

G -Mapper: Learning a Cover in the Mapper Construction

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Abstract

The Mapper algorithm is a visualization technique in topological data analysis (TDA) that outputs a graph reflecting the structure of a given dataset. However, the Mapper algorithm requires tuning several parameters in order to generate a “nice” Mapper graph. This paper focuses on selecting the cover parameter. We present an algorithm that optimizes the cover of a Mapper graph by splitting a cover repeatedly according to a statistical test for normality. Our algorithm is based on G -means clustering which searches for the optimal number of clusters in k -means by iteratively applying the Anderson-Darling test. Our splitting procedure employs a Gaussian mixture model to carefully choose the cover according to the distribution of the given data. Experiments for synthetic and real-world datasets demonstrate that our algorithm generates covers so that the Mapper graphs retain the essence of the datasets, while also running significantly fast.

1 Introduction

Topological data analysis (TDA) utilizes techniques from topology in order to extract valuable insights from a dataset. Topology, the major branches of mathematics, studies the shape of a space, and TDA uncovers the shape of the dataset using topology. We refer the reader to [6] for an overview of this area. This paper focuses on the *Mapper* algorithm introduced in [38] by Singh, Mémoli, and Carlsson, one of the fundamental visualization tools in TDA. Mapper has been shown to be useful in various applications such as analyzing breast cancer microarray data [29], identifying diabetes subgroups [26], and studying divergence of COVID-19 trends [45].

Mapper is a network-based visualization technique of high-dimensional data. The algorithm takes as input a point cloud dataset and produces as output a graph reflecting the structure of the underlying data. To apply the Mapper algorithm, the user needs to determine the following parameters that include choosing a *lens* (or *filter*) function $f : X \rightarrow Y$ from a high-dimensional point cloud X to a lower-dimensional space Y , an (*open*) *cover* of the target space Y , and a *clustering* algorithm for cover elements. Optimizing these parameters is essential for generating a “nice” Mapper graph. We concentrate on tuning a *cover* given by a collection of overlapping intervals. While the traditional Mapper algorithm takes a uniform cover with the number of intervals and the same overlapping percent between consecutive intervals to be specified by the user [38], sophisticated methods have recently been applied to optimize the cover of Mapper.

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This paper is concerned with *clustering* methods which have been utilized for selection of a cover. Motivated by the *X-means* algorithm [30] for estimating the number of clusters in *k-means* according to the *Bayesian Information Criterion* (BIC), Chalapathi, Zhou, and Wang devised an algorithm which repeatedly splits intervals of a coarse cover [8] according to information criteria. This Mapper algorithm is called *Multipass AIC/BIC*. Our work is primarily inspired by this algorithm. We develop a Mapper algorithm based on another iterative clustering algorithm (*G-means* [19]) utilizing a statistical test. Additionally, employing the *Fuzzy C-means* algorithm [15, 3], a centroid-based overlapping clustering method, Bui et al. presented a Mapper construction called *F-Mapper* that takes clusters obtained by the algorithm applied to $f(X)$ as a cover of Mapper [5].

1.1 Contributions

We propose a new Mapper construction algorithm called *G-Mapper* for optimizing a cover of the Mapper graph based on *G-means* clustering [19]. The *G-means* clustering algorithm aims to learn the number k of clusters in the *k-means* clustering algorithm according to a statistical test, called the *Anderson–Darling* test, for the hypothesis that the points in a cluster follow a *Gaussian* distribution. Our algorithm splits a cover element iteratively, with our splitting decision determined by the Anderson–Darling score. For further elaboration, we split each cover element into two overlapping intervals by employing a *Gaussian mixture model* (GMM) so that the splits are made according to the characteristics of the cover element rather than yielding uniform intervals. This procedure allows us to take variance into account when forming cover elements, making our algorithm perform well without the initialization of a cover.

G-Mapper integrates ideas from the current state-of-the-art techniques to fill in gaps from each method. To find the number of intervals in a cover, the *Multipass AIC/BIC* method iteratively splits cover elements using information criteria. However, experiments reveal that *X-means* based on the criteria does not perform well when a given dataset is non-spherical or high-dimensional [19, 20, 37] and it has computational issues [21]. Additionally, when a cover element splits, two intervals are created to have a set uniform length. In contrast, *F-Mapper* takes into account the data to determine where intervals in the cover should be located, but the number of intervals must be predetermined. *G-Mapper* finds the number of intervals by applying an iterative splitting procedure with the Anderson–Darling test. *G-means* works well experimentally even for non-spherical data and high-dimensional data, performing considerably faster than *X-means* [19]. Moreover, our method splits a cover element into two intervals using a GMM, considering the distribution of the data.

