DISCERN: Diversity-based Selection of Centroids for k-Estimation and Rapid Non-stochastic Clustering

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Abstract. As one of the most ubiquitously applied unsupervised learning methods, clustering has also been known to have a few disadvantages. More specifically, parameters such as the number of clusters and neighborhood radius are what call the “unsupervised” nature of these algorithms into question. Moreover, the stochastic nature of a great number of these algorithms is also a considerable point of weakness. In order to address these issues, we propose DISCERN which can serve as an initialization algorithm for K-Means, finding suitable centroids that increase the performance of K-Means. Following that, the algorithm can estimate the number of clusters if need be. The algorithm does all of that, while maintaining complete robustness and returning the same results at each separate run. We ran experiments on the proposed method processing multiple datasets and the results show its undeniable superiority in terms of results, computational time and robustness when compared to the randomized K-Means and K-Means++ initialization. In addition, the superiority in estimating the number of clusters is also discussed and we prove the lower complexity when compared to methods such as the elbow and silhouette methods in estimating the number of clusters.

Keywords: Clustering, Machine Learning, K-Means initialization, Deep Clustering, Estimating the number of clusters.

1. Introduction

One of the most prominent methods in data analysis and unsupervised methods of machine learning is data clustering. This is basically a process of dividing data into separate groups, the number of which is usually the initial parameter. Nevertheless, the number of groups is usually unknown in practical cases, leaving the determination or estimation of this number open to discussion, as many have proposed measures to address this problem [2][21]. Therefore, most clustering algorithms are however, not exactly as “unsupervised” as one would imagine, as they require at least one parameter to be set prior to learning, i.e. the number of clusters. An instance of that can be a dataset of image data of people’s faces, the number of people is usually unknown, and sometimes even impossible to estimate by conventionally analyzing the data.

Multiple clustering algorithms have been introduced during the past years, each with varying input parameters. Partitioning algorithms compute specific center points or centroids for each group. Any given record can then be assigned to the nearest centroid’s corresponding cluster. K-Means [27][38][25] is one of the oldest and most commonly used partitional clustering algorithms, and has been widely used in subjects such as patent detection [24].

Methods such as K-Means require the number of clusters or “K” as the initial parameter. The algorithm then starts with K random points in the data space as centroids and then recomputes the centroids by setting them each to the mean point of the records in their cluster. Therefore, the entire algorithm operates based on an optimal estimation of this number which has been debated. Moreover, even though the power of stochastic measures is undeniable in most cases, nevertheless their lack of robustness can be troubling.

Density-based methods such as DBSCAN [12] and OPTICS [1] require two parameters in particular in order to operate, which help the algorithm detect cluster shapes and outliers. Consequently, the overall results vary depending on correctly setting these parameters.

One key parameter in clustering algorithms is the distance metric which depends entirely on the features and the data. The most frequently used metric is Euclidean distance. Nevertheless, in specific applications other distance metrics such as cosine distance (spherical clustering) will yield more desirable results.

A few instances are expressed in figure 1.

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In spherical clustering cosine similarity of data is used to cluster them. In regular clustering using Euclidean distance, any two vectors $v_1$ and $v_2$ have distance which is expressed below:

$$\text{distance}(v_1, v_2) = \|v_1\|_2^2 - 2(v_1^T v_2) + \|v_2\|_2^2.$$  (1)

As a result, more distance yields less similarity.

Cosine distance on the other hand can be expressed as

$$\cos(\theta(v_1, v_2)) = \frac{v_1^T v_2}{\|v_1\|_2\|v_2\|_2}.$$  (2)

Since the cosine function has a range of [-1,1], this scalar value can easily be mapped to the range [0,1], consequently yielding a percentage-based similarity metric. Higher cosine value equals higher similarity between vectors. Cosine similarity and spherical clustering have been applied to text mining [11] and document clustering [18][23].

Spherical clustering using cosine normalization of data and directional variance has also been applied previously to K-Means initialization [10]. Furthermore, spherical K-Means has also been used for the segmentation of pathology images [29] as well as intrusion detection [35].

In order to efficiently cluster data with no parameters, specifically the number of clusters, we propose a diversity-based approach in order to initialize K-Means appropriately by selecting the most diverse records as centroids. The limit of the number of these clusters can be recognized based on their diversity as well. After these initial records are selected, the algorithm passes them to K-Means which selects the final coordinates for each centroid, in order to improve future predictability. The similarity metric is in the form of cosine similarity which is mapped to the range of [0,1]. As this method does not rely on any random values, it is completely robust, yielding exactly the same results at each separate run.

2. Related Work

Many methods have been introduced as initializers to K-Means, which usually select the initial cluster coordinates rather than setting them to random values in order to address the unreliable stochastic nature of K-Means. A good and very commonly practiced example is K-Means++ [4] which was introduced in order to precompute centroids as to increase performance. Despite being over a decade old, K-Means++ is still considered one of the most prominent partitional clustering methods, as it has been applied in many cases such as recommendation systems [6] and image processing [37]. Moreover, improvements to this measure have also been proposed recently [50][51]. This extension to K-Means nevertheless also relies on the number of clusters given as input, on top of being also stochastic in nature.

Furthermore, methods such as the elbow method [42] and silhouette method [34] have been employed to estimate an optimal number of clusters. These measures require sequential runs of algorithms such as K-Means in order to evaluate each run and select the most appropriate one. Consequently, these metrics are time-consuming and impractical, as each run is costly. Another point of weakness in these methods, which will be further discussed in detail is that their results, which are contingent on appropriate convergence of K-Means at each run.
X-Means [32] has also been used in estimating an optimal number of clusters as it runs K-Means on each cluster’s records separately, and stops when a stopping criterion is met. Zhang et al. [52] proposed a deep constrained clustering method which uses constrained variations of clustering methods such as K-Means and used deep learning in order to map images to a latent space suitable for clustering. In our experiments, we also employed a deep network in order to compress facial image data into a latent 128-dimensional space which is very suitable for the clustering of different faces. Other methods such as I-nice (Identifying the number of clusters and initial cluster centers) [28] were also proposed as metrics that estimate both the correct number of clusters as well as the initial centroids for K-Means. I-nice in particular uses a hill peak observation measure, which also relies on a stochastic initialization of observations and therefore the results may vary. As stated, many clustering algorithms exist which have eliminated one or multiple issues with the standard K-Means algorithm specifically, as it can be argued that K-Means is a very suitable clustering method for many cases when it is provided with a near-optimal or optimal set of initial clusters. As some algorithms estimate an optimal number of clusters, some more optimal cluster centroids, and most usually depend on random numbers, we sought to develop an algorithm which can achieve both without having to rely on random numbers, and doing it more efficiently with less complexity.

3. Proposed Approach

As previously stated, K-Means is a clustering method which depends entirely on the initial set of cluster centers, as well as the number of clusters. In this paper, we propose DISCERN (DisCriminate REmoval of Clusters by sElecting) as a centroid initialization measure, somewhat similar to K-Means++, which selects a number of records from the original dataset as the initial centroids and helps increase the probability of K-Means reaching better results without relying on stochastic measures. Moreover, this approach can estimate a suitable number of clusters based on the diversity of the records it chooses.

The idea behind this approach is similar to its name, which is to discriminate between records and select the most diverse records possible, and later choosing them as centroids, and then passing them to K-Means where each cluster centroid is set to the mean coordinates of its corresponding cluster’s members.

Assume we are given the dataset \( X \) (\( n \times d \), \( n \) is the number of records, \( d \) is the number of features), and \( X_i \) is the i-th row and record of \( X \) and its membership to a specific cluster (assuming there are \( K \) clusters) is defined in Eq. (3).

\[
X_i \in \text{Cluster}_l, \quad (3)
\]

\[
l = \arg\min_{1 \leq j \leq K} \left( \text{distance}(X_i, C_j) \right), \quad \text{when using Euclidean distance}
\]

\[
l = \arg\max_{1 \leq j \leq K} \left( \text{similarity}(X_i, C_j) \right), \quad \text{when using cosine distance}.
\]

\( C_l \) is the centroid (cluster center) of \( \text{Cluster}_l \) and \( |\text{Cluster}_l| \) is the number of records in \( \text{Cluster}_l \).

