Characterizing N-Dimension Data Clusters: A Density-based Metric for Compactness and Homogeneity Evaluation

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Abstract: The new challenges Science is facing nowadays are legion; they mostly focus on high level technology, and more specifically *Robotics*, *Internet of Things*, *Smart Automation* (cities, houses, plants, buildings, etc.), and more recently *Cyber-Physical Systems* and *Industry 4.0*. For a long time, cognitive systems have been seen as a mere dream only worth of Science Fiction. Even though there is much to be done, the researches and progress made in *Artificial Intelligence* have let cognition-based systems make a great leap forward, which is now an actual great area of interest for many scientists and industrialists. Nonetheless, there are two main obstacles to system's smartness: computational limitations and the infinite number of states to define; Machine Learning-based algorithms are perfectly suitable to Cognition and Automation, for they allow an automatic – and accurate – identification of the systems, usable as knowledge for later regulation. In this paper, we discuss the benefits of Machine Learning, and we present some new avenues of reflection for automatic behavior correctness identification through space partitioning, and density conceptualization and computation.

1 INTRODUCTION

While the XIXth century is that of industrial processes and the beginning of production line, and the XXth century is characterized by mass production and assembly line, the actual XXIst century is that of Robotics, Automation and Hyper-Connectivity. A great many of projects related to these topics are current active areas of research: self-driving vehicles[1] (Shan and Englot, 2018), domotics, exoskeletons, smart robots able to interact with human beings (Russo, 2020), self-adaptable systems, telecommunications (IoT, 5G), etc.

Robotics and Automation are getting more and more accurate and reliable; there are two ways to achieve great performances: 1- By defining explicitly how a system should behave in a certain context (*Expert System* paradigm); 2- By letting the system learn by itself and self-adapt through examples and observations (*Machine Learning* paradigm).

The former has been considered so far as the most reliable, since every possible state the system can enter in is explicitly defined by some experts or users; nonetheless, it suffers from a severe limitation: defining any possible behavior is an unfeasible task, and thus severely hinders the self-adaptation capability.

A piece of solution comes along a possible usage of the examples encountered by the system in order to let it study from them and learn how to react in the already known contexts. Once more, encountering any possible situation is merely unfeasible; it is though greatly easier to cover many more cases through observations and experience than to list them manually. Letting the system learn ever more through time allows to hypothetically cover any possible scenario.

It is the *Machine Learning* ML paradigm; it can be used to identify, characterize and eventually model a system, what can serve several purposes, among which its monitoring and its semi-manual regulation.

In general, the first step of any ML-based identification technique is an exploration of the data to point out what can be. This procedure is often blind – *unsupervised* – and is processed to automatically extract information from the data. The most common *Data Mining* task is space-partitioning, also called *clustering*, which consists in gathering the data into compact groups within those they share similarities. This step can be used to identify the system's local behaviors, optimize the processes by gathering similar tasks, etc.

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[1] Automated Vehicle AV and Advanced Driver Assistance Systems ADAS as well.

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A great area of interest for clustering could be the modeling of a system. Indeed, each cluster should contain similar data and thus can be assumed to represent a local behavior: a local model can therefore be built upon it. This is the *Multi-Models* paradigm. This decomposition of the feature space, and thus of the system as a whole, is very suitable to an Automation and Industry 4.0 application; indeed, the cornerstone of any network – such as an Industry 4.0 Cyber-Physical System – is to treat every unit as a part of a wider process. Clustering could help to identify the elementary units of an industrial system, either physically (subprocesses) or theoretically (behaviors).

There exists plenty of clustering methods, but they do not all perform alike. Their accuracy greatly depends on the studied data; as such, two clustering algorithms can be similar while achieving very different results. The remaining question would be to know how to automatically distinguish a good decomposition from a poor one. This knowledge can be very important and relevant for the further steps of the modeling process; indeed, how to expect a good model when the first step, *i.e.* clustering, has achieved poor results, and has gathered (very) dissimilar data?

In this paper, we will present a new way to quantify the compactness of a cluster of data, which is very useful as an indicator of data homogeneity. In the next section, we will present both some Machine Learning models and some Machine Learning-based clustering methods; in section 3, we will detail both that used and our homogeneity quantifier. Section 4 will display some examples of results and how one can interpret them for further understanding of the systems. Finally, section 5 is the conclusion of this paper.

2 STATE OF THE ART

Whether it is artificial or biological (brain), a Neural Network NN is somehow a graph where the nodes are a sort of activator and the branches linking the nodes to one another are a channel, whose span lets a signal go through with a high or low amplitude, like a nozzle would do. By analogy with the brain, the nodes are called the *neurons* and the channels are the *synapses*.

Training an Artificial Neural Network means to adapt ”the span” of its channels; a weighting coefficient (called *weight*) is responsible for this adaptation, which is modified in such a way it fits the known data.

More generally, the *Machine Learning* paradigm exploits data and experience to train a system, and to teach it how to behave within certain situations. It relies on several approaches: Multi-Layer Perceptron MLP (Rumelhart et al., 1986a), Radial Basis Function RBF (Broomhead and Lowe, 1988), Multi-Expert System MES (Thiaw, 2008), Multi-Agent System MAS (Rumelhart et al., 1986b), Support Vector Machine SVM (Boser et al., 1996), etc. The most common model in use is the MLP, which is somehow a representation of the biological brain; they are often long to train however. Thus, some other models can be preferred, depending on the context of application.

Though less widespread, another paradigm in use is the Multi-Expert System MES: it is anew a Neural Network, with the main difference that the neurons are local experts. The output of the whole model is a combination of the outputs of the local models. It is an extension of the very widespread Expert System paradigm (Buchanan and Feigenbaum, 1978). The local experts can take many shapes, from expert systems to Machine Learning-based models (MLP, RBF, SVM, etc.). Though still depending on the data and on the context, MESs are capable of achieving great accuracy, for the sub-models are trained to correctly model and represent each of the system’s sub-parts.

As a consequence, to use the MES paradigm, the feature space must be split upstream. As such, we need a clustering method to make the framework ready for this step. There exists several clustering algorithms, mostly based on Machine Learning; this avoids to have to rely on human experts charged to manually describe the system, what can be hard and time-greedy. Machine Learning lets a (smart) algorithm do the job instead; the inquiry is mainly to know whether or not one can trust the so-obtained clusters.

Once more, clustering can be driven by some knowledge – *supervised* learning – or be totally blind – *unsupervised* learning. However, supervised learning requires some often manual expertise of the data (or given by an unsupervised algorithm upstream) and is therefore not suitable to a blind data mining procedure. Among the existing clustering algorithms, it is worth mentioning: K-Means (Jain, 2010), Self-Organizing Maps (Kohonen, 1982), Neural Gas (Martinetz and Schulten, 1991), Fuzzy Clustering (Dunn, 1973) and Support Vector Machine (Boser et al., 1996). The first three are unsupervised, and are perfectly suitable to a data mining application.

