Sparsification on Parallel Spectral Clustering*

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Abstract. Spectral clustering is one of the most relevant unsupervised method able to gather data without a priori information on shapes or locality. A parallel strategy based on domain decomposition with overlapping interface is reminded. By investigating sparsification techniques and introducing sparse structures, this parallel method is adapted to treat very large data set in fields of Pattern Recognition and Image Segmentation.

1 Introduction

Spectral clustering selects dominant eigenvectors of a parametrized affinity matrix in order to build a low-dimensional data space wherein data points are grouped into clusters [1]. This method based on eigendecomposition of affinity matrix is used in Pattern Recognition or image segmentation to cluster non-convex domains without a priori on the shapes. The main difficulties of this method could be summarized by the two following questions: how to automatically separate clusters one from the other and how to perform clustering on large dataset, for example on image segmentation. This means that we look for some full-unsupervising process with parallelization. Several studies exist for defining a parallel implementation which exploits linear algebra [3], [4] for the affinity computation of the whole data set [2]. But the input parameters which are the affinity parameter and the number of clusters limit these methods. To address this limitation, a fully unsupervised parallel strategy based on domain decomposition was proposed in [6] which preserves the quality of global partition thanks to overlapping interface. From the first results, we have observed that the main part of the time is spent in the spectral clustering step and we encountered memory limitation with large problems.

In this paper, we study the robustness of the parallel spectral clustering with overlapping interface presented in [6] by investigating sparsification techniques and introducing sparse structures and adapted eigensolvers in order to treat larger problems. Then we test this improvements on geometrical examples and image segmentations.

2 Parallel Spectral Clustering

Let consider a data set $S = \{x_i\}_{i=1..n} \in \mathbb{R}^p$. Assume that the number of targeted clusters k is known. First, the spectral clustering consists in constructing the

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affinity matrix based on the Gaussian affinity measure between points of the dataset S. After a normalization step, the k largest eigenvectors are extracted. So every data point x_i is plotted in a spectral embedding space of $\mathbb{R}^k$ and the clustering is made in this space by applying $K-means$ method. Finally, thanks to an equivalence relation, the final partition of data set is defined from the clustering in the embedded space. Algorithm 1 presents the different steps of spectral clustering.

Algorithm 1. Spectral Clustering Algorithm

Input: data set S, number of clusters k

1. Form the affinity matrix $A \in \mathbb{R}^{n\times n}$ defined by:

$$A_{ij} = \begin{cases} \exp\left(-\frac{\|x_i - x_j\|^2}{(\sigma/2)^2}\right) & \text{if } i \neq j, \\ 0 \text{ otherwise,} \end{cases} \tag{1}$$

2. Construct the normalized matrix: $L = D^{-1/2}AD^{-1/2}$ with $D_{i,i} = \sum_{j=1}^{n} A_{ij}$,
3. Assemble the matrix $X = [X_1 X_2 .. X_k] \in \mathbb{R}^{n\times k}$ by stacking the eigenvectors associated with the k largest eigenvalues of L,
4. Form the matrix Y by normalizing each row in the $n \times k$ matrix X,
5. Treat each row of Y as a point in $\mathbb{R}^k$, and group them in k clusters via the *K-means* method,
6. Assign the original point x_i to cluster j when row i of matrix Y belongs to cluster j.

This spectral clustering method could be adapted for parallel implementation [6] as a fully unsupervised method (see Figure 1). This avoid extracting the largest eigenvectors of a fully affinity matrix which complexity is of $O(n^3)$ [5].

The principle is based on domain decomposition with overlaps. By dividing the data set S in q sub-domains, each processor applies independently the spectral clustering algorithm on the subsets and provide a local partition. For each subdomain, a quality measure which exploits the block structure of indexed affinity matrix per cluster is used to determine the number of clusters. This heuristic avoids us to fix the targeted of clusters k. The final number of clusters k will be provided after the grouping step. The gathering step is dedicated to link the local partitions from the sub-domains thanks to the overlapping interface and the following transitive relation: $\forall x_{i_1}, x_{i_2}, x_{i_3} \in S$,

$$\text{if } \; x_{i_1}, x_{i_2} \in C^1 \text{ and } x_{i_2}, x_{i_3} \in C^2 \text{ then } C^1 \cup C^2 = P \text{ and } x_{i_1}, x_{i_2}, x_{i_3} \in P \tag{2}$$

where S is a data set, C^1 and C^2 two distinct clusters and P a larger cluster which includes both C^1 and C^2. By applying this transitive relation (2) on the overlapping interface, the connection between subsets of data is established and