Applying the *G-Mapper* algorithm to various synthetic and real-world datasets, we demonstrate that the algorithm generates covers such that the corresponding Mapper graphs preserve the essence of the datasets. A comparison of Mapper graphs, generated by *G-Mapper* and *Multipass BIC*, indicates that our algorithm captures characteristics of the datasets that are not detected by the other algorithms, performs better even for high-dimensional datasets, and runs significantly faster. Experiments also reveal that while *Multipass BIC* requires initialization of a cover, *G-Mapper* does not due to utilizing a GMM. In addition, we illustrate that the number of intervals in the cover produced by *G-Mapper* could be utilized as input for other Mapper algorithms such as *F-Mapper*. We provide an open-source implementation (<https://github.com/MRC-Mapper/G-Mapper>) and we are working on distributing it as a stand-alone Python package.

1.2 Related Work

Following the original Mapper construction algorithm [38], most implementations of Mapper including [42, 40] construct the cover using open intervals or hypercubes of a fixed length with a fixed amount of overlap. However, the optimal number of intervals or amount of overlap to use is often unknown and the Mapper output is very sensitive to these parameters.

The implementation of Mapper in Giotto TDA [40] has a *balanced cover* method in which the user specifies the number of intervals and the algorithm finds a cover with the given number of intervals so that each interval covers the same number of points. This parameter is also difficult to know a priori and the method may not be elaborate on generating an optimal cover.

Statistical methods are utilized for optimizing a cover of the Mapper construction algorithm. Carrière, Michel, and Oudot introduced a statistical method to select these parameters [7]. The main idea is to sweep through various Mapper parameters to find the “best” Mapper graph that is structurally stable and close to a particular *Reeb graph* [34]. *Extended persistence* [12] developed by Cohen-Steiner, Edelsbrunner, and Harer is used to find this optimal Mapper graph. This method requires the user to know the Reeb graph to compare the Mapper graph against and relies on independent sampling conditions of the point cloud.

Clustering methods such as Fuzzy C -means [15, 3] and X -means [30] have been used for optimizing an open cover [5, 8]. These methods were already mentioned in the third paragraph of Section 1. The cover optimizing algorithm we propose is motivated by a clustering method called the G -means clustering [19].

2 Background

This section is devoted to reviewing the Mapper construction and statistical tools used in our proposed G -Mapper algorithm to tune the cover parameter. Section 2.1 describes the Mapper construction and we focus on a cover constructed from a set of points in \mathbb{R} . The central idea of our algorithm is to form cover elements (intervals) around points that appear to be normally distributed. In order to test if a set of points in an interval follows a Gaussian distribution, we apply the Anderson-Darling test that we explain in Section 2.2. If the statistical test indicates the points do not follow a Gaussian distribution, we split the interval into two intervals using a Gaussian mixture model reviewed in Section 2.3. In Section 2.4, we describe the G -means clustering algorithm that inspires our G -Mapper algorithm.

2.1 Mapper

The Mapper algorithm was first introduced in [38] and generates a graph or a network. The output is called a Mapper graph. For a given dataset X , constructing a Mapper graph consists of the following procedure that we illustrate in Example 2.1.

1. Define a lens (or filter) function $f : X \rightarrow Y$ from the point cloud X to a lower-dimensional space Y . In this paper, we focus on the case that the target space Y is a subset of \mathbb{R} , i.e., the space Y is of dimension 1.
2. Construct a cover $\mathcal{U} = \{U_i \mid U_i \text{ is open for } i \in I\}$ of the target space Y given in Step 1, i.e., $Y \subset \bigcup_{i \in I} U_i$. For a one-dimensional space Y , a cover of Y consists of overlapping intervals.
3. For each element U_i of the cover, apply a clustering algorithm to the pre-image $f^{-1}(U_i)$ of U_i under the lens function f . We use a density-based clustering algorithm called DBSCAN [17]. The algorithm is popularly chosen for Mapper because it does not require the number of clusters to be pre-determined and it detects arbitrarily shaped clusters. DBSCAN has two main parameters: epsilon, ε , and minimum samples, `MinPts`.
4. Create the Mapper graph whose vertices are the clusters found in Step 3, and an edge between two vertices exists if the two corresponding clusters share data points. The output is a simplified representation of the dataset X . Note that the Mapper graph is the 1-skeleton of the nerve of the cover of X generated in Step 3.