The K-Means iteratively aggregate the data points around some ”seeds” (random points drawn from the database), and update them again and again until satisfying some criterion. They are easy to implement, but are unable to cluster nonlinearly separable datasets. The Kernel K-Means use a kernel (a projection of the data from an Euclidean space into a non-Euclidean one, called *kernel space*) to compensate that, but they are very resource-consuming and are prone to achieve only local optima.

The Self-Organizing Maps are an ingenious extension of the K-Means, by linking the seeds with each other, forming somehow a grid; it is now the whole grid which is updated to fit any data. They converge quicker, and by using a nonlinear learning function (*cf.* section 3.1), they are able to separate even nonlinear databases, while still operating in an Euclidean space. A Neural Gas is an evolution of the SOMs, by allowing a possible pruning of the grid (in case a node represents no data), or by adding new nodes; the grid can evolve to better represent the feature space, and its evolution through time. Neural Gases are thus great to represent very changing and dynamic systems.

Sometimes, the datasets are not easily distinguishable, for they boundaries are blurry: some data can belong to several clusters at the same time. To take that into account, one can assign a probability to any data, to represent how it belongs to each cluster. This is the *Fuzzy* paradigm, which is very useful to represent compact databases, with overlapping groups; it is nonetheless a more complicated paradigm, which changes how one deals with a database – any further work should be fuzzy based. The Fuzzy C-Means are a fuzzy version of the regular K-Means.

Support Vector Machine is an accurate approach, which aims at interpolating the best boundaries (linear for the regular SVM, but can also be a kernel), by finding the points which are at the same time the outermost of a cluster and the nearest of another cluster. SVMs are accurate, but are limited to the separation of two clusters only, and are slightly hard to compute.

When only focusing on unsupervised learning, we are totally blind and have no clue on the actually existing classes to be identified; it would therefore be relevant to use an indicator to quantify the accuracy and the relevancy of the detected clusters. Indeed, since there is no available clue on the real class of a data, it is impossible to say whether the data has been correctly clustered or not. With a weak quantifier, a cluster could be considered as good whereas it could contain several types of data and would be worth being split. On the other hand, if the data are scattered due to a lack of instances, a real unique class of data could be split into several smaller clusters.

To validate a clustering while having no specific knowledge on the actual classes, one can rely on *Intrinsic Methods*, which are unsupervised metrics to quantify the clustering's quality. Unfortunately, most of the metrics of the literature are quite old (70s-90s), and it is why we want to propose an innovative new effective and efficient qualifying metric. From the literature, it is worth mentioning the Dunn Index DI (Dunn, 1974), the Davies-Bouldin Index DB (Davies and Bouldin, 1979) and the Silhouette Coefficient SC (Rousseeuw, 1987). All three compare the inter-cluster distances and the intra-cluster distances to estimate the cluster's *density*; they differ from one another by how they operate this comparison (ratio, average, min/max, etc.). They all have their drawback: the first and the third suffer from a high computational cost, while the second is not always reliable (a good value can be retrieved with a poor clustering).

Nowadays, there is no universal indicator of clustering's correctness, and there will probably never be. Nonetheless, in this paper, we take our chance and we propose an indicator based on the compactness of the clusters to decide if it is relevant for consideration.

3 CLUSTERING AND PROPOSAL

In the following, let $\mathcal{D} = \{x_i\}_{i\in[\![1,N]\!]}$ be the database, with N the total number of points, and let d be a n-dimension distance, such as the Euclidean distance. Let also $t \in \mathbb{N}$ refer to an iteration number, and $k \in [\![1,K]\!]$ be a cluster's issue, with K the total number of clusters obtained after processing (or expected).

3.1 Clustering Algorithm

Since the purpose of this paper is to propose a compactness measurement, we will limit ourselves to the Kohonen's Self-Organizing Maps. Indeed, it is an unsupervised algorithm, thus suitable for Data Mining and blind knowledge extraction. It is also efficient and effective, and achieves good results, while also being simple and resource-saving.

Self-Organizing Maps SOMs. Somehow an extension of the K-Means where the clusters are artificially linked to each other under the shape of a grid. When a cluster's mean is updated, so are its connected clusters. A notion of neighborhood is therefore added; this allows a quicker convergence and the preservation of the feature space topology. When a new data x is drawn, the whole grid is updated, neighbor after neighbor. This update is the strongest for the nearest cluster's pattern (*node*) of x, called the *Best Matching Unit* and denoted as k^*, and decreases when moving away from it; this procedure is embodied by the neighborhood function h defined by (1). The learning stops after T_{max} iterations.

$$h_k^{(t)}(k^*) = \exp\left(-\frac{d^2(k,k^*)}{2\sigma^{(t)^2}}\right) \qquad (1)$$

where $\sigma^{(t)}$ is the neighborhood rate at iteration t, which aims at decreasing the neighborhood impact through time, and defined by (2), where σ_0 is its initial value ($t = 0$).

$$\sigma^{(t)} = \sigma_0 \exp\left(-\frac{t}{T_{max}}\right) \quad (2)$$

We also define the learning rate $\varepsilon^{(t)}$ at iteration t, which aims at decreasing the learning of the grid through time (to avoid oscillations), and is defined by (3), where ε_0 is anew its initial value ($t = 0$).

$$\varepsilon^{(t)} = \varepsilon_0 \exp\left(-\frac{t}{T_{max}}\right) \quad (3)$$

Finally, the pattern of cluster k, here represented by an attraction coefficient called *weight* $w_k^{(t)}$ at iteration t, is updated by (4).

$$w_k^{(t+1)} = w_k^{(t)} + \varepsilon^{(t)} \times h_k^{(t)}(k^*) \times \left(w_k^{(t)} - x\right) \quad (4)$$

Note that we are no longer talking about "mean", but about "pattern"; the pattern of a cluster (or a node) is its aggregation center, and often differs from the mean of its data. It is generally more representative, since it is updated through the learning procedure (4) and not by the data themselves.

3.2 Compactness Measurement

An indicator of the correctness of the generated clusters is a very relevant knowledge for more advanced purposes, such as a MES model. Unfortunately, an accurate and, especially, a relevant measure is not easy to define, since it strongly depends on the data and on the context. Indeed, a cluster can be seen as "correct" through a weak quantifier, while it is not in reality.

Let $C_k^{(t)}$ and $m_k^{(t)}$ be respectively the k^{th} cluster itself and its aggregation center (mean or any pattern) at iteration t. The clusters are formed following (5), and their mean is given by (6) (or (4) for the SOMs).

$$C_k^{(t)} = \left\{ x \in \mathcal{D} : d(x, m_k^{(t)}) = \min_{i \in [\![1,K]\!]} d\left(x, m_i^{(t)}\right) \right\} \quad (5)$$

$$m_k^{(t)} = \frac{1}{\left|C_k^{(t)}\right|} \sum_{x \in C_k^{(t)}} x \quad (6)$$

From now on, we will set aside the notion of iteration for readability concerns: the expressions are more general and do not precise a given timestamp. When we will refer to an above equation, we will assume this will be true for any $t \in \mathbb{N}$.

