Spaces of Clusterings

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Abstract

We propose two algorithms to cluster a set of clusterings of a fixed dataset, such as sets of clusterings produced by running a clustering algorithm with a range of parameters, or with many initializations. We use these to study the effects of varying the parameters of HDBSCAN, and to study methods for initializing $k$-means.

1 Introduction

Often, a clustering algorithm, rather than producing a single clustering of a dataset, produces a set of clusterings. For example, one gets a set of clusterings by running a clustering algorithm with a range of parameters, or with many initializations. Given a set $S$ of clusterings of a dataset $X$, one may want to know how many different kinds of clusterings the set $S$ contains, ignoring small differences between elements of $S$. In effect, one may want to cluster $S$. This paper proposes two clustering algorithms, specifically for use on sets of clusterings of a fixed dataset.

The starting point is the observation that sets of clusterings have geometric structure. Indeed, there are many ways, described in the literature, to define a metric on the set of all clusterings of a fixed dataset, and it is a natural idea to use such metrics to cluster a set of clusterings. See, e.g., [Mei07]. However, this is not our approach. Rather than using a metric on the set of all clusterings of a dataset $X$, we define pseudometrics on any given set $S$ of clusterings of $X$, so that the distance between two clusterings $C, D \in S$ depends on $S$. The clustering algorithms we propose are based on these notions of distance in $S$.

In Section 2, we describe these clustering algorithms, and in Section 3, we give two examples. In the first, we apply the clustering algorithm HDBSCAN to a synthetic dataset, and use our algorithms to understand the
effect of varying HDBSCAN’s parameters. In the second, we apply \( k \)-means to two datasets from the UCI Machine Learning Repository, and use our algorithms to study different methods of initializing \( k \)-means.

Implementations of our proposed clustering algorithms are available at [RS19].

2 Choosing representative pairs

By a clustering of a set \( X \), we mean a set of disjoint subsets of \( X \). Points of \( X \) that do not belong to any subset in a clustering of \( X \) are called noise points. Given a set \( S \) of clusterings of \( X \), there is an embedding \( M : S \rightarrow 2^P \), where \( 2 = \{0, 1\} \), \( P \) is the set of unordered pairs with repetition of points of \( X \), and \( 2^P \) is the set of binary vectors indexed by \( P \). For \( C \in S \), let \( M(C)_{(x,y)} = 0 \) if \( C \) clusters \( x \) and \( y \) together, and \( M(C)_{(x,y)} = 1 \) otherwise.

We allow pairs with repetition to distinguish noise points from one-point clusters: if \( x \in X \) is a noise point of \( C \), then \( M(C)_{(x,x)} = 1 \), but if \( \{x\} \) is a cluster of \( C \), then \( M(C)_{(x,x)} = 0 \). Write \( n = |S| \) and \( p = |P| = \binom{|X|}{2} + |X| \). We’ll think of \( M(S) \) as an \( n \times p \) matrix, so that a row of \( M(S) \) is \( M(C) \) for some \( C \in S \). Each column of \( M(S) \) corresponds to a pair of points of \( X \).

In many cases of interest, it is not possible to consider all pairs of data points when constructing the matrix \( M(S) \). Instead, one can first sample pairs from the dataset, then construct \( M(S) \) with columns corresponding only to the sampled pairs.

In this section, we describe two feature selection procedures for \( M(S) \), and use these procedures to partition \( S \) into classes.

2.1 A simple approach

In cases of interest, the matrix \( M(S) \) has many repeated columns: given a pair of points \((x, y)\) of \( X \), if \( x' \) is a point close to \( x \), and \( y' \) is a point close to \( y \), then most “reasonable” clusterings of \( X \) will cluster together \( x \) and \( y \) if and only if they cluster together \( x' \) and \( y' \). So, if \( x \) and \( y \) are in dense regions of \( X \), one expects to have many columns of \( M(S) \) that are equal to the column corresponding to \((x, y)\).