In Step 2, the conventional Mapper algorithm [38] employs covers consisting of intervals of uniform length and the overlap g between each two consecutive intervals. The parameter g and the number r of intervals are referred to as the *gain* and the *resolution*, respectively. The user should tune these two parameters to optimize a cover in the conventional Mapper algorithm.

We illustrate the Mapper construction algorithm by applying it to a toy dataset in Example 2.1.

Example 2.1 (Mapper Graph). Let X be the set of points sampled from a circle of radius $1/2$ with center at $(1/2, 1/2)$. Refer to Figure 1.

1. We define the lens function $f : X \rightarrow Y$ to be the projection map onto the first coordinate with the target space $Y = [-0.03, 1.05]$.
2. The cover $\{U_i\}_{i=1}^3$ is chosen to be three overlapping intervals of Y . Specifically, we set $U_1 = [-0.03, 0.39)$, $U_2 = (0.30, 0.72)$, and $U_3 = (0.64, 1.05]$. Consecutive intervals are overlapping by 20%.
3. The DBSCAN clustering algorithm generates four clusters where each of $f^{-1}(U_1)$ and $f^{-1}(U_3)$ forms a cluster and $f^{-1}(U_2)$ is separated into two clusters based on whether the points are in the upper or lower part of the circle.
4. The Mapper graph constructed in Step 4 is a cycle graph with four vertices and four edges. The color of each vertex in the Mapper graph is the average value of the lens function with the rainbow color map.

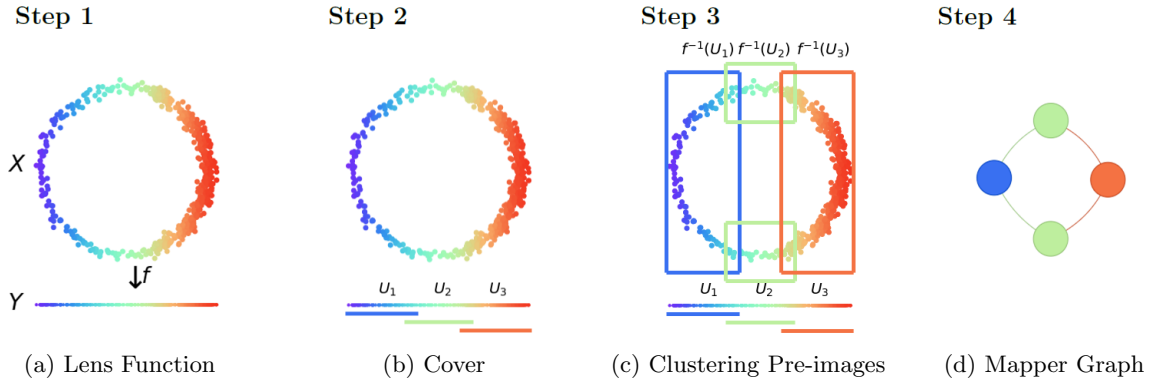


Figure 1: Mapper Construction. The dataset X consists of points sampled from a circle of radius $1/2$ with center at $(1/2, 1/2)$. Constructing a Mapper graph requires selecting a lens function f (Figure 1a) and cover $\{U_i\}$ (Figure 1b), and applying a clustering algorithm to $\{f^{-1}(U_i)\}$ (Figure 1c). The parameters are specified in Example 2.1, and the generated Mapper graph is a cycle graph with four vertices and four edges (Figure 1d).

2.2 Statistical test for a Gaussian distribution

The Anderson-Darling test is a statistical test to determine if data follows a Gaussian distribution [1, 39]. The test is similar to two other normality tests, the Komologorov-Smirnov test [28] and the Shapiro-Wilk test [36] in that it is computing test statistics based on the empirical distribution function (EDF).