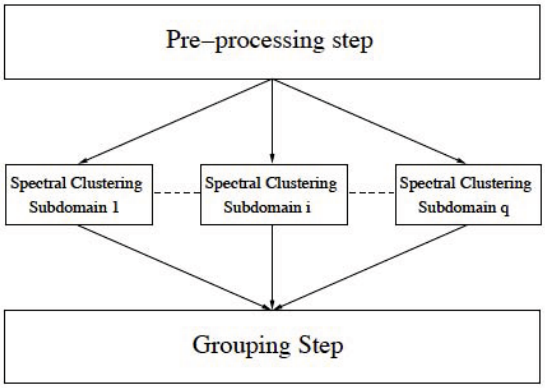


Fig. 1. Principle of the parallel spectral clustering

provides a global partition. We can summarize this Master-Slave implementation with Algorithm 2 and Algorithm 3.

We can notice that when we split the original data set into overlapping sub-pieces of data set, we gain on two aspects:

- *memory consumption:* the local spectral clustering analysis of each sub-piece involves the creation of a local affinity matrix. The size of the matrix is n^2, n being the cardinal of the data subset. The sum of the memory needs for all these local affinity matrix is much less than that needed for the affinity matrix covering the global data set. The consequence is that we can manage bigger data set, data set whose size cannot permit us to run with only one processor.
- *floating point operations:* the analysis of each subproblem is made from the extraction of eigenvectors in the scaled affinity sub-matrix: one extracted eigenvector for each identified cluster of the data subset. In that respect, the parallel approach enables us to decrease drastically the cost of this eigenvector computation: each subproblem will include a number of clusters much less than the total number of clusters in the whole data set.

Nevertheless, as we want to be able to consider larger and larger data sets, as, for instance, in image segmentation (see 4.2) or genomic applications, we still encounter memory limitation when the number of points in a local data subset is too much for the memory capacity of one processor.

3 Sparsification of Spectral Clustering

Despite the domain decomposition, the most time consuming is dedicated to the spectral clustering algorithm. To address this limitation and the memory consumption ones, we investigate a thresholding as sparsification technique.

Algorithm 2. Parallel Algorithm: Master

1: Pre-processing step
  1.1 Read the global data and the parameters
  1.2 Split the data into q subsets
  1.3 Compute the affinity parameter σ with the formula given in paper [6]; the bandwidth of the overlapping is fixed to $3 \times \sigma$
2: Send the sigma value and the data subsets to the other processors (MPI_SEND)
3: Perform the Spectral Clustering Algorithm on its subset
  3.1 Computation of the spectrum of the affinity matrix (1): classical routines from LAPACK library [7] are used to compute selected eigenvalues, eigenvectors of the normalized affinity matrix A for its subset of data points
  3.2 Number of clusters: the number of clusters k with the heuristic [6]
  3.3 Spectral embedding: the centers for K-means initialization in the spectral embedding are chosen to be the furthest from each other along a direction
4: Receive the local partitions and the number of clusters from each processor (MPI_RECV)
5: Grouping Step
  5.1 Gather the local partitions in a global partition thanks to the transitive relation given in paper [6]
  5.2 Output a partition of the whole data set S and the final number of clusters k

Algorithm 3. Parallel Algorithm: Slave

1: Receive the sigma value and its data subset from the Master processor (MPI CALL)
2: Perform the Spectral Clustering Algorithm on its subset
3: Send the local partition and its number of clusters to the Master processor (MPI CALL)

3.1 Theoretical Interpretation

From the definitions of both the Gaussian affinity A_{ij} between two data points x_i and x_j and the Heat kernel $K_t(x) = (4\pi t)^{-\frac{p}{2}} \exp\left(-\|x\|^2/4t\right)$ in free space $\mathbb{R}_+^* \times \mathbb{R}^p$, we can interpret the gaussian affinity matrix as discretization of heat kernel by the following equation:

$$A_{ij} = (2\pi\sigma^2)^{\frac{p}{2}} K_t\left(\sigma^2/2, x_i - x_j\right). \tag{3}$$

So, we can prove that eigenfunctions for bounded and free space Heat equation are asymptotically close [8]. With Finite Elements theory, we can also prove that the difference between eigenvectors of A and discretized eigenfunctions of K_t is of an order of the distance between points include inside the same cluster. This means that applying spectral clustering into subdomains resumes in restricting the support of these L^2 eigenfunctions which have a geometrical property: their supports are included in only one connected component. In fact, the domain decomposition by overlapping interface does not alter the global partition because the eigenvectors carry the geometrical property and so, the clustering property.