Average Standard Deviation AvStd. Proposed by (Rybnik, 2004), the relevancy of a cluster is quantified by the standard deviation of the data contained within: the highest, the worst. This technique has the advantage to diminish the impact of the outliers, with the condition there are enough data[2]. The drawback is that it is essentially an indicator of data scattering. The standard deviation is computed feature by feature, and the AvStd measurement is their average. Let m_k be the mean of the k^{th} cluster, defined by (6), whose data are defined by (5). The standard deviation σ_k is defined by (7).

$$\sigma_k^{(i)} = \frac{1}{|C_k|} \sum_{x \in C_k} \left(m_k^{(i)} - x^{(i)}\right)^2 \quad (7)$$

where $i \in [\![1, n]\!]$ is the current feature, with n the feature space's dimension. The AvStd measure of cluster k is finally given by (8).

$$\text{AvStd}_k = \overline{\sigma}_k = \frac{1}{n} \sum_{i=1}^{n} \sigma_k^{(i)} \quad (8)$$

3.3 Proposal: Density Estimation

The idea is to estimate the density of a cluster, and to use this value as an indicator of compactness, and therefore of homogeneity: the higher, the better. We first evaluate its volume, and we multiply its reciprocal by the number of points within the cluster.

This is the regular definition of *density*. The main difficulty is to define and compute the *volume* of a cluster; indeed, what do we call a volume in dimension n? There are several ways to answer this question; one can be the hyper-volume theory.

For instance, in dimension 3, to evaluate the volume occupied by a set of 3D points, one can search for the minimal sphere containing all these points, and use the sphere's volume as the cluster's volume. Theoretically, it should not be a hard task, at least in dimension 3; but when the dimension increases, the regular 3D volumes are not sufficient, and from there appear the benefits of using a hyper-volume, and especially a hyper-sphere.

The density $\rho_k^{(n)}$ of cluster k is therefore computed by dividing the number N_k of data instances contained within by its volume $v_s^{(n)}$; the density is given by (9).

$$\rho_k^{(n)} = \frac{N_k}{v_s^{(n)}} \quad (9)$$

The cluster's volume can be estimated by searching its outermost points, then interpolating the surface[3] containing all these points, and finally estimating the so-called n-dimensional volume.

[2] It is the Cesàro mean.

[3] It would therefore be a hyper-plane of dimension $n-1$.

This approach fits the best the data instances representing the corresponding cluster, but has two major drawbacks: 1- It is computationally very demanding; 2- The hyper-volume obtained will be defined only with the encountered data instances: a data could belong to it, but if its features are outer those of the outermost points of the cluster, this data will not be considered as belonging to this cluster. This way of evaluating the volume is too strict for it exactly fits to the database's instances only.

To avoid that, one can decrease the strictness of the hyper-volume's shape by using a more conventional and flexible hyper-volume, such as a hyper-cube or a hyper-sphere. The former has the advantage to cut the n-dimension space into a set of hyper-cubes, whose union is the space itself; the latter has the advantage to be more compact and to avoid any possible clusters' overlap. For this reason, hyper-spheres seem more relevant to represent random clusters.

Let $r \in \mathbb{R}^+$ be the radius of a n-hyper-sphere (*i.e.* the distance from its mean to any point on its surface); its volume $v_s^{(n)}$ is given by (10) (Lawrence, 2001).

$$v_s^{(n)}\left(r\right) = r^n v_s^{(n)}\left(r=1\right) = \frac{r^n.\pi^{n/2}}{\Gamma\left(\frac{n}{2}+1\right)} \quad (10)$$

where Γ is the Gamma function, defined by (11).

$$\forall z \in \left\{\mathbb{C} : \mathfrak{Re}(z) > 0\right\}, \Gamma(z) = \int_0^{+\infty} x^{z-1} e^{-z} dx \quad (11)$$

The last concern is to evaluate the radius r: which hyper-sphere should be chosen to best fit, contain and represent a cluster of data?

To answer this question, several constraints might be considered, particularly the accuracy and the computational complexity. The former is about choosing a cluster's shape, such as a hyper-volume, which best includes the data, while having a high generalization capability. The latter is about computational efficiency; indeed, some techniques and algorithms have a high computational requirement – whether it is about clustering or about cluster's compactness estimation – and as such might not be suitable for embedded systems, and especially in an Industry 4.0 context.

The last point severely hinders a perfect interpolation of the cluster's boundaries, since it generally requires very complex approaches. Therefore, a simpler and more resource-saving approach should be preferred in an embedded system context, even though it might also mean a slight decrease in accuracy.

In a 1-dimension space, the span of a group of data is defined by the largest distance[4] between two of its points. It is more easily visualization with a line (1D), but the idea remains the same for a higher dimension. As such, a possible span estimate of a cluster in dimension n could be the maximal distance between any couple of its points, in any dimension.

This idea is quite natural, but suffers from a high computational cost: it requires the distances between any couple of data. Let N_k be the number of points contained within cluster C_k; there is thus $N_k(N_k-1)/2$ couples and as many distances to be computed. The complexity is therefore in $O(N_k^2)$, which can be too high for some embedded system contexts.

For this reason, alternative approaches might be investigated, with a linear complexity at best. The solution we propose is to take benefit from the cluster's statistics. Indeed, instead of comparing any point to any other, the idea would be to compare them to an only one reference. The complexity would therefore be in $O(N_k)$, since there would only be the distances from any point to this reference to be computed.

This reference must be chosen wisely: we propose the cluster's mean (or its pattern for the SOMs), since it is the best indicator of its attraction capability[5]. As a consequence, the cluster's span is therefore the double of the maximal distance between any point and its mean, as (12), which requires only N_k distances. Only the mean remains to be computed, but either that has already been done through the clustering, or it is only the summation of the data, divided by the cluster's cardinal, what has once more a complexity in $O(N_k)$.

$$s_k = 2 \times \max_{x \in \mathcal{C}_k} \left\{d(x, m_k)\right\} \quad (12)$$

where $\mathcal{C}_k$ refers to the cluster's data, defined by (5), and m_k is the cluster's mean, defined by (6).

In order to decrease the impact an unique outlier could have, one can also identify several most distant points from the mean, and then compute their average.