Let $X = \{x_i\}_{i=1}^n$ be a given dataset. We standardize the data to yield a set $X' = \{x'_i\}_{i=1}^n$ such that X' has a mean of 0 and a variance of 1. Let $x'_{(i)}$ be the i^{th} ordered value of X' . Define $z_i = F(x'_{(i)})$, where F is the cumulative distribution function of the standard normal distribution. Let F_n be the sample cumulative distribution function. Then the *Anderson-Darling (AD)* statistic is defined to be the quadratic EDF statistic measuring differences between F and F_n :

$$A^2(X) = n \int_{-\infty}^{\infty} (F_n(x) - F(x))^2 w(x) dF(x),$$

where $w(x)$ is a weighting function given by $w(x) = (F(x)(1 - F(x)))^{-1}$. This weighting function places more weight on observations in the tails. Computing the integration results in

$$A^2(X) = -\frac{1}{n} \sum_{i=1}^n (2i - 1) (\log(z_i) + \log(1 - z_{n+1-i})) - n.$$

In the case where both μ and σ are unknown and estimated from the data, a modification of the statistic was suggested in [39] as follows:

$$A_*^2(X) = A^2(Z)(1 + 4/n - 25/n^2).$$

The user selects a critical threshold, which we call the *AD threshold*. The set of values exceeding the critical threshold is called the critical region. The null hypothesis H_0 , asserting that the data follows a Gaussian distribution, is rejected for values $A_*^2(X)$ in the critical region, and H_0 is not rejected for values below the AD threshold. The probability of A_*^2 occurring in the critical region under the null hypothesis is the *significance level* α . A table of critical values for varying significance levels can be found in [16].

2.3 Gaussian mixture models

A Gaussian mixture model (GMM) is a probabilistic model representing a probability density function as a finite weighted sum of Gaussian distributions (refer to Section 9.2.2 of [4]). The model learns a mixture model distribution with K components. The probability density function $p(x)$ of a real-valued vector x is given by

$$p(x) = \sum_{k=1}^K \pi_k N[x|m_k, \Sigma_k],$$

where π_k is a mixture probability with $\sum_{k=1}^K \pi_k = 1$, and $N[x|m_k, \Sigma_k]$ is the k^{th} Gaussian distribution with mean m_k and covariance Σ_k . See Example 2.2 for an illustration of the GMM. In order to fit the model, the GMM implements the expectation-maximization (EM) algorithm searching for the maximum likelihood estimators of model parameters. Since the GMM takes into account the covariance structure of the given data as well as the centers of the components, it is considered a generalization of k -means clustering. We will use the means and the variances generated by the GMM to create two overlapping intervals for the cover parameter in Mapper.

Example 2.2 (AD Statistic and GMM). Let X be a one-dimensional dataset whose histogram is shown in Figure 2. The AD statistic of the dataset X is 53.85. If we apply a GMM with two components on this dataset X , we get means $m_1 = 0.21$, $m_2 = 0.68$ and variances $\sigma_1 = 0.10$, $\sigma_2 = 0.16$. We divide the dataset into two sets based on if a point has a value less than 0.41 or not. The AD statistics of the left and right sides are 1.66 and 3.40, respectively. These values are much smaller than the AD statistic of the entire dataset X .

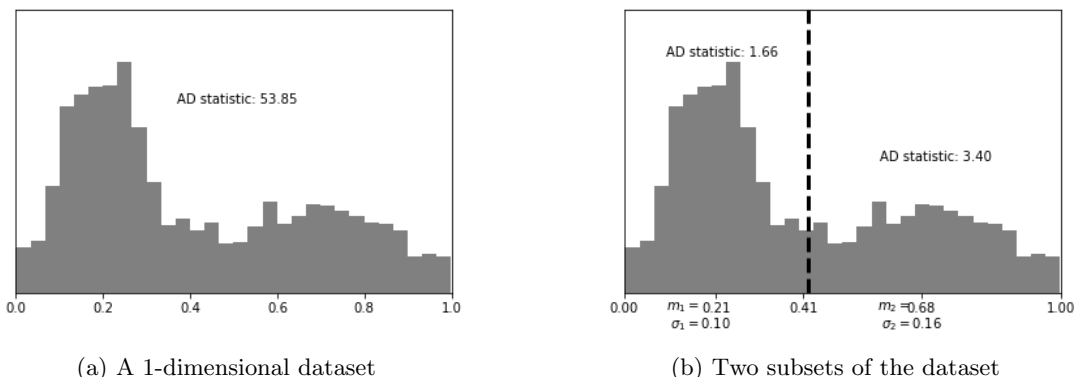


Figure 2: Anderson-Darling statistics and a Gaussian mixture model. Figure 2a. The histogram of a 1-dimensional dataset whose AD statistic is 53.85. Figure 2b. The GMM is applied to the dataset and the AD statistics of the left and right sides are much smaller than the AD statistic of the entire dataset.

