ECD Test: An Empirical Way based on the Cumulative Distributions to Evaluate the Number of Clusters for Unsupervised Clustering

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Abstract: Unsupervised clustering consists in blindly gathering unknown data into compact and homogeneous groups; it is one of the very first steps of any Machine Learning approach, whether it is about Data Mining, Knowledge Extraction, Anomaly Detection or System Modeling. Unfortunately, unsupervised clustering suffers from the major drawback of requiring manual parameters to perform accurately; one of them is the expected number of clusters. This parameter often determines whether the clusters will relevantly represent the system or not. From literature, there is no universal fashion to estimate this value; in this paper, we address this problem through a novel approach. To do so, we rely on a unique, blind clustering, then we characterize the so-built clusters by their Empirical Cumulative Distributions that we compare to one another using the Modified Hausdorff Distance, and we finally regroup the clusters by Region Growing, driven by these characteristics. This allows to rebuild the feature space's regions: the number of expected clusters is the number of regions found. We apply this methodology to both academic and real industrial data, and show that it provides very good estimates of the number of clusters, no matter the dataset's complexity nor the clustering method used.

1 INTRODUCTION

In the area of Machine Learning, clustering is a major cornerstone: it is often used to preprocess data, or to highlight hidden information. Maybe one of the most interesting applications of clustering is the automatic labeling of data, which allows the use of supervised (learning) methods downstream – the automatic labeling performed by unsupervised clustering aims to replace a manual labeling (Molinié et al., 2021).

Although promising, clustering has some limits. The first is the accuracy of the results: since we deal with blind methods, it is very hard to state on the accuracy – and on the relevance alike – of the obtained clusters. To handle that, we proposed BSOM, a two-level clustering method based on the averaging of several clusterings, so as to diminish the scattering of the results whilst maximizing the number of scenarios taken into account (Molinié and Madani, 2022).

The second limitation of clustering is related to the meta-parameters. Actually, alike most unsupervised approaches, some parameters must be set manually, which greatly impacts the results, especially in a blind, unsupervised context. As a consequence, the parameters should be chosen very wisely; but the question remains quite simple: how to do so?

Indeed, the true reason for using unsupervised learning is that one needs no previous information on the data; ironically, the meta-parameters are the paradox of unsupervised learning, for they require some specific knowledge to be set correctly. Even though every method has its own meta-parameters, there is one required by most of them: the (expected) number of clusters; for instance, it is the K of the K-Means, or the grid's size of the Self-Organizing Maps. This parameter is incontestably the most sensitive one, for it may change the results in depth. Note that some methods do not need this parameter, such as hierarchical approaches (e.g., Ascending Hierarchical Classification, Tree-like Divide To Simplify); however, they suffer from another drawback with their thresholds and split criteria (when to isolate data from others).

As a consequence, finding a way to estimate the optimal value to set the meta-parameters to – and especially the number of clusters – becomes crucial, even though there exists no such tool. A piece of solution may come along an upstream analysis of the database before processing; for instance, one may study the relation between data in order to see if any

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redundancies appear, which could drive the choice of the number of clusters. Unfortunately, attempting to find a universal characteristic suitable to any database is just a waste of effort (Molinié et al., 2022).

In this paper, we address that actual problem, through an empirical fashion. Indeed, whilst it is very hard to find a universal criterion to any database, nothing prevents from applying a first, raw clustering, at a fine grain for instance, and then refine it further, and eventually use the refined version of the clustering as an indicator of a good candidate for the number of clusters. Note that refining a database such way and proceeding to a clustering with a good value for the number of clusters are two different things, since redoing a clustering with the correct meta-parameters takes benefit from the intrinsic ability of the clustering method for data organization, i.e., the learning step, which is lost when only refining the clusters.

First, we will begin with a short overview of some already-existing methods to evaluate the number of clusters, and we will move on to the detailed description of the proposed method. Then, we will assess this technique with both academic and real industrial data, and we will eventually conclude this paper.

2 STATE-OF-THE-ART

There exists two ways of evaluating the optimal parameters of an algorithm: 1- By a deep upstream analysis, based on heavy mathematical tools; 2- Through an empirical approach based on the example. The former has the advantage of leading to more accurate results (mathematically "optimal"), but has the major drawback of being very heavy to perform, and lowly generalizable (which tool to use?); on the contrary, the latter has the advantage of being easier and more universal, but has the limitation of achieving less accurate results (empirically adapted, but not optimal)[1].

Unfortunately, thus far, no mathematically optimal solution has been proposed to the problem of determining the number of clusters of a dataset; one generally has to content oneself with heuristics, i.e., acceptable estimates with respect to the observed data.

These heuristics can be gathered into two groups: 1- The theoretical ones, which apply some tools to the database so as to estimate the empirically "optimal" number of clusters; 2- The true empirical ones, which simply cluster the database several times by varying the value of the number of clusters, and eventually select the clustering (and thus the number of clusters) which minimizes any criterion. Most of the methods of the literature belong to the second category.

From the rare methods of the first category, it is worth mentioning (Honarkhah and Caers, 2010). The authors assumed that any dataset can be linearly clustered in an appropriate space, called kernel space[2]; to do so, one must have recourse to a dedicated transition matrix, called kernel matrix, which projects the data from the original space to the kernel space. The authors suggested that this matrix would contain much information, and especially that plotting its eigenvalues, sorted and weighted by the normalized dot product of their eigenvectors, would lead to a good estimate of the number of clusters as of the curve's knee. They got good results on simple examples, but this method suffers from two major drawbacks: firstly, the projection into the kernel space is a complex and time-consuming operation; secondly, the kernel to use must be defined manually upstream, which requires some kind of knowledge (such as the possible data's distribution), and thus we are replacing a knowledge (the number of clusters) by another (the kernel).

Otherwise, some methods rely on the Akaike or the Bayesian Information Criteria (AIC and BIC, respectively (Goutte et al., 2001; Pelleg and Moore, 2002). Based on a pure statistical estimation of the information contained within a dataset, these criteria can be used in some fashion so as to provide an estimate of the number of clusters. Nonetheless they are generally used as simple indicators of clustering quality in an empirical fashion by running the clustering several times, incrementing each time the number of clusters, and by eventually selecting the value maximizing these information criteria.