The two major benefits of this estimation of the cluster's span is its computational efficiency, and that it ensures any of its points is contained within the so-built hyper-volume (hyper-sphere or hyper-cube). The drawback is that it is an estimate in excess of the span, since it takes the (or some) most distant point(s) from the mean and uses this distance as the half of the maximal distance separating any couple of points. For instance, let's imagine the perfect case where the two farthest points are aligned with the cluster's mean in between. The distance separating the farthest of these two points from the mean is therefore s_k, as defined by (12), but the distance separating the second point from the mean is necessarily smaller; otherwise, it would be this point which would be the farthest one. As a

[4] According to a distance: Manhattan, Euclidean, etc.

[5] A cluster is generally represented either by a learned pattern (SOMs) or its mean (K-Means).

consequence, the summation of these two distances is smaller than the double of s_k, meaning that it is an estimate in excess.

It is not a big deal howsoever, since the boundaries of a cluster are data driven and are delimited by the only known data. A cluster could actually be larger in reality than its data let presume, and for this reason, a higher estimate of the cluster's span is not really a problem, since it leaves more freedom by decreasing the constraints set by the data.

As the little too large estimate is not a real issue there, and that the complexity is only linear, we will use this way to estimate the maximal span of a cluster, and use this value as the radius of the hyper-sphere incorporating all the cluster's data. We will eventually evaluate the cluster's density with (9), which indicates the compactness of the cluster, through a relevant and computationally efficient indicator.

4 RESULTS

In this section, we introduce two academical datasets, and apply our density measure ρ (9) on them in order to evaluate its relevancy, and the AvStd $\overline{\sigma}$ (8) for comparison as well. We will also apply both on some data provided to us by one of our partners involved in the project HyperCOG (*cf.* section "Acknowledgements") in order to illustrate the applicability of our density measure to a real Industry 4.0 use-case.

The first example is a set of three 2D strips. While the strips are clearly different for a human being, they overlap each other; that has been done in order to study what happens in such conditions, more representative of a real use-case, where data are very likely to be not so easily distinct and separable.

The second example is a set of n-dimension Gaussian distributions, with randomly generated clusters in a n-dimension feature space. Both gaps and overlaps are greatly possible: some clusters are therefore easily separable, even by a linear clustering approach, whereas some other are painful, for their respective boundaries are not clear.

Finally, the real data were provided by a chemistry plant specialized in Rare Earth extraction, and belonging to Solvay Opérations®, located at 26 Rue du Chef de Baie, 17000 La Rochelle, France.

We will mainly remain in dimensions 2 and 3 for representation concerns, but we will also study a set of 25-dimension Gaussian distributions, to show the generalization capability of our metric.

The results are gathered within tables, where the first column is the list of the real distributions ("dbai") and of the obtained clusters ("clti"). For each one of them, some measures have been applied: the "Density" tag refers to the density measure (9), "σ_α" is the Standard Deviation along axis α, and "$\overline{\sigma}$" is the AvStd measure (8), *i.e.* the average of the σ_α. These measures have been applied to the original groups ("dbai") to serve as references. The lines "Min", "Max", "Q1", "Med", "Q3" and "Mean" are respectively the minimum, maximum, first quantile, median, third quantile and finally the statistical mean of the clusters only lines ("clti").

Please note that the density measure scale is somehow arbitrary for it depends on the scale of the feature space – similarly to the Standard Deviation as well. For a given cluster, its density should be compared to those of the other clusters; this is the reason why the above mentioned statistics are represented.

4.1 Strip Distributions

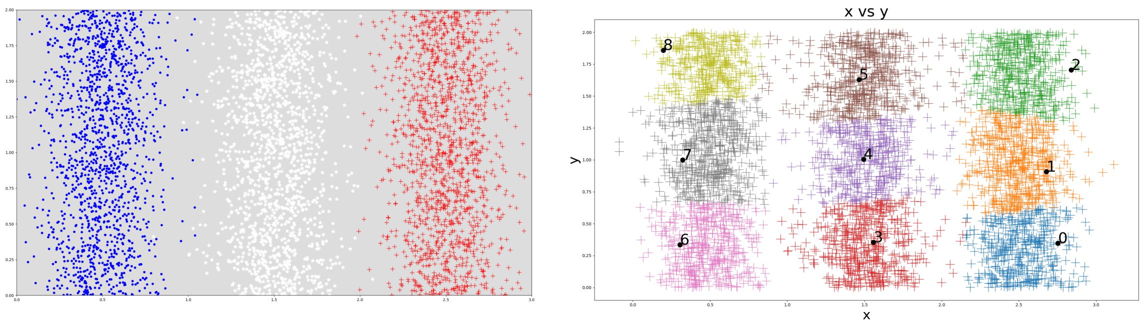
The first example is a set of three strips, generated following a Gaussian distribution along the x-axis and an uniform distribution along the y-axis. The purpose of such a mixture is to create an overlap along the x-axis, and since the strips are side-by-side along the x-axis, there is no possible overlap along the y-axis.

Each strip contains 1500 points, centered around $(1,0.5)$, $(1,1.5)$ and $(1,2.5)$ respectively, with a standard deviation of 0.175 unit along x-axis; they are displayed on Figure 1a, and Figure 1b represents the clustered dataset, projected onto a 3×3 grid by the SOMs. The results are gathered within Table 1.

The database has been split into 9 pretty compact groups, but some overlaps can be observed, especially in the middle strip. Indeed, the patterns of the nodes #0, #1 and #2 are on the extreme right of the image, while the patterns of the nodes #6, #7 and #8 are on the extreme left. That lets the middle nodes, namely #3, #4 and #5, attract some points from the two other strips. These points are the farthest from their respective node and thus are caught by those in the middle of the feature space (along the x-axis).

For instance, consider the blue cluster, at the bottom right of Figure 1b and represented by node's pattern #0: its farthest points, *i.e.* those at its extreme left, are too far from it and are caught by the red cluster, at the bottom middle and with node's pattern #3.

This observation can also be drawn from Table 1. Indeed, the density of the obtained groups is around 500 units for clusters #0, #1 and #2 (right) and #6, #7 and #8 (left). As we said above, this value has no real meaning, but if we compare it with those of the three remaining clusters, #3, #4 and #5, which are around 370, we can notice a great gap in value: there is a density decrease of 26%. As such, one can understand



(a) The three distinct but slightly overlapping strips. (b) The three strips projected onto a 3x3 grid.

Figure 1: The overlapping 2D-strips.

Table 1: Density and AvStd of the three 2D-strips.

Strips	**Density**	**Standard deviation**		
		σ_x	σ_y	$\overline{\sigma}$
dba0	407.44	0.17	0.59	0.38
dba1	388.88	0.18	0.58	0.38
dba2	403.13	0.17	0.58	0.38
clt0	534.39	0.17	0.18	0.17
clt1	463.67	0.16	0.22	0.19
clt2	503.95	0.16	0.19	0.18
clt3	382.01	0.19	0.20	0.19
clt4	378.72	0.19	0.18	0.19
clt5	347.15	0.22	0.20	0.21
clt6	507.68	0.16	0.19	0.18
clt7	539.01	0.17	0.23	0.20
clt8	531.27	0.15	0.15	0.15
Min	347.15	0.15	0.15	0.15
Max	539.01	0.22	0.23	0.21
Q1	382.01	0.16	0.18	0.18
Med	503.95	0.17	0.19	0.19
Q3	531.27	0.19	0.20	0.19
Mean	465.32	0.17	0.19	0.18

there is something weird with these three clusters.