2.4 *G*-means clustering

The *G*-means clustering algorithm [19] automatically detects the number k of clusters by employing the Anderson-Darling test to decide if a cluster should be split into two clusters. The algorithm starts by applying k -means to a dataset of vectors with a small number of centers. The algorithm is initialized with $k = 1$, or a larger k can be selected if there is some advance knowledge of the range of values of k .

Let \mathcal{C} be the set of derived clusters. Choose a cluster $C \in \mathcal{C}$ to be tested. Applying k -means with two components to C splits the cluster into two clusters C_1 and C_2 . Let ℓ be the line connecting the two centers of C_1 and C_2 and project the points of the cluster C onto ℓ . If the corrected Anderson-Darling statistic for the projected points is below the user-specified AD threshold, the cluster C is kept. Otherwise, the cluster C is deleted from \mathcal{C} and C_1 and C_2 are added. These steps are repeated until no more clusters are added.

3 Methods

We devise a method (*G*-Mapper) for learning a cover in the Mapper construction based on the *G*-means algorithm for learning the parameter k in identifying the correct number k of clusters.

3.1 *G*-Mapper Algorithm

The input for *G*-Mapper consists of (1) the image of a dataset X under the 1-dimensional lens f , i.e., $f(X)$, (2) the AD threshold, and (3) the percentage of overlap for intervals when an interval is split into two. This parameter is denoted by `g_overlap`.

The main differences between the *G*-Mapper algorithm and the *G*-means clustering algorithm are (1) we are interested in finding overlapping clusters (intervals) rather than disjoint clusters, (2) we design overlapping intervals using variances generated by the GMM rather than applying k -means, and (3) the *G*-Mapper algorithm also does not require a projection of points for performing the Anderson-Darling test since the lens employed in our algorithm is 1-dimensional.

For *G*-Mapper, we begin with the cover consisting of one interval containing $f(X)$, i.e., the interval $[\min\{f(X)\}, \max\{f(X)\}]$. The *G*-Mapper algorithm is iterative and proceeds as follows:

1. Select an interval from the current cover (a collection of intervals).
2. For the data points in the interval, perform a statistical test to determine if it follows a Gaussian distribution. For the test, we use the corrected Anderson-Darling statistic.
3. If the computed statistic is smaller than the AD threshold, keep the original interval.
4. Otherwise, split the interval into two overlapping intervals. We utilize the means and variances derived from the GMM, as described in detail in the following paragraph.

Repeat Steps 1-4 until no more intervals split.

See Example 3.1 for a step-by-step illustration of the *G*-Mapper algorithm.

We now provide the details of the splitting procedure in Step 4. Let m_1, m_2 and σ_1, σ_2 be the two means and the two standard deviations discovered from the GMM. An interval (a, b) is split into the following two intervals:

$$(a, \min\{m_1 + (1 + \text{g_overlap})\sigma_1/(\sigma_1 + \sigma_2)(m_2 - m_1), m_2\}), \text{ and} \\ (\max\{m_2 - (1 + \text{g_overlap})\sigma_2/(\sigma_1 + \sigma_2)(m_2 - m_1), m_1\}, b).$$

These two intervals are formed by considering a value [18]

$$\frac{\sigma_2}{\sigma_1 + \sigma_2}m_1 + \frac{\sigma_1}{\sigma_1 + \sigma_2}m_2 = m_1 + \frac{\sigma_1}{\sigma_1 + \sigma_2}(m_2 - m_1) = m_2 - \frac{\sigma_2}{\sigma_1 + \sigma_2}(m_2 - m_1)$$

dividing the two means m_1 and m_2 in the ratio $\sigma_1 : \sigma_2$ based on the minimum-error decision boundary between two Gaussian distributions [14] and extending the length between this value and each mean by `g_overlap`, respectively.

When applying the GMM algorithm to an interval, we take as two initial centers $c \pm \sqrt{2\lambda/\pi}$, where c and λ are the mean and variance of data points in the interval, respectively. This method is the 1-dimensional version of a recommended initialization using principal component analysis (PCA) [19]. However, even though we have a consistent way of initializing the centers, the initialization of the variances and mixing coefficients may be different each time we implement the *G-Mapper* algorithm on the same dataset. Thus, this can result in different *G-Mapper* graphs with the same parameters on the dataset.