This suggests the following feature selection procedure. Assume we are given \( d \in \mathbb{N} \).
1. Let $N(S)$ be the matrix obtained by dropping all columns from $M(S)$ that are equal to the zero vector or to the vector with every component equal to one;

2. Drop all duplicate columns from $N(S)$;

3. If $N(S)$ has less than $d$ columns, fail;

4. Let the multiplicity of a column of $N(S)$ be the number of times that this column appears in $M(S)$;

5. Let $M'(S)$ be the matrix obtained by keeping only the $d$ columns of $N(S)$ with the greatest multiplicity.

We can interpret $M'$ as a function $M' : S \rightarrow 2^d$. To partition $S$ into classes, say that two clusterings $C, D \in S$ are in the same class if and only if $M'(C) = M'(D)$. We will refer to this clustering algorithm as Algorithm 1.

More generally, any feature selection procedure $M' : S \rightarrow 2^d$ can be used to define a pseudometric on $S$, given by

$$\rho(C, D) = \rho_{\text{ham}}(M'(C), M'(D)) \text{ for } C, D \in S,$$

where $\rho_{\text{ham}}$ is the hamming distance between binary vectors. This is the notion of distance underlying Algorithm 1.

### 2.2 An approach based on latent class models

In this section, we describe a more involved feature selection procedure, which aims to address the case that the matrix $M(S)$ has many columns that are very similar, but not equal. Notice that any clustering of the columns of $M(S)$ gives a feature selection procedure: to choose $d$ features, take the $d$ largest clusters of columns, then pick a representative of each cluster. We use complete-linkage clustering to cluster the columns of $M(S)$, so we need to choose a distance scale parameter $\epsilon$. In order to choose $\epsilon$, we quantify how well a choice of features represents the matrix $M(S)$. We do this by associating a latent class model for $M(S)$ to each choice of features. Such a model comes with a likelihood function, and we choose the parameter $\epsilon$ that maximizes the likelihood function of the associated latent class model.

We now recall the notion of a latent class model, following [BKM11]. Suppose given a random vector $Z$ of dimension $p$, and a random variable $Y$ taking values in a set $\mathbb{Y}$. If, for each $y \in \mathbb{Y}$ and $1 \leq i, j \leq p$ with $i \neq j$, we
assume that the random variable \((Z_i \mid Y = y)\) is independent of the random variable \((Z_j \mid Y = y)\), we call this a latent variable model. If \(Z_i\) and \(Y\) are assumed to be discrete random variables with finitely many possible values, we call each possible value of \(Y\) a class, and the model a latent class model. Under these assumptions, the log-likelihood for a sample \(Z^1, \cdots, Z^n\) is given by

\[
L = \sum_{h=1}^{n} \ln \left( \sum_{y \in Y} P(Y = y) \prod_{i=1}^{p} P(Z_i = Z_i^h \mid Y = y) \right). \tag{1}
\]

Now, we explain how to associate a latent class model for \(M(S)\) to a choice of features. Given a choice of \(d\) columns of \(M(S)\), let \(M'(S)\) be the \(n \times d\) matrix obtained from \(M(S)\) by keeping only the \(d\) chosen columns. Write \(S'\) for the set of rows of \(M'(S)\), and let \(f : S \to S'\) be the obvious projection. To construct a latent class model, we have to describe \(Z\) and \(Y\). We let \(Z\) be a binary random vector of dimension \(p\), so that each \(Z_i\) is a Bernoulli variable, and we let \(Y\) be a random variable taking values in the set \(2^d\). We interpret \(S\) as a set of samples of \(Z\), and \(S'\) as a set of samples of \(Y\). We can then estimate the log-likelihood of the model as follows.

For \(0 \leq i \leq p\) and \(y \in 2^d\), let \(\hat{\eta}_y = P(Y = y)\) and \(\hat{\pi}_{i,y} = P(Z_i = 1 \mid Y = y)\). These can be estimated as

\[
\hat{\eta}_y = \frac{|f^{-1}(y)|}{n}, \quad \hat{\pi}_{i,y} = \frac{\text{mean}_{v \in f^{-1}(y)} (v_i)}. \tag{2}
\]

Then \(P(Z_i = Z_i^h \mid Y = y)\) can be estimated by the formula

\[
\hat{\pi}_{i,y}^{Z_i^h} (1 - \hat{\pi}_{i,y})^{1 - Z_i^h}. \tag{3}
\]

Using estimates 2 and 3 together with Eq. (1), we get an estimate for the log-likelihood of the model.