It is what we were talking about in the above paragraph: clusters #3, #4 and #5 overlap the others, what makes them less dense. As all these clusters have a similar shape, they should all have a similar density, but the overlaps increase the density of the left and right clusters and decrease that of the middle clusters.

This observation does not manifest itself with the AvStd: 0.19, 0.19 and 0.21 for clusters #3, #4 and #5, respectively. These values are slightly consistent with those of the other clusters. This is due to the fact that the outermost points, caught by the middle nodes, are somehow outliers to them; the standard deviation is little sensitive to outliers, reason of this consistency.

As a conclusion, through this example, the density measure has an advantage on the AvStd measure, since it has allowed to point out the three overlapping clusters, what the AvStd has not been able to do.

4.2 Gaussian Distributions

The second example is a set of Gaussian distributions, in dimension n. We will start in dimension 3; then we will move on to the greatly higher dimension 25 to show the generalization capability of our metric.

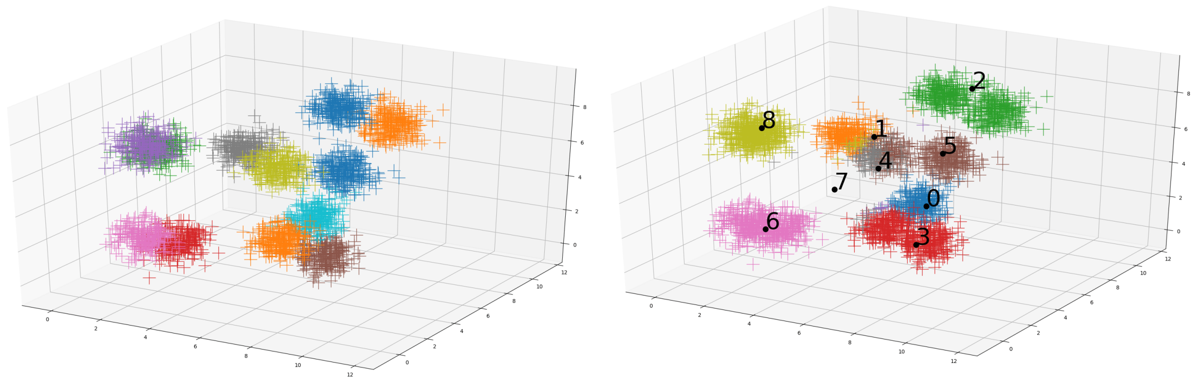
4.2.1 Dimension 3

Let us start in dimension 3, with a set of twelve groups of data, each generated with a Gaussian distribution. The mean of any cluster is randomly drawn following an uniform distribution within the feature space, ranging from 0 to 10 units for each of the 3 dimensions. Each 3D-Gaussian distribution contains 250 data instances, with a standard deviation of 0.5 unit. Even though this value is not prone to great overlaps, the random drawing of the groups' means makes possible and even probable some overlaps however.

This dataset mainly aims at showing the results obtained within a 3-dimension feature space, and how an overlap can be pointed out with our density measure, while not that easily with the AvStd measure.

The so-generated database is shown on Figure 2a and the clustered database projected onto a (too small) grid of size 3×3 is displayed on Figure 2b. The opposition of any possible couple of dimensions $\big((x,y)$, (x,z) and $(y,z)\big)$ is represented as Figure 3, in order to give a greater insight on the relations and overlaps of the clusters, in any dimension. The results of the quantifying measures are gathered within Table 2.

The first thing is that several Gaussian distributions have been merged as a unique cluster, which is not surprising, since the grid is too small (nine nodes for twelve distributions): nodes #2, #3, #6 and #8 of Figure 2b are such a merging. For some, this is not a problem, since the groups are very close in the original database: according to Figure 3, we can see that cluster #3 is perfectly compact, and that its merging is not a problem at all. But for the three remaining clus-



(a) The original 3D-Gaussian distributions, as random compact groups of data, but with some local overlaps.

(b) The clustered 3D-Gaussian distributions, projected onto a too small 3x3 grid, causing the merging or the splitting of some groups whereas they should not be.

Figure 2: The 3D-Gaussian distributions.

Table 2: Density and AvStd of the twelve 3D-Gaussians.

Gauss	Density	Standard deviation			
		σ_x	σ_y	σ_z	$\overline{\sigma}$
dba0	8.36	0.51	0.51	0.52	0.51
dba1	8.12	0.51	0.54	0.55	0.53
dba2	9.89	0.49	0.55	0.48	0.51
dba3	5.75	0.51	0.52	0.51	0.51
dba4	7.19	0.52	0.50	0.51	0.51
dba5	11.87	0.52	0.51	0.53	0.52
dba6	6.97	0.49	0.46	0.52	0.49
dba7	8.90	0.54	0.51	0.50	0.52
dba8	11.79	0.51	0.48	0.49	0.49
dba9	6.56	0.46	0.52	0.52	0.50
dba10	11.75	0.45	0.52	0.49	0.48
dba11	11.83	0.44	0.50	0.48	0.47
clt0	6.56	0.46	0.52	0.52	0.50
clt1	0.82	0.57	0.52	0.52	0.54
clt2	3.79	1.47	0.86	0.52	0.95
clt3	9.70	0.77	0.65	0.65	0.69
clt4	0.03	0.25	1.13	1.16	0.85
clt5	4.72	1.14	0.50	0.50	0.71
clt6	4.65	0.52	1.01	0.71	0.75
clt7	0.31	0.67	0.54	1.18	0.80
clt8	1.67	0.83	0.53	0.50	0.62
Min	0.03	0.25	0.50	0.50	0.50
Max	9.70	1.47	1.13	1.18	0.95
Q1	0.82	0.52	0.52	0.52	0.62
Med	3.79	0.67	0.54	0.52	0.71
Q3	4.72	0.83	0.86	0.71	0.80
Mean	3.58	0.74	0.70	0.70	0.71

ters, #2, #6 and #8, a gap between the original distributions can be observed: the clusters are not compact.

