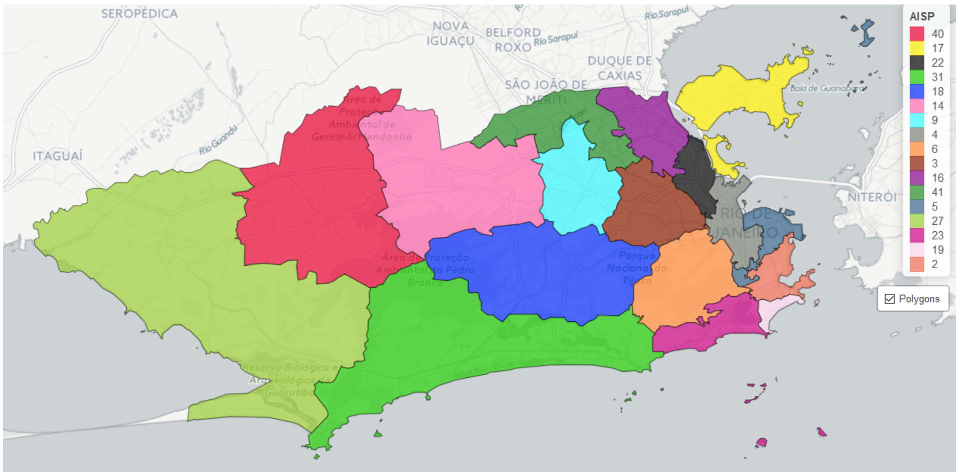


Figure 5.6: Map of AISP regions in Rio de Janeiro Capital.

In conclusion, the DPs inside the AIPS have different behaviours.

5.2.2
Exploring the HDI Dataset

The Human Development Index as part of the United Nations program has been created, among other objectives, to compare and characterize the countries according to their development level. As stated by [5], “The Human Development Index (HDI) is a summary measure of average achievement in key dimensions of human development: a long and healthy life, being knowledgeable and having a decent standard of living. The HDI is the geometric mean of normalized indices for each of the three dimensions.”

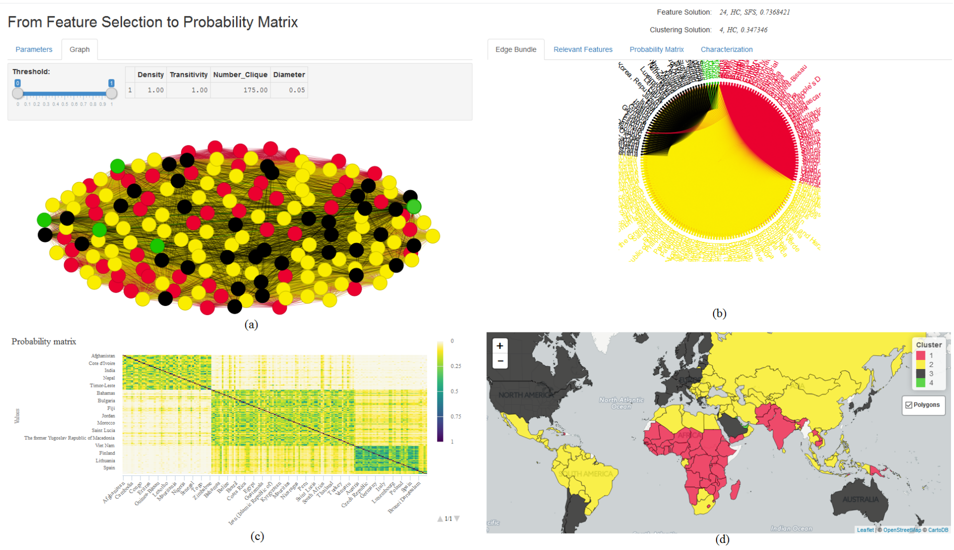
On the website of Human Development Report these data are publicly available. The online data are organized by year and for each year it contains a set of features to compute the index. Table C.1 lists the variables used to build the dataset.

The first four variables from Table C.1 were removed before the analysis of the dataset. The first one is the ranking of the countries in the ONU based on the results obtained from the HDI. The second variable is the name of the country. The third one is a clusterization of the countries in four groups: *very high, high, medium and low*, which therefore divide the dataset in four well defined groups. The last feature removed was the fourth variable, which contains the HDI as a numeric value calculated using the remaining features.

The method was applied using the following parameters:

- K varying from 2 to 28.
- The Features Selection Methods applied were SFS, and SBS.
- The clustering methods were K-Means, PAM, and HC-AL.

The best solution is shown in Figure 5.7.