We now describe the feature selection procedure. Let \(d \in \mathbb{N}\).

1. For each \(\epsilon \geq 0\), let \(K(\epsilon)\) be the clustering of the columns of \(M(S)\) obtained using complete linkage-clustering with respect to the hamming distance, and distance scale parameter \(\epsilon\);

2. Drop the clusterings \(K(\epsilon)\) that contain less than \(d\) clusters;

3. For each remaining \(K(\epsilon)\), drop all but the \(d\) largest clusters;
4. For each $K(\epsilon)$, let $R(\epsilon)$ be the set of $d$ columns obtained by taking the medoid$^1$ of each cluster in $K(\epsilon)$;

5. Keep the set of columns $R(\epsilon_0)$ that maximizes the log-likelihood of the associated latent class model, and let $M'(S)$ be the matrix obtained by keeping only the columns in $R(\epsilon_0)$.

As in Section 2.1, we say that two clusterings $C, D \in S$ are in the same class if and only if $M'(C) = M'(D)$. We refer to this clustering algorithm as Algorithm 2.

3 Examples

3.1 Varying the parameters of HDBSCAN

The following example illustrates the way in which our method can identify clusterings of interest. Let $X$ be the 2-dimensional synthetic dataset of Fig. 1. There appears to be one cluster on the bottom right, however, on the top left, one might see one or two clusters.

![Figure 1: Gaussian mixture with 154 points.](image)

We run HDBSCAN on $X$ with a range of parameters. HDBSCAN is a density-based clustering algorithm, first proposed in [CMS13], [CMZS15], which takes two parameters: a minimum cluster size $m \geq 2$, and a density threshold $k \geq 1$. Rather than returning a partition of a dataset, HDBSCAN may designate some points as noise. For more information see [MH18] and

$^1$That is, the vector that minimizes the sum of the distances to the rest of the columns in the cluster. Recall that we are using the hamming distance.
We start by considering a large range of parameters, \((m, k) \in [2, \cdots, 40] \times [1, \cdots, 40]\). Let \(S\) be the set of clusterings of \(X\) obtained by running HDBSCAN with these parameters.

Using Algorithm 1 with \(d = 4\), we obtain the partitioning of \(S\) shown in Fig. 2. As is usual with HDBSCAN, very small values of both \(m\) and \(k\) return very “unstable” results, with many clusters. These values appear in the bottom left corner. If we want to ignore these unstable results, we can delete them from \(S\) to obtain a new set of clusterings \(S'\), and run Algorithm 1 again, this time with \(d = 3\). See Fig. 2.

To better understand the partitioning of \(S'\), we display in Fig. 3 a representative example of each class. The light blue and green classes are easy to understand: every clustering in these classes is equal to the representative displayed in Fig. 3. The red class contains 5 distinct clusterings of \(X\); each clustering in the red class has exactly two clusters, one on the bottom right of the dataset, one on the top left, but they differ as to which points are regarded as noise. The brown class contains 36 distinct clusterings of \(X\); each clustering in the brown class designates the bottom right corner of the dataset as noise, and finds exactly two clusterings in the top left portion of the dataset.

Recall that, running Algorithm 1 with \(d = 3\), we get a function \(M' : S' \rightarrow 2^3\); clusterings \(C, D \in S'\) are in the same class if and only if \(M'(C) = M'(D)\). Each dimension of \(2^3\) corresponds to a set of pairs of points in \(X\). In Fig. 4,
Figure 3: Clockwise from top left, HDBSCAN with \((m,k) = (5,8), (5,9), (40,15), (32,20)\). Grey points are noise. Still clockwise from top left, these clusterings represent the light blue, red, green, and brown classes of \(S'\), as in Fig. 2.

we show a representative pair for each dimension.