This statement can also be drawn from Table 2: ”clt3” has the highest density (9.70 units, 46% greater than the second highest value 6.56 units), meaning it

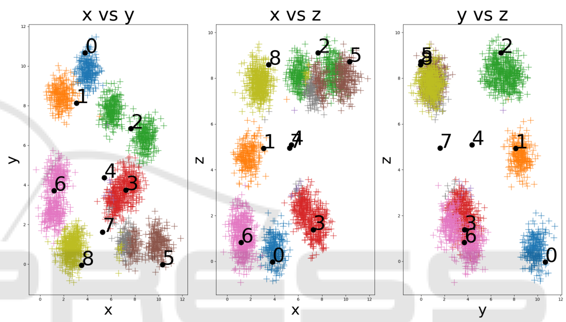


Figure 3: The 3D-Gaussian clusters projected onto any possible 2-dimension feature set.

is very compact; but this observation does not work with the AvStd measure, since its value 0.69 is very close to the mean 0.71. The density indicates here that this cluster #3 is very well-built, since very compact, whereas the AvStd says only to us that it is in the average, neither good nor bad. Nonetheless, our above qualitative observations validate the density measure.

That is also true for clusters #2, #6 and #8: the two first have an average density, while the third has a very poor one. For clusters #2 and #6, that is because the two original Gaussian distributions are close from each other, thus their merging is not really dreadful (Figure 4). Cluster #8 has a very low density however, justified by a bad overlap with another cluster (Figure 5). On the contrary, the AvStd measure indicates that its average standard deviation is very good – equal to the first quantile. This is due to the fact that cluster #8 has a little overlap, with few data belonging to a very distinct – and distant – cluster. Since the AvStd measure is lowly affected by outliers, its average standard deviation is very good, while its density is not, since that one is severely affected by outliers.

What happens to cluster #8 is also true for cluster

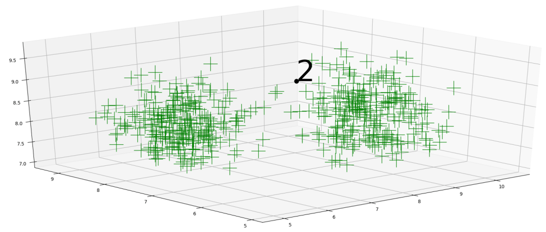


Figure 4: Zoom on cluster #2: it is not compact since it gathers two independent, but near, distributions.

#1: it contains some distant outliers (should belong to cluster #2), what greatly decreases its density.

The lowest density is achieved by cluster #4, which contains very few data, dispatched within several Gaussian distributions. This cluster is more an outlier itself, what can be verified for its pattern is nowhere, in between several clusters. Actually, it is the middle node of the grid, reason why it finds itself somehow in the middle of the feature space.

Finally, the last observation we can make is about the two remaining clusters #5 and #7. A zoom on them and on cluster #8 is displayed on Figure 5.

Indeed, these three clusters have some problems: as already discussed, cluster #8 contains some outliers, what greatly decreases its density; cluster #5 overlaps another Gaussian distribution; and cluster #7 is alike #1: its pattern is nowhere, in the middle of the figure, catching some points from here and there.

On Figure 5, one can notice that the Gaussian distribution right next to (the main part of) cluster #5 is split into 3 sub-parts, one for each cluster among #5, #7 and #8. Nonetheless, this distribution is very close to cluster #5, as can be seen on Figure 3: a merging of these two distributions is therefore not a big deal, similarly to clusters #2 and #6.

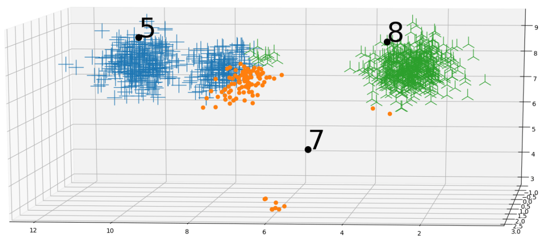


Figure 5: Zoom on clusters #5, #7 and #8 as they all overlap an independent, but unidentified, group. Note that cluster #7 overlaps 3 different clusters (middle bottom, middle right and left), what causes it to have a very poor density, even though its AvStd measure is perfectly acceptable.

All these observations can be understood from Table 2 too: the density of clusters #7 and #8 are very low, which means they are poorly compact. Unfortunately, their AvStd, 0.8 and 0.62 respectively, are anew in the average and acceptable compared to the others: they do not really help to identify a possible problem with these clusters, what their density, 0.31 and 1.67 respectively, did on the contrary.

As a conclusion, all our qualitative observations have been validated by the density measure, and can independently be made from them. This was rarely the case with the AvStd measure, which is less affected by outliers, but also less likely to point out compactness and homogeneity troubles.

4.2.2 Dimension 25

Let's now finish with a high dimension feature space. The database is built following the same methodology than that of section 4.2.1: twelve Gaussian distributions, ranging from 0 to 10 in every dimension, a standard deviation of 0.5 unit, with 250 points each, but this time in dimension 25 instead of 3.

The purpose of such a database is to illustrate the generalization capability of our metric, as blind users. Indeed, as we are in a too highly dimensional feature space for 2D or 3D representation, we will only give quantitative avenues of reflection, without a real possibility to directly validate them through qualitative observations. This represents a real blind – *unsupervised* – evaluation for a Machine Learning application within an Industry 4.0 context for instance.

Once more, the results obtained after clustering are gathered within Table 3; "None" entry represents the absence of value, in case of the corresponding cluster is empty (and might be pruned).

This example is interesting for is works on a perfect clustering of the database: any of the twelve Gaussian distributions has been perfectly identified and is represented by a unique node of the SOM's 4×4 grid. One can be convinced of this by comparing the "dba" lines to the "clt" lines: there is a perfect correspondence for each, *e.g.* "dba0" is "clt4".

So, what can we learn from this table? The mean standard deviation, *i.e.* the AvStd measure, is consistent within the twelve clusters, and is approximately equal to 0.5 (which is coherent when compared to the standard deviation used to generate the Gaussian distributions), thus the clusters seem coherent and compact. This observation is also slightly true based on the density measure, which is quite consistent too, varying from 85.24 to 102.70 – an increase of 20.5 %.

The effective difference in the densities can be explained by the span of the clusters: even though they share a very similar standard deviation, their outermost points are not all as distant from their respective cluster's mean. The density measure is sensitive to that, what explains the small but real variation. As such, in order to correctly use this measure, only very

Table 3: Density and AvStd of the twelve 25D-Gaussians.

