Extending the SACOC algorithm through the Nyström method for Dense Manifold Data Analysis

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Abstract: Data analysis has become an important field over the last decades. The growing amount of data demands new analytical methodologies in order to extract relevant knowledge. Clustering is one of the most competitive techniques in this context. Using a dataset as a starting point, these techniques aim to blindly group the data by similarity. Among the different areas, manifold identification is currently gaining importance. Spectral-based methods, which are the mostly used methodologies in this area, are however sensitive to metric parameters and noise. In order to solve these problems, new bio-inspired techniques have been combined with different heuristics to perform the clustering solutions and stability, specially for dense datasets. Ant Colony Optimization (ACO) is one of these new bio-inspired methodologies. This paper presents an extension of a previous algorithm named Spectral-based ACO Clustering (SACOC). SACOC is a spectral-based clustering methodology used for manifold identification. This work is focused on improving this algorithm through the Nyström extension. The new algorithm, named SACON, is able to deal with Dense Data problems. We have evaluated the performance of this new approach comparing it with online clustering algorithms and the Nyström extension of the Spectral Clustering algorithm using several datasets.

Keywords: Ant Colony Optimization, Clustering, Data Mining, Machine Learning, Spectral, Nyström, SACON, SACOC

1 Introduction

Data analysis is currently a growing field [1]. The importance of analysing these data quantities is growing as a consequence of Social interactions, smart devices, WiFi and networks, etc. Several methodologies have been extended in order to deal with these problems. Two of the most recent methodologies in Data Mining are based on MapReduce [1] and online algorithms [2]. The former is an approach which was designed for parallelizing computation. Using several nodes it distributes some calculus in two steps the mapper and the reducer step. Online analysis is a methodology where data instances are only processed once and the system keeps no information about old instances. This reduces the memory usage and allows the algorithms to work with Dense Data.

There are several Data Mining approaches which deal with Dense Data. The most relevant are those based on Supervised [3] and Unsupervised Learning [3]. Because supervised techniques usually need human assistant by a manual labelling process, and this is costly, unsupervised techniques are gaining importance in this area [2]. One of the most relevant unsupervised techniques is clustering. Clustering is defined as the process of grouping data blindly, using a similarity criterion. These methods have been extensively used in several and heterogeneous fields [3].

Clustering techniques can be divided in several sub-areas [3] such as centroid-based, medoid-based, hierarchical and continuity-based among others. This work is based on the latter. Continuity-based clustering is a methodology focused on the identification of manifolds within the data. These manifolds are structures which are defined by the data points inside their search space [4]. The main idea behind this work is to extend a previous continuity-based algorithm to a

Dense Data approach. The algorithm, named SACOC (Spectral-based ACO Clustering algorithm) [5], is a bio-inspired clustering algorithm based on Ant Colony Optimization.

Ant Colony Optimization [6] algorithms are based on the foraging behaviour of the ants when they need to find the shortest path between their nest and the food source. The ants use a methodology based on pheromones to indicate the path that they have followed. The evaporation of these pheromones is used to choose the best path. This idea can be extended to optimization problems and has been successfully applied in several fields, such as Data Mining [7, 8].

This work aims to extend a previous SACOC the Nyström extension [9]. This extension applies a space reduction using a subset of the dataset. It guarantees accurate solutions even when the reduction has been applied. The new algorithm designed, called SACON, has been evaluated using several continuity-based datasets and it has been compared against Online Clustering algorithms and the Nyström extension of Spectral Clustering.

The paper is structured as follows: Section 2 presents the related work, Section 3 introduces the SACOC algorithm which is extended in Section 4 to create the new SACON algorithm. Section 5 shows the experimental setup applied in the experiments of Section 6. Finally, the last section explains the conclusions.

2 Related Work

Following sections will be focused on provide a general description of the clustering problem, include some issues about ACO for classification and clustering.

2.1 Clustering Large Data

Clustering has been widely used in several and heterogeneous fields. Important challenges of large data analysis is the online analysis. Clustering methods have become promising techniques in this field, as these algorithms can deal with unlabelled data.

The idea behind online clustering algorithm is to analyse this data using real-time techniques. These techniques usually need to deal with large data quantities. The main problem of these algorithms is that they need a specific space to update the information. This limits the possibilities of the new algorithm, producing for example, that some clustering algorithms might not be easily adapted to this kind of analysis [2].

One of the main tools used for online clustering analysis is the Massive On-line Analysis (MOA) tool. This framework provides the following online clustering algorithms:

- Online K-means [2]: This online algorithm updates the centroid position when a new instance arrives. Only one centroid is updated per iteration. It is similar to classical K-means algorithm.
- ClusTree [10]: This online algorithm iteratively updates the information of the clusters. It is able to consider the speed of the data stream generating the concept of the age of the object. It also maintains stream summaries.
- CluStream [11]: This algorithm combines offline clustering and online clustering in order to provide partial clustering solutions which measure the evolution of the clusters.

All of these algorithms have been designed in order to identify more properties of the data stream than the final clusters in a specific moment.