From Feature Selection to Probability Matrix

Feature Solution: 24, HC, SFS, 0.7368421

Clustering Solution: 4, HC, 0.347346

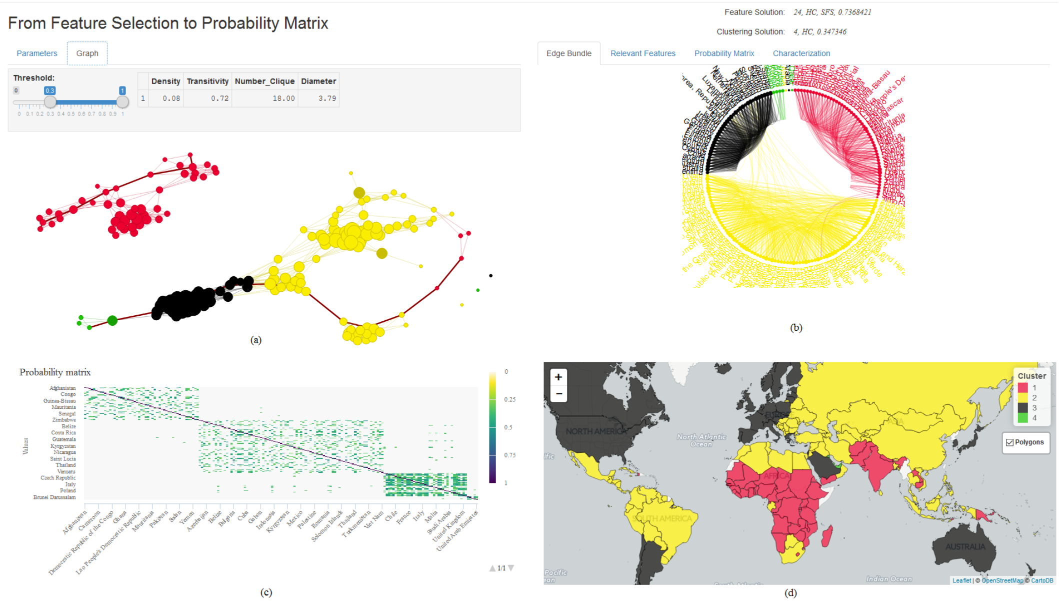
Threshold: 0 – 1

	Density	Transitivity	Number_Clique	Diameter
1	1.00	1.00	175.00	0.05

Figure 5.7: Visualization of the suggested solution for the HDI dataset.

One can see that the green cluster contains outliers of the dataset, such as Qatar and United Emirates. The countries with very high are located in the black cluster. The countries with high are in the yellow cluster and the poor countries are in the red cluster. The countries with medium development are mixed between the yellow and red cluster. Our method reveals that the most important feature was Mean Years of Schooling.

In the Figure 5.7c, it is possible to see three well defined blocks 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 them. In order to highlight this fact, the threshold was set to 0.30, as illustrated by Figure 5.8.



From Feature Selection to Probability Matrix

Parameters | Graph

Threshold: 0.3 (range 0 – 1)

	Density	Transitivity	Number_Clique	Diameter
1	0.08	0.72	18.00	3.79

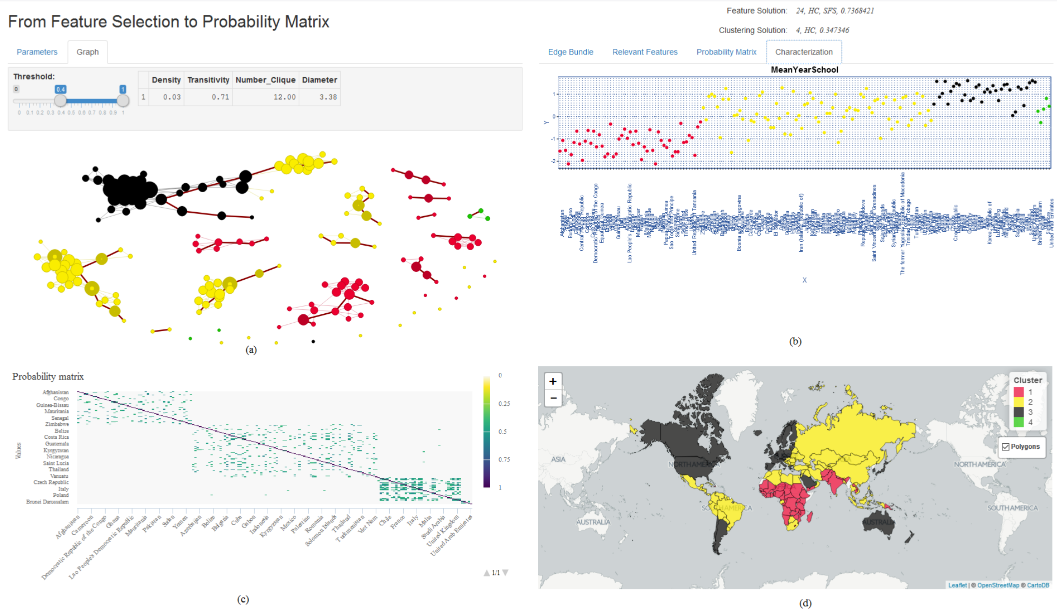
Feature Solution: *24, HC, SFS, 0.7368421*

Clustering Solution: *4, HC, 0.347346*

Edge Bundle | Relevant Features | Probability Matrix | Characterization

Figure 5.8: Visualization of the suggested solution for the HDI dataset with a threshold of 0.30.

In Figure 5.8, one can notice that the edge bundling is almost empty in the middle and there are few connections between elements in different clusters. In the graph, one can also see that there are only three isolated countries, the largest clique is 18 and the transitivity is 0.72. So the elements have strong connections between them. Notice that there is a diameter with elements in the four clusters so the threshold was again modified to 0.40, as shown in the Figure 5.9.



From Feature Selection to Probability Matrix

Feature Solution: 24, HC, SFS, 0.7368421

Clustering Solution: 4, HC, 0.347346

Parameters | Graph

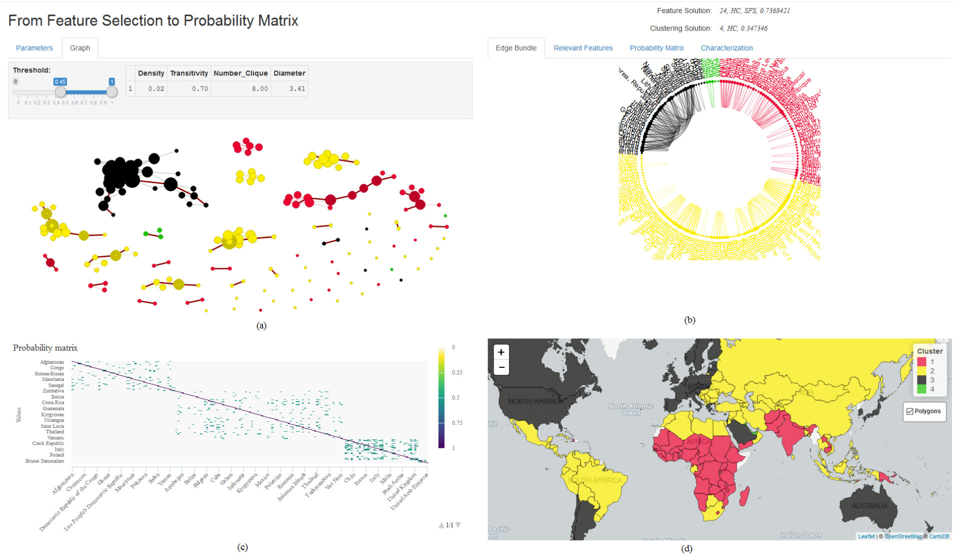
Edge Bundle | Relevant Features | Probability Matrix | Characterization

Threshold: 0.4

	Density	Transitivity	Number_Clique	Diameter
1	0.03	0.71	12.00	3.38

Figure 5.9: Visualization of the suggested solution for the HDI dataset with a threshold of 0.40.