On the opposite, the second category's methods operate much simpler: they cluster the data with different values for the number of clusters, compute some quality criteria, and eventually select that with the best results. Notice that even though these techniques claim that they are able to find a good candidate for the number of clusters, they are actually not *sensu stricto*; indeed, they actually think and operate the other way round: the interest in finding a good candidate for the number of clusters is precisely to obtain a good clustering, but there is no need for this parameter if one already has the best results just by chance or by brute force. These methods are more an empirical way to find the best clustered version of a database rather than a true way to estimate the optimal number of clusters.

[1] This limitation is not a real one in Physics and Machine Learning, for an optimized solution is generally well-suited for models, but often not applicable to real situations. Moreover, an experimental dataset can differ from a record to another, thus the optimal solution may vary between both.

[2] For instance, two circles can be linearly separated if the space is circular, since a line in this space is a true circle.

That being said, they propose some variations, and especially a quantification of the information brought by the addition of new clusters; indeed, very likely when adding new clusters, they should be more compact, and thus should carry more information, but there is often a point from which adding new clusters is not really useful. For instance, consider a database with 5 classes: clustering it with 5 clusters should be the best option, but using 10 clusters will probably lead to more compact groups, thus the quality of that last clustering will be better. Most techniques from the literature aim to address that problem of information, by proposing an empirical trade-off: which value to use to get the most information, while also not degrading the clustering relevance too much?

This is for instance the Elbow method's purpose (Marutho et al., 2018): it plots the explained variance against the number of clusters, and selects as best candidate (trade-off) for the number of clusters the curve's knee (also called elbow). Simple method, it can provide a correct estimate, but there is no certitude that such inflection point actually exists.

Similarly, instead of using the explained variance, (Amorim and Hennig, 2015) proposed to use the Silhouette Coefficients, a compactness quantifier popular in clustering (Rousseeuw, 1987), while keeping the same methodology, i.e., plotting the mean Silhouettes against the number of clusters, and eventually return the curve's knee. These coefficients are highly representative of the quality of the clustering (Molinié et al., 2022), but are very long to compute: the method is slightly more representative, but longer to perform.

A last work to mention may be (Tibshirani et al., 2001), which processes the same way than the two previous methods, but this time replacing the metrics by the explained variation, i.e., the part of the observed variance in the theoretical variance of a model. To do so, the idea is to build a "ground truth" model under the null hypothesis, i.e., with the same characteristics (particularly the mean and variance) than the database, cluster it several times and finally compare how close to the clustering performed over the real data it is. This procedure is repeated with several values set for the number of clusters, and that obtaining the less dissimilarity between the clustered "ground truth" and the real clustered database is chosen as the best candidate. This method led to quite good results, but requires a model to build the ground truth upon and is incredibly complex for such a simple purpose.

As a summary, there are two ways to estimate the number of clusters: by a theoretical analysis or by testing several values and selecting that minimizing any criterion. In this paper, we propose a third kind of methodology, halfway between both.

3 PROPOSED SOLUTION

The main problem with fully theoretical approaches is that they are generally very complex, often too complex for the user's real purposes. Indeed, it is not rare that a mathematically optimal solution to a physical problem is not applicable as it is to real situations, due to the intrinsic imperfections of the real system. An optimal solution suits well simulations, but an only approximated solution is often more than enough for real systems. Of course, that is not always true, such as in aviation or with critical systems for instance, where an exact solution is absolutely necessary; but where unsupervised learning can be used, such accuracy is generally not mandatory, whence the use of empirical approaches can be justified.

Moreover, empirical methods have another great advantage over theoretical ones: they perfectly suit the observed data in a given context; they actually are more practical and data oriented.

For these reasons, we have favored an empirical approach for the estimation of the number of clusters contained within a database. Nonetheless, we did not want to propose another clustering method, which is somehow what the Elbow method and assimilated do in testing several clusterings and eventually selecting that minimizing any criterion. As a consequence, we thought about a different methodology which would provide a true empirical value for the number of clusters but without unnecessarily testing many.

In short, our methodology can be summarized as follows: 1- Cluster the database only once, but with a large number of clusters; 2- Characterize the clusters in some fashion; 3- Regroup the clusters according to the closeness of their characteristics computed in the previous point; 4- Return the estimated number of clusters as of the number of so-built "super-groups".

Remark that this is not a new clustering, but actually a true estimation of the number of clusters. So as to get a true clustering method, we could have merged repeatedly the clusters in a hierarchical fashion, but that already exists and is entitled agglomerative clustering (Sibson, 1973; Defays, 1977). Getting a good estimate for the number of clusters aims to put everything in place for the true Machine Learning clustering step thereafter. Indeed, the learning step would be lost in the clusters merging, whilst setting the optimal parameters to the clustering method would take advantage of all its abilities.

In all the following, we will refer to the real number of clusters as K, the estimated number as K', the database as $\mathcal{D} = \{x_n\}_{n \in [\![1,N]\!]}$ with $N = |\mathcal{D}|$ the number of data within, the clustering $\mathcal{C} = \{C_k\}_{k \in [\![1,K]\!]}$ with C_k the cluster k, and denote d as a distance.

3.1 Clustering

In our methodology, the very first step is clustering: it consists in gathering data into compact and homogeneous groups, within which they share similarities, while differing from a group to another. In practice, most unsupervised clustering methods aim to minimize the statistical "error" between the clusters and data. As an example, by considering that the distance between a data and the barycenter of its corresponding cluster is such an error, the total error of the clustering is the sum of these local distances, for all the data, for all the clusters: clustering aims to reduce this sum. Actually, it is mostly a matter of optimization, but hidden behind a dedicated formalism.

There exists plenty of clustering methods, either supervised (SVM, Random Forests) or totally blind (K-Means, SOMs). The choice of the method to use depends on the context and on the objectives.

Supervised clustering consists in searching for the best borders between different, already-labeled classes, by adapting a shape (line, curve) to the space between them; note that, here, the classes are known, whence the use of "class" instead of "cluster". Unsupervised clustering consists in blindly regrouping data into compact groups, with no previous assumption on them; neither the barycenters of the classes, nor even their number are known, whence the term unsupervised. The former achieves better results, but assumes much information on the data (their true classes), whereas the latter is more universal, but the quality and relevance of its output is not certain.

In an Industry 4.0 context, we study the relevance of using Data Mining methods to dig into data, and extract whatever knowledge can be found. As such, we mainly rely on unsupervised learning, for we aim to investigate highly generalizable works. For these reasons, we will only present unsupervised clustering.