The number of clusters, \( K \), is assumed to be unknown, which as mentioned the algorithm will be able to estimate. Nevertheless, the number of clusters can be confined to a specific value.

3.1. Similarity precomputation

DISCERN operates based on record-by-record similarity and starts by precomputing a similarity matrix, \( S = [s_{ij}] \in \mathbb{R}^{n \times n} \):

\[
s_{ij} = \text{similarity}(X_i, X_j), \quad i, j \in \{1, 2, ..., n\}. \quad (4)
\]

This matrix represents the similarity or proximity of each pair of records. It is self-evident that this matrix is symmetric and that \( \text{tr}(S) = n \) since the main diagonal consists of ones (full similarity between a record and itself). This matrix is computed using cosine similarity with a complexity of \( O(dn^2) \), and requires storing the values, which yields a space complexity of \( O(n^2) \). Nevertheless, the actual computation time is reduced by precomputing each record’s norm value, as well as storing the matrix in a symmetrical data structure, requiring only about half of the values to be actually stored. In order to make the actual computations less time-consuming and more uniform, each record of the dataset (row of \( X \)) is divided by its norm value instantly after being computed. As a result, a simple dot product of any two vectors will yield their cosine similarity:

\[
X_i' = \frac{X_i}{\|X_i\|_2}, \quad i = 1, 2, ..., n, \quad (5)
\]

\[
X_i'^T X_j' = \frac{X_i^T X_j}{\|X_i\|_2 \times \|X_j\|_2}. \quad (6)
\]
3.2. DISCERN and the Diversity-Based Selection

The main idea behind DISCERN, as previously discussed, is finding the most diverse records possible and selecting them as the initial centroids. For instance, in a human face dataset, consisting of multiple images of each person, the algorithm attempts to find one image of each person’s face while avoiding the selection of a specific person more than once. As a result, with each person’s face being selected as the centroid, it is highly expected of K-Means to cluster each person’s images with each other, resulting in a distinction between different people. Such a measure is designed to be discerning in the selection of the aforementioned centroids, and would help estimate a near-optimal number of clusters in the meantime.

In order to make this achievement, firstly we choose the two most diverse records possible, which can be akin to finding the most distanced records. This is mathematically equivalent to finding the minimum similarity in the matrix $S$ and selecting the corresponding records. Therefore:

$$ (r_1, r_2) = \arg\min_{(i,j)} (s_{ij}), $$

$$ (i,j) \in \{1,2,...,n\} \times \{1,2,...,n\}. $$

(7)

Since the minimum number of clusters in any given problem is 2, these two records $X_{r_1}$ and $X_{r_2}$ are the first of $K$ cluster centroids, where $K$ is usually unknown and is yet to be estimated.

Now we start with an iterative approach, the first two steps of which are already completed. This approach selects one record per iteration which is expected to be the most different record from the ones which are already selected. In other words, $X_{r_3}$ will be one of the records from $X$, except for $X_{r_1}$ and $X_{r_2}$, which has the least similarity to both. In order to achieve this, we start by creating a submatrix of $S$, named $S_3 \in \mathbb{R}^{2 \times n}$ at step 3:

$$ (S_3)_{ij} := s_{ij}, \quad i \in \{r_1, r_2\}, \quad j \in \{1,2,...,n\} \setminus \{r_1, r_2\}, $$

$$ (S_3)_{ij} := \delta_{ij}, \quad i,j \in \{r_1, r_2\}. $$

(8)

The matrix $S_3$ basically shows the similarity between the selected records $X_{r_1}$ and $X_{r_2}$ to the others. Since the idea is to select the record with the least similarity from the two, one idea for this multi-objective optimization problem may be considering each similarity between each record and the selected records as an objective. However, this is proven to be not suitable, as the results will not necessarily yield diverse records. For instance, a record may be different drastically from all of the selected records, but however very similar to only one. Since in this case the objectives consist of equal weights, the lone high similarity may go unnoticed.

In order to solve this problem, we introduce the Estimated Membership Vector at step $\ell$, $p_\ell$, $\ell \geq 3$, which computes a diversity factor for each record compared to the selected ones and thus helps the selection of truly diverse records. This vector therefore depends on the selected and not selected records and their similarities. Therefore, the $p_3$ vector at step three uses the values of $S_3$ as input and is computed using the Hadamard product of some vectors.

Hadamard product of two matrices $H$ and $J$ of the same size is defined as:

$$ H \odot J := [H_{ij} \ast J_{ij}], $$

where $H = [H_{ij}]$ and $J = [J_{ij}]$.

(9)

Now, $p_3$ vector can be defined as:

$$ p_3 := (M_3) \odot (M_3) \odot m_3 \odot (M_3 - m_3), $$

where

$$ M_3 := [\max((S_3)_1), \max((S_3)_2), ..., \max((S_3)_n)], $$

$$ m_3 := [\min((S_3)_1), \min((S_3)_2), ..., \min((S_3)_n)], $$

and $(S_3)_j$ is the $j$-th column of $S_3$.

(10)

Following that, $r_3$ is simply selected by finding the record with the minimum value of $p_3$ vector, which resembles a membership rate of the record and the selected records. Therefore, the record with the least membership is the most diverse:

$$ r_3 = \arg\min (p_3). $$

(11)
Now, we assume that the method has proceeded up to step ℓ-1, and step ℓ requires $S_\ell \in \mathbb{R}^{(\ell-1) \times n}$ to be computed:

$$(S_\ell)_{ij} := s_{ij}, \quad i \in \{r_1, r_2, ..., r_{\ell-1}\}, \quad j \in \{1, 2, ..., n\} \setminus \{r_1, r_2, ..., r_{\ell-1}\},$$

and

$$(S_\ell)_{ij} := \delta_{ij}, \quad i, j \in \{r_1, r_2, ..., r_{\ell-1}\}. \quad (12)$$

Following that, $p_\ell$ is computed:

$$p_\ell := (M_\ell) \circ (M_\ell) \circ m_\ell \circ (M_\ell - m_\ell),$$

where

$$M_\ell := [\max((S_\ell)_1), \max((S_\ell)_2), ..., \max((S_\ell)_n)],$$

$$m_\ell := [\min((S_\ell)_1), \min((S_\ell)_2), ..., \min((S_\ell)_n)],$$

and $(S_\ell)_j$ is the $j$-th column of $S_\ell$. \quad (13)

Afterwards, $r_\ell$ is selected:

$$r_\ell := \text{argmin}(p_\ell), \quad (14)$$

When the number of clusters is unknown, we define the **Membership Rate Function**, $R$:

$$R : \{1, 2, ..., n\} \rightarrow [0, 1], \quad (15)$$

where

$$R(1) = R(2) = 0, \quad R(\ell) = \min(p_\ell), \quad \ell = 3, 4, ..., n.$$ 

By minimizing the vector $p_\ell$, the algorithm is set to minimize the maximum and minimum similarities of any given record with the selected clusters, as well as the range of similarities.

### 3.3. DISCERN and cluster number estimation

![Figure 2](image-url)

**Figure 2:** The function $R$ and the target number of clusters (red point) of the dataset a) CPMP, b) Wine and c) FEI Face Database

As we introduced the vector $p_\ell$ in Eq. (13) in order to minimize possible similarities to any cluster centroids, we also adjusted this formula in order to be able to notice the change in the function $R$ in Eq. (15) which points to an optimal number of clusters. Instances of this function on three real datasets [43][15][41] are presented in Figure 2.