Let now interpret a thresholding of the affinity matrix on the clustering result. This leads to restrict the approximation to the finite elements which satisfy

homogeneity mesh condition in the interpretation. In other words, this means that it strengthens the piece-wise constancy of the dominant eigenvectors from the normalized Gaussian affinity matrix. But the threshold should be well-chosen and should be coherent according to the data distribution. So it should be defined function of both dimension of the data and number of data as defined in [8].

(a) Without thresholding (b) With thresholding

Fig. 2. Thresholding of the weighted adjacency graph

From another point of view, the affinity matrix could be also interpreted as a Gaussian weighted adjacency graph. The thresholding will control the width of the neighborhoods. This parameter chosen according to the affinity parameter plays a similar role as the parameter ϵ in case of the ϵ-neighborhood graph. A thresholding of the largest distances is equivalent to cancel edges which connect data points very distant from each other as represented in Figure 2. So it strengthens the affinity between points among the same cluster and, so, the separability between clusters.

3.2 Thresholding

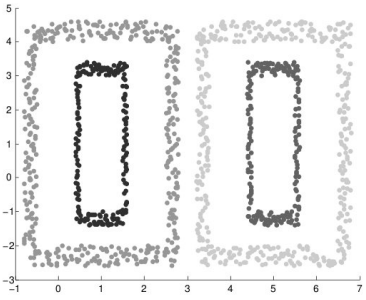
However a threshold should be heuristically defined to build an automatic sparsified matrix. We define the threshold that should represents a distance adapted to any distribution of input data. To do so, we start by defining a distance D_{unif} as the distance in the case of the uniform distribution of n points in this enclosing p-th dimensional box in which the data are equidistant each other. This uniform distribution is reached when dividing the box in n smaller boxes all of the same size, each with a volume of order $D_{\max}^p/n$ where $D_{\max}$ is the maximum of the distance between two data point x_i and x_j, $\forall i, j \in \{1, .., n\}$. The corresponding edge size which defines D_{unif} is given by:

$$D_{unif} = \frac{D_{\max}}{n^{\frac{1}{p}}} \tag{4}$$

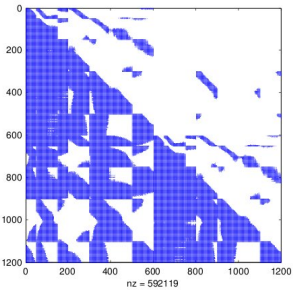
The thresholding will be function of D_{unif} for any kind of data distribution S.

4 Numerical Experiments

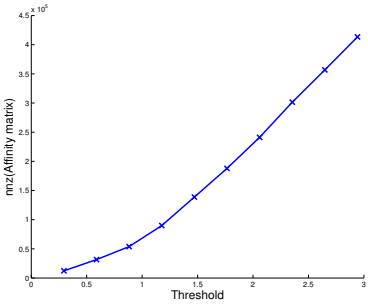
As numerical experiments, we first begin by testing the thresholding on geometrical examples for data set of small size. Then some tests on larger data set are investigated on image segmentation examples.



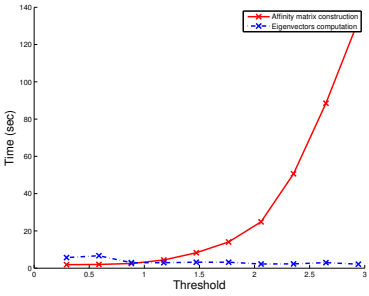
(a) Clustering result with thresholding



(b) Affinity matrix : lower triangular without threshold, upper triangular with threshold



(c) Memory cost function of the threshold



(d) Timings function of the threshold

Fig. 3. Example 1: data set, sparsity of the affinity matrix, memory cost and timings

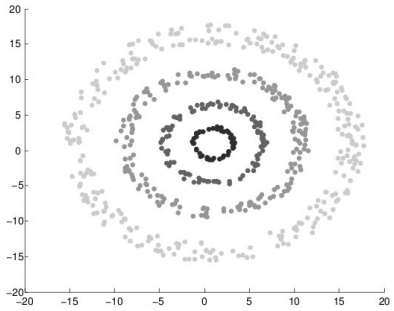
4.1 First Validations

For first validations, we consider two geometrical examples represented in Fig. 3 (a) and Fig. 4 (a) in which the clusters could not be separated by hyperplanes: the first one with four rectangles of $n = 1200$ points and the second one with a target of $n = 600$ points. The eigenvectors were provided by the reverse communication required by the Fortran library ARPACK [9].