The first to be introduced is the K-Means, the reference clustering method (Lloyd, 1982): it draws K points as barycenters, aggregates the surrounding data around these points according to their respective closeness, and then updates the barycenters as the true means of the so-built groups; this operation is repeated a certain number of times or until satisfying any criterion. The K-Means is a very-well known clustering algorithm, but also very naive and simple: it has the major limitation of being able to separate only linearly separable datasets, and therefore poorly suitable for real situations such as industrial systems.

To compensate that, one may operate in a kernel space, where the data would be "linearly" separable, provided that a line in such space is a nonlinear curve in the original space. Once the data projected into this nonlinear space, one may apply the K-Means to them; this method is called Kernel K-Means (Dhillon et al., 2004). Notice that this kernel version also exists for many methods (Kernel SOM, SVM, etc.).

Better than the K-Means and more adapted to nonlinearly separable datasets, one may also consider the Self-Organizing Maps (SOMs) (Kohonen, 1982); they can be seen as a generalization of the K-Means in which the learning step is nonlinear, and where the different clusters are connected to each other within a map, called a grid. This linkage aims to maintain the topology of the database, while also accelerating the learning by using a notion of neighborhood.

In (Molinié et al., 2021), we tested the K-Means, Kernel K-Means and SOMs on real industrial data, and concluded that the last method is that which works best, by providing the most representative clusters, i.e., the closest to the real system's behaviors.

In (Molinié and Madani, 2022), we proposed an improvement to the SOMs as of the Bi-Level Self-Organizing Maps (BSOMs), a two-level clustering aiming to reduce the scattering of the results, while also improving their accuracy and relevance. Indeed, alike any unsupervised method, the initialization should be random so as to avoid bias; but doing so may scatter the results: there is no certitude that two runs of the same algorithm give the same results. To compensate that, we proposed to build several maps, with different initializations and learnings (first level), and eventually project all of them into a final map using the SOMs (second level), giving birth to what we called BSOM. We tested it on real industrial data anew, and, compared to the K-Means and to the original SOMs, BSOM proved to be more accurate, less volatile (more consistent results between the runs) and closer to the real objective clusters, i.e., the real behaviors of the industrial system we considered.

In this paper, we will use the K-Means, the SOMs and BSOM to assess our methodology of determining the best candidate for the number of clusters, i.e., K for the first, and the grid's size for the two others. Figure 1 gives an example of results for each method, applied to a handful of Gaussian distributions; even though it is pretty subjective, BSOM seems to give the best clustering, with the most consistent regional groups, then SOM and finally the K-Means.

3.2 Cumulative Distributions

Once the clusters built, they must be characterized; this can be done in many fashions: feature vector, compactness, homogeneity, etc. Some of these indicators aim to measure the quality of the clusters, i.e., how similar the data within are, and/or how far

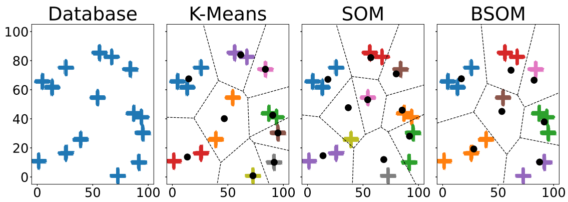


Figure 1: Example of clustering with different methods.

from the other clusters they are; this is for instance the case with the Silhouette Coefficients. On the contrary, some of these quantifiers aim to describe the clusters, i.e., propose a characteristic unique to them and allowing to find them back or compare them between each other: this is for example the case with descriptor vectors, which are commonly used in computer vision so as to simplify the comparison of images, or to search for the same object in different images.

In order to evaluate the quality of the clustering, the first category of methods is the most appropriate; on the opposite, if the purpose is to compare the clusters with each other, the second category of methods should be considered first. In our case, since we want to estimate how similar the clusters are, so as to link them in some fashion, the second category of methods is the most appropriate for us.

Consequently, we are looking for a characteristic unique to every cluster, which would indicate that two clusters are very close (or distant) in the feature space, but without necessarily taking account their inner quality. To that purpose, the Average Standard Deviation (Rybnik, 2004), the Hyper-Density (Molinié and Madani, 2021) or the Silhouettes (Rousseeuw, 1987) would be of little help; in fact, we need more a characteristic than a true compactness measure.

There exists thousands of tools to characterize (or just compare) groups of data: mathematical moments (mean, variance, etc.), intercluster distances, linkages (single, complete, Ward, etc.), correlation, etc. Each one of them has its own advantages and drawbacks: for instance, correlation is only able to detect linear similarity between groups of data; a linkage does not necessarily take into account the outliers; and a statistical moment can be routed by the physical proximity of the clusters in the feature space.

As such, inspired by the Kolmogorov-Smirnov (KS) Test (Simard and L'Ecuyer, 2011; Hassani and Silva, 2015), we propose to use the Empirical Cumulative Distributions (ECDs) of the clusters. Indeed, they are highly representative of the clusters: they indicate how the data within are distributed, with the great advantage of considering the data's intrinsic values, contrary to most of the metrics discussed earlier.

The ECD of a cluster represents the empirical probability that its data are lower than a threshold; for cluster C_k, this probability P_k is given by formula (1).

$$\forall x \in \mathbb{R},\ P_k(x) = \frac{1}{|C_k|} \sum_{x_n \in C_k} \mathbb{1}_{x_n \leq x} \qquad (1)$$

with $\mathbb{1}_{x_n \leq x}$ the indicator function of $\{x_n \in \mathbb{R} \mid x_n \leq x\}$, and defined by (2).

$$\forall x_n, x \in \mathbb{R},\ \mathbb{1}_{x_n \leq x} = \begin{cases} 1, & \text{if } x_n \leq x \\ 0, & \text{else} \end{cases} \qquad (2)$$

Notice that one may derive function $\mathbb{1}_{x_n \leq x}$ from the (delayed) Heaviside step function H, as of (3).

$$\forall x_n, x \in \mathbb{R},\ \mathbb{1}_{x_n \leq x} = 1 - H(x_n - x) \qquad (3)$$

Finally, the ECD of cluster C_k is defined as the set of all the empirical probabilities, as of (4).

$$\text{ECD}_k = \{P_k(x)\}_{x \in \mathbb{R}} \qquad (4)$$

Notice that the ECD should not be computed for any real value, but only for that belonging to the domain of the database; in practice, this set is computed for a finite number of x, ranging from the database's minimum to its maximum with a given step.