2.2 Continuity-based and Spectral Clustering

This section explains the Spectral Clustering Algorithm (see Algorithm 1) which is one of the most relevant continuity-based clustering algorithms. The algorithm starts generating a Similarity Graph among the data instances (line 1 of Algorithm 1), pair to pair. There are three main methodologies, i.e., graphs, which are used in these techniques [12]:

1. **The ϵ-neighbourhood graph**: all the components whose pairwise distance is smaller than ϵ are connected.
2. **The k-nearest neighbour graphs**: the vertex v_i is connected with vertex v_j if v_j is among the k-nearest neighbours of v_i.
3. **The fully connected graph**: all points with positive similarity are connected with each other.

This work is centred in the fully connected graph. One of the most important metrics used in Spectral Clustering is the RBF kernel [14] defined by:

$$s(x_i, x_j) = e^{-\sigma||x_i - x_j||^2} \tag{1}$$

The second step is related to the study of the eigenvectors of the Laplacian Matrix of the Similarity Graph (lines 2 and 3 of Algorithm 1). Depending on the Laplacian Matrix calculation, there are three different techniques related to Spectral Clustering [12]:

1. **Unnormalized Spectral Clustering** It defines the Laplacian matrix as: $L = D - W$
2. **Normalized Spectral Clustering** It defines the Laplacian matrix as: $L_{sym} = D^{-1/2}LD^{-1/2} = I - D^{-1/2}WD^{-1/2}$
3. **Random Walks-based Normalized Spectral Clustering** It defines the Laplacian matrix as: $L_{rw} = D^{-1}L = I - D^{-1}W$

In these equations I is the identity matrix, D represents the diagonal matrix whose (i, i)-element is the sum of the Similarity Matrix ith row and W represents the Similarity Graph (see Algorithm 1, line 2). Once the

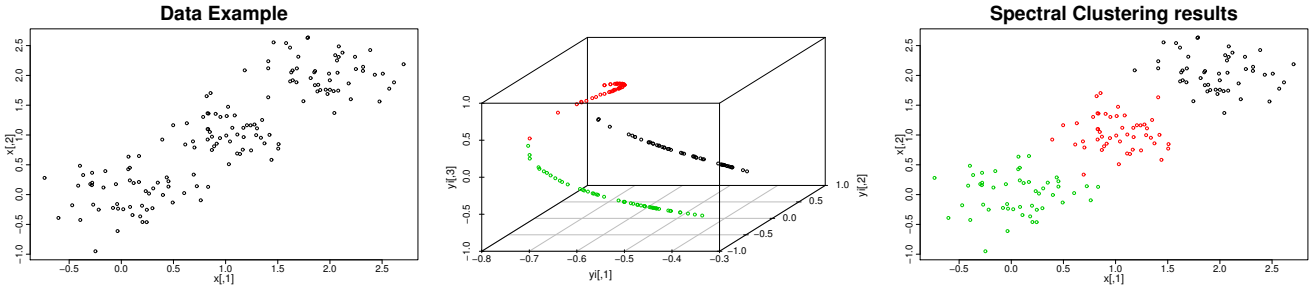


Figure 1 Spectral Clustering process from the original dataset to the final clustering results (left to right): the original data, the partition in the projective space and the final discrimination.

Algorithm 1 Normalized Spectral Clustering according to Ng et al. (2001)[13]

Require: A dataset of n elements $X = \{x_1, \ldots, x_n\}$ and a fixed number of clusters k.

Ensure: A set of clusters $C = \{C_1, \ldots, C_k\}$ which is a partition of X

1: Form the Similarity Graph $W \in R^{n \times n}$ defined by $W_{ij} = e^{-\sigma ||x_i - x_j||^2}$ if $i \neq j$, and $W_{ii} = 0$.
2: Define D to be the diagonal matrix whose (i,i)-element is the sum of the i-th row of W.
3: Construct the matrix $L = D^{-1/2} W D^{-1/2}$.
4: Find $v_1, \ldots, v_k$, the k largest eigenvectors of L (chosen to be orthogonal to each other in the case of repeated eigenvalues) and form the matrix $V = [v_1 v_2 \ldots v_k] \in R^{n \times k}$ by stacking the eigenvectors in columns.
5: Form the matrix Y from V by renormalizing each row of V to have unit length (i.e. $Y_{ij} = V_{ij} / (\sum_j V_{ij}^2)^{1/2}$).
6: Apply K-means (or any other algorithm) treating each row of Y as a point in R^k.
7: Assign the points x_i to cluster C_j if and only if the row i of the matrix Y was assigned to cluster j.
8: **return** C

Laplacian is calculated (in Algorithm 1 the Normalized Spectral Clustering algorithm is used), its eigenvectors are extracted (see lines 4 and 5 of Algorithm 1). Some of the main problems of Spectral Clustering are related to the consistency of the two classical methods used in the analysis: normalized and un-normalized Spectral Clustering. A deep analysis about the theoretical effectiveness of normalized clustering over un-normalized can be found in [15].

The graph cut problem is closely related to Spectral Clustering. In the graph cut literature this problem has two classical solutions [12]: RadioCut and NCut. Von Luxburg et al. [12] describe the connection between the different approaches of Spectral Clustering (focused on the Laplacian Matrices), RadioCut and NCut. They also show that Unnormalized Spectral Clustering converges to RadioCut and the Normalized methods converge to NCut.