Gauss25	**Density**	**Standard deviation**		
		min	mean	max
dba0	102.70	0.46	0.50	0.53
dba1	97.07	0.45	0.49	0.52
dba2	95.98	0.47	0.50	0.54
dba3	92.12	0.47	0.50	0.54
dba4	85.24	0.46	0.50	0.56
dba5	99.00	0.46	0.50	0.54
dba6	99.28	0.47	0.50	0.55
dba7	94.34	0.46	0.50	0.55
dba8	94.68	0.47	0.50	0.54
dba9	97.75	0.43	0.50	0.54
dba10	88.45	0.45	0.49	0.53
dba11	94.64	0.47	0.50	0.56
clt0	94.34	0.46	0.50	0.55
clt1	95.98	0.47	0.50	0.54
clt2	94.64	0.47	0.50	0.56
clt3	99.28	0.47	0.50	0.55
clt4	102.70	0.46	0.50	0.53
clt5	None	None	None	None
clt6	92.12	0.47	0.50	0.54
clt7	94.68	0.47	0.50	0.54
clt8	None	None	None	None
clt9	None	None	None	None
clt10	None	None	None	None
clt11	88.45	0.45	0.49	0.53
clt12	99.00	0.46	0.50	0.54
clt13	97.75	0.43	0.50	0.54
clt14	97.07	0.45	0.49	0.52
clt15	85.24	0.46	0.50	0.56
Min	85.24	0.43	0.49	0.52
Max	102.70	0.47	0.50	0.56
Q1	93.78	0.46	0.50	0.54
Med	95.33	0.46	0.50	0.54
Q3	98.06	0.47	0.50	0.55
Mean	95.10	0.46	0.50	0.54

noticeable differences should be considered, that is to mean higher than 20 % from min to max for instance.

Nonetheless, this variation could indicate a not so compact cluster, which might be worth being split for a higher homogeneity anyway. Unfortunately, this conclusion strongly depends on the context and on the data themselves: there is no real absolute answer, especially when using an unsupervised paradigm.

This example shows that the density measure is as reliable as the AvStd in high dimensions, at least for a perfect clustering. Added to the previous observations, it seems that our density measure is reliable to both point out issuing clusters and qualify compact clusters, in every dimension.

4.3 Industrial Data: Solvay Opérations

Our last example is a real use-case, in order to validate the relevancy of our metric on real Industry 4.0 data. For confidentiality concerns, we won't explain in details how the Solvay Opérations®'s plant works; we will remain general, what is not a big deal, since we want to study automatic knowledge extraction from unsupervised Machine Learning-based clustering.

We let just the reader know that the plant features hundreds of sensors, for many purposes; according to the Solvay's experts, some are more relevant than the others. Indeed, during the production procedure, some steps are essential, and a small local disturbance can have a huge impact and totally disturb the whole system. In the following, for representativeness concerns, only some of these most *important* sensors are depicted. As such, the feature space is the n-dimension Euclidean space represented by the n most important sensors. We will limit ourselves to only 3 sensors to be able to represent the results.

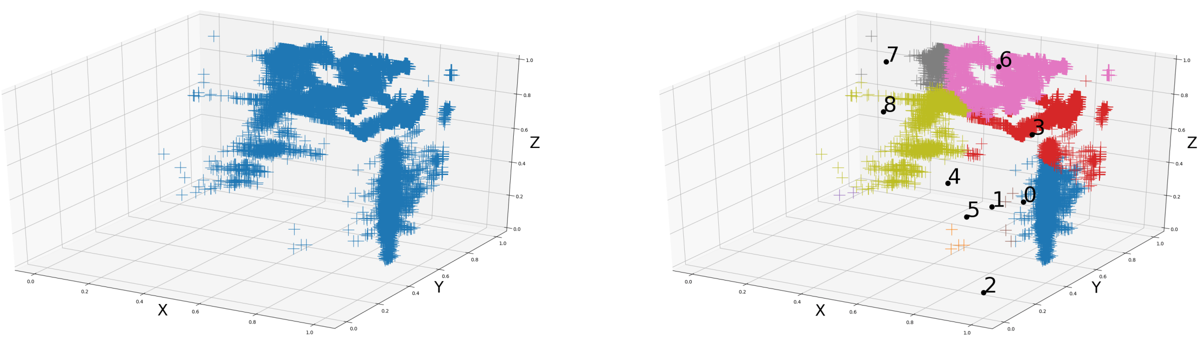
The raw 3D sensor's data are represented on Figure 6a, and the clustered data on Figure 6b. The results are gathered within Table 4, and Figure 7 shows any couple of dimensions to give a clearer insight on the relation between the data and the clusters as well.

Table 4: Density and AvStd of the Solvay's data.

Solvay	**Den.**	**Standard deviation**			
		σ_x	σ_y	σ_z	$\overline{\sigma}$
dba	4701	0.17	0.19	0.24	0.2
clt0	6290	0.01	0.01	0.10	0.04
clt1	2.7	0.03	0.00	0.05	0.03
clt2	None	None	None	None	None
clt3	1118	0.14	0.08	0.11	0.11
clt4	4.9	0.02	0.01	0.00	0.01
clt5	1.6	0.02	0.01	0.12	0.05
clt6	2948	0.04	0.10	0.11	0.08
clt7	137	0.03	0.02	0.05	0.03
clt8	2840	0.06	0.05	0.13	0.08
Min	1.6	0.01	0.00	0.00	0.01
Max	6290	0.14	0.10	0.13	0.11
Q1	4.3	0.02	0.01	0.05	0.03
Med	211	0.03	0.02	0.11	0.04
Q3	1576	0.04	0.06	0.11	0.08
Mean	1348	0.04	0.03	0.08	0.05

On Figure 6a and Figure 7, we can distinguish several compact groups of data, from at least two and up to perhaps four or five. This incertitude we have in counting the clusters, even as human beings, is the exact reason why a density, or similar, measure is essential to understand the structure of the data. Indeed, there are only 3 dimensions, and that is enough to disseminate a doubt; imagine a hundred of dimensions: for a human being, and even worse for a machine, identifying the number of clusters is an impossible task without an accurate and reliable criterion!

Howsoever, without taking into account the actually found clusters, Figure 7 displays 2 clusters for ”x vs y”, 2 or 3 for ”x vs z”, and 2 or 3 too for ”y vs z”. On Figure 6a, we can see 3, maybe 4, clusters: one



(a) The original 3D Solvay's data. (b) The 3D Solvay's data projected onto a 3x3 grid.

Figure 6: Example of application on a real Industry 4.0 use-case: the Solvay's data.

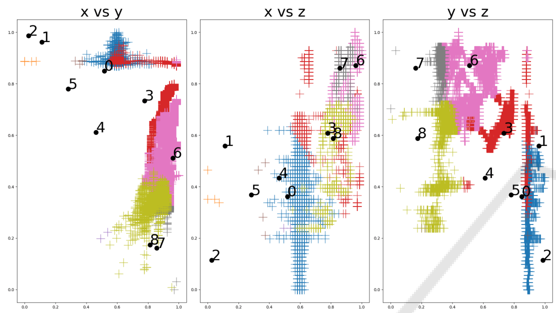


Figure 7: The Solvay's clusters projected onto any possible 2-dimension feature set.

along Y-axis, one or two along Z-axis, and another one along Y-axis anew, but shifted along X-axis.