It is self-evident that the range of an optimal $K$ is within a concave curve. As a result, we used the definition of curvature in order to detect this point. The signed curvature of $R$ is defined as:

$$\kappa(R) = \frac{R''}{(1 + R'^2)^{3/2}}, \quad (16)$$
The derivative and second derivatives of R were calculated using central finite differences. The results showed that an optimum \( K \) is usually the minimum value of curvature (\( \kappa(R) \)). In the following, the graphs of \( \kappa(R) \) on the three instances in Figure 2 are expressed in Figure 3.

![The curvature of R, the target number of clusters (red points) and the estimated number of clusters (if different from red, green points).](image)

The red points in these graphs represent the target number of clusters, which is the same as the minimum value of the signed curvature of R in figure 3.a and 3.b. In figure 3.c, the minimum of curvature of R is the green point which is different from the exact target (the target being 199 clusters and the minimum of \( \kappa(R) \) being at 201). It goes without saying that finding the minimum requires finding the values of R for all possible records, except for \( X_{r_1} \) and \( X_{r_2} \). Nevertheless, we can set one constraint that can further decrease computation by detecting convergence. Convergence can be defined for certain cases in which the function R converges almost immediately after it reaches the optimum curve. An instance is presented in figure 2.a. This convergence can be easily detected by using finite differences, which are already being computed for the computation of curvature later on, and comparing them to the finite differences seen before. As previously mentioned, the minimum value of \( \kappa(R) \) points to an optimal number of clusters, which is selected by the proposed approach. The reason for this selection of the optimum is that drastic increases in R can be interpreted as the selection of records that belong to clusters whose centroids have not already been selected. In other words, a significant increase in R shows the significance in diversity. When diversity starts to dissipate, the function starts to converge. In brief, the optimal number of clusters is estimated as:

\[
K = \text{argmin}(\kappa(R)).
\]  

The resulting centroids that DISCERN computes are:

\[
\text{Centroids} = \{X_{r_1}, X_{r_2}, \ldots, X_{r_K}\}, \quad K \geq 2,
\]  

which are the initial centroids that can guide K-Means to converge to the appropriate results. Meanwhile, it has estimated an optimal number of clusters, which is expressed in Eq. (17).

Another notable feature of DISCERN is that since it isn’t stochastic, it yields the same results each time, regardless of the arrangement of the data, therefore maintaining a deviation of zero in its results, unlike K-Means and K-Means++. As a result, this method doesn’t require multiple runs in order to find an optimal clustering of the data. We also present the worst-case complexity order of DISCERN below. Since the worst case is the case in which early no stopping takes place, that would result in the algorithm calculating the function R for all \( n \) records.

| Algorithm 1. DISCERN without early stopping |
|---------------------------------------------|
| **Input:** The set of data \( X_{n \times d} \) |
| **Output:** \( K, \text{Centroids} \) |
| Compute(\( S_{n \times n} \)) \( (r_1, r_2) = \text{argmin}(S) \) |
| R(1) = R(2) = 0 \( O(dn^2) \) |
| for \( \ell = 3:n \) \( O(n) \) |
| Create \( S_\ell \in M_{\ell-1 \times n} \), according to Eq. (12) \( O(n\ell) \) |
| \( (M_\ell, m_\ell) = \max, \min(S_\ell) \), according to Eq. (13) \( O(n\ell) \) |
| \( p_\ell := (M_\ell) \circ (M_\ell) \ast m_\ell \ast (M_\ell \ast m_\ell) \) \( O(n\ell) \) |
| \( R(\ell), r_\ell = (\min(p_\ell), \arg\min(p_\ell)) \) \( O(n) \) |
| Compute(\( \kappa(R) \)) according to Eq. (16) \( O(n) \) |
| \( K = \text{argmin}(\kappa(R)) \) \( O(n) \) |
| Centroids = \( \{X_{r_1}, X_{r_2}, \ldots, X_{r_K}\} \) \( O(n) \) |

This would yield that:

\[
\text{DISCERN} \in O(n^3 + dn^2).
\]  

(19)
However, in the case that \( K \) is not required to be estimated, the loop would run for exactly \( K \) iterations and the resulting complexity can be expressed as:

\[
DISCERN(K) \in O(K^2 n + dn^2) .
\]  

What is notable about the proposed method’s difference between other initializations such as K-Means++ is that the former essentially maps the \( d \)-dimensional data points to a one-dimensional similarity space which when precomputed has less complexity (\( O(K^2 n) \) instead of \( O(dK^2 n) \)). Nevertheless, this precomputation itself, as discussed previously, has a complexity of \( O(dn^2) \) which in the case of a small \( d \) and large \( n \) is computationally more complex than the latter. This comparison of complexity will be further discussed in the next section.

4. Experiment Details

In this section, we present the details of the experiments we conducted in order to compare each aspect of the proposed approach to other known methods. We firstly compared other methods that estimate the number of clusters that are currently used in terms of the estimation and the computational complexity and time. The methods we compared are: silhouette method which uses the Average Silhouette Coefficient (ASC) [34] and the elbow method using the Calinski-Harabaz Index (CH) [7], the elbow method using sum of errors, and X-Means [32]. Average Silhouette Coefficient (ASC) was defined as the mean of the silhouette score for each record in a clustering, which is calculated using inter-cluster and outer-cluster distances. In order to do that, assuming that:

\[
X_i \in \text{Cluster}_j \text{ and } |\text{Cluster}_j| \geq 2,
\]

inter-cluster distances of \( X_i \) is defined as:

\[
a(X_i) := \frac{1}{|\text{Cluster}_j| - 1} \sum_{X_j \in \text{Cluster}_j, j \neq i} \text{distance}(X_i, X_j),
\]  

and outer-cluster distances of \( X_i \) is defined as:

\[
b(X_i) := \min_{t \in \{1,2,\ldots,K\} \setminus j} \frac{1}{|\text{Cluster}_t|} \sum_{X_j \in \text{Cluster}_t} \text{distance}(X_i, X_j).
\]  

Finally, the silhouette of \( X_i \) is defined:

\[
s(X_i) := \begin{cases} 
b(X_i) - a(X_i) & \text{if } |\text{Cluster}_j| > 1, \\
\max\{a(X_i), b(X_i)\} & \text{if } |\text{Cluster}_j| = 1. 
\end{cases}
\]  

It is also self-evident that: \( \forall x, s(x) \in [-1,1] \). In the silhouette method, a range of cluster numbers is defined (usually starting at a minimum of 2) and each integer within is given to a clustering algorithm (in our experiments, K-Means and K-Means++), and then the clustering is evaluated using the ASC score. Finally, the clustering with the maximum ASC score is selected, since the higher ASC represents better clustering, and therefore its number of clusters is estimated as the optimal \( K \).

Calinski-Harabaz Index (CH) on the other hand operates by calculating the overall within-cluster variance (\( W \)):

\[
W := \sum_{i=1}^{K} \sum_{X \notin \text{Cluster}_i} \text{distance}(C_i, X),
\]  

and the overall between-cluster variance:

\[
B := \sum_{i=1}^{K} |\text{Cluster}_i| \text{distance}(C_i, \bar{X}),
\]  

where \( \bar{X} \) is the center (mean) of all records (rows) in \( X \).
Finally, CH is defined as:

$$CH = \frac{B}{W} \times \frac{n - K}{K - 1}.$$  \hspace{1cm} (26)

The Calinski-Harabaz method is similar to the silhouette method as it also selects the clustering with the highest CH score and therefore its number of clusters as the optimal K.

The elbow method on the other hand uses the overall within-cluster variance, expressed in Eq. (24), and attempts to find the point from which this variance converges. In other words, the first point from which the results do not improve much is selected as the optimal K. X-Means [32] explores the space of cluster locations by running K-Means on each cluster’s records separately, and attempts to optimize the number of clusters using the Bayesian Information Criterion (BIC) or other similar measures.