Figure 1 shows an example where the Laplacian Matrix has a maximum of 150 different eigenvectors. According to the leader eigenvalues (those eigenvalues with the highest values) their associated eigenvectors are chosen. Since this example has three clusters (see Figure 1), the 3 leader eigenvectors are chosen.

The last step is the application of a clustering algorithm to the projective space formed by the normalized eigenvectors (see Figure 1 considering each row of the matrix as a point (see lines 6 and 7 of Algorithm 1). The most frequently applied algorithm is K-means. There are several versions of Spectral Clustering according to the algorithm that is used in this step, e.g., the SACOC [5] algorithm is a Spectral-based algorithm which applies an ACO clustering algorithm instead of K-means. Figure 1 shows the application of K-means to the previous example. The figure shows the distribution of the data in the space generated by the chosen eigenvector. In this case, each point could be interpreted as a projection of the original points. The results of the application of the algorithm to this data are also shown in Figure **??** (right). The data in the projective space is easier to separate than in the original space. This shows the results of the algorithm in the original space.

The main problem of Spectral Clustering is how to compute the eigenvectors and the eigenvalues of the Laplacian Matrix of the Similarity Graph avoiding the huge memory that it consumes. For example, when large datasets are analysed, the Similarity Graph of the SC algorithm requires a high memory storage and it makes extremely hard the eigenvalues and eigenvectors computation.

2.3 Ant Colony Optimization in Classification and Clustering

One of the current perspectives which deals with Machine Learning problems is Ant Colony Optimization [6]. ACO approaches have been used to improve local minima convergence problems. These algorithms are designed to look for an optimal solution. These approaches have been applied for both, classification [3] and clustering [3] algorithms.

In ACO there are also some adaptations of classification algorithms—e.g., Otero et al. introduce an ACO algorithm for decision tree induction [7]; Blum and Socha introduce a neural network ACO model [16] and

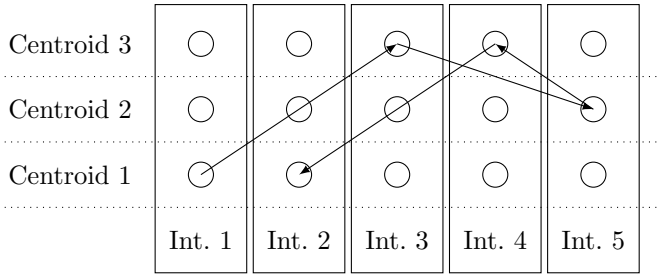


Figure 2 The construction graph of SACOC. The arrows represent a trail of an ant.

Borrotti and Poli focused their work on the Naïve Bayes model [17].

There are also some clustering algorithms which have produced promising results—e.g., Kao and Cheng designed a centroid-based ACO clustering algorithm [18]; Ashok and Messinger focused their work on graph-based clustering [19]; Menéndez et al. designed a Medoid-based ACO Clustering algorithm called MACOC [8] focused on improving the results of ACOC; and, finally, several other approaches are discussed in [20]. It is interesting to remark that both MACOC and SACOC are based on ACOC algorithm. The logic of the algorithms is similar (also the parameters), but the goal and search space are different.

3 Spectral-based ACO Clustering Algorithm (SACOC)

This section presents the Spectral-based ACO Clustering Algorithm (SACOC) [5]. This algorithm is similar to Spectral Clustering. The goal of the algorithm is to choose the data discrimination representing the information as a Similarity Graph, and cutting it in different clusters.

3.1 ACOC algorithm

The ACOC algorithm (see Algorithm 2) is the base of SACOC (see Algorithm 3). It has a search space based on instances and centroids, and can be defined as a graph whose associated matrix is a N×k matrix, where N is the number of instances and k is the number of centroids (clusters).

The algorithm works with several ants looking for the best path in the graph (see Fig. 2). Each ant (a) has the following features: a list of visited objects (tb^a), a set of chosen centroids C^a and a Weighted matrix W^a (related to the assignment of objects to clusters).
An ant a has two possible strategies: exploration and exploitation. It chooses the strategy according to the following equation:

$$j = \begin{cases} argmax_{u \in N_i}\{[\tau(i,u)][\eta^a(i,u)]^\beta\}, & \text{if } q \leq q_0 \\ S, & \text{otherwise} \end{cases} \quad (2)$$

where N_i is the set of nodes associated to object i, j is the chosen cluster, $\tau(i,u)$ is the pheromone value between i and u, q_0 is the exploitation probability, q is a random number for strategy selection,β is a parameter, $\eta^k(i,u)$ is the heuristic value between i and u for ant a defined by the formula: $\eta^a(i,u) = 1/d(x_i, c_j^a)$.
where x_i is a data instance and c_j^k is a centroid from the ant centroid list. and S is the exploration defined by:

$$S = P^a(i,u) = \frac{[\tau(i,u)][\eta^a(i,u)]^\beta}{\sum_{j=1}^{m}[\tau(i,j)][\eta^a(i,j)]^\beta} \ . \quad (3)$$

The algorithm steps can be divided by:

1. Initialize pheromone matrix (see line 1 of Algorithm 2).

2. Initialize ants (see line 3 of Algorithm 2): (tb^a, C^a, W^a), for each ant a in the colony. Then, each ant repeats until tb^a is full:

   (a) Select (randomly) a data object i satisfying $i \notin tb^a$ (see line 6 of Algorithm 2).