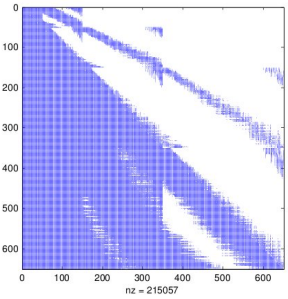
We measure the timings in seconds, in function of the threshold, of the construction of the affinity matrix and of the computation of eigenvectors. The memory cost is evaluated in function of the threshold by the number of non-zeros elements in the affinity matrix.

We can notice on (c) sub-figure that we gain a lot of memory when we decrease the threshold i.e. when we drop the connections of points at a distance larger than it. In fact, this sub-figure shows the memory space required for the storage of the affinity matrix by using a sparse structure $(i, j, value(A_{ij}))$.

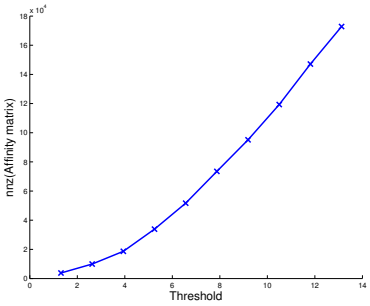
We also remark on (d) sub-figure that the time to construct the affinity matrix decreases in this case. Indeed, the computation of the component A_{ij} requires to



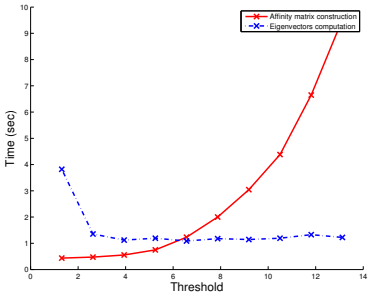
(a) Clustering result with thresholding



(b) Affinity matrix : lower triangular without threshold, upper triangular with threshold



(c) Memory cost function of the threshold



(d) Timings function of the threshold

Fig. 4. Example 2: data set, sparsity of the affinity matrix, memory cost and timings

compute an exponential (1). So because the selection of the connections we keep is done only with the distance, we don't compute the non-useful components and save a lot of floating point operations.

So we have a response to the memory consumption and timing limitations we mentioned previously. As we can see on the first validations, a thresholding strategy allows for considerable gains in terms of memory requirements and computational performance.

If we look the timing for the extraction of the eigenvectors, the time remains the same for acceptable values of the threshold. But we encounter a limit to the sparsification technique with example 2: a strong threshold could imply a very sparsified affinity matrix and an ill-conditioned matrix. In this case, the eigenvector computation becomes the most time consuming task in the sense that the algorithm from Arnoldi method does not converge.

4.2 Another Application: Image Segmentation

For image segmentation, the domain decomposition is applied geometrically on the image and also on the brightness distribution (or color levels) as shown in the figure 5. In fact, we include both 2D geometrical information and 1D brightness (or 3D color levels) information in the spectral clustering method in the sense that there does not exist some privileged directions with very different magnitudes in the distances between points along theses directions. The step between pixels and brightness (or color levels) are about the same magnitude. Thus, a new distance in the affinity measure is defined for image. In the same way, a global heuristic for the Gaussian affinity parameter is proposed in which both dimension of the problem as well as the density of points in the given 3D (or 5D for colored image) are integrated. By considering the size of the image I, the Gaussian affinity A_{ir} is defined as follows:

$$A_{ir} = \begin{cases} \exp\left(-\frac{d(I_{ij},I_{rs})^2}{(\sigma/2)^2}\right) & \text{if } (ij) \neq (rs), \\ 0 \text{ otherwise,} \end{cases}$$

with the distance between the pixel (ij) and (rs) defined by:

$$d\left(I_{ij}, I_{rs}\right) = \sqrt{\left(\frac{i-r}{l}\right)^2 + \left(\frac{j-s}{m}\right)^2 + \left(\frac{I_{ij}-I_{rs}}{256}\right)^2} \tag{5}$$

Parallel spectral clustering was used for image segmentation [6] and we present now the first results of the sparsified parallel spectral clustering applied on image segmentation.