After estimating an optimal number of clusters using each of the aforementioned methods, and selecting the top methods, we compared clustering results on each set of estimate cluster numbers. We compared both K-Means and K-Means++ to the proposed method. The metrics used for comparison are the ASC, Davies-Bouldin Index (DBI) [8], purity index (classification accuracy), Adjusted Rand Index (ARI) [22] and Normalized Mutual Information (NMI).

DBI is an internal evaluation metric for clustering, like the ASC, as both analyze the clusters without any supervision. On the other hand, DBI yields a lower score for better clustering, transforming the best possible clustering to a score of zero. In order to measure DBI, firstly, each cluster’s inter-cluster distance is measured:

$$T_i := \frac{1}{|Cluster_i|} \sum_{j \in cluster_i} distance(C_i, X_j).$$ \hspace{1cm} (27)

Following that, is defined to measure the quality of clustering:

$$Q_{ij} := \frac{T_i + T_j}{distance(C_i, C_j)}.$$ \hspace{1cm} (28)

Finally, DBI is measured simply using the following equation:

$$DBI := \frac{1}{K} \sum_{i=1}^{K} \max_{j \neq i} Q_{ij}.$$ \hspace{1cm} (29)

Purity, on the other hand is an external evaluation metric, which can only be applied in the case of using classification datasets in which the target is known. It is measured using Eq. (30).

$$Purity := \frac{1}{n} \sum_{i=1}^{K} \max_{j} |Cluster_i \cap Target_j|,$$ \hspace{1cm} (30)

where Target_j is the set of the records (rows) of X in Class j.

This metric can serve as an accuracy index for clustering algorithms. ARI is another external metric for cluster analysis, which is expressed in Eq. (31).

ARI is measured using:

$$ARI := \frac{\sum_{i<j}^{n_{ij}} \left( \frac{n_{ij}}{2} \right) - \left[ \frac{\sum_i^{(a_i)} \sum_j^{(b_j)}}{n_2} \right]}{\frac{1}{2} \left[ \sum_i^{(a_i)} + \sum_j^{(b_j)} \right] - \left[ \frac{\sum_i^{(a_i)} \sum_j^{(b_j)}}{n_2} \right]}$$ \hspace{1cm} (31)

in which

$$n_{ij} = |Cluster_i \cap Target_j|.$$ 

$$a_i = \sum_{j=1}^{T} n_{ij}, T is the number of classes$$

$$b_j = \sum_{i=1}^{K} n_{ij}.$$
NMI is also an external metric, and can be best described as a normalization of the Mutual Information index to a scale of [0,1] in which 1 yields the best possible clustering, with regard to the target classes.

We also analyzed the robustness of the proposed approach compared to that of others based on the standard deviation of the number of clusters estimated by other methods. We will also discuss possible downsides of the proposed approach on specific datasets.

The datasets we used to evaluate and compare the methods can be divided into two groups: multivariate datasets and facial image data. The multivariate datasets were retrieved from OpenML [45] and UCI Machine Learning Repository [9], which are summarized in Table 1.

### Table 1

**Multivariate Datasets and Their Characteristics**

| Dataset             | Abbreviation | Features | Samples | Classes |
|---------------------|--------------|----------|---------|---------|
| CPMP [43]           | CPMP         | 22       | 527     | 4       |
| Wine [15]           | WINE         | 13       | 178     | 3       |
| Iris [14]           | IRIS         | 4        | 150     | 3       |
| Banana [5]          | BNN          | 2        | 5300    | 2       |
| Wap [47] *           | WAP          | 8460     | 1560    | 20      |

* We used Principle Component Analysis (PCA) to reduce WAP and mapped its original set to \( \mathbb{R}^{36} \) prior to running the tests as it was then better suited for clustering.

The facial images were retrieved from multiple sources and are discussed in Table 2. For processing facial images, we used a convolutional neural network trained with an online triplet selection method and optimized with triplet loss proposed by Schroff et al. named FaceNet [36]. This network maps each image of a person’s face into the 128-dimensional latent space so that each person’s different images are mapped to two very close points. We used the pre-trained weights of the aforementioned network from a GitHub repository [39] which was trained on the Microsoft’s “MS-Celeb-1M” dataset [19].

### Table 2

**Facial Images Datasets and Their Characteristics**

| Dataset            | Abbreviation | People | Images |
|--------------------|--------------|--------|--------|
| Yale Face Database [49] | YALE        | 15     | 165    |
| MIT-CBCL [13]      | MIT          | 10     | 59     |
| GeorgiaTech Face Database [17] | GA       | 50     | 750    |
| AT&T Faces [40]    | ATT          | 40     | 400    |
| Caltech Faces [48] | CA           | 31     | 450    |
| FEI Face Database [41] | FEI        | 199    | 400    |

In the experiments, facial data are clustered using spherical clustering (cosine similarity), as they go through FaceNet [36] which according to the paper constraints the resulting mappings to existing on the 128-dimensional hypersphere. Iris and Wap were also clustered using cosine similarity, while the rest were clustered using Euclidean distance.

All experimental tests were implemented using Python 3, and were conducted on a Windows 10 computer with a 64-bit Intel Core-i7 quad-core processor clocked at 2.6 GHz with 16 GB of memory. Experiments including stochastic measures were conducted multiple times and their results were averaged. The Python libraries used in conducting the tests are: Numpy [46], Scikit-Learn [31], and PyClustering [30].

### 5. Analysis of DISCERN in estimating K

In this section, we estimated an optimum K for each dataset using different methods. The silhouette and Calinski-Harabaz methods were used with both randomized K-Means and K-Means++ as they performed differently. The elbow method and X-Means were implemented using K-Means++ only. It should be noted that all of these methods require a minimum and maximum number of clusters to be set, and each were set to a specific maximum number based on some previous knowledge of the datasets in order to reduce computational time, but this is rarely the case in real-life examples. In our charts and tables, we’ll refer to the silhouette and Calinski-Harabaz methods which used K-Means++ as \( K++ \) Silhouette and \( K++ \) Calinski-Harabaz. Even though these algorithms explore a much smaller set of numbers for an optimum K when compared to the proposed approach, the approach shows considerable significance both in terms of performance in estimation of K as well as computational time. The estimated K and the real number of classes are discussed in Table 3. It should be noted that the other methods estimate different values for K every time as they are stochastic in nature. Therefore, each method was evaluated multiple times and the results were averaged, and rounded to the nearest integer.
TABLE 3

ESTIMATED K COMPARISON BETWEEN THE PROPOSED APPROACH AND OTHER MEASURES.

| Dataset | K | Silhouette | Calinski-Harabaz | X-Means | Elbow | DISCERN |
|---------|---|------------|------------------|---------|-------|---------|
|         |   | Random     | K-Means++        |         |       |         |
| Yale    | 15| 13         | 16               | 17      | 17    | 15      |
| MIT     | 10| 13         | 13               | 13      | 17    | 14      |
| GA      | 50| 59         | 56               | 2       | 9     | 52      |
| ATT     | 40| 50         | 44               | 52      | 49    | 4       |
| CA      | 31| 27         | 29               | 36      | 32    | 25      |
| FEI     | 199| 221       | 216              | 2       | 2     | 2       |
| CPMP    | 4 | 2          | 2                | 2       | 2     | 10      |
| WINE    | 3 | 2          | 2                | 7       | 9     | 10      |
| IRIS    | 3 | 2          | 2                | 2       | 2     | 6       |
| BNN     | 4 | 2          | 2                | 6       | 7     | 4       |
| WAP     | 20| 27         | 28               | 2       | 2     | 40      |

The results from the table above were used in a Friedman test [16] in order to rank the algorithms. The resulting rankings are presented in Figure 4.

As it can be seen, the proposed approach exceeds the rest in this rank-based test. Furthermore, the p-value comparison of these methods to the proposed approach are presented in Table 4.