   (b) Select a cluster j: first the ant chooses a strategy; then, it calculates the transition probability and, finally, it visits a node (see line 7 of Algorithm 2).

   (c) Update tb^a, C^a and W^a (see lines 9 and 10 of Algorithm 2).

3. Choose the best solution. First, calculate the objective function for each ant (see lines 14 and 15 of Algorithm 2):

$$J^k = \sum_{i=1}^{n}\sum_{j=1}^{m} w_{ij}^a d(x_i, c_j^a) \ , \quad (4)$$

   where w_{ij}^a is a weight value of the assignment matrix W^a. Next, rank ants solutions. Choose the iteration-best solution, apply local search (for more details of local search see [21]), to improve the solution and, finally, compare it with the best-so-far solution and update this value with their maximum.

4. Update pheromone trails (global updating rule). Only the best r ants are able to add pheromones. Let ρ be the pheromone evaporation rate, ($0 < \rho < 1$), t the iteration number, r is the number of elitism ants and $\Delta\tau_{ij}^h = 1/J^h$ (see line 17 of Algorithm 2):

$$\tau_{ij}(t+1) = (1-\rho)\tau_{ij}(t) + \sum_{h=1}^{r} w_{ij}^h \Delta\tau_{ij}^h \ . \quad (5)$$

5. Check the termination condition: if the number of iterations is greater than the maximum limit, finish; otherwise, go to step 2.

Algorithm 2 ACOC algorithm.

Require: $X = x_1, \ldots, x_n$ and k number of clusters
Ensure: $c_1, \ldots, c_k$ best k centroids
1: Initialize the pheromone matrix τ_0.
2: **for** generation $g = 0$ **to** *maxGenerations* **do**
3: Initialize ants: $C^a = \emptyset$ and $tb^a = \emptyset$
4: **for all** ant $a \in A$ (the ants set) **do**
5: **while** $|tb^a| == n$ or $|C^a| == k$ **do**
6: Select the next data object i
7: Choose a strategy (exploration, exploitation)
8: Select $c_{q^*} \in C^a$ as the closest centroid
9: Set $W^a_{i,q^*} = 1$
10: addInstance(i) to tb^a
11: **end while**
12: Calculate the objective function for each ant: $J^a = \sum_{i=1}^{n} \min_{j=1}^{|M|} d(x_i, m^a_j)$
13: **end for**
14: Rank the ants according to J^a.
15: Choose the best ant a^* (iteration-best solution).
16: Compare it with the best-so-far solution (a^{**}) and update this value with the maximum between them.
17: $\tau_{g+1}(i,u) = (1-\rho)\tau_g(i,u) + \sum_{h=1}^{r} w^h_{iu} \cdot \Delta\tau_g(i,u)^h$
18: **end for**
19: Re-centralize a^{**}.

3.2 The Spectral hybridisation

The original ACOC algorithm uses the Euclidean space as a search space. However, the algorithm can be modified to consider any kernel in a similar way that K-means is modified to generate the Spectral Clustering algorithm. Consider a graph G and its associated weighted matrix W, which is a pairwise Similarity Graph amongst the data. The similarity is calculated using a similarity function defined by a kernel $k(x_i, x_j)$ (see line 1 of Algorithm 3). The Spectrum of the graph is calculated in a similar fashion used by Ng et al. [13] (see lines 2 and 3 of Algorithm 3) to create the original Spectral Clustering algorithm. First, we calculate the Laplacian matrix defined by: $L_{sym} = I - D^{-1/2}WD^{-1/2}$, where I is the identity matrix and D represents the diagonal matrix whose (i,i)-element is the sum of the similarity matrix i-th row. After the creation of the Laplacian matrix, we extract the $v_1, \ldots, v_z$, (see line 4 of Algorithm 3) which corresponds with the z largest eigenvectors of L—chosen to be orthogonal to each other in the case of repeated eigenvalues—and form the matrix $V = [v_1\, v_2\, \ldots\, v_z] \in \mathbb{R}^{n \times z}$ by stacking the eigenvectors in columns. Finally, we form the matrix Y from V by renormalizing each row of V to have unit length (i.e., $Y_{ij} = V_{ij}/(\sum_j V^2_{ij})^{1/2}$) (see line 5 of Algorithm 3). Then, we can consider Y as a projection of the original space and apply ACOC (see line 6 of Algorithm 3) to the representation of each point.

Algorithm 3 SACOC algorithm. [5]

Require: $X = x_1, \ldots, x_n$ and k number of clusters
Ensure: $c_1, \ldots, c_k$ best k clusters
1: Form the Similarity Graph $W \in R^{n \times n}$ defined by $W_{ij} = e^{-||x_i - x_j||^2/2\sigma^2}$ if $i \neq j$, and $W_{ii} = 0$.
2: Define D to be the diagonal matrix whose (i,i)-element is the sum of the i-th row of W.
3: Construct the matrix $L = D^{-1/2}WD^{-1/2}$.
4: Find $v_1, \ldots, v_k$, the k largest eigenvectors of L (chosen to be orthogonal to each other in the case of repeated eigenvalues) and form the matrix $V = [v_1 v_2 \ldots v_k] \in R^{n \times k}$ by stacking the eigenvectors in columns.
5: Form the matrix Y from V by renormalizing each row of V to have unit length (i.e. $Y_{ij} = V_{ij}/(\sum_j V^2_{ij})^{1/2}$).
6: ACOC(Y,k).