The splitting algorithm has three variations based on deciding which unprocessed interval to check for Step 1. The following three search methods include:

- The *depth-first search* (DFS) method iteratively splits as deep as possible by choosing an interval with a bigger Anderson-Darling statistic. Once a chosen interval does not split, the method backtracks and explores an unchecked interval.
- The *breadth-first search* (BFS) method checks all intervals in the current cover. The interval with the biggest Anderson-Darling statistic is split. This process is repeated with the newly updated cover.
- The *randomized* method randomly selects an interval where intervals with a bigger Anderson-Darling statistic have a higher probability of being chosen.

In this paper, we adopted the DFS method for generating *G-Mapper* graphs, which is more time-efficient than the BFS method and more reproducible than the randomized method.

Example 3.1 (The *G-Mapper* Algorithm). We apply the *G-Mapper* algorithm to the circle dataset given in Example 2.1. We initialize the algorithm by selecting an AD threshold equal to 10, `g_overlap` equal to 0.2, and the DBSCAN clustering algorithm. The *G-Mapper* algorithm starts with the cover $\{U_0\}$ consisting of one interval, the entire target space $U_0 = Y = [-0.03, 1.05]$. The Mapper graph at this iteration is a single vertex. In the first iteration, the AD statistic of U_0 is 32.09. Since $32.09 > 10$, the first interval is split into two intervals $U'_0 = [-0.03, 0.65)$ and $U''_0 = (0.52, 1.05]$. The Mapper graph at this iteration is an edge. In the second iteration, the AD statistics of U'_0 and U''_0 are 3.30 and 10.64, respectively. Since $10.64 > 10$, the interval U''_0 is split into $U_2 = (0.52, 0.89)$ and $U_3 = (0.84, 1.05]$ so that $\{U_1, U_2, U_3\}$ is a cover of Y with $U_1 = U'_0 = [-0.03, 0.65)$. The Mapper graph is a cycle graph with 4 vertices.

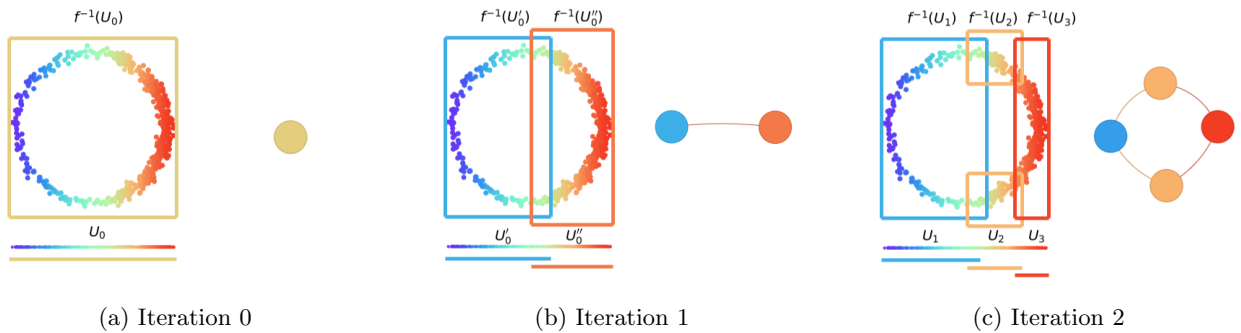


Figure 3: *G-Mapper*. The initialization and first two iterations of the splitting procedure are represented in Figure 3a, Figure 3b, and Figure 3c respectively. The cover, the pre-images of the cover elements, and the corresponding Mapper graph are located on the lower left side, the upper left side, and the right side, respectively. The final Mapper graph is a cycle graph with 4 vertices.

3.2 Parameter Selection for the G -Mapper Algorithm

The G -Mapper algorithm involves two key user-specified parameters: `AD.threshold`, the critical value corresponding to the significance level α for the statistical test, and `g_overlap`, the amount of overlap when an interval is split in two. One important thing to note is that unlike the Multipass AIC/BIC algorithm, the G -Mapper algorithm does not require the user to initialize an open cover. In the next section, we show G -Mapper performs well without this initialization.