TABLE 4

P-VALUE COMPARISON OF THE METHODS TO DISCERN

| Algorithm          | p-value  |
|--------------------|----------|
| Silhouette         | 0.023212 |
| K-Means++          | 0.084146 |
| Calinski-Harabaz   | 0.000097 |
| X-Means            | 0.000119 |
| Elbow              | 0.182744 |

The values that are bolded are those below the limit of 0.05 which yields that the proposed approach shows significant improvement over these methods (Silhouette method using random-based K-Means, Calinski-Harabaz Method and X-Means). However, the significance of the improvement over the Elbow method and Silhouette method using K-Means++ cannot be inferred with certainty. Therefore, we compared the performance of these two methods to the proposed method.

In terms of complexity order, both Silhouette and Elbow methods use K-Means++ and in a completely unsupervised manner, would have to cluster data by incrementing the number of clusters from 2 to n. K-Means++ initialization has a complexity order of $O(nK^2d)$:

Algorithm 2. K-Means++ Initialization

Input: The set of data $X_{n \times d}$, The number of clusters $K$

Output: Centroids

Select $C_i$ randomly

for $i = 2:K$

Compute distance($X$, $\{C_1, \ldots, C_{i-1}\}$)

Compute probability proportional to $D(x)^2$

Select $C_i$ based on probability proportional to $D(x)^2$

Centroids = $\{X_{C_1}, X_{C_2}, \ldots, X_{C_K}\}$

$O(nKd)$
Furthermore, a single K-Means run using Lloyd’s algorithm [26] afterwards has an average complexity order of $O(nKdT)$ [20] in which $T$ is the number of iterations it goes through prior to convergence. As a result, both the silhouette and elbow methods have the same complexity which is expressed in Eq. (32) and Eq. (33).

$$K - ESTIMATE \in O \left( \sum_{i=2}^{n} n_i^2d + n_i dT_i \right), \quad (32)$$

$$= O \left( nd \sum_{i=2}^{n} i^2 + iT_i \right)$$

$$= O \left( nd \sum_{i=2}^{n} i^2 + nd \sum_{i=2}^{n} iT_i \right)$$

$$= O \left( nd \frac{(n)(n+1)(2n+1)}{6} + nd \sum_{i=2}^{n} iT_i \right)$$

$$= O \left( ndn^3 + nd \sum_{i=2}^{n} iT_i \right)$$

$$= O \left( n^4d + nd \sum_{i=2}^{n} iT_i \right).$$

Assuming that every $T_i$ has a limit of $\bar{T}$:

$$= O \left( n^4d + nd \bar{T} \sum_{i=2}^{n} i \right)$$

$$= O \left( n^4d + nd \bar{T} \frac{n(n+1)}{2} \right),$$

which yields that:

$$K - ESTIMATE \in O \left( dn^4 + dn^3\bar{T} \right). \quad (33)$$

As previously mentioned, the proposed approach has a worst-case complexity of $O(n^3 + dn^2)$ in the case that $K$ is unknown, which when added to K-Means becomes $O\left(n^3 + dn^2 + dn^2\bar{T}\right)$ which can be simplified as $O\left(n^3 + dn^2\bar{T}\right)$.

It is also clear that:

$$d \in \mathbb{N} \text{ and } n \in \mathbb{N} \setminus \{1\}$$

$$dn^4 > n^3,$$

$$dn^3 > dn^2,$$

and since $\bar{T} \in \mathbb{N}$, we can conclude that:

$$dn^3\bar{T} > dn^2\bar{T}. \quad (34)$$

Therefore, we can infer from Eq. (34) that:

$$\left( dn^4 + dn^3\bar{T} \right) > \left( n^3 + dn^2\bar{T} \right). \quad (35)$$

Eq. (35) shows that the complexity of elbow and silhouette which run consecutive K-Means++ is higher than that of the proposed method, therefore making the latter superior in terms of time.
The comparison between the average computational times of the methods also point toward the same conclusion, which can be observed in Table 5.

| Dataset | K++ Silhouette | Elbow | DISCERN |
|---------|----------------|-------|---------|
| YALE    | 156.231        | 160.667 | 0.34    |
| MIT     | 43.133         | 49.308 | 0.066   |
| GA      | 15994.29       | 18778.89 | 6.367   |
| ATT     | 6515.039       | 8169.401 | 2.082   |
| CA      | 8305.744       | 9975.593 | 4.325   |
| FEI     | ***            | ***    | 7.158   |
| CPMP    | 5.401          | 27.812 | 0.814   |
| WINE    | 2.418          | 6.288  | 0.094   |
| IRIS    | 13.89          | 11.688 | 0.078   |
| BNN     | 55.921         | 537.933 | 42.629  |
| WAP     | 7592.106       | 5884.55 | 10.585  |

*The numbers are rounded to 3 decimal points. The cells marked with *** are greater than 30,000 seconds.*

The two methods took significantly more time as the number of clusters increased, and therefore exceeded the time limit in the case of the dataset FEI. Since the timing of this particular dataset containing almost 200 classes (which is therefore the target $K$) greatly affects the standard statistical tests, we removed this particular dataset from the results prior to running a Friedman Aligned test. The rankings are presented in Figure 5.

![Figure 5](image-url)

*Figure 5. Friedman aligned ranking test on the 2 chosen methods and the proposed method*

The p-values for silhouette method vs DISCERN and elbow method vs DISCERN are 0.001372 and 0.000074 respectively. The p-values are both under the value of 0.05 which yield significant improvement of the proposed method in computational time over the other 2 methods with great certainty. In the next section, we will compare the results of K-Means, K-Means++ and the proposed approach with the number of clusters set to the estimated $K$ values of the proposed method and the two methods mentioned above; Silhouette and elbow methods.

6. Analysis of DISCERN as a centroid initialization method for K-Means

In this section, we compared the results of K-Means clustering on the datasets using 3 initializations: Randomized K-Means, K-Means++ and DISCERN. We tried 4 set of clusters numbers:

- True $K$: The number of classes
- DISCERN $K$: estimated by the proposed method
- Elbow $K$: estimated by the elbow method
- Silhouette $K$: estimated by the silhouette method using K-Means++ (K++ Silhouette)

These $K$ values are presented in Table 6.
6.1. Clustering using True K

When clustering using True K, we added “True Centers” [28] to our tables which shows the results of setting the mean of the records of different classes as centroids prior to running K-Means. This helps understand how well a classification dataset can be clustered, meaning how well the feature space separates the records of a specific class from others. This can also serve as a grasp on the maximum expectation of a clustering algorithm. The results are provided in Table 7 and Table 8. The resulting numbers are rounded to 3 decimal points.

Table 6
DIFFERENT SETS THAT WERE SET AS THE NUMBER OF CLUSTERS WHEN COMPARING CLUSTERING METHODS

| Dataset | True K | Silhouette K | Elbow K | DISCERN K |
|---------|--------|-------------|---------|-----------|
| YALE    | 15     | 16          | 14      | 15        |
| MIT     | 10     | 13          | 11      | 12        |
| GA      | 50     | 56          | 32      | 54        |
| ATT     | 40     | 44          | 44      | 40        |
| CA      | 31     | 29          | 34      | 41        |
| FEI     | 199    | 216         | 69      | 201       |
| CPMP    | 4      | 2           | 4       | 4         |
| WINE    | 3      | 2           | 4       | 3         |
| IRIS    | 3      | 2           | 4       | 3         |
| BNN     | 2      | 6           | 5       | 2         |
| WAP     | 20     | 28          | 17      | 18        |