4 SACON: Improving the SACOC algorithm through the Nyström Method

The goal of this methodology is to reduce the dimensions sampling the Similarity Matrix. We are going to choose a subset of points $S = \{s_1, \ldots, s_n\} \in X = \{x_1, \ldots, x_N\}$ (see line 1 of Algorithm 4). If W is the Similarity Matrix (related to the Similarity Graph), we need to extract the eigenvectors of its Spectrum in order to project the data. The Spectrum we are going to consider in this work is defined by: L_{sym} (see Section 3.2). Because it is difficult to scale the original Similarity Matrix, we need to use the subsample S and reformulate the whole process to describe how to extract approximate eigenvectors of the Spectrum using less information related to the original Similarity Matrix.

For this approximation, we are going to apply the Nyström extension [9], defined as follows:

Nyström Extension: Let $k(x_i, x_j)$ be a kernel whose Gram matrix K is symmetry and positive semi-definite satisfying $K_{i,j} = k(x_i, x_j)$. We assume that the eigendescomposition is $KU = U\Lambda$ with U orthogonal. Then, the Nyström extension for a new instance x is the eigenvector approximation $\bar{u}^k(x)$ to the real $u^k(x)$ given by:

$$\bar{u}^k(x) = \frac{1}{\lambda^u_k} \sum_{j=1}^{N} k(x, x_j) u^k_j \tag{6}$$

In order to apply the extension to calculate the eigenvectors of L_{sym} we need to simplify the problem. First, $L_{sym} = I - D^{-1/2}WD^{-1/2}$, so it is equivalent to calculate the eigenvectors for $P = D^{-1/2}WD^{-1/2}$.

In order to approximate the eigenvectors, we are going to follow the scheme of Figure 3. In this case, we use W, and we take the subsamples set S, which defines a submatrix of W called A. These matrices satisfy:

$$W = \begin{pmatrix} A & B \\ B^t & C \end{pmatrix}$$

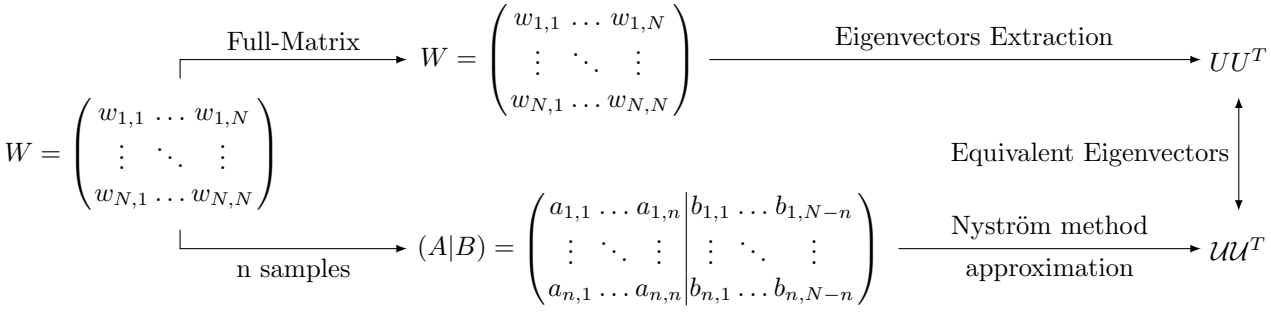


Figure 3 Eigenvector decomposition applying the Nyström extension. The original Similarity Matrix W is subsampled in the augmented matrix $(A|B)$. Using only this information the Nyström extension is able to approximate the eigenvectors U of W as the eigenvectors $\mathcal{U}$.

Algorithm 4 SACOC+Nystrom (SACON) algorithm.

Require: $X = x_1, \ldots, x_N$ and k number of clusters
Ensure: $c_1, \ldots, c_k$ best k clusters

1: Select a subsample of the data instances: $S = \{s_1, \ldots, s_n\} \in X = \{x_1, \ldots, x_N\}$ where, $n << N$.
2: Form the Similarity Graph $A \in R^{n \times n}$ defined by $A_{ij} = e^{-\sigma||s_i - s_j||^2}$ if $i \neq j$, and $A_{ii} = 0$.
3: Calculate the Matrix B formed by the similarities among the elements of A and the rest of data instances.
4: Calculate the eigenvectors of A, named $\bar{U}$ and the eigenvalues, named $\bar{\Lambda}$.
5: Calculate the approximate eigenvectors $\mathcal{U}$ of W which try to approximate the real eigenvectors, named U, as:

$$\mathcal{U} = \begin{pmatrix} \bar{U} \\ B^t \bar{U} \bar{\Lambda}^{-1} \end{pmatrix}$$