The ECDs are very useful to understand how the data are distributed within a cluster. Moreover, since they are based on absolute values, they also have a physical meaning, related to achieved values; indeed, if two datasets have close ECDs, it means that their data distributions are close alike, both in compactness and in absolute values. To keep it simple, the slope of an ECD indicates the compactness (the larger the slope, the more compact the data), whilst its position indicates the position of the data within the space. That last point is the core of our methodology, and the main reason why we chose the ECDs over any other metric: by comparing two of them, it is possible to decide if two clusters are similar (density, compactness), but also if they are just close in the space.

Notice that there is one ECD by dimension, which must be fused in some fashion so as to provide a scalar as of the number of clusters. One may think about taking their average, computed over all the dimensions, but this could create false correspondence. For instance, assuming x and y belong to the same interval I, the function $f_1(x,y) = x$ and the function $f_2(x,y) = y$ are very different, but have the same mean over the two dimensions. This is a good example of the limit of averaging; to avoid such case, we propose to state that two distributions are very close if that is true for all the dimensions at the same time.

As an example, Figure 2 depicts the ECDs of both dimensions of the clusters given by BSOM (rightmost image on Figure 1); this gives an idea about what does an ECD look like. Our methodology consists in identifying the very similar and very close curves, which would indicate that the two distributions are very close in the feature space, and thus the clusters alike. On the contrary, having no such proximity would indicate that the clusters are very different (may be considered as a pledge of quality).

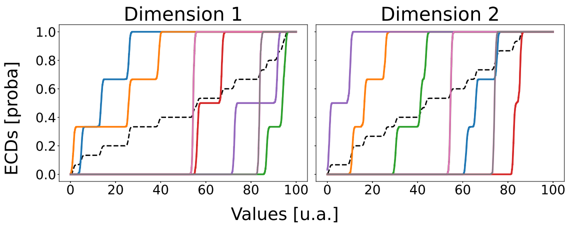


Figure 2: Example of ECDs, computed over BSOM's clusters (see rightmost image of Figure 1 for the clustering). The dot black curve is the mean of all the colored ones.

3.3 Gathering of the Clusters

Once the clusters obtained and characterized, it is time to process the results and see how to draw the number of clusters from them.

As mentioned earlier, comparing two clusterings *sensu stricto* is very difficult, for there is no true universal indicator; we propose to use the Empirical Cumulative Distributions instead, so as to describe the clusters, and therefore use these characteristics for our comparison. That being said, a problem remains: how to compare two ECDs? Indeed, they are sets of values, and, as such, what characteristic to use to state on their closeness? One may think about comparing their mean through a distance measure, but this is very weak; since we told that the position and the angle of the slope are great indicators, they may also be worth being compared, but this is not really clear, nor really easy though (should the slope position weight more than its angle? Is 5° a small or large difference?).

Therefore, we preferred interpreting the results as graphical curves, which they actually are. To take all their characteristics into account in a simple and very representative fashion, we decided to compare their shapes themselves: to do so, we followed the feeling of Dubuisson and Jain, who consider the Hausdorff distance as one of the most appropriate distance functions for shape recognition (Dubuisson and Jain, 1994). The Hausdorff distance compares two graphical shapes (such as curves), and gives a closeness score, the lower the closer. This distance is therefore very-well adapted to our purposes, and has the advantage of being simple while also highly representative.

For two discretized shapes $P = \{p_i\}_{i \in [\![1,N_1]\!]}$ and $Q = \{q_j\}_{j \in [\![1,N_2]\!]}$, the Hausdorff distance sets a point in P and searches for the minimal distance between it and any point in Q; it does so for any point in P and takes the maximal value among all of these minimal distances. Since the minimum and maximum are not symmetric, this operation must be done the other way round by exchanging P and Q. Finally, so as to obtain a symmetric distance, the Hausdorff distance takes the maximum between both. It is given by formula (5).

$$d_h\big(P,Q\big) = \max\big\{h(P,Q), h(Q,P)\big\} \tag{5}$$

where $h(X,Y)$ is the maximal value of the minimal distances between sets X and Y, as given by 6. Notice that generally $h(X,Y) \neq h(Y,X)$ (no symmetry).

$$h(X,Y) = \max_{x\in X}\left\{\min_{y\in Y}\big\{d(x,y)\big\}\right\} \tag{6}$$

This definition has the drawback of ignoring most values (only the maximum is considered); to compensate that, (Dubuisson and Jain, 1994) proposed the Modified Hausdorff Distance (MHD), which replaces the maximum by a mean in the definition of h, more representative of the shapes, as given by (7).

$$h_{MHD}(X,Y) = \frac{1}{|X|}\sum_{x\in X}\min_{y\in Y}\big\{d(x,y)\big\} \tag{7}$$

The final definition of the MHD remains (5), but using h_{MHD} instead of h.

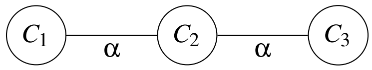
The (Modified) Hausdorff Distance is just an indicator on the resemblance of two shapes: it is pairwise. In our case, we have K clusters, therefore this distance must be computed for any pair of cluster's empirical cumulative distributions, and that in any of the space's dimension. As a consequence, all these distances can be gathered in a square matrix $M \in \mathbb{R}^{K\times K}$; since the MHD is built to be symmetric, the matrix will be symmetric as well, and since the MHD between a shape and itself is null $\big(d_h(X,X) = 0\big)$, its diagonal will be full of zeroes, as shown by (8).

$$M = \begin{array}{c} \\ \text{ECD}_1 \\ \text{ECD}_2 \\ \vdots \\ \text{ECD}_K \end{array} \begin{array}{c} \begin{array}{cccc} \text{ECD}_1 & \text{ECD}_2 & \cdots & \text{ECD}_K \end{array} \\ \begin{pmatrix} 0 & d_h^{(1,2)} & \cdots & d_h^{(1,K)} \\ d_h^{(2,1)} & 0 & \cdots & d_h^{(2,K)} \\ \vdots & \vdots & \ddots & \vdots \\ d_h^{(K,1)} & d_h^{(K,2)} & \cdots & 0 \end{pmatrix} \end{array} \tag{8}$$

where $d_h^{(i,j)}$ is the (Modified) Hausdorff Distance between ECD_i and ECD_j: $d_h^{(i,j)} = d_h\big(\text{ECD}_i, \text{ECD}_j\big)$.