Table 7
INTERNAL METRICS COMPARED WHEN USING TRUE K

| Dataset | DISCERN | True Centers | K-Means | K-Means++ |
|---------|---------|--------------|---------|-----------|
| YALE    | 0.544   | 0.723        | 1.168   | 0.795     |
| MIT     | 0.493   | 0.653        | 1.167   | 0.817     |
| GA      | 0.494   | 0.625        | 1.33    | 0.619     |
| ATT     | 0.569   | 0.771        | 1.173   | 0.817     |
| CA      | 0.595   | 0.83         | 1.251   | 0.619     |
| FEI     | 0.47    | 0.796        | 0.845   | 0.53      |
| CPMP    | 0.57    | 0.623        | 0.988   | 0.919     |
| WINE    | 0.728   | 0.732        | 0.539   | 0.534     |
| IRIS    | 0.752   | 0.748        | 0.842   | 0.768     |
| BNN     | 0.553   | 0.553        | 1.046   | 1.046     |
| WAP     | 0.316   | 0.333        | 1.703   | 1.465     |

Table 8
EXTERNAL METRICS COMPARED WHEN USING TRUE K

| Dataset | DISCERN | True Centers | K-Means | K-Means++ |
|---------|---------|--------------|---------|-----------|
| YALE    | 0.544   | 0.723        | 1.168   | 0.795     |
| MIT     | 0.493   | 0.653        | 1.167   | 0.817     |
| GA      | 0.494   | 0.625        | 1.33    | 0.619     |
| ATT     | 0.569   | 0.771        | 1.173   | 0.817     |
| CA      | 0.595   | 0.83         | 1.251   | 0.619     |
| FEI     | 0.47    | 0.796        | 0.845   | 0.53      |
| CPMP    | 0.57    | 0.623        | 0.988   | 0.919     |
| WINE    | 0.728   | 0.732        | 0.539   | 0.534     |
| IRIS    | 0.752   | 0.748        | 0.842   | 0.768     |
| BNN     | 0.553   | 0.553        | 1.046   | 1.046     |
| WAP     | 0.316   | 0.333        | 1.703   | 1.465     |
We also conducted Quade statistical analysis [33] on these results. Figure 6 presents the rankings of the Quade test, and Table 9 presents the p-value results.

![Figure 6. Quade rankings of the methods using True K](image)

**Table 9**

| Method       | ASC  | DBI  | Purity | ARI  | NMI  |
|--------------|------|------|--------|------|------|
| K-Means      | 0.004| 0.005| 0.002  | 0.002| 0.003|
| K-Means++    | 0.070| 0.077| 0.024  | 0.009| 0.012|
| DISCERN      | 0.647| 0.858| 0.499  | 0.350| 0.591|

As expected, the top ranked method is True Centers. Nevertheless, True Centers is a target, not an algorithm, which is why we used it to compare p-values. The p-values indicate no significant improvement when comparing DISCERN’s results to that of True Centers, which is not necessarily true when it comes to K-Means and K-Means++. In fact, the p-values show with good certainty that True Centers had significant improvement over the two, but not over DISCERN.

### 6.2. Clustering using DISCERN K

The results are provided in Table 10 and Table 11. The resulting numbers are rounded to 3 decimal points.

| Dataset | ASC  | DBI  | Purity | ARI  | NMI  |
|---------|------|------|--------|------|------|
| YALE    | 0.534| 0.599| 0.723  |      |      |
| MIT     | 0.504| 0.54  | 0.667  |      |      |
| GA      | 0.492| 0.521| 0.607  |      |      |
| ATT     | 0.572| 0.622| 0.751  |      |      |
| CA      | 0.515| 0.588| 0.775  |      |      |
| FEI     | 0.469| 0.609| 0.793  |      |      |
| CPMP    | 0.573| 0.584| 0.55   |      |      |
| WINE    | 0.73  | 0.73  | 0.732  |      |      |
| IRIS    | 0.764| 0.756| 0.748  |      |      |
| BNN     | 0.553| 0.553| 0.553  |      |      |
| WAP     | 0.313| 0.299| 0.319  |      |      |

**Table 10**

**Internal metrics compared when using DISCERN K**
### Table 11

**EXTERNAL METRICS COMPARED WHEN USING DISCERN K**

| Dataset | Purity | ARI | NMI |
|---------|--------|-----|-----|
|         | K-Means | K-Means++ | DISCERN | K-Means | K-Means++ | DISCERN | K-Means | K-Means++ | DISCERN |
| YALE    | 0.815   | 0.868       | 1       | 0.759   | 0.822       | 1       | 0.929   | 0.95       | 1       |
| MIT     | 0.878   | 0.917       | 0.966   | 0.756   | 0.799       | 0.887   | 0.902   | 0.916       | 0.94    |
| GA      | 0.863   | 0.882       | 0.96    | 0.806   | 0.809       | 0.919   | 0.955   | 0.958       | 0.98    |
| ATT     | 0.851   | 0.888       | 1       | 0.808   | 0.853       | 1       | 0.955   | 0.966       | 1       |
| CA      | 0.947   | 0.985       | 1       | 0.816   | 0.873       | 0.956   | 0.935   | 0.952       | 0.981   |
| FEI     | 0.843   | 0.909       | 1       | 0.634   | 0.769       | 0.995   | 0.961   | 0.977       | 0.999   |
| CPM     | 0.534   | 0.526       | 0.545   | 0.162   | 0.165       | 0.15    | 0.13    | 0.126       | 0.137   |
| WINE    | 0.697   | 0.695       | 0.702   | 0.366   | 0.362       | 0.371   | 0.427   | 0.426       | 0.429   |
| IRIS    | 0.819   | 0.924       | 0.973   | 0.681   | 0.847       | 0.922   | 0.783   | 0.873       | 0.914   |
| BNN     | 0.566   | 0.566       | 0.566   | 0.017   | 0.017       | 0.017   | 0.015   | 0.015       | 0.015   |
| WAP     | 0.616   | 0.596       | 0.626   | 0.287   | 0.261       | 0.406   | 0.536   | 0.524       | 0.549   |

Quade statistical analysis on these results was also conducted. The rankings are presented in Figure 7.

![Figure 7. Quade rankings of the methods using DISCERN K](image)

The p-values compared to the highest-ranking method (DISCERN) are provided in Table 12.

### Table 12

**QUADE TEST P-VALUES WHEN USING DISCERN K**

| Method     | ASC   | DBI   | Purity | ARI   | NMI   |
|------------|-------|-------|--------|-------|-------|
| K-Means    | 0.002 | 0.000 | 0.000  | 0.000 | 0.000 |
| K-Means++  | 0.123 | 0.041 | 0.020  | 0.041 | 0.019 |

The results yield that the proposed method shows significant improvement with great certainty in DBI, Purity, ARI and NMI. When taking silhouette into consideration, significant improvement is still certain over K-Means, but not however over K-Means++. That means that while improvement over K-Means++ in silhouette score may not be significant, the proposed method still has a better rank. In brief, the proposed method shows significant improvement in all other scores, while not necessarily showing significant improvement in silhouette score. This can be interpreted as the prevalence of the proposed method over K-Means with great certainty in all of the 5 scores, while the same standard over K-Means++ can only be confirmed in all scores other than silhouette. In that case, while significant improvement is not certain, the proposed method is still ranked better than K-Means++.

### 6.3. Clustering using Elbow K

In the two previous subsections, we compared the clustering results when setting the number of clusters to the number of classes and the estimated numbers of the proposed approach which are very similar, as discussed in the previous section’s statistical tests. In this and the next subsections, we present the results when the number of clusters is set to those estimated by the top two methods ranked closely with the proposed method: Elbow and Silhouette.
The results of Elbow are provided in Table 13 and Table 14. The resulting numbers are rounded to 3 decimal points.