6: Define D to be the diagonal matrix whose (i,i)-element is the sum of the i-th row of W.
7: Construct the matrix $L' = D^{-1/2} W' D^{-1/2}$.
8: Separate $L' = \begin{pmatrix} A' & B' \\ (B')^t & (B')^t (A')^{-1} B' \end{pmatrix}$
9: Set $R = A' + (A')^{-1/2} B' (B')^t (A')^{-1/2}$, and calculate its eigenvector decomposition $R = U_R \Lambda_R U_R^t$.
10: Set $\mathcal{V} = \begin{bmatrix} A' \\ (B')^t \end{bmatrix} (A')^{-1/2} U_R \Lambda_R^{-1/2}$.
11: Find $v_1, \ldots, v_k$, the k largest eigenvectors of L' and form $V = [v_1 v_2 \ldots v_k] \in R^{n \times k}$ by stacking the eigenvectors in columns.
12: Form the matrix Y from V by renormalizing each row of V to have unit length (i.e. $Y_{ij} = V_{ij} / (\sum_j V_{ij}^2)^{1/2}$).
13: ACOC(Y,k).

where $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times (N-n)}$ and $C \in R^{(N-n) \times (N-n)}$ (see line 3 of Algorithm 4). The Nyström Extension will only need the augmented matrix formed by A and B: $(A|B)$. The matrix C is the part that we want to approximate and satisfies that has more elements than A, due to $n << N$. Using this matrix it will be able to approximate eigenvectors of U calculating the eigenvectors of A, denoted by $\bar{U}$ (see line 4 of Algorithm 4). These eigenvectors $\bar{U}$ will be extended to form the approximation $\mathcal{U}$ which is close to the original U. Once the eigenvectors $\bar{U}$ have been calculated, we have the eigendecomposition of A as $A = \bar{U} \bar{\Lambda} \bar{U}^T$ because U is orthonormal. Equation 6 provides a methodology to calculate $\mathcal{U}$ as (see line 5 of Algorithm 4):

$$\mathcal{U} = \begin{pmatrix} \bar{U} \\ B^t \bar{U} \bar{\Lambda}^{-1} \end{pmatrix} \tag{7}$$

which is the approximation of the K first eigenvectors of W.

Now, we need to extract the Laplacian eigenvectors, which are extracted from the approximate matrix (see line 7 of Algorithm 4): $L' = D^{-1/2} W' D^{-1/2}$, where $W' = \mathcal{U} \widehat{\Lambda} \mathcal{U}$, $\widehat{\Lambda} = \frac{n}{l} \bar{\Lambda}$. Setting $D_{i,i} = \sum_{j=1}^{N} w'_{i,j}$ we can restructure D as

$$D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix}$$

where $D_1 \in \mathbb{R}^{n \times n}$ and $D_2 \in \mathbb{R}^{(N-n) \times (N-n)}$ and L can be approximated by (see lines 7 and 8 of Algorithm 4):

$$L' = \begin{pmatrix} A' & B' \\ (B')^t & (B')^t (A')^{-1} B' \end{pmatrix}$$

where $A' = D_1 A$ and $B' = D_2 B$. In order to approximate the eigenvectors of L' we will use the same methodology that we have used to approximate W- In this case, we are going to use A' as the base, supposing that the eigenvectors of A' and eigenvalues are $\mathcal{V}^o$ and Λ^o.

$$\Lambda' = \frac{n}{l} \Lambda^o, \quad \mathcal{V} = \sqrt{\frac{l}{n}} \begin{bmatrix} A' \\ (B')^t \end{bmatrix} V^o \Lambda^o$$

where $\mathcal{V}$ and Λ' are the extended eigenvectors and eigenvalues of L'. Due to $\mathcal{V}$ is not orthogonal, which is required by the Spectral Clustering algorithm, we apply the transformation of Fowlkes et al. [9] and defined the matrix (see line 9 of Algorithm 4):

$$R = A' + (A')^{-1/2} B' (B')^t (A')^{-1/2}$$

This matrix can be decomposed as $R = U_R \Lambda_R U_R^t$ due to A' is positive define. Then, we set (see line 10 of Algorithm 4):

$$\mathcal{V} = \begin{bmatrix} A' \\ (B')^t \end{bmatrix} (A')^{-1/2} U_R \Lambda_R^{-1/2}$$

And, finally,

$$D^{-1/2} W' D^{-1/2} = \mathcal{V} \Lambda_R \mathcal{V}^t$$

which means that $\mathcal{V}$ are the eigenvectors which will be used for the ACOC clustering algorithm (see line 11 of Algorithm 4).

5 Experimental Setup

The evaluation of the clustering algorithm is a sensitive process, specially when the algorithm deals with large datasets. In this work we have focused the evaluation on comparing the algorithm with other Big Data algorithms. This evaluation has been performed using 8 datasets with 50.000 instances.

The experiments have been carried out using the Nyström extension of Spectral Clustering [9] (SC+N), CluStream, Online K-means and ClusTree.

The parameters of SACON are: the subsample size (fixed to 500), and the sigma value that has been calculated using the methodology described by Ng et al. in [13] (for SC + Nyström is the same); the ants number is 10, the elitism is 1, the exploitation probability is 0.0001, the initial pheromone values have been set to $1/k$—where k is the number of clusters, $\beta = 2.0$, $\rho = 0.1$, the local search probability is 0.001 and the maximum number of iterations is 1000.