Finally, once this matrix fulfilled, we propose to use it to estimate the empirically optimal number of clusters of the database. Indeed, if a value is low, it means that the curves are graphically close, and thus the data distributions are physically close alike, and therefore the clusters very likely belong to the same database's sub-region: merging them would probably increase the clustering's representativeness.

From there raises the question of how to connect the ECDs with each other; indeed, there is often many possible configurations. Consider the scenario of three clusters aligned, regularly spaced of a Hausdorff distance α, as shown below:



The corresponding matrix of the ECDs would therefore be the following:

$$M = \begin{pmatrix} 0 & \alpha & 2\alpha \\ \alpha & 0 & \alpha \\ 2\alpha & \alpha & 0 \end{pmatrix}$$

Assuming α is low, pairs $\{C_1, C_2\}$ and $\{C_2, C_3\}$ are two possible candidates for merging. Nonetheless, the question to know what to do with C_2 remains: since it belongs to two different pairs, should it be merged with C_1 or with C_3? From there, four possibilities appear: 1- Do nothing; 2- Fuse C_2 with C_1; 3- Fuse C_2 with C_3; 4- Fuse the three clusters as one (but is 2α a low enough distance?). This simple example shows the problematic we are facing: there are different cases, and there is no universal solution to it (incidentally, this is the main problem with hierarchical clustering). To handle that, we propose to adopt a Region Growing approach (Rabbani et al., 2006).

Indeed, this hierarchical clustering method draws a point, assimilates it to a cluster's barycenter, then aggregates all the surrounding points at a maximum distance of ρ, repeats this procedure for each one of these neighbors, and continues to do so until there is no more point at a maximum distance of ρ from any point of this cluster not belonging to it or to any other cluster. Once this cluster built, the procedure is repeated anew with another not-yet-assigned point, until all the database's points are categorized. This procedure can be serial (concurrent), by starting a new cluster only when the last one has been completely built, or it can be parallel, by building several clusters at the same time. The first ensures large clusters, whilst the second leads to more, smaller of them.

Region growing can be considered in two ways: either the data are truly fused into real entities (clusters), or they can just be linked to one another, somehow forming a map. Even though the two methods are all the same, the second is more graphical, and thus can ease the reading; in our case, the idea is to create a graph whose nodes are the ECDs (or equivalently the clusters), and the edges represent the connections between them when they are less distant than ρ.

We propose to use this procedure to gather the ECDs, which has the advantage of being efficient and proposing a solution to the above problem. In our case, assuming α is low (i.e., $\alpha \leq \rho$), C_1 will be linked to C_2 on the one hand, and C_2 will be linked to C_3 on the other hand. As a consequence, we will get the organized set $\{C_1, C_2, C_3\}$, meaning that C_1 will be indirectly linked to C_3 through the intermediary of C_2.

Following this procedure, Figure 3 gives an example of configurations we could have (assuming the arrows represent distances lower that ρ).

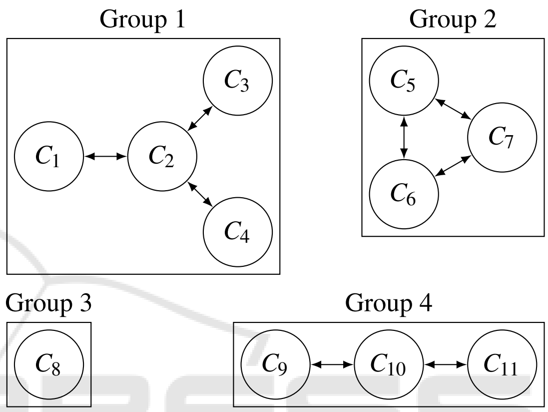


Figure 3: Example of region growing clustering and the resulting cluster's ECDs mapping.

Region growing clustering aims to identify the sub-regions of the feature space, which is actually the basis of the estimation of the number of clusters. Indeed, blindly attempting to find the correct clusters, with no knowledge provided upstream, is like trying to find a needle in a haystack: nonetheless, it is much easier to just search for the sub-regions of the space instead of the true clusters. In reality, most clustering methods work this way: they are based on the notion of attraction, represented by the barycenters; that is called their Region Of Influence (ROI), i.e., the area around them within which any point can be aggregated to them. This last point justifies our choice in the gathering of the ECDs by region growing.

Finally, our estimation of the number of clusters is the number of subgroups built from the ECDs, eventually gathered by following a region growing approach.

This can be done by just reading the matrix of the ECDs M; indeed, if a value is low (according to a threshold), it means that the two corresponding ECDs (and thus clusters) can be connected to one another. As such, to operate the region growing clustering, one just has to create a map of all the clusters and link them within; to do so, just find the lowest values of the matrix and add the corresponding connections to the map. Once done, the map can be easily read, and the estimated optimal number of clusters is simply the number of disconnected groups (regions).

3.4 Summary of the Proposal

To make clearer our methodology, this subsection aims to summarize the previous ones. Its different steps can be enumerated as follows:

1. Cluster a database using an unsupervised, data-driven clustering method from the state-of-the-art, with a high value set for the number of clusters. It may be the K-Means, the Self-Organizing Maps or the Bi-Level SOMs for instance.
2. Compute the ECDs for every cluster, in every dimension, using (4).
3. Compute the MHDs between any pair of ECDs using (5) and (7), and gather all of them within a matrix, such as shown in (8).
4. Gather all the MHDs of the matrix into compact and similar regions using Region Growing clustering, as shown in Figure 3.
5. Read the so-built cluster's ECDs mapping: the estimated number of clusters K' of the database is the number of regions identified.

All this methodology is graphically summarized in a flowchart as of Figure 4.