Computational Environment
The parallel numerical experiments were carried out on the Hyperion supercomputer[1]. Hyperion is the latest supercomputer of the CICT (Centre Interuniversitaire de Calcul de Toulouse). With its 352 bi-Intel "Nehalem" EP quad-core nodes it can develop a peak of 33TFlops. Each node has 4.5 GB memory dedicated for each of the cores and an overall of 32 GB fully available memory on the node that is shared between the cores.

3D Image Segmentation
The first example is a Mahua illustration of Benjamin Zhang Bin which presents some continuous degradation of grayscale levels. This grayscale image of 232764 data points is divided in 20 subdomains. We perform experiments with different values of the factor. The threshold is given by the product of the factor with D_{unif} defined by (4). Fig. 6 summarizes the memory consumption (black: maximum consumption on one sub-domain, red: average consumption, blue: minimum).

[1] `http://www.calmip.cict.fr/spip/spip.php?rubrique90`

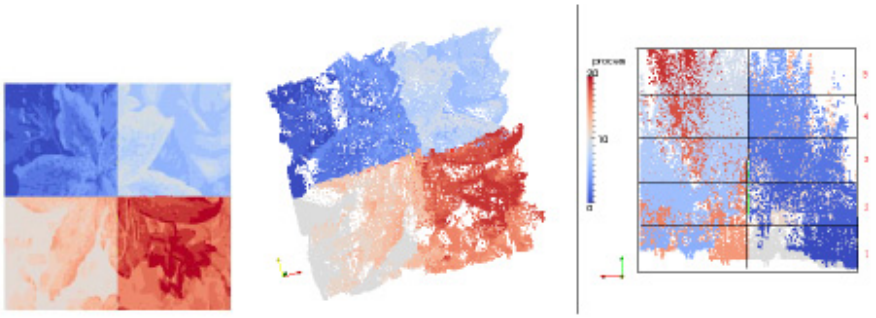


Fig. 5. Example of domain decomposition for image segmentation : geometrical decomposition on the left, brightness distribution and decomposition on the right

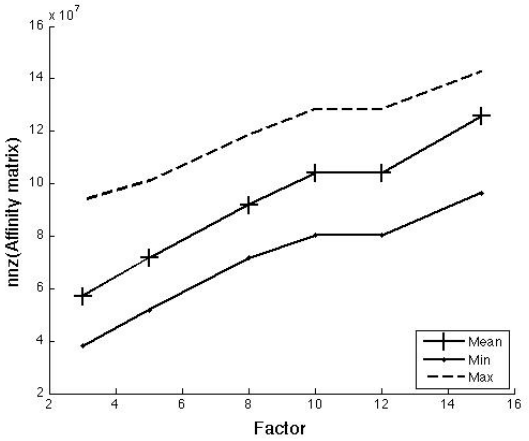


Fig. 6. Example of image segmentation in grayscale: memory cost function of the factor

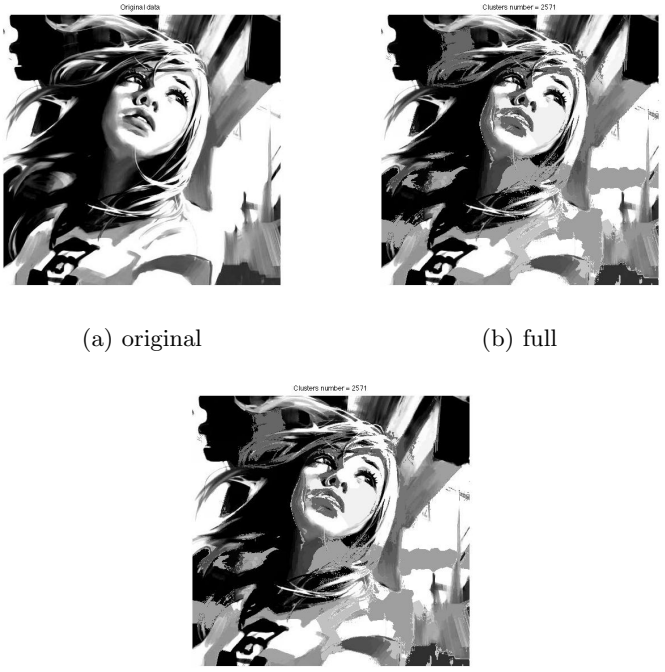
As we can observe, we are able to decrease this memory consumption by a factor two on average without losing the quality of image segmentation as we can see in Fig. 7. There is no significant difference between the result with the full matrix and the one with sparsification with a factor 3.

5D Image Segmentation

The second example represents a photo of Yann Arthus Bertrand of colored fields in Vaucluse. This is a color image of 128612 points which is also divided in 20 subdomains. In Fig. 8, the memory consumption is plotted.