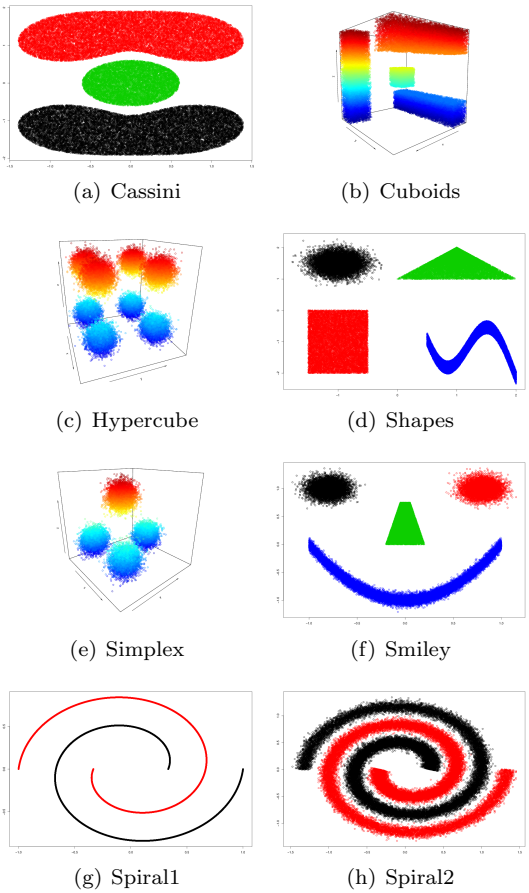
The metrics used are the Euclidean Distance for online algorithms, and the RBF for the spectral-based algorithms. The evaluation is performed comparing the results with the ideal labels. The evaluation is performed with the accuracy metric, defined by:

$$sim(C_i, C_j) = \frac{\sum_{q=1}^{n} \delta_{C_i}(x_q) \delta_{C_j}(x_q)}{2} \left(\frac{1}{|C_i|} + \frac{1}{|C_j|} \right) \quad (8)$$

where $|C_i|$ is the number of elements of cluster C_i and $\delta_{C_i}(x_q)$ is the Kronecker δ defined by:

$$\delta_{C_i}(x_q) = \begin{cases} 0 \text{ if } x_q \notin C_i \\ 1 \text{ if } x_q \in C_i \end{cases}$$

All the experiments have been executed 100 times. The statistical test which has been performed is the Wilcoxon test, because we can not guarantee that the distributions are normal. It compares SACON with SC+Nyström since these algorithms are very similar to each other. We have considered that there is statistically difference when the p-value of the test is lesser than 0.05 (5% significance level).



(a) Cassini (b) Cuboids (c) Hypercube (d) Shapes (e) Simplex (f) Smiley (g) Spiral1 (h) Spiral2

Figure 4 The original images of the synthetic datasets

5.1 Dataset Description

The datasets have been generated using the R package mlbench [22] which allows to generate dense datasets with a specific form. The datasets—all composed by 50.000 instances—that have been generated are the following (see Figure 4):

- **Cassini**: This dataset is formed by 3 clusters which are continuity-based.
- **Cuboids**: This dataset has four cuboids in three dimensions.
- **Hypercube**: This datasets is composed by eight spheres distributed as the vertex of a cube.
- **Shapes**: This dataset has 4 different shapes.
- **Simplex**: This dataset has four spheres well separated.
- **Smiley**: This dataset is formed by four clusters which define a smiley face.
- **Spirals1**: This dataset has two spirals without noise.
- **Spirals2**: This dataset has two noisy spirals.

6 Experimental Results

This section presents the evaluation process of SACON. Table 1 shows the results for the algorithms applied to the datasets. As we can appreciate, SACON obtains overall good results, but it is important to analyse the algorithm according to each dataset in order to identify its weaknesses.

In the case of **Cassini** dataset, SACON obtains the best results. SC+Nyström also obtains good results. It is important to remark that the SD of SACON is 0, which means that these results are stable. The rest of the algorithms obtain worse results. It should be because the dataset (see Figure 4 (a)) has two sections which can be easily defined using a Gaussian distribution, and when the number of instances is high, the boundaries between these distributions are harder for the discrimination process. SC is also sensitive to the noise produced in this situation. The statistical test shows that SACON is significantly better than SC + Nyström.

For **Cuboids** dataset, Clustream obtains the best Median results (100.0%) followed by SC+Nyström (99.74%). However SACON obtains close results (99.33%). This dataset produces the lesser stable results for SACON (0.0066 of SD), however, the algorithm is the most stable of the algorithms group. These results suggest that the algorithm is also able to deal with volume identification problems (see Figure 4 (b)). The Wilcoxon test shows that there is not statistical difference between the spectral-based algorithms.

Hypercube results show that SACON is able to discriminate the clusters perfectly. Clustream also obtains good results during the discrimination process. SC+Nyström, Clustree and Online K-means have more problems to discriminate the cluster distribution. It might be because the algorithms have to deal with large data quantities and that introduces noise during the calculation (see Figure 4 (c)). The algorithms are also less stable than SACON (the SD of SACON is 0). Again, SACON is significantly better than SC+Nyström approach.

In the case of **Shapes**, the best results according to the Mean and Median are achieved by Clustream, and the best for Median by Clustree and Online K-means. SACON obtains worse but close results (99.98%) because the algorithm is more stable (the SD is 0.0002). SC+Nyström obtains the worst results of the iteration (68.71%). According to the statistical test, SACON is better again.