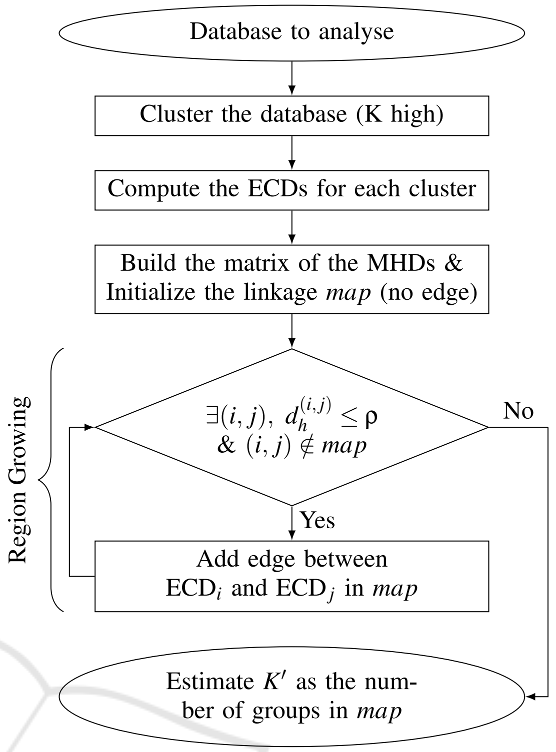


Figure 4: Flowchart of the proposed method for empirical estimation of the number of clusters in a database.

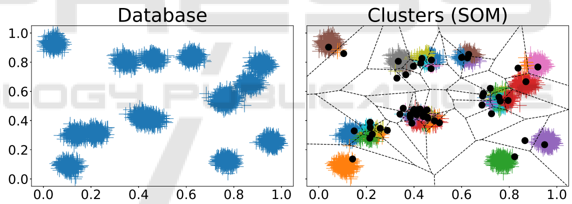


Figure 5: Results of the SOMs with a 10×10 grid.

4 RESULTS

In this section, we will apply the proposed method to an academic dataset in order to show how it works step by step and how to interpret each of them. We will then apply this methodology to real industrial data to show its potential in real conditions.

4.1 Academic Dataset

To illustrate our approach, consider first a simple but truly didactic example: a set of fifteen 2D Gaussian distributions. We will mainly use the Self-Organizing Map, but we will also try the K-Means and BSOM. Figure 5 depicts both the original database (left) and the clustered data using a 10×10 SOM (right). We remind that the first step is to break the input database in very small pieces, whence the large number of SOM's grid's nodes (100). Notice that the objective number of clusters should be a dozen, depending on the accuracy one wants to achieve; indeed, for instance, on the right of the leftmost image on the figure (the dataset), three clusters are clearly overlapping, thus should they be considered as different or as one unique data group? Depending on the accuracy, one may identify up to 9-12 different groups; this range of numbers is the objective of our proposed method.

The SOM led to 48 empty clusters (this is made possible by the learning procedure), which will not be considered in the following. As such, Figure 6 depicts the Empirical Cumulative Distributions of the 52 nonempty clusters. There are too many curves to clearly identify the different groups; nonetheless, this image is interesting for it shows what do ECDs look like with real data, and to remember that they must be computed in any dimension, whence the two subgraphs. Moreover, in our approach, an important thing to remind is that to consider two ECDs as close, they must be in all dimensions. For instance, the pink and violet curves at the extreme right in the leftmost image are very close in that dimension, but not in the

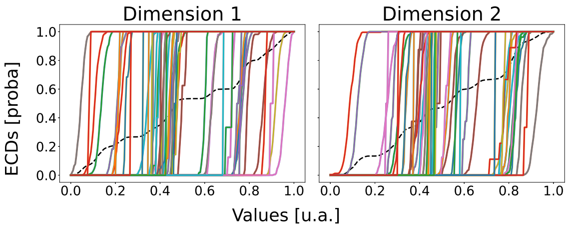


Figure 6: ECDs of the clustering (rightmost image of Figure 5). The dot black curve is the mean of all the colored curves, each corresponding to the ECDs of a unique cluster.

second one: therefore, they can not be considered as close, whence the validation of the closeness in every dimension, and the final comparison of the matrices of the MHDs in all dimensions.

Now that the clusters have been built and that their ECDs have been computed, their Modified Hausdorff Distances must be computed and gathered within the MHD Matrices, for each dimension. Table 1 presents a part of these matrices: M_1^T and M_2^T are these matrices compared term by term to a threshold ρ, following region growing clustering; if a pair of ECDs has a MHD lower than ρ, this pair is tagged with the Boolean True (noted T in the rightmost matrices), and False else (noted F). Finally, to test if two ECDs are actually close, the final matrix of the pairs is given by logical and &: $M = M_1^T \,\&\, M_2^T$, as depicted on Table 2.

This matrix allows to gather the pairs into full groups of ECDs, by region growing clustering: two pairs are connected if they share at least one common ECD. For instance, $\{11, 19\}$ and $\{11, 22\}$ are two such pairs, since they share ECD_{11}. Finally, the formed groups are the following: $\{10, 18\}$ in red, $\{11, 19, 22\}$ in green, $\{14, 15, 20\}$ in orange, and $\{12, 16, 21, 23, 24\}$ in blue. These pairs are mapped as of Figure 7; notice that connections are completed with dot edges with the whole matrix (for instance, ECD_{14} and ECD_{15} are not connected in Table 2, but they actually are in the full matrix). In short words, that means that for 14 clusters considered here, they actually form 5 groups: the number of clusters here should therefore be 5 (the blue, red, green and orange ones, plus the isolated cluster 13).

Finally, by reading the full matrix and creating the full map, we obtain the following groups: {1}, {2}, {3}, {4, 44}, {5, 41}, {6, 31}, {14, 15, 20}, {0, 11, 19, 22, 28, 39, 51}, {7, 10, 18, 27, 29, 36, 45, 48}, {8, 9, 13, 32, 34, 40, 42, 47}, {12, 16, 17, 21, 23, 24, 25, 26, 30, 33, 35, 37, 38, 43, 46, 49, 50}. These groups are the final ones, i.e., the compact regions of the space; by enumerating these regions (thus groups), we obtain our estimate for the number of clusters, whence $K' = 11$, which is in our objective range of 9-12, and especially very close to the real number of non-overlapping clusters.

Finally, to generalize a little, Table 3 gathers the mean estimated number of clusters using SOM, BSOM and K-Means. Each method has been run 100 times, and some statistics are presented in the table.

The three methods provide similar estimates, living in the same range. It is hard to state on which is the best, for it depends on the user's needs. Indeed, as discussed with Figure 5, several numbers of clusters can be accepted: 9-10 if one only thinks by full regions (possible clusters' overlapping), or 12-14 if one wants more accurate groups. As such, depending on the accuracy, one method can be preferred over the two others. For instance, the K-Means gave the lowest number of clusters, with a very low standard deviation: it can be used to get consistent results; on the contrary, BSOM gave about 12 clusters, which is actually the closest to the reality (cluster by cluster): it can be used to get clearer clusters, with finer borders. Moreover, we have not talked about cluster's quality, but maybe these values are all great and are the most appropriate for their respecting clustering method.