The first parameter is `AD.threshold` corresponding to the significance level α for the statistical test. The significance level is the probability of making a Type I error meaning we incorrectly reject the null hypothesis H_0 . As the parameter (resolution) for the number of intervals of a cover in the conventional Mapper algorithm, `AD.threshold` influences the number of nodes of the output graph. Setting a lower threshold segments the given data into more pieces, which produces a more detailed Mapper graph with more nodes. Taking a high threshold yields a coarse-grained visualization with the graph having fewer nodes.

The second parameter is `g_overlap` which specifies how much two intervals should overlap when applying a split. In the G -Mapper algorithm, a split is made utilizing the means and variances estimated by the GMM together with this parameter. As the overlap parameter (gain) in the conventional Mapper algorithm, `g_overlap` controls relationships between overlapping clusters. Increasing this parameter generates more edges between nodes in the Mapper graph, which results in a more compact graph representation. Decreasing this parameter makes the output Mapper graph less connected, segmenting nodes in the graph into smaller groups.

4 Experimental Results

In this section, we present the results of applying the G -Mapper algorithm to both synthetic and real-world datasets compared to fine-tuned Mapper graphs resulting from the conventional Mapper algorithm. We call the fine-tuned Mapper graphs the *reference Mapper graphs*. This is followed by a comparison to the current state-of-the-art Mapper construction algorithms (Multipass BIC, F -Mapper, and balanced cover). We explore how Mapper graphs built from G -Mapper and Multipass BIC are different. For the latter two algorithms, we utilize the number of intervals detected by G -Mapper as an input parameter. Finally, we close the section by providing a runtime comparison between all methods.

4.1 Synthetic Datasets

We first applied the G -Mapper algorithm to three synthetic datasets (two circles, human, and Klein bottle datasets). Our experiments reveal that G -Mapper generates Mapper graphs that aptly describe the intrinsic structure of the original datasets. Furthermore, the output G -Mapper graphs turn out to be close to the reference Mapper graphs. For each dataset, three figures for the original dataset and these two Mapper graphs will be presented together.

We describe the two main parameters (`g_overlap` and `AD.threshold`) of G -Mapper for the synthetic datasets. For all datasets, we set the parameter `g_overlap` to 0.1. We pick different Anderson-Darling (AD) thresholds according to the datasets. We use 10 as the thresholds for the two circles and human datasets, and a larger value of 15 for the Klein bottle dataset to prevent generating an overly detailed Mapper graph.

In order to better visualize the characteristics of nodes in Mapper graphs, we color nodes with the rainbow colormap. In all Mapper graphs of synthetic datasets, the color of a node represents the average value of the lens function over all data points in the node.

4.1.1 Two Circles Dataset

The two circles dataset comprises 5,000 sampled points from two concentric circles. The lens function is the sum of the x and y coordinates normalized. The reference Mapper graph consists of two concentric circles. The G -Mapper graph also consists of two concentric circles and the graph was found in 7 iterations. Note that the generated Mapper graphs retain the homological features of the underlying space. In Figure 4, we present Mapper graphs along with the parameters used.

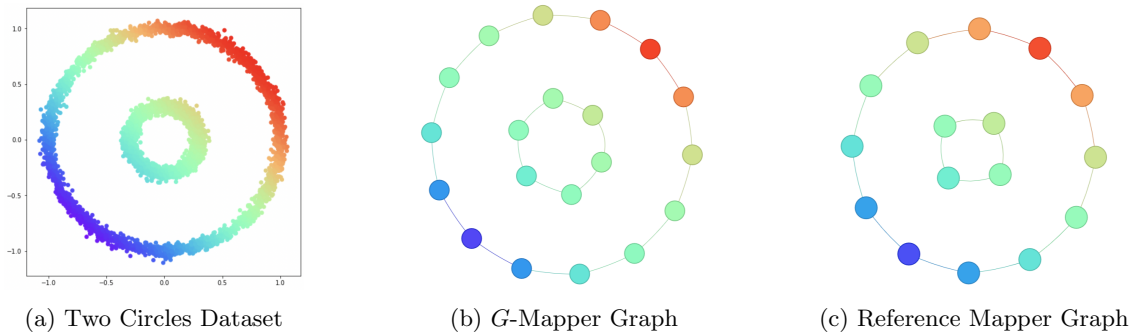


Figure 4: Two Circles Dataset. G -Mapper Parameters: AD threshold = 10, $g_overlap$ = 0.1, clustering algorithm = DBSCAN with ϵ = 0.1 and $MinPts$ = 5, and search method = DFS. The cover was found in 7 iterations and consists of 8 intervals. Reference Mapper Parameters: number of intervals = 7, overlap = 0.2, and the same DBSCAN parameters.