With a 0.40 threshold (Figure 5.9a), the elements look sparse, but still the yellow and black are connected by an articulation point. Particularly, in the characterization of the most important variables one can see that there is a clear difference between the red and the black cluster.



From Feature Selection to Probability Matrix

Feature Solution: 24, HC, SFS, 0.7368421

Clustering Solution: 4, HC, 0.347346

Parameters | Graph

Edge Bundle | Relevant Features | Probability Matrix | Characterization

Threshold: 0.45

	Density	Transitivity	Number_Clique	Diameter
1	0.02	0.70	8.00	3.41

Figure 5.10: Visualization of the suggested solution for the HDI dataset with a threshold of 0.45.

In Figure 5.10, to split the cluster, the threshold was set to 0.45 and there is still a full graph with eight nodes, and only five elements isolated in the black group of the countries with very high HDI. On the other hand the relationships between the red and yellow countries is less visible and there are a lot more isolated countries from these categories.

5.3 Discussion

In the comparison with individual clustering methods during the evaluation of our method (in other words, using less computational resources), the Iris and Wine datasets have the best results while Glass, Breast Cancer, Seeds and Segmentation get similar results. The worst results were obtained with the Yeast dataset.

Finally, the experiments reveal a detailed analysis of the datasets, but aims at the relationships rather than the groups, allowing a more selective case of study. They combine different points of view of the similarity matrix giving a flexible tool to attack a wide range of problems. The use of the method and the visual tools came in handy, highlighting key details that can solve or turn the interest of a research and shed light beyond the clustering.

6
Conclusion and Future Work

This work presented a new method based on ensemble clustering, which creates a similarity matrix combining multiple partitions of the dataset using feature selection and clustering methods. Finally, it joined all partitions in order to obtain a consensus one that uses a transformation of the previously computed similarity matrix as a distance matrix input in an other clustering process. Also, it proposed a visual tool prototype that is capable to explore the dataset from different points of view. This prototype shows to be a useful tool to deeply analyze the connection between the elements, characterize the instances and locate them on the map. This is an interesting approach for spatial analysis where the number of elements is reduced. With all the results, the proposed objectives had been accomplished in the research.

The experiments reveal a good performance of our method. They show that it is better or similar when compared with the individual clustering methods. Moreover, when it is compared with the ensemble clustering methods, it also has better results.

For future research, some suggestions that may improve the quality of our method are listed below:

- It would be interesting to study a voting mechanism to suggest the most important variables, as well as to create a similarity matrix between the variables to apply network analysis.
- There are several of metrics to measure the quality of the clusters, such as the Davies-Buldin index, the Dunn's index and the Calinsky-Harabasz index. And would be interesting to see the quality of a clustering process as a combination of these measures, giving the chance to enhance the characteristics of the metrics, unbalance the results and customize the method according to the scenario.
- The method is independent of the clustering method and feature selection algorithms, but it would be interesting to compare the results of other methods, such as Diana and DBSCAN as well as other feature selection techniques, such as Simulated Annealing or Principal Feature Component.

- Sometimes the best solution, even when it has the best quality coefficient, is not the expected or desired result. So it would be extremely useful to set a ranking and return the top 10 recommended clusterings.
- To validate the visual tool, use the observational techniques and interviews.

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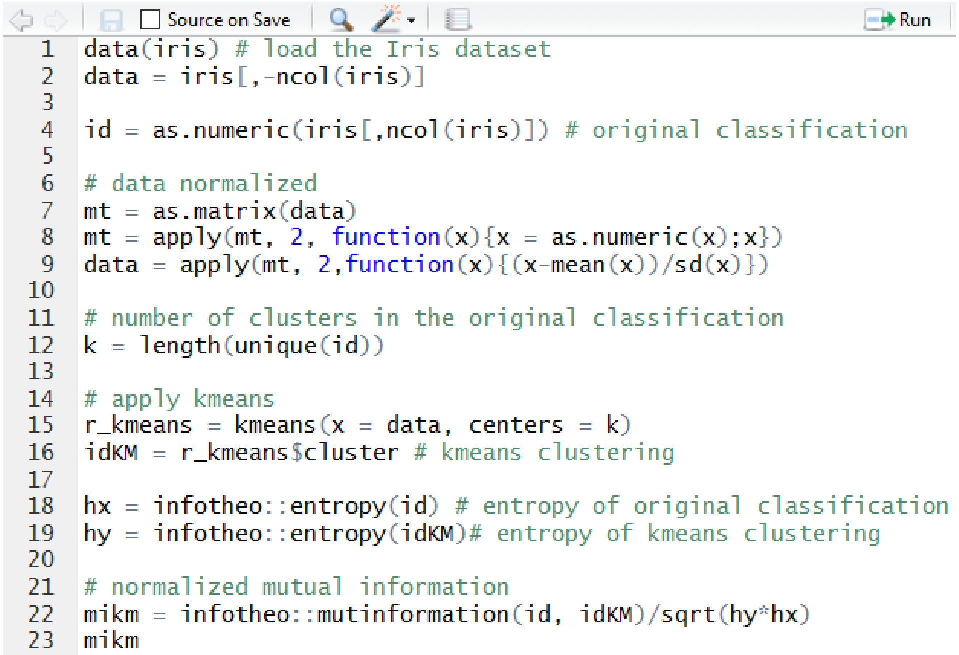
A
Appendix



```r
data(iris) # load the Iris dataset
data = iris[,-ncol(iris)]

id = as.numeric(iris[,ncol(iris)]) # original classification

# data normalized
mt = as.matrix(data)
mt = apply(mt, 2, function(x){x = as.numeric(x);x})
data = apply(mt, 2,function(x){(x-mean(x))/sd(x)})

# number of clusters in the original classification
k = length(unique(id))

# apply kmeans
r_kmeans = kmeans(x = data, centers = k)
idKM = r_kmeans$cluster # kmeans clustering

hx = infotheo::entropy(id) # entropy of original classification
hy = infotheo::entropy(idKM)# entropy of kmeans clustering

# normalized mutual information
mikm = infotheo::mutinformation(id, idKM)/sqrt(hy*hx)
mikm
```