The light blue class is the preimage of the vector \((1,0,0)\), the red class is the preimage of the vector \((0,0,0)\), the green class is the preimage of the vector \((1,1,1)\), and the brown class is the preimage of the vector \((1,0,1)\). The first component of these vectors, corresponding to the leftmost image in Fig. 4, is checking whether the two potential clusters on the top left of the dataset are merged or not. The second component, corresponding to the middle image in Fig. 4, checks whether the whole dataset is regarded as noise, and, similarly, the third component, corresponding to the rightmost image in Fig. 4, checks whether the cluster on the bottom right is regarded as noise.

We see that Algorithm 1 successfully partitions \(S\) into classes with very similar outcomes, and that pairs of points in \(X\) can be used to explain the partitioning.

Algorithm 2 does not perform as well in this case. Although it finds much of the same structure, in both \(S\) and \(S'\) it fails to distinguish between the light blue and brown classes of Fig. 2.
3.2 Choosing initial centers for $k$-means

Given a finite set of points in euclidean space, the $k$-means problem is to choose $k$ centers that minimize $\phi$, the sum of the squared distance between each point and its closest center. A commonly used algorithm to find approximate solutions to the $k$-means problem is due to Lloyd [Llo82]. The algorithm begins by choosing $k$ centers at random from the dataset. It then assigns each data point to its closest center, and recomputes each center as the center of mass of the points assigned to it. This step is repeated until the process stabilizes, to obtain $k$ centers $x_1, \ldots, x_k$. This produces a clustering with $k$ clusters, for which a point $x$ belongs to the $i^{th}$ cluster if the closest center to $x$ is $x_i$.

Of course, the outcome of Lloyd’s algorithm depends on the choice of the initial centers. A common approach is to choose these initial centers uniformly at random from the dataset. In [AV07], Arthur and Vassilvitskii propose a more sophisticated approach: choosing the initial centers at random from the dataset, but weighing data points according to their squared distance from the closest center already chosen.

Following [AV07], we’ll refer to Lloyd’s algorithm, with initial centers chosen uniformly at random from the dataset, as $k$-means, and we’ll refer to Lloyd’s algorithm, with initial centers chosen according to the method of [AV07], as $k$-means++.

In [AV07], Arthur and Vassilvitskii compare the performance of $k$-means and $k$-means++ on four datasets, including the Cloud and Intrusion datasets from the University of California – Irvine Machine Learning Repository [Col89, Dat].

The Cloud dataset consists of 1024 vectors in $\mathbb{R}^{10}$, encoding information about two images of the atmosphere. We consider a set $T$ of 40 clusterings of the Cloud dataset, with 20 produced by $k$-means and 20 produced by $k$-means++, both with $k = 10$. Information about the associated values of $\phi$...
is in Table 1.

While \texttt{k-means++} produces clusterings with very similar values of $\phi$, the output of \texttt{k-means} is quite varied. Algorithm 2, with $d = 3$ and a sample of 100,000 pairs of points from the dataset, finds interesting structure in the output of \texttt{k-means}. It partitions $T$ into 4 classes: class 0 consists of the 20 outputs of \texttt{k-means++}, and the outputs of \texttt{k-means} are distributed among classes 1, 2, and 3. See Table 2. In this case, the classes produced by Algorithm 2 correspond well to the values of $\phi$. The dimension $d = 3$ is the smallest such that Algorithm 2 separates the outputs of \texttt{k-means} and \texttt{k-means++}.

If we apply Algorithm 1 to $T$, we need to select more features to separate the \texttt{k-means++} output from the \texttt{k-means} output. We use $d = 6$, the smallest value of $d$ for which Algorithm 1 separates these outputs, and a sample of 100,000 pairs. See Table 3.

The partitioning of $T$ given by Algorithm 1 is a refinement of the partitioning given by Algorithm 2. Class 0 is equal to the union of classes 4 and 5, class 1 is equal to the union of classes 6 and 7, class 2 is equal to class 8, and class 3 is equal to class 9.