Anyway, these results seem very promising, and indicate that the proposed method works very well, at least with this academic example. Moreover, it proved to be resilient to the clustering method used: there is no huge gap with the results when using a method or another, which is somehow reassuring.

4.2 Real Industrial Data

Now that the method has been validated over an academic dataset, so as to test it and also to show step by step how it works, it is time to apply it to a real context, i.e., real industrial data. These data were provided to us by Solvay®, a chemistry plant specialized in Rare Earth specialties extraction. They are one of the HyperCOG partners, a H2020 European project whose main aim is to study the feasibility of the Cognitive plant, i.e., the intelligent and autonomous industry of tomorrow (Industry 4.0).

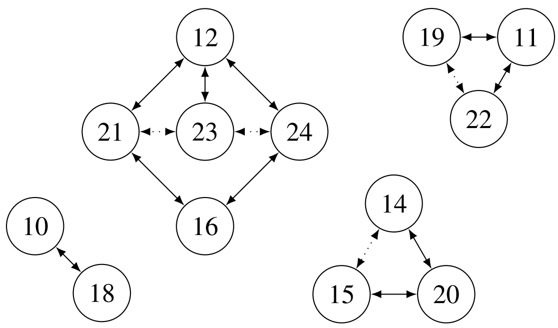


Figure 7: Mapping of the MHDs.

Table 2: Final matrix of the closeness of the ECDs, for all dimensions, given as the logical and between all the corresponding matrices in any dimension. The *True* T have been regrouped by color, following region growing clustering: one color per final group (region).

M_1^T & M_2^T =

	18	*19*	*20*	*21*	*22*	*23*	*24*
10	*T*	*F*	*F*	*F*	*F*	*F*	*F*
11	*F*	*T*	*F*	*F*	*T*	*F*	*F*
12	*F*	*F*	*F*	*T*	*F*	*T*	*T*
13	*F*	*F*	*F*	*F*	*F*	*F*	*F*
14	*F*	*F*	*T*	*F*	*F*	*F*	*F*
15	*F*	*F*	*T*	*F*	*F*	*F*	*F*
16	*F*	*F*	*F*	*T*	*F*	*F*	*T*

The process we are studying at Solvay® is the Rare Earth separation from raw material; this step is performed in what is called a ”battery”. The data we will work with in this section came from one of these batteries: they were recorded over seven work weeks, at a rate of one per minute, for a total of 65,505 data samples, over 14 sensors (and thus as many dimensions in the feature space). For confidentiality concerns, these data have been normalized. Following our work (Molinié et al., 2022), there should be about 7-10 real behaviors in this battery, and thus as many objective clusters (one per real system's behavior).

Table 3: Estimated number of clusters using different clustering methods after 100 runs each, with 100-node grids for SOM and BSOM, and $K = 50$ for the K-Means.

Method	Mean	Std	Min	Max
K-Means	10.04	0.86	9	12
SOM	10.21	1.44	8	14
BSOM	12.21	1.18	10	16

This range of values is therefore our objective here.

Figure 8 depicts two of these sensors over time (left), their respective feature space on the top right hand corner (sensor 2's data against sensor 1's), and the corresponding clustering below, using the BSOM. Notice that the clustering was performed using all the sensors/dimensions, but only two are depicted for the sake of conciseness.

BSOM used 10 SOMs, with 100 nodes each; the final clustering contains 61 nonempty clusters, with which we will deal. The ECDs have been computed for every cluster, and then compared to one another using the MHD, and the final state matrix of all the pairs' MHDs has been built. Table 4 gives a portion of that matrix, where, anew, T corresponds to a close pair, and F to a distant one. The sensors' tag numbers have been added on the top and left as small italic numbers. The colors corresponds to the

Table 1: Part of the MHDs matrices for every dimension (left) and the state on the closeness for every pair of ECDs (right), in which T means that the two ECDs involved in the corresponding pair are close, and F else. The indexes of the cluster's ECDs are indicated at the very start of every row, and at the top of every column as small italic numbers.

Dimension 1 M_1

M_1^T =

	18	*19*	*20*	*21*	*22*	*23*	*24*
10	0.90	9.20	2.50	0.30	10.2	1.20	1.60
11	7.00	0.40	17.0	9.10	0.50	5.60	4.50
12	0.50	7.90	3.10	0.50	8.90	0.60	1.00
13	16.3	37.9	5.60	12.7	39.8	17.7	19.3
14	6.20	21.0	0.80	4.00	22.4	6.90	7.90
15	6.20	21.1	0.70	4.00	22.6	7.00	8.00
16	0.50	5.40	4.50	1.10	6.30	0.40	0.50

$\leq \rho$ =

	18	*19*	*20*	*21*	*22*	*23*	*24*
10	*T*	*F*	*F*	*T*	*F*	*T*	*T*
11	*F*	*T*	*F*	*F*	*T*	*F*	*F*
12	*T*	*F*	*F*	*T*	*F*	*T*	*T*
13	*F*	*F*	*F*	*F*	*F*	*F*	*F*
14	*F*	*F*	*T*	*F*	*F*	*F*	*F*
15	*F*	*F*	*T*	*F*	*F*	*F*	*F*
16	*T*	*F*	*F*	*T*	*F*	*T*	*T*

Dimension 2 M_2

M_2^T =

	18	*19*	*20*	*21*	*22*	*23*	*24*
10	0.40	26.9	0.30	22.9	33.8	23.1	19.5
11	32.3	0.60	31.1	1.90	0.60	1.30	2.10
12	23.0	1.00	22.1	0.50	2.60	0.40	0.50
13	12.3	6.30	11.6	4.50	9.80	4.60	3.10
14	0.60	25.8	0.50	21.9	32.7	22.2	18.5
15	0.50	30.3	0.60	26.1	37.7	26.4	22.4
16	19.6	1.70	18.7	0.80	3.70	3.50	0.30

$\leq \rho$ =

	18	*19*	*20*	*21*	*22*	*23*	*24*
10	*T*	*F*	*T*	*F*	*F*	*F*	*F*
11	*F*	*T*	*F*	*F*	*T*	*T*	*F*
12	*F*	*T*	*F*	*T*	*F*	*T*	*T*
13	*F*	*F*	*F*	*F*	*F*	*F*	*F*
14	*T*	*F*	*T*	*F*	*F*	*F*	*F*
15	*T*	*F*	*T*	*F*	*F*	*F*	*F*
16	*F*	*F*	*F*	*T*	*F*	*F*	*T*