Figure A.1: An example of how we calculate the Normalized Mutual Information.

B
Appendix

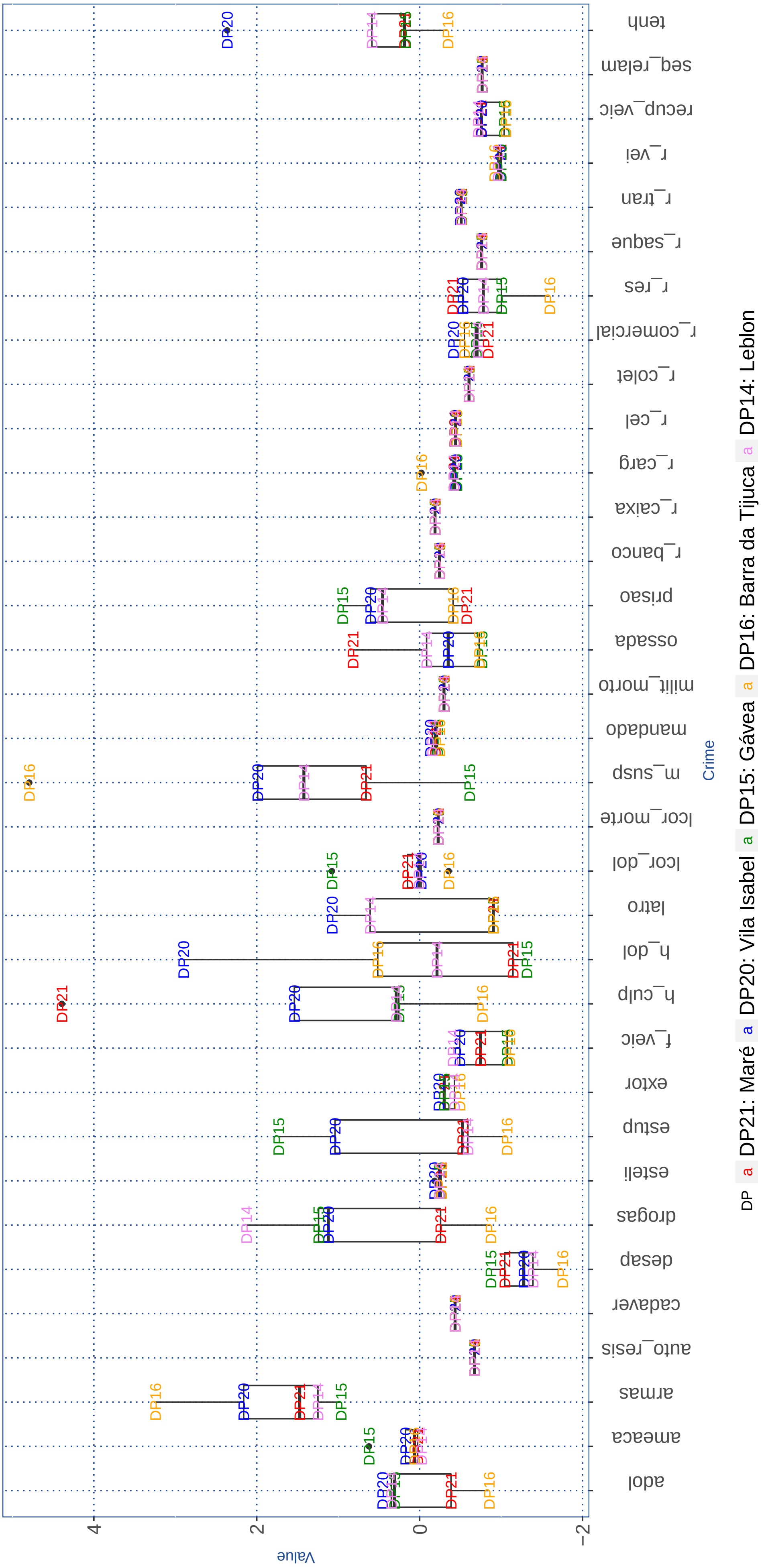


Figure B.1: Characterization of the variables in the cluster formed by *Gávea, Vila Isabel, Maré, Barra da Tijuca and Leblon.*