**TABLE 13**  
INTERNAL METRICS COMPARED WHEN USING ELBOW K

| Dataset | ASC  | DBI  |   | ASC  | DBI  |
|---------|------|------|---|------|------|
|         | K-Means | K-Means++ | DISCERN | K-Means | K-Means++ | DISCERN |
| YALE    | 0.52 | 0.585 | 0.724 | 1.205 | 1.08 | 0.773 |
| MIT     | 0.535 | 0.56 | 0.657 | 1.066 | 1.021 | 0.924 |
| GA      | 0.408 | 0.431 | 0.485 | 1.467 | 1.416 | 1.325 |
| ATT     | 0.58 | 0.629 | 0.739 | 1.148 | 1.083 | 0.83 |
| CA      | 0.584 | 0.648 | 0.809 | 1.306 | 1.146 | 0.594 |
| FEI     | 0.189 | 0.207 | 0.246 | 1.735 | 1.704 | 1.637 |
| CPMP    | 0.563 | 0.565 | 0.55 | 1.005 | 0.984 | 1.036 |
| WINE    | 0.727 | 0.727 | 0.727 | 0.543 | 0.538 | 0.546 |
| IRIS    | 0.668 | 0.64 | 0.644 | 1.513 | 1.465 | 1.415 |
| BNN     | 0.529 | 0.529 | 0.528 | 0.838 | 0.839 | 0.836 |
| WAP     | 0.309 | 0.3 | 0.309 | 1.754 | 1.783 | 1.59 |

Quade statistical analysis on these results was also conducted. The rankings are presented in Figure 8. The p-values compared to the highest-ranking method (DISCERN) are provided in Table 15.

**Figure 8.** Quade rankings of the methods using Elbow K

**TABLE 14**  
EXTERNAL METRICS COMPARED WHEN USING ELBOW K

| Dataset | K-Means | Purity | K-Means++ | ARI  | Purity | ARI  | NMI  |
|---------|---------|--------|-----------|------|--------|------|------|
|         | ASC  | DBI  | DISCERN | ASC  | DBI  | DISCERN | ASC  | DBI  | DISCERN |
| YALE    | 0.781 | 0.815 | 0.933 | 0.724 | 0.754 | 0.927 | 0.919 | 0.933 | 0.983 |
| MIT     | 0.888 | 0.897 | 0.966 | 0.792 | 0.804 | 0.912 | 0.917 | 0.92 | 0.952 |
| GA      | 0.619 | 0.621 | 0.64 | 0.603 | 0.585 | 0.648 | 0.908 | 0.91 | 0.921 |
| ATT     | 0.885 | 0.924 | 0.956 | 0.828 | 0.876 | 0.981 | 0.958 | 0.969 | 0.993 |
| CA      | 0.927 | 0.97 | 0.956 | 0.843 | 0.896 | 0.936 | 0.946 | 0.961 | 0.982 |
| FEI     | 0.347 | 0.349 | 0.35 | 0.246 | 0.248 | 0.245 | 0.866 | 0.868 | 0.866 |
| CPMP    | 0.53 | 0.535 | 0.545 | 0.158 | 0.157 | 0.15 | 0.128 | 0.132 | 0.137 |
| WINE    | 0.722 | 0.72 | 0.725 | 0.304 | 0.307 | 0.303 | 0.386 | 0.39 | 0.382 |
| IRIS    | 0.916 | 0.952 | 0.96 | 0.728 | 0.781 | 0.785 | 0.78 | 0.81 | 0.801 |
| BNN     | 0.597 | 0.601 | 0.572 | 0.019 | 0.021 | 0.009 | 0.025 | 0.027 | 0.013 |
| WAP     | 0.612 | 0.597 | 0.622 | 0.3 | 0.269 | 0.405 | 0.536 | 0.527 | 0.556 |

**TABLE 15**  
QUADE TEST P-VALUES WHEN USING ELBOW K

| Method | ASC  | DBI  | Purity | ARI  | NMI  |
|--------|------|------|--------|------|------|
| K-Means | 0.005 | 0.000 | 0.002 | 0.008 | 0.003 |
| K-Means++ | 0.120 | 0.059 | 0.197 | 0.090 | 0.278 |
The proposed approach shows significantly improved results in all scores over K-Means with great certainty, while being closely ranked with K-Means++. Therefore, the proposed approach doesn’t show significant improvement in results when compared to K-Means++ in this test, but it is still ranked the best of the three.

6.4. Clustering using Silhouette K

The results are provided in Table 16 and Table 17. The resulting numbers are rounded to 3 decimal points.

Table 16

| Dataset | Silhouette | DBI |
|---------|------------|-----|
|         | K-Means    |     | K-Means    |     | DISCERN  |
|         | K-Means++  |     | K-Means    |     | DISCERN  |
| YALE    | 0.535      | 0.606 | 0.693      | 1.158 | 1.011    | 0.864 |
| MIT     | 0.504      | 0.57  | 0.676      | 1.021 | 0.95     | 0.85  |
| GA      | 0.501      | 0.526 | 0.594      | 1.306 | 1.25     | 1.099 |
| ATT     | 0.577      | 0.643 | 0.739      | 1.145 | 1.05     | 0.83  |
| CA      | 0.613      | 0.701 | 0.799      | 1.227 | 1.041    | 0.667 |
| FEI     | 0.481      | 0.616 | 0.744      | 0.774 | 0.69     | 0.441 |
| CPMP    | 0.725      | 0.725 | 0.723      | 0.694 | 0.697    | 0.688 |
| WINE    | 0.82       | 0.82  | 0.821      | 0.481 | 0.481    | 0.479 |
| IRIS    | 0.958      | 0.958 | 0.958      | 0.384 | 0.384    | 0.384 |
| BNN     | 0.529      | 0.528 | 0.524      | 0.833 | 0.837    | 0.847 |
| WAP     | 0.314      | 0.327 | 0.357      | 1.644 | 1.628    | 1.527 |

Table 17

| Dataset | Purity | ARI | NMI |
|---------|--------|-----|-----|
|         | K-Means |     |     | K-Means |     | DISCERN |
|         | K-Means++|    |    | K-Means |     | DISCERN |
| YALE    | 0.85    | 0.895 | 1   | 0.798  | 0.839 | 0.988 | 0.938 | 0.954 | 0.994 |
| MIT     | 0.904   | 0.944 | 0.966 | 0.749 | 0.809 | 0.843 | 0.899 | 0.922 | 0.927 |
| GA      | 0.879   | 0.894 | 0.98  | 0.822 | 0.813 | 0.941 | 0.958 | 0.958 | 0.984 |
| ATT     | 0.882   | 0.931 | 1   | 0.823 | 0.882 | 0.981 | 0.957 | 0.971 | 0.993 |
| CA      | 0.887   | 0.938 | 0.909 | 0.824 | 0.898 | 0.898 | 0.942 | 0.964 | 0.976 |
| FEI     | 0.878   | 0.941 | 1 | 0.666 | 0.805 | 0.956 | 0.965 | 0.98  | 0.994 |
| CPMP    | 0.513   | 0.507 | 0.528 | 0.157 | 0.151 | 0.172 | 0.135 | 0.128 | 0.152 |
| WINE    | 0.657   | 0.657 | 0.657 | 0.366 | 0.366 | 0.369 | 0.43  | 0.43  | 0.443 |
| IRIS    | 0.667   | 0.667 | 0.667 | 0.568 | 0.568 | 0.568 | 0.761 | 0.761 | 0.761 |
| BNN     | 0.693   | 0.684 | 0.674 | 0.062 | 0.055 | 0.049 | 0.093 | 0.081 | 0.066 |
| WAP     | 0.678   | 0.647 | 0.663 | 0.261 | 0.221 | 0.233 | 0.551 | 0.534 | 0.546 |

Quade statistical analysis on these results were also conducted. The rankings are presented in Figure 9.

![Quade rankings of the methods using Silhouette K](image)

The p-values compared to the highest-ranking method (DISCERN) are provided in Table 18.
The proposed approach is again significantly improving K-Means with great certainty in both internal and external measures, while only being closely ranked with K-Means++ and not showing significant improvement with great certainty in most of the scores.

7. Analysis of Robustness

Both randomized K-Means and K-Means++ are stochastic based. Randomized versions of K-Means include randomly selecting records or randomly selecting points in the d-dimensional space as the initial centroids. K-Means++ on the other hand starts with a random centroid as the first, and uses probability-based metrics in selecting the rest. This obviously yields different results each time. Nevertheless, the power of K-Means++ at reducing standard deviation in results in undeniable.