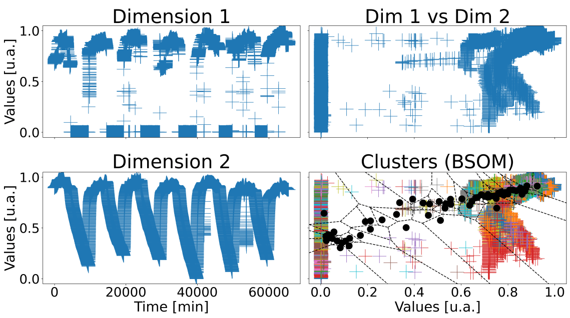


Figure 8: Possible clustering obtained with real industrial data. On the left, the two sensor's data over time; on the right, their corresponding feature space (sensor 2's data against sensor 1's) and the clustering given by BSOM.

Table 4: Example of the all-dimension state matrix.

$$
\begin{array}{cc}
 & \begin{array}{ccccccc} 44 & 45 & 46 & 47 & 48 & 49 & 50 \end{array} \\
M = \begin{array}{c} 33 \\ 34 \\ 35 \\ 36 \\ 37 \\ 38 \\ 39 \end{array} &
\begin{pmatrix}
F & F & F & F & F & T & T \\
F & F & F & F & F & F & T \\
F & T & F & F & F & F & F \\
F & F & F & F & F & F & T \\
F & F & F & F & F & F & F \\
F & T & F & F & F & F & F \\
T & F & F & T & F & F & F
\end{pmatrix}
\end{array}
$$

groups formed by region growing: $\{33,34,36,49,50\}$ in blue, $\{35,38,45\}$ in green, and $\{39,44,47\}$ in red.

The corresponding map is depicted on Figure 9, where the numbers correspond to the ECDs (e.g., "34" means ECD_{34}); the plain edges are that drawn from the matrix, and the dotted edges are that drawn when considering all the 61 clusters.

The results mean that there actually are 5 groups: the colored ones, plus the isolated {37} and {48}. Finally, the full groups are the following ("x-y" means all values between x and y): {37}, {43}, {53}, {27, 42, 48}, {28, 35, 38, 45, 60}, {2-5, 16, 18, 19, 23, 30, 32, 41, 46, 54, 58}, {0, 1, 6-15, 17, 20-22, 24-26, 29, 31, 33, 34, 36, 39, 40, 44, 47, 49-52, 55-57, 59}. As a consequence, there are 7 groups of clusters, and therefore, the estimated number of clusters is $K' = 7$, which is actually the one we were expecting.

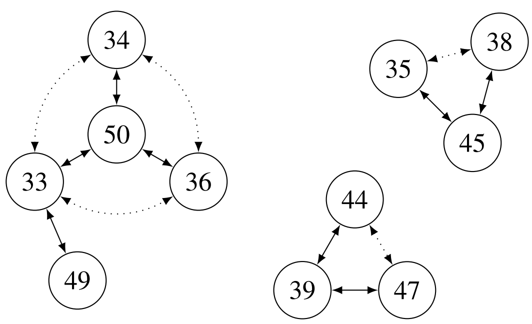


Figure 9: Example of mapping of the Battery.

Table 5: Number of regions obtained with the Solvay's data, using each of the three clustering methods, run 100 times, with 100 nodes for SOM and BSOM, and 50 for K-Means.

Method	Mean	Std	Min	Max
K-Means	3.9	0.98	2	6
SOM	7.98	2.05	3	12
BSOM	8.46	2.54	4	15

Eventually, Table 5 compares the results obtained when using the three clustering methods introduced earlier, run 100 times: the mean, standard deviation, minimum and maximum for each method.

The results of this table are close to that drawn from the academic dataset: BSOM is the closest to reality, with the best range, but a high scattering, closely followed by SOM; the K-Means has the least scattered results, but the number of regions identified is a little low. That being said, all the three methods have provided acceptable estimates (no aberration nor outliers), which confirms the universality of our method.

5 CONCLUSION

Unsupervised clustering is a blind approach which aims to point out the similarities and hidden patterns of an unknown database. They are automatic, but generally require an important parameter as of the expected number of clusters. This parameter must be set manually, and the choice of one value over another may change the clustering's representativeness in depth. In this paper, we have addressed the problem of the automatic estimation of the empirical optimal number of clusters to be set as meta-parameter for an unsupervised, data-driven clustering method.

To that purpose, we propose the ECD Test, which aims to estimate the empirically most suited number of clusters. Whilst most approaches from literature operate several clusterings by varying the number of clusters, and by selecting that achieving the best results, we rejected that idea, for it is closer to a true brute-force clustering rather than a real estimation of the number of clusters. Our method relies on a hierarchical aggregation of the characteristics of the database so as to propose a judicious estimate.

Indeed, we propose to operate a unique clustering, with a high number of clusters, compute the Empirical Cumulative Distributions to characterize the clusters, and finally bring the clusters together according to the closeness of their respective ECDs. To do so, we compute the Modified Hausdorff Distance between any couple of two ECDs, and gather all these measures into a unique matrix, whose values are compared to a threshold: if a value is low, then the involved ECDs (and then clusters) are considered as close. Finally, all these measures are linked to one another into a map by region growing clustering, allowing to rebuild the regions of the feature space. The number of isolated groups of clusters is somehow the number of regions of the feature space, and therefore a very good estimate for the optimal number of clusters.

We assessed this methodology over an academic dataset consisting in fifteen 2D-Gaussian Distributions, and then over real industrial data. In both cases, we found back about the number of clusters we had expected, i.e., a ten in both cases. We tested three clustering methods (K-Means, SOMs and Bi-Level SOMs) to show the resilience of our methodology, which proved to be highly reliable in any context, even with unsupervised data-driven approaches.

The ECD Test tool is very helpful to prepare the ground for some sort of next steps. In our next works, we will endeavor to use it in wider situations, and to use it so as to get the best clustering as possible on real datasets. A great and accurate clustering is of major importance in many contexts, such as multi-modeling the system under consideration (one local model for each cluster): this is the solution we are actually working on, and the reason why we addressed the problem raised in this paper.

ACKNOWLEDGEMENTS

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