The \textit{Intrusion} dataset simulates features available to an intrusion detection system. We used the full dataset available at the UCI Machine Learning Repository, which consists of 4,898,431 points. We kept the 34 continuous features, ignoring the 8 categorical features. We consider a set $U$ of 40 clusterings of the \textit{Intrusion} dataset, with 20 produced by \texttt{k-means} and 20 produced by \texttt{k-means++}, both with $k = 25$. Information about the associated values of $\phi$ is in Table 4.

Taking $d = 1$ and a sample of 5,000 pairs of data points, Algorithms 1 and 2 produce the same result: they find two clusters, one containing the output of \texttt{k-means}, and the other the output of \texttt{k-means++}. So, the most repeated column of the matrix $M(U)$ says exactly whether a clustering in $U$ was produced by \texttt{k-means} or \texttt{k-means++}.

To get a finer partitioning of $U$, we ran Algorithm 2, with $d = 3$ and a sample of 5,000 pairs of data points, on the set of outputs of \texttt{k-means}. The results are displayed in Table 5. One gets a similar result using Algorithm 1.

On both datasets, our algorithms distinguish between the outputs of \texttt{k-means} and \texttt{k-means++}. Furthermore, they produce classes that correspond well to the $\phi$ values of the clusterings.
| clusterings   | number of clusterings | $\phi$ mean | $\phi$ min. | $\phi$ max. | std. deviation |
|--------------|-----------------------|-------------|-------------|-------------|----------------|
| $T$          | 40                    | $6.059 \cdot 10^6$ | $5.761 \cdot 10^6$ | $6.582 \cdot 10^6$ | $2.996 \cdot 10^5$ |
| k-means      | 20                    | $6.353 \cdot 10^6$ | $6.223 \cdot 10^6$ | $6.582 \cdot 10^6$ | $8.806 \cdot 10^4$ |
| k-means++    | 20                    | $5.766 \cdot 10^6$ | $5.761 \cdot 10^6$ | $5.776 \cdot 10^4$ | $4.417 \cdot 10^3$ |

Table 1: Experimental results of k-means and k-means++ on the Cloud dataset, with $k = 10$.

| class | number of clusterings | $\phi$ mean | $\phi$ min. | $\phi$ max. | $\phi$ std. deviation |
|-------|-----------------------|-------------|-------------|-------------|-----------------------|
| 0     | 20                    | $5.766 \cdot 10^6$ | $5.761 \cdot 10^6$ | $5.776 \cdot 10^6$ | $4.417 \cdot 10^4$ |
| 1     | 12                    | $6.287 \cdot 10^6$ | $6.223 \cdot 10^6$ | $6.314 \cdot 10^6$ | $2.144 \cdot 10^4$ |
| 2     | 7                     | $6.433 \cdot 10^6$ | $6.423 \cdot 10^6$ | $6.434 \cdot 10^6$ | $3.767 \cdot 10^3$ |
| 3     | 1                     | $6.582 \cdot 10^6$ | $6.582 \cdot 10^6$ | $6.582 \cdot 10^6$ | – |

Table 2: Partitioning $T$ into classes using Algorithm 2, with $d = 3$.

| class | number of clusterings | $\phi$ mean | $\phi$ min. | $\phi$ max. | $\phi$ std. deviation |
|-------|-----------------------|-------------|-------------|-------------|-----------------------|
| 4     | 18                    | $5.766 \cdot 10^6$ | $5.761 \cdot 10^6$ | $5.776 \cdot 10^6$ | $3.735 \cdot 10^4$ |
| 5     | 2                     | $5.774 \cdot 10^6$ | $5.773 \cdot 10^6$ | $5.775 \cdot 10^6$ | $1.248 \cdot 10^4$ |
| 6     | 9                     | $6.290 \cdot 10^6$ | $6.286 \cdot 10^6$ | $6.314 \cdot 10^6$ | $8.658 \cdot 10^4$ |
| 7     | 3                     | $6.278 \cdot 10^6$ | $6.223 \cdot 10^6$ | $6.307 \cdot 10^6$ | $3.881 \cdot 10^4$ |
| 8     | 7                     | $6.433 \cdot 10^6$ | $6.423 \cdot 10^6$ | $6.434 \cdot 10^6$ | $3.767 \cdot 10^3$ |
| 9     | 1                     | $6.582 \cdot 10^6$ | $6.582 \cdot 10^6$ | $6.582 \cdot 10^6$ | – |