Simplex is easy for all algorithms. The Median value shows that they obtain the maximum results. However, according to the Mean, only SACON, Clustream and SC+Nyström keep these results in all the iterations. These results are a consequence of the data structure (see Figure 4 (e)), in this case, they only need to discriminate spheres which is the simplest clustering problem. There is not statistical difference between them.

Smiley results show that SACON obtains the best discrimination results (99.59%). The rest of the algorithms have more problems generating the clusters. This dataset is a continuity-based problem, therefore only SC+Nyström, Clustream and SACON can discriminate the boundaries (see Figure 4 (f)). SACON is statistically better than SC + Nyström.

The **Spiral1** dataset tests show how the algorithms can deal with continuity datasets without noise (see Figure 4 (g)). In this case, SACON and SC+Nyström obtain the best results (100.0%). In this case, Online K-means, Clustree and Clustream have more problems discriminating the spirals which means that these algorithms are not able to deal with pure continuity-based problems. There is not statistically difference between them.

The **Spiral2** dataset introduces noise to the previous one (see Figure 4 (h)). In this case, the results of SACON are worse than in the previous datasets, but it also obtains the best and more stable results. The results of the rest algorithms show that there is a good minimal solution and all of them are close to this solution (around the 59%), however, they still find problems discriminating the spirals. SACON is significantly better than SC + Nyström.

6.1 Discussion

SACON shows competitive results when it is applied to continuity-based data, such as Cassini, Shapes, Smiley and Spirals while the rest have more problems, e.g., with Spirals which is a pure continuity-based problem. It also performs better than the rest when we add noise to the dataset. The algorithm also obtains more stable results than the others according to the standard deviation. The spectral transformation is probably the main reason of the algorithm improvements. The performance is correlated to the type of clustering that this algorithm can face.

In order to compare the memory usage of the current algorithm against SACOC (its predecessor), it is important to remark that SACON uses a matrix of $50,000 \times 500$ instances, whereas SACOC uses $50,000 \times 50,000$ instances. The memory usage of the former is around 0.18 GB while the latter consumes around 18.63 GB. The memory consume of SACON grows linearly whereas SACOC grows exponentially. The rest of the algorithm are not spectral algorithm, i.e., they do not use a Similarity Matrix. According to the memory consumption, the online algorithms only keep memory about the centroids they are using (similar to K-means), i.e., the memory grows according to the number of centroids, while ACOC keep memory of the assignation of the instance to the centroid, i.e., its memory usage grows linearly according to the product of instances and centroids number.

Dataset	**SACON**	**SC+Nystrom**	**Online K-means**	**Clustree**	**Clustream**
Cassini	▲ **99.98%** ± 0.0000	*98.61%* ± 0.1681	65.47% ± 0.0003	66.97% ± 0.1301	67.39% ± 0.0478
Cuboids	99.33% ± 0.0066	*99.74%* ± 0.1736	88.84% ± 0.1219	72.74% ± 0.1108	**100.0%** ± 0.1157
Hypercube	▲ **100.0%** ± 0.0000	76.71% ± 0.1565	81.36% ± 0.1122	82.29% ± 0.1126	**100.0%** ± 0.0541
Shapes	▲ 99.98% ± 0.0002	68.71% ± 0.4425	**100.0%** ± 0.1389	**100.0%** ± 0.1765	**100.0%** ± 0.0001
Simplex	**100.0%** ± 0.0000	**100.0%** ± 0.0000	**100.0%** ± 0.1508	**100.0%** ± 0.1703	**100.0%** ± 0.0000
Smiley	▲ **99.56%** ± 0.0003	74.99% ± 0.1627	62.54% ± 0.1729	64.41% ± 0.1608	*91.60%* ± 0.1451
Spirals1	**100.0%** ± 0.0000	**100.0%** ± 0.0991	50.00% ± 0.0000	50.01% ± 0.0002	50.01% ± 0.0006
Spirals2	▲ **63.03%** ± 0.0001	*59.59%* ± 0.0392	59.36% ± 0.0000	58.84% ± 0.0295	*59.59%* ± 0.0392

Table 1 Median and Standard Deviation accuracy results of the application of the algorithms to the datasets. Values in bold shows the best results while italics shows the second. The ▲ symbol shows those datasets where the results of SACON are statically better than the results of the benchmark algorithm SC + Nystrom.

7 Conclusions

This paper presents an evolution of the SACOC algorithm [5] using the a Nyström extension [9]. The new algorithm, called SACON, applies the spectral transformations and the Nyström extension to the original search space in order to apply the clustering in the projective space. The transformation consists on transforming the original data into a graph-based representation (through a similarity graph) and calculate its Laplacian matrix, during this calculation, the Nyström extension guarantees that the Laplacian calculation is accurate enough using less information. Once the Laplacian has been obtained, the eigenvectors are extracted and normalized to generate the projective space, this extraction also applies the Nyström extension in order to reduce the memory usage.

The proposed SACON algorithm shows good results for the studied datasets. It is able to discriminate continuity-based clusters with more stable results, when compared to Spectral Clustering using the Nyström extension (SC+Nyström) and modern online clustering algorithms.

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