	Type of Crime	Crime
1	VÍTIMAS DE CRIMES VIOLENTOS	Homicídio Doloso
2		Lesão Corporal Seguida de Morte
3		Latrocínio (Roubo seguido de morte)
4		Tentativa de Homicídio
5		Lesão Corporal Dolosa
6		Estupro
7		Atentado Violento ao Pudor
8	VÍTIMAS DE MORTES COM TIPIFICAÇÃO PROVISÓRIA	Encontro de Cadáver
9		Morte Suspeita
10		Encontro de Ossada
11		Homicídio Culposo
12		Lesão Corporal Culposa
13	REGISTROS DE CRIMES CONTRA O PATRIMÔNIO	Roubo a Estabelecimento Comercial
14		Roubo a Residência
15		Roubo de Veículo
16		Roubo de Carga
17		Roubo a Transeunte
18		Roubo em Coletivo
19		Roubo a Banco
20		Roubo de Caixa Eletrônico
21		Roubo de Aparelho Celular
22		Roubo com condução da vítima para saque em I.F.
23		Furto de Veículos
24		Extorsão Mediante Sequestro (Sequestro Clássico)
25		Extorsão
26		Extorsão com momentânea privação da liberdade (Sequestro Relâmpago)
27		Estelionato
28	ATIVIDADE POLICIAL	Apreensão de Drogas
29		Armas Apreendidas
30		Prisões
31		Apreensão de adolescente
32		Recuperação de veículo
33		Cumprimento de Mandado de Prisão
34	OUTROS REGISTROS	Ameaça (vítimas)
35		Pessoas Desaparecidas
36		Homícídio Decorrente de Intervenção Policial - Auto de Resistência / Resistência com morte do opositor - Auto de Resistência
37		Policiais Militares Mortos em Serviço
38		Policiais Civis Mortos em Serviço

Table B.1: Type of crimes in CrimesRJ dataset.

	h_dol	cor_morte	latro	tent_h
1	Min. : 0.000	Min. : 0.0000	Min. :0.0000	Min. : 0.00
2	1st Qu.: 9.775	1st Qu.: 0.0000	1st Qu.:0.0000	1st Qu.: 17.33
3	Median :20.962	Median : 0.0000	Median :0.4774	Median : 30.81
4	Mean :25.589	Mean : 0.3936	Mean :0.8866	Mean : 37.47
5	3rd Qu.:36.610	3rd Qu.: 0.0000	3rd Qu.:1.3411	3rd Qu.: 48.89
6	Max. :83.605	Max. :19.3050	Max. :6.5125	Max. :152.42

	lcor_dol	estup	atv_pudor	h_culp
1	Min. : 247.1	Min. : 5.698	Min. : NA	Min. : 0.000
2	1st Qu.: 445.9	1st Qu.: 22.685	1st Qu.: NA	1st Qu.: 1.225
3	Median : 560.0	Median : 34.284	Median : NA	Median : 3.224
4	Mean : 598.5	Mean : 35.707	Mean :NaN	Mean : 4.277
5	3rd Qu.: 661.0	3rd Qu.: 44.203	3rd Qu.: NA	3rd Qu.: 6.232
6	Max. :2370.6	Max. :115.830	Max. : NA	Max. :27.996
7			NA's :138	

	lcor_cul	cadaver	m_susp	ossada
1	Min. : NA	Min. :0.0000	Min. : 0.000	Min. : 72.05
2	1st Qu.: NA	1st Qu.:0.0000	1st Qu.: 6.338	1st Qu.: 193.23
3	Median : NA	Median :0.0000	Median : 11.378	Median : 260.40
4	Mean :NaN	Mean :0.1771	Mean : 17.378	Mean : 309.71
5	3rd Qu.: NA	3rd Qu.:0.0000	3rd Qu.: 22.293	3rd Qu.: 344.01
6	Max. : NA	Max. :2.4470	Max. :159.206	Max. :2220.47
7	NA's :138			

	r_comercial	r_res	r_vei	r_carg
1	Min. : 0.00	Min. : 0.000	Min. : 0.00	Min. : 0.000
2	1st Qu.: 13.37	1st Qu.: 3.643	1st Qu.: 12.77	1st Qu.: 5.063
3	Median : 33.15	Median : 6.844	Median : 72.77	Median : 10.791
4	Mean : 43.80	Mean : 8.403	Mean :139.54	Mean : 33.995
5	3rd Qu.: 59.18	3rd Qu.:11.151	3rd Qu.:221.92	3rd Qu.: 34.807
6	Max. :501.93	Max. :39.888	Max. :859.40	Max. :965.251

Table B.2: Summary of CrimesRJ dataset.

	r_tran	r_colet	r_banco	r_caixa
1	Min. : 0.00	Min. : 0.000	Min. : 0.0000	Min. : 0.0000
2	1st Qu.: 15.54	1st Qu.: 1.202	1st Qu.: 0.0000	1st Qu.: 0.0000
3	Median : 191.02	Median : 15.126	Median : 0.0000	Median : 0.0000
4	Mean : 470.13	Mean : 44.081	Mean : 0.3231	Mean : 0.5175
5	3rd Qu.: 597.03	3rd Qu.: 50.754	3rd Qu.: 0.0000	3rd Qu.: 0.0000
6	Max. :10212.35	Max. :791.506	Max. :19.3050	Max. :38.6100

	r_cel	r_saque_2014	f_veic_2014	e_seq_2014
1	Min. : 0.000	Min. :0.0000	Min. : 0.00	Min. :0.00000
2	1st Qu.: 2.222	1st Qu.:0.0000	1st Qu.: 50.10	1st Qu.:0.00000
3	Median : 15.133	Median :0.0000	Median : 75.66	Median :0.00000
4	Mean : 52.887	Mean :0.5183	Mean : 98.58	Mean :0.02486
5	3rd Qu.: 54.058	3rd Qu.:0.6140	3rd Qu.:129.36	3rd Qu.:0.00000
6	Max. :1428.571	Max. :9.7688	Max. :579.15	Max. :3.43053

	extor	seq_relam	esteli	drogas
1	Min. : 0.000	Min. : 0.0000	Min. : 19.44	Min. : 7.069
2	1st Qu.: 4.976	1st Qu.: 0.0000	1st Qu.: 78.80	1st Qu.: 78.864
3	Median : 7.800	Median : 0.0000	Median : 123.06	Median : 154.105
4	Mean : 12.463	Mean : 0.8638	Mean : 311.55	Mean : 266.637
5	3rd Qu.: 13.147	3rd Qu.: 1.0842	3rd Qu.: 207.45	3rd Qu.: 234.173
6	Max. :193.050	Max. :14.2596	Max. :13474.90	Max. :5284.923

	armas	prisao	adol	recup_veic
1	Min. : 11.01	Min. : 0.00	Min. : 0.000	Min. : 2.825
2	1st Qu.: 34.32	1st Qu.: 80.93	1st Qu.: 6.124	1st Qu.: 40.743
3	Median : 50.27	Median : 154.07	Median : 22.797	Median : 75.707
4	Mean : 60.08	Mean : 227.69	Mean : 49.004	Mean :116.252
5	3rd Qu.: 72.77	3rd Qu.: 283.58	3rd Qu.: 57.189	3rd Qu.:161.804
6	Max. :209.57	Max. :3702.38	Max. :716.379	Max. :767.654