In Table 19, we present the standard deviation of the estimated K values of the silhouette method using K-Means and K-Means++ as well as that of the proposed method.

Table 19

| Dataset | Silhouette | K++ Silhouette | DISCERN |
|---------|------------|----------------|---------|
| YALE    | 3.038811   | 2.291288       | 0       |
| MIT     | 1.713914   | 1.713914       | 0       |
| GA      | 6.781178   | 4.520785       | 0       |
| ATT     | 5.218656   | 3.427827       | 0       |
| CA      | 5.53963    | 4.768058       | 0       |
| FEI     | 12.31868   | 9.82026        | 0       |
| CPMP    | 0          | 0              | 0       |
| WINE    | 0          | 0              | 0       |
| IRIS    | 0          | 0              | 0       |
| BNN     | 1.964529   | 2.05776        | 0       |
| WAP     | 6.036348   | 2.061553       | 0       |

Quade statistical analysis on these results were also conducted. The rankings are presented in Figure 10. As it can be observed, DISCERN is ranked at close to 1 which is far better than the other two, while the rankings of K-Means and K-Means++ are noticeably different, highlighting K-Means++’s improvement.
The p-values of silhouette method using K-Means and K-Means++ compared to the highest-ranking method (DISCERN) are 0.000382 and 0.035193 respectively. The p-values clearly indicate significant improvement over the two with great certainty. Moreover, we present similar information regarding the two methods chosen for K-estimation: the elbow method and silhouette method (using K-Means++). The results are presented in Table 20.

### Table 20

| Dataset | $\sigma(K)$ Elbow | $\sigma(K)$ K++ Silhouette | $\sigma(K)$ DISCERN |
|---------|------------------|----------------------------|---------------------|
| YALE    | 2.277608         | 2.291288                   | 0                   |
| MIT     | 1.414214         | 1.713914                   | 0                   |
| GA      | 3.705992         | 4.520785                   | 0                   |
| ATT     | 3.119996         | 3.427827                   | 0                   |
| CA      | 4.044672         | 4.768058                   | 0                   |
| FEI     | 13.52544         | 9.82026                    | 0                   |
| CPMP    | 0.968246         | 0                          | 0                   |
| WINE    | 0                | 0                          | 0                   |
| IRIS    | 0.5              | 0                          | 0                   |
| BNN     | 0.5              | 2.05776                    | 0                   |
| WAP     | 2.146946         | 2.061553                   | 0                   |

Quade statistical analysis on these results were also conducted. The rankings are presented in Figure 11.

As it can be observed, DISCERN is again ranked better than the other two methods in robustness. The p-values of elbow method and silhouette method compared to the highest-ranking method (DISCERN) are 0.001205 and 0.007902 respectively and clearly indicate significant improvement over the two with great certainty.

8. Evaluation Summary and Interpretation

As we discussed in the previous section, the proposed method values diversity, and picks the most diverse records as centroids. This can be a bit problematic when noisy data exists. In the facial datasets specifically, we noticed that those with noisier images (rotated angles, dark lighting, and the like) were sometimes being clustered alone. An instance of the dataset MIT-CBCL [13] being clustered by DISCERN is presented in Figure 12. Moreover, the t-SNE [44] visualization of MIT-CBCL is also presented in Figure 13.a.

We should note that in all of our t-SNE visualizations, the numbers represent the class number and the different colors represent different clusters.
Figure 12. MIT dataset clustered using DISCERN. Centroids selected by DISCERN are placed in the middle and highlighted with a red border.

This dataset includes 10 individuals each with a different number of images and from different angles. It should be noted that the neural network that we used to compress facial images [36] was trained on a more standard dataset and is therefore sensitive to face angles. In other words, the neural net cannot map the side of a subject’s face close enough to the rest of the subject’s facial images. As it can be seen, while the proposed method clusters data well enough up to the 10th cluster, the 11th and 12th centroids which are unnecessary are those of two particular subject’s sides (Subjects 9 and 0), and as a result of the clustering, subject 9’s side image as centroid drew other side images of similar-looking subjects (subjects 4 and 2) into its this cluster. It is also noticeable that in some clusters, particularly the first two (whose centroids are picked based on least similarity from the matrix S), the centroids are those least similar and therefore most noisy (images of sides). While this can be a disadvantage in datasets with noisy data present, it serves also as the most obvious advantage in the rest. To summarize, while K-Means and K-Means++ as partitionial clustering measures are sensitive to noise, the proposed approach may be even more in specific cases. Datasets such as Yale Face Database [49] on the other hand are perfectly clustered by DISCERN, with 100% percent accuracy. T-SNE visualization of Yale is presented in Figure 13.b.
Moreover, t-SNE visualization of some of the more accurately clustered (based on external metrics) datasets used in our experiments are provided in Figure 14.

On the other hand, some datasets such as Banana (t-SNE provided in Figure 15) are not well represented by their features and therefore cannot be clustered well by any partitional clustering algorithms.
9. Conclusions

One of the most prominently used partitional clustering algorithms, K-Means is notorious for being sensitive to its centroid initialization. While a number of methods improved the random-based initialization, K-Means++ however has proven to be the most efficient, effective and applicable initialization. Nevertheless, the problem of setting the number of clusters still exists in real-time applications. Many methods such as X-Means, the elbow and silhouette methods have been used previously, but they either fail to estimate a number close to the optimal number or are inapplicable when there exists no knowledge of the minimum and maximum number of clusters. These methods often require multiple runs of an initialization algorithm on top of what can be a super-polynomial algorithm (K-Means) [3] which is highly inefficient. Moreover, these methods are stochastic in nature which would make their results lack robustness at times.

As a result, we introduced DISCERN which is an initialization algorithm that attempts to solve all three of these issues. Firstly, DISCERN operates based on actual record-by-record similarity which eliminates any use of stochastic measures and therefore yields the same results at every run, and essentially maps the data from a d-dimensional space to a 1-dimensional Euclidean space and then processes them. Secondly, through this similarity, the algorithm chooses the most diverse records as the initial centroids which is then passed on to K-Means. This process increases the probability of a suitable clustering result in most cases. Finally, by tracking the level of similarity, it can detect a convergence pattern and easily estimate an optimal number of clusters. We compared DISCERN in both in estimating an optimal number of clusters, and as a clustering initialization method and found that it is mostly ranked either higher or alongside K-Means++ in terms of suitable clustering, and ranked the best in robustness with an obvious standard deviation of zero. Finally, in terms of complexity order, it is self-evident that this measure is more efficient than other K-estimating metrics that are ranked close to it, and that is further visible when comparing computational time.

However, the point in which this algorithm lacks the most is its strength as well, which is diversity-based selection. Because this algorithm selects the most diverse records as initial centroids, it may not yield suitable results in datasets which include a noisy data. When noisy records are selected as centroids, that offsets attention to the actual data and may result in incorrect clustering. However, in the event that noisy records, for instance dark lighted images exist and their feature space places them far away from the actual records, the algorithm clusters the noisy data together in a separate group.

Further improvements of this method may include mini-batches of data being process first, as the computation of the similarity matrix can be very costly.

One future application of the proposed method is undoubtedly in deep learning. In our experiments, we used a pretrained deep
network trained with triplet loss in order to cluster facial data, and observed very good results even in the cases where the number of unique faces surpassed 100 (FEI). Following that, clustering methods can play an essential role in unsupervised and semi-supervised learning using deep learning, where deep learning finds a suitable feature representation, and the actual clustering or classification is done afterwards.

In summary, this method, like other clustering methods relies on a suitable feature representation which can be provided using matrix methods and deep network latent representations, but when that representation is suitable, it serves as a completely parameterless learning algorithm, taking only the data as input.

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