Table 3: Partitioning $T$ into classes using Algorithm 1, with $d = 6$.

| clusterings | number of clusterings | $\phi$ mean | $\phi$ min. | $\phi$ max. | $\phi$ std. deviation |
|-------------|-----------------------|-------------|-------------|-------------|-----------------------|
| $U$         | 40                    | $3.537 \cdot 10^{14}$ | $7.827 \cdot 10^{13}$ | $7.339 \cdot 10^{14}$ | $2.915 \cdot 10^{14}$ |
| k-means     | 20                    | $6.279 \cdot 10^{14}$ | $2.286 \cdot 10^{14}$ | $7.339 \cdot 10^{14}$ | $1.397 \cdot 10^{14}$ |
| k-means++   | 20                    | $7.946 \cdot 10^{13}$ | $7.827 \cdot 10^{13}$ | $8.335 \cdot 10^{13}$ | $1.935 \cdot 10^{13}$ |

Table 4: Experimental results of k-means and k-means++ on the Intrusion dataset, with $k = 25$.
Table 5: Partitioning the k-means clusterings of $U$ into classes, using Algorithm 2, with $d = 3$.

| class | number of clusterings | $\phi$ mean | $\phi$ min. | $\phi$ max. | std. deviation |
|-------|-----------------------|--------------|-------------|-------------|---------------|
| 0     | 4                     | $6.227 \cdot 10^{14}$ | $6.191 \cdot 10^{14}$ | $6.336 \cdot 10^{14}$ | $6.242 \cdot 10^{12}$ |
| 1     | 13                    | $6.839 \cdot 10^{14}$ | $6.114 \cdot 10^{14}$ | $7.339 \cdot 10^{14}$ | $4.140 \cdot 10^{13}$ |
| 2     | 1                     | $2.288 \cdot 10^{14}$ | $2.288 \cdot 10^{14}$ | $2.288 \cdot 10^{14}$ | $-$ |
| 3     | 1                     | $2.286 \cdot 10^{14}$ | $2.286 \cdot 10^{14}$ | $2.286 \cdot 10^{14}$ | $-$ |
| 4     | 1                     | $7.188 \cdot 10^{14}$ | $7.188 \cdot 10^{14}$ | $7.188 \cdot 10^{14}$ | $-$ |

4 Conclusions and future work

Given a set $S$ of clusterings of a fixed dataset, we have encoded $S$ as a binary matrix $M(S)$, and proposed two feature selection procedures for this matrix. We used these to define two clustering algorithms, specifically for use on sets of clusterings. Using these algorithms, we found meaningful structure in sets of clusterings produced by running HDBSCAN with a range of parameters on a synthetic dataset, and in sets of clusterings produced by running $k$-means with different initializations on two datasets from the UCI Machine Learning Repository. We also illustrated, in Section 3.1, how the partitionings of $S$ produced by our algorithms can be interpreted in terms of pairs of data points.

In the examples, we have compared the performance of our proposed clustering algorithms. Algorithm 1 is fast and produced good results in all of our experiments. It is also easy to understand and implement. Algorithm 2 performed well in the experiments of Section 3.2, finding the same structure as Algorithm 1 using fewer features. Algorithm 2 is designed to be more robust to outliers in $S$, which might reduce the number of repeated columns in $M(S)$. However, it takes much longer to compute, because of the complexity in computing the log-likelihood of the statistical model involved. And it sometimes fails to find small, interesting classes of clusterings, as in Section 3.1.

Algorithm 2 uses the hierarchical clustering of the feature space of $M(S)$ produced by complete-linkage with the hamming distance, and a statistical model to automatically choose features from this hierarchy. In forthcoming work, we will use topological and persistence methods to study the feature space, as in e.g. [CG18]. Instead of flat clusterings of $S$, we will produce more flexible structures, such as hierarchical clusterings and graphs.
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