Table B.3: Summary of CrimesRJ dataset (continued).

	mandado	ameaca	desap	auto_resis
1	Min. : 6.126	Min. : 266.1	Min. : 0.00	Min. : 0.0000
2	1st Qu.: 70.312	1st Qu.: 430.6	1st Qu.: 14.09	1st Qu.: 0.0000
3	Median : 96.399	Median : 542.0	Median : 24.85	Median : 0.6793
4	Mean : 140.589	Mean : 587.1	Mean : 26.54	Mean : 2.4317
5	3rd Qu.: 149.686	3rd Qu.: 648.2	3rd Qu.: 33.96	3rd Qu.: 3.1065
6	Max. :2211.166	Max. :2625.5	Max. :133.29	Max. :23.7647

	milit_morto	civ_morto
1	Min. :0.00000	Min. :0
2	1st Qu.:0.00000	1st Qu.:0
3	Median :0.00000	Median :0
4	Mean :0.09661	Mean :0
5	3rd Qu.:0.00000	3rd Qu.:0
6	Max. :2.82554	Max. :0

Table B.4: Summary of CrimesRJ dataset (continued).

	h_dol	lcor_morte	latro	tenh	lcor_dol	estup	h_culp	cadaver
h_dol	1.00	0.14	0.25	0.32	0.19	0.37	-0.01	0.09
lcor_morte	0.14	1.00	-0.13	0.09	0.91	0.61	-0.14	-0.06
latro	0.25	-0.13	1.00	0.11	-0.10	0.15	-0.17	-0.13
tenh	0.32	0.09	0.11	1.00	0.27	0.20	0.12	0.03
lcor_dol	0.19	0.91	-0.10	0.27	1.00	0.73	-0.04	0.04
estup	0.37	0.61	0.15	0.20	0.73	1.00	0.00	-0.08
h_culp	-0.01	-0.14	-0.17	0.12	-0.04	0.00	1.00	0.32
cadaver	0.09	-0.06	-0.13	0.03	0.04	-0.08	0.32	1.00
m_susp	0.31	-0.17	-0.03	0.11	-0.11	-0.08	0.24	0.14
ossada	0.12	0.74	-0.19	0.25	0.80	0.39	0.04	0.24
r_comercial	0.12	0.90	-0.09	0.13	0.83	0.47	-0.26	0.01
r_res	0.13	0.39	-0.02	0.07	0.41	0.43	0.17	0.24
r_vei	0.25	-0.01	0.56	-0.01	0.01	0.02	-0.37	-0.05
r_carg	0.22	0.91	-0.05	0.10	0.85	0.53	-0.25	-0.08
r_tran	0.15	0.95	-0.02	0.14	0.89	0.55	-0.24	-0.05
r_colet	0.21	0.86	0.01	0.15	0.85	0.49	-0.25	0.11
r_banco	0.10	0.98	-0.11	0.18	0.91	0.58	-0.15	-0.10
r_caixa	0.14	0.99	-0.14	0.12	0.91	0.62	-0.13	-0.07
r_cel	0.08	0.94	-0.06	0.08	0.87	0.54	-0.22	-0.06
r_saque	-0.23	-0.13	0.04	-0.18	-0.15	-0.29	-0.15	0.20
f_veic	0.17	0.75	-0.06	0.06	0.66	0.43	-0.09	0.19
extor	0.08	0.96	-0.16	0.13	0.89	0.57	-0.18	-0.04
seq_relam	-0.22	-0.13	0.16	-0.09	-0.21	-0.26	-0.26	-0.05
esteli	0.11	0.99	-0.14	0.10	0.91	0.59	-0.14	-0.05
drogas	0.15	0.56	-0.09	0.35	0.63	0.40	0.07	0.04
armas	0.52	0.36	-0.02	0.27	0.45	0.29	0.19	0.01
prisao	0.34	-0.17	0.00	0.16	-0.00	0.02	0.05	0.39
adol	0.33	-0.15	-0.00	0.12	-0.03	-0.03	0.04	0.19
recup_veic	0.43	0.06	0.31	0.06	0.09	0.00	-0.31	0.03
mandado	-0.00	0.20	-0.09	-0.02	0.23	0.04	0.02	-0.05
ameaca	0.23	0.93	-0.12	0.22	0.96	0.75	-0.02	-0.01
desap	0.34	0.68	-0.03	0.15	0.69	0.52	-0.25	0.06
auto_resis	0.38	-0.09	0.15	-0.11	-0.13	-0.14	-0.32	-0.03
milit_morto	0.04	-0.06	0.01	0.20	0.01	-0.07	-0.15	0.15

Table B.5: Correlation matrix for CrimesRJ dataset.