The clustering method used is a 3×3 SOM, as depicted on Figure 6b and Figure 7; five nodes seem very large. Does this mean there are indeed 5 clusters in the data? Let's check this assumption out with the results of Table 4.

Among all the nodes, cluster #2 is empty, and #1, #4 and #5 have a poor density (they contain very few data actually). The five remaining clusters, #0, #3, #6, #7 and #8, have a small AvStd and a high density, except #7, which is compact but contains some outliers.

Indeed, on Figure 6b and Figure 7, we can see that these clusters are actually compact and acceptable, except #3, which spans across clusters #0 and #6. This cluster should be split, and its two parts should be merged with these two clusters. This observation can also be drawn from Table 4: cluster #3 has the lowest density among the four valid, *i.e.* #0, #3, #6 and #8, with a very noticeable gap, from 6290 units for the most dense to 1118 units for it – a decrease of 82%. Moreover, cluster #3 has the highest AvStd, which means that its outermost data instances are not outliers, but are real part of the cluster: that is because it spans across two clusters.

Therefore, if we couple a low density with a high AvStd, we can understand that cluster #3 has some issues, and should be split to gain in homogeneity!

Cluster #0 is the only one to have a high density and a very low AvStd, and can be trusted as representative of a local behavior of the system. Clusters #6 and #8 have a good density, but a quite high AvStd, which means they are not real outliers, but they are more likely spanning across several sub-regions of the feature space: they might be worth being split!

As a conclusion, we have applied our density metric on Industry 4.0 real data, and we have been able to identify from 1 (sure) to 3 (very likely) and perhaps 4 (low probability) local behaviors. This short example illustrates the potential of the density metric in a real situation, that is to point out issuing clusters, especially when used alongside the AvStd measure (to compensate its high sensitiveness to outliers).

Future Work. Now this metric is validated and trustful, the next step of our work would be to apply it on very wider databases related to Industry 4.0, in order to extract knowledge by using data mining approaches, such as local behavior identification. Once done, the next step is to train a MES network, whose neurons are local experts trained upon the data within the identified local behaviors, and validated by a compactness metric.

5 CONCLUSION

In this paper, we have introduced a compactness density-based measure to quantify and validate the quality of a n-dimension cluster.

This measure is computationally efficient, since it computes the cluster's mean, searches for the farthest point from it, and doubles this distance to obtain an estimate of the cluster's span. This value is then used as the radius of a n-hyper-sphere, which is built to contain all the data of the cluster, and to provide a n-

dimension boundaries estimate. Its volume is then assimilated to that of the cluster. The density measure is eventually defined as the ratio of the number of points contained within by that hyper-sphere's volume.

We then compared and validated this measure to a reference one, namely the Average Standard Deviation AvStd. We applied both on several academical datasets, before and after clustering, in order to show the relevancy and the accuracy of both metrics. We also studied the data provided by a real Industry 4.0 use-case – Solvay Opérations®'s plant.

While the AvStd showed some good results, there are several cases where it failed to identify an underlying issue within the clusters, such as an almost empty cluster or a small but real overlap of several clusters.

On the contrary, the density measure displayed good results in both identifying clustering issues and in indicating a cluster is compact and homogeneous.

Nonetheless, we also showed that the density measure is sensitive to outliers; that can be a problem for some applications. This measure is therefore not perfect, and has its drawbacks. To better understand the data, especially in a data mining context, one could use both (or more) measures, namely AvStd and our density measure, to qualify the clusters and evaluate their compactness, how representative they are, etc.

Indeed, the AvStd measure indicates if a group of data is centered around its mean, and is lowly sensitive to outliers; the density is the reverse, since it indicates if the group is compact, but is affected by outliers. A high density with a small AvStd means a very compact group. A low density with a high AvStd indicates scattered data. A high density with a high AvStd means there are few outliers, but the data are scattered nonetheless: it indicates a cluster is spanning across several classes and thus not homogeneous.

Perhaps the best way to take benefit from our metric is to use it alongside some others, and to merge their respective outputs. This trend is often true, since there is no perfect method, especially with an unsupervised Machine Learning-based approach like ours.

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REFERENCES

Boser, B., Guyon, I., and Vapnik, V. (1996). A training algorithm for optimal margin classifier. *Proceedings of the Fifth Annual ACM Workshop on Computational Learning Theory*, 5.

Broomhead, D. and Lowe, D. (1988). Radial basis functions, multi-variable functional interpolation and adaptive networks. *Royal Signals and Radar Establishment Malvern (UK)*, RSRE-MEMO-4148.

Buchanan, B. and Feigenbaum, E. (1978). Dendral and meta-dendral: Their applications dimension. *Artificial Intelligence*, 11(1):5–24. Applications to the Sciences and Medicine.

Davies, D. and Bouldin, D. (1979). A cluster separation measure. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, PAMI-1:224–227.

Dunn, J. (1974). Well-separated clusters and optimal fuzzy partitions. *Cybernetics and Systems*, 4:95–104.

Dunn, J. C. (1973). A fuzzy relative of the isodata process and its use in detecting compact well-separated clusters. *Journal of Cybernetics*, 3(3):32–57.

Jain, A. K. (2010). Data clustering: 50 years beyond k-means. *Pattern Recognition Letters*, 31(8):651–666.

Kohonen, T. (1982). Self-organized formation of topologically correct feature maps. *Biological Cybernetics*, 43(1):59–69.

Lawrence, A. E. (2001). The volume of an *n*-dimensional hypersphere. University of Loughborough.

Martinetz, T. and Schulten, K. (1991). A "neural-gas" network learns topologies. *Artificial neural networks*, 1:397–402.

Rousseeuw, P. (1987). Silhouettes: A graphical aid to the interpretation and validation of cluster analysis. *Journal of Computational and Applied Mathematics*, 20:53–65.

Rumelhart, D., Hinton, G., and Williams, R. (1986a). *Learning Internal Representations by Error Propagation*, pages 318–362. MIT Press.

Rumelhart, D., McClelland, J., and PDP Research Group, C., editors (1986b). *Parallel Distributed Processing: Explorations in the Microstructure of Cognition, Vol. 1: Foundations*. MIT Press, Cambridge, MA, USA.

Russo, C. (2020). *Knowledge design and conceptualization in autonomous robotics*. PhD thesis, Universities Paris-Est XII, France and Naples Federico II, Italy.

Rybnik, M. (2004). *Contribution to the modelling and the exploitation of hybrid multiple neural networks systems : application to intelligent processing of information*. PhD thesis, University Paris-Est XII, France.

Shan, T. and Englot, B. (2018). Lego-loam: Lightweight and ground-optimized lidar odometry and mapping on variable terrain. In *2018 IEEE/RSJ International Conference on Intelligent Robots and Systems*, pages 4758–4765.

Thiaw, L. (2008). *Identification of non linear dynamical system by neural networks and multiple models*. PhD thesis, University Paris-Est XII, France. (in French).