With this example we are able to divide by 10 this consumption when we take a factor of 1 without loss of quality as we can see in Fig. 9.

However with this example, we tried to further reduce the factor. We experiment that with the value 1, we reach a limit because with factors lower than 1 we notice a significant loss of quality in the segmentation as we can see in subfigure



(a) original (b) full

(c) factor=3

Fig. 7. Example of 3D image segmentation: original data set, clustering result without thresholding and with thresholding (factor 3)

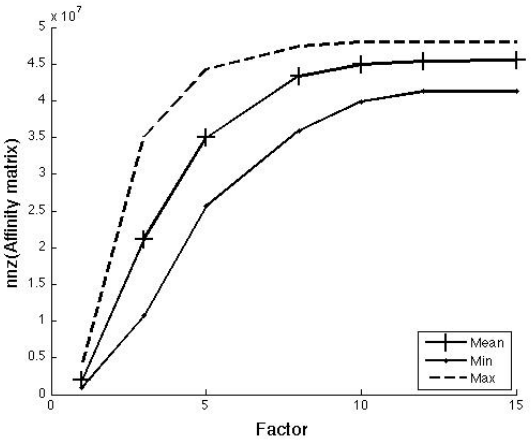
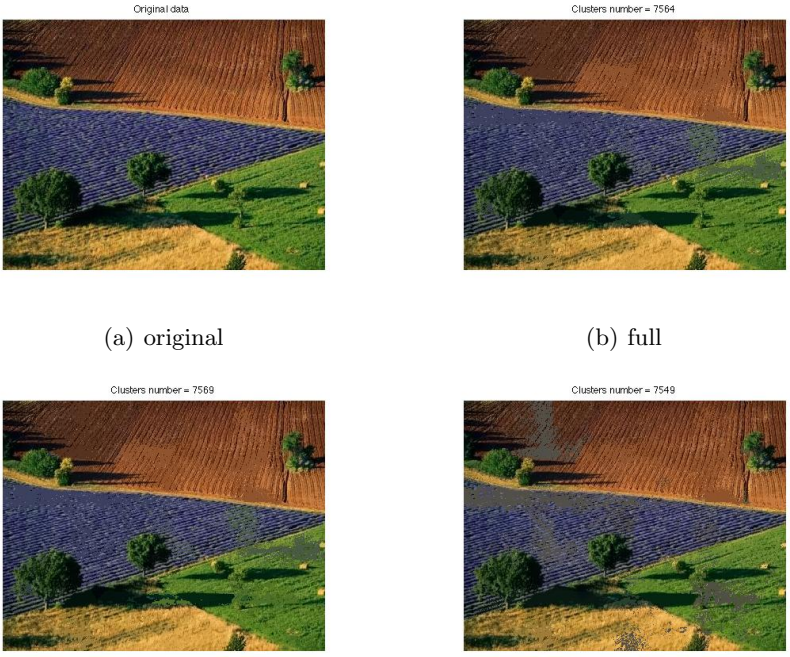


Fig. 8. Example of 5D image segmentation in colors: memory cost function of the factor



(a) original (b) full

(c) factor=1 (d) factor=0.9

Fig. 9. Example of image segmentation: original data set, clustering result without and with thresholding (factor = 1 and factor = 0.9)

(d) of Fig. 9 that presents the results with a factor of 0.9. As D_{unif} defined by (4) represents the distance for an uniform distribution, clusters may exis if there are data points which are separated by a fraction of D_{unif}. So for a value of factor lower than 1, the thresholding could affect the clustering result.

5 Conclusion and Ongoing Works

As we mentioned in the conclusion of our work at the previous VECPAR conference [6], we have begun to study sparsification techniques in the construction of affinity matrix by dropping some components that correspond to points at a distance larger than a threshold. We validate this approach in matlab by showing that the number of non zero of the affinity matrix decreases with still some good results in terms of spectral clustering and even some gains in the time spent to compute the affinity matrix.

These results are confirmed when we use sparsification with our parallel spectral clustering solver. We are able to show that we are able to reduce significantly the size of the affinity matrix without loosing the quality of the segmentation solution.

We have still more experiments to perform and some improvements to achieve. First, we have to investigate in all the available tunings in ARPACK to be sure to use the less memory when computing the eigenvectors and eigenvalues. We will then be able to compare the timings with or without sparsification. And finally, we have to perform experiments with bigger images for which we can't have solution if we don't use sparsification.

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