	m_susp	ossada	r_comercial	r_res	r_vei	r_carg	r_tran	r_colet
h_dol	0.31	0.12	0.12	0.13	0.25	0.22	0.15	0.21
lcor_morte	-0.17	0.74	0.90	0.39	-0.01	0.91	0.95	0.86
latro	-0.03	-0.19	-0.09	-0.02	0.56	-0.05	-0.02	0.01
tenh	0.11	0.25	0.13	0.07	-0.01	0.10	0.14	0.15
lcor_dol	-0.11	0.80	0.83	0.41	0.01	0.85	0.89	0.85
estup	-0.08	0.39	0.47	0.43	0.02	0.53	0.55	0.49
h_culp	0.24	0.04	-0.26	0.17	-0.37	-0.25	-0.24	-0.25
cadaver	0.14	0.24	0.01	0.24	-0.05	-0.08	-0.05	0.11
m_susp	1.00	-0.03	-0.30	-0.17	-0.31	-0.19	-0.27	-0.23
ossada	-0.03	1.00	0.75	0.45	0.01	0.71	0.78	0.82
r_comercial	-0.30	0.75	1.00	0.45	0.22	0.90	0.97	0.91
r_res	-0.17	0.45	0.45	1.00	0.19	0.36	0.42	0.38
r_vei	-0.31	0.01	0.22	0.19	1.00	0.23	0.22	0.29
r_carg	-0.19	0.71	0.90	0.36	0.23	1.00	0.94	0.92
r_tran	-0.27	0.78	0.97	0.42	0.22	0.94	1.00	0.94
r_colet	-0.23	0.82	0.91	0.38	0.29	0.92	0.94	1.00
r_banco	-0.20	0.76	0.90	0.37	0.00	0.91	0.95	0.87
r_caixa	-0.18	0.74	0.91	0.40	-0.01	0.93	0.96	0.87
r_cel	-0.27	0.75	0.95	0.43	0.15	0.91	0.98	0.90
r_saque	-0.23	0.10	0.14	0.03	0.15	-0.09	0.04	0.06
f_veic	-0.22	0.71	0.82	0.61	0.26	0.74	0.80	0.75
extor	-0.24	0.77	0.94	0.41	0.02	0.91	0.96	0.89
seq_relam	-0.35	-0.09	0.08	0.02	0.29	-0.09	0.03	-0.03
esteli	-0.19	0.76	0.93	0.41	-0.01	0.92	0.97	0.88
drogas	0.04	0.53	0.47	0.10	-0.24	0.51	0.52	0.56
armas	0.59	0.30	0.26	-0.08	-0.04	0.43	0.33	0.36
prisao	0.13	0.04	-0.07	-0.07	-0.03	-0.10	-0.11	0.05
adol	0.02	0.02	0.01	0.05	0.09	-0.07	-0.06	0.06
recup_veic	-0.25	0.16	0.23	0.09	0.72	0.40	0.24	0.43
mandado	-0.10	0.20	0.23	0.15	-0.06	0.21	0.22	0.26
ameaca	-0.05	0.75	0.83	0.45	-0.04	0.84	0.89	0.80
desap	-0.39	0.64	0.73	0.45	0.33	0.74	0.75	0.79
auto_resis	-0.22	-0.11	0.04	-0.04	0.59	0.22	0.03	0.16
milit_morto	-0.02	0.16	0.11	-0.07	0.21	0.10	0.04	0.13

Table B.6: Correlation matrix for CrimesRJ dataset (continued).

	r_banco	r_caixa	r_cel	r_saque	f_veic	extor	seq_relam	esteli
h_dol	0.10	0.14	0.08	-0.23	0.17	0.08	-0.22	0.11
lcor_morte	0.98	0.99	0.94	-0.13	0.75	0.96	-0.13	0.99
latro	-0.11	-0.14	-0.06	0.04	-0.06	-0.16	0.16	-0.14
tenh	0.18	0.12	0.08	-0.18	0.06	0.13	-0.09	0.10
lcor_dol	0.91	0.91	0.87	-0.15	0.66	0.89	-0.21	0.91
estup	0.58	0.62	0.54	-0.29	0.43	0.57	-0.26	0.59
h_culp	-0.15	-0.13	-0.22	-0.15	-0.09	-0.18	-0.26	-0.14
cadaver	-0.10	-0.07	-0.06	0.20	0.19	-0.04	-0.05	-0.05
m_susp	-0.20	-0.18	-0.27	-0.23	-0.22	-0.24	-0.35	-0.19
ossada	0.76	0.74	0.75	0.10	0.71	0.77	-0.09	0.76
r_comercial	0.90	0.91	0.95	0.14	0.82	0.94	0.08	0.93
r_res	0.37	0.40	0.43	0.03	0.61	0.41	0.02	0.41
r_vei	0.00	-0.01	0.15	0.15	0.26	0.02	0.29	-0.01
r_carg	0.91	0.93	0.91	-0.09	0.74	0.91	-0.09	0.92
r_tran	0.95	0.96	0.98	0.04	0.80	0.96	0.03	0.97
r_colet	0.87	0.87	0.90	0.06	0.75	0.89	-0.03	0.88
r_banco	1.00	0.98	0.94	-0.14	0.75	0.96	-0.08	0.98
r_caixa	0.98	1.00	0.95	-0.10	0.76	0.97	-0.11	0.99
r_cel	0.94	0.95	1.00	0.09	0.79	0.96	0.08	0.97
r_saque	-0.14	-0.10	0.09	1.00	0.07	0.01	0.54	-0.05
f_veic	0.75	0.76	0.79	0.07	1.00	0.77	0.03	0.77
extor	0.96	0.97	0.96	0.01	0.77	1.00	0.04	0.98
seq_relam	-0.08	-0.11	0.08	0.54	0.03	0.04	1.00	-0.05
esteli	0.98	0.99	0.97	-0.05	0.77	0.98	-0.05	1.00
drogas	0.57	0.57	0.48	-0.20	0.30	0.54	-0.33	0.56
armas	0.34	0.38	0.29	-0.30	0.15	0.31	-0.32	0.36
prisao	-0.19	-0.16	-0.18	0.09	-0.15	-0.11	-0.14	-0.16
adol	-0.16	-0.13	-0.13	0.07	-0.10	-0.06	-0.06	-0.12
recup_veic	0.08	0.08	0.15	0.08	0.20	0.09	0.09	0.07
mandado	0.24	0.20	0.22	-0.06	0.04	0.22	-0.11	0.21
ameaca	0.92	0.94	0.89	-0.16	0.71	0.91	-0.16	0.94
desap	0.68	0.69	0.70	0.01	0.62	0.71	-0.04	0.69
auto_resis	-0.12	-0.09	-0.04	0.01	0.04	-0.08	0.07	-0.11
milit_morto	-0.05	-0.05	-0.03	0.14	0.07	-0.01	-0.06	-0.04

Table B.7: Correlation matrix for CrimesRJ dataset (continued).

	drogas	armas	prisao	adol	recup_veic	mandado	ameaca	desap
h_dol	0.15	0.52	0.34	0.33	0.43	-0.00	0.23	0.34
lcor_morte	0.56	0.36	-0.17	-0.15	0.06	0.20	0.93	0.68
latro	-0.09	-0.02	0.00	-0.00	0.31	-0.09	-0.12	-0.03
tenh	0.35	0.27	0.16	0.12	0.06	-0.02	0.22	0.15
lcor_dol	0.63	0.45	-0.00	-0.03	0.09	0.23	0.96	0.69
estup	0.40	0.29	0.02	-0.03	0.00	0.04	0.75	0.52
h_culp	0.07	0.19	0.05	0.04	-0.31	0.02	-0.02	-0.25
cadaver	0.04	0.01	0.39	0.19	0.03	-0.05	-0.01	0.06
m_susp	0.04	0.59	0.13	0.02	-0.25	-0.10	-0.05	-0.39
ossada	0.53	0.30	0.04	0.02	0.16	0.20	0.75	0.64
r_comercial	0.47	0.26	-0.07	0.01	0.23	0.23	0.83	0.73
r_res	0.10	-0.08	-0.07	0.05	0.09	0.15	0.45	0.45
r_vei	-0.24	-0.04	-0.03	0.09	0.72	-0.06	-0.04	0.33
r_carg	0.51	0.43	-0.10	-0.07	0.40	0.21	0.84	0.74
r_tran	0.52	0.33	-0.11	-0.06	0.24	0.22	0.89	0.75
r_colet	0.56	0.36	0.05	0.06	0.43	0.26	0.80	0.79
r_banco	0.57	0.34	-0.19	-0.16	0.08	0.24	0.92	0.68
r_caixa	0.57	0.38	-0.16	-0.13	0.08	0.20	0.94	0.69
r_cel	0.48	0.29	-0.18	-0.13	0.15	0.22	0.89	0.70
r_saque	-0.20	-0.30	0.09	0.07	0.08	-0.06	-0.16	0.01
f_veic	0.30	0.15	-0.15	-0.10	0.20	0.04	0.71	0.62
extor	0.54	0.31	-0.11	-0.06	0.09	0.22	0.91	0.71
seq_relam	-0.33	-0.32	-0.14	-0.06	0.09	-0.11	-0.16	-0.04
esteli	0.56	0.36	-0.16	-0.12	0.07	0.21	0.94	0.69
drogas	1.00	0.45	0.37	0.35	0.06	0.53	0.55	0.35
armas	0.45	1.00	0.29	0.20	0.18	0.09	0.46	0.09
prisao	0.37	0.29	1.00	0.88	0.30	0.41	-0.09	0.04
adol	0.35	0.20	0.88	1.00	0.35	0.55	-0.09	0.14
recup_veic	0.06	0.18	0.30	0.35	1.00	0.14	-0.00	0.46
mandado	0.53	0.09	0.41	0.55	0.14	1.00	0.17	0.21
ameaca	0.55	0.46	-0.09	-0.09	-0.00	0.17	1.00	0.67
desap	0.35	0.09	0.04	0.14	0.46	0.21	0.67	1.00
auto_resis	-0.16	0.13	0.25	0.27	0.84	-0.05	-0.20	0.24
milit_morto	0.03	0.01	0.27	0.20	0.30	-0.03	-0.06	0.10

Table B.8: Correlation matrix for CrimesRJ dataset (continued).

C
Appendix

	Variables
1	HDI rank
2	Country
3	HD
4	Human development index - 2014
5	Infant mortality rate (per 1,000 live births) - 2013
6	Gross national income (GNI) per capita (2011 PPP$) - 2014
7	Labour force participation rate (% ages 15 and older) - 2013
8	Mean years of schooling - 2014
9	Expected years of schooling - 2014
10	Life expectancy at birth - 2014

Table C.1: Variables of HDI dataset.

	Rank	Country	HD	HDI
1	Min. : 1.00	Afghanistan: 1	h :50	Min. :0.3500
2	1st Qu.: 47.50	Albania : 1	l :42	1st Qu.:0.5650
3	Median : 96.00	Algeria : 1	m :37	Median :0.7200
4	Mean : 95.18	Angola : 1	vh:46	Mean :0.6905
5	3rd Qu.:142.50	Argentina : 1		3rd Qu.:0.8200
6	Max. :188.00	Armenia : 1		Max. :0.9400
7		(Other) :169		

	IMR	GNI	LF	MeanYearSchool
1	Min. : 1.60	Min. : 580.7	Min. :37.90	Min. : 1.400
2	1st Qu.: 7.00	1st Qu.: 3647.1	1st Qu.:56.60	1st Qu.: 5.500
3	Median : 14.60	Median : 10404.5	Median :63.70	Median : 8.400
4	Mean : 25.64	Mean : 16615.5	Mean :63.84	Mean : 8.054
5	3rd Qu.: 40.00	3rd Qu.: 22557.0	3rd Qu.:70.25	3rd Qu.:10.750
6	Max. :107.20	Max. :123124.4	Max. :89.10	Max. :13.100

	ExpSchool	LifeExp
1	Min. : 4.10	Min. :49.00
2	1st Qu.:11.05	1st Qu.:64.90
3	Median :13.10	Median :73.10
4	Mean :12.89	Mean :70.99
5	3rd Qu.:15.10	3rd Qu.:76.80
6	Max. :20.20	Max. :83.50

Table C.2: Summary of HDI dataset.