4.1.2 Human Dataset

The next point cloud dataset we explored is a 3D human shape from [9] that consists of 4,706 points. The lens function is the height function normalized. In Figure 5, we present Mapper graphs along with the parameters used. The cover for G -Mapper was found in 11 iterations. Both the reference Mapper graph and the G -Mapper graph represent human skeletons consisting of a head, two arms, and two legs. While each body part in the G -Mapper graph has fewer nodes than its counterpart in the reference Mapper graph, the ratios of any pairs of the body parts are consistent.

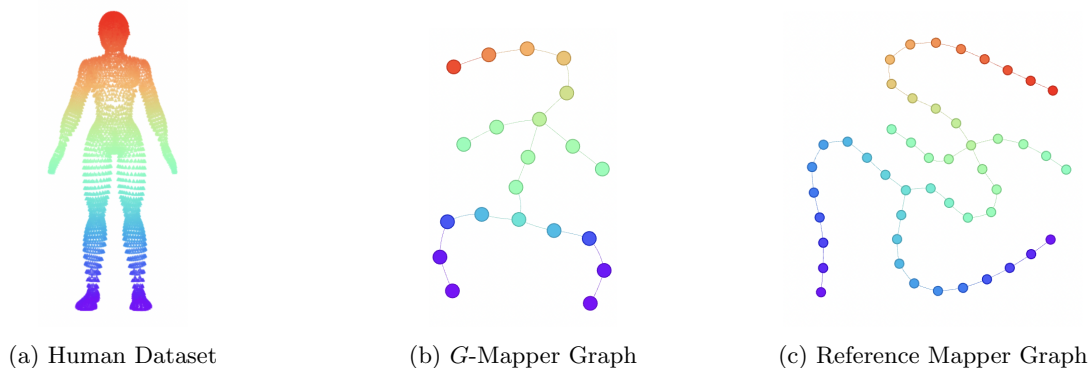


Figure 5: Human Dataset. G -Mapper Parameters: AD threshold = 10, $g_overlap$ = 0.1, clustering algorithm = DBSCAN with ϵ = 0.1 and $MinPts$ = 5, and search method = DFS. The cover was found in 11 iterations and consists of 12 intervals. Reference Mapper Parameters: number of intervals = 30, overlap = 0.4, and the same DBSCAN parameters.

4.1.3 Klein Bottle Dataset

The Klein bottle dataset consists of 15,875 points sampled from the Klein Bottle embedded in \mathbb{R}^5 . The dataset is obtained from the Gudhi library [27]. The lens function is the projection map onto the first coordinate normalized. In Figure 6, we present Mapper graphs along with the parameters used. The reference Mapper graph exhibits a long cycle with several flares (branches). The G -Mapper algorithm produces a highly similar graph in 16 iterations.

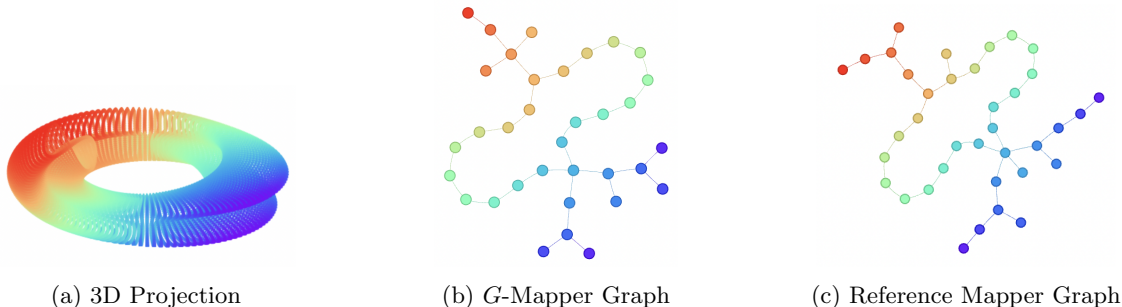


Figure 6: Klein Bottle Dataset. G -Mapper Parameters: AD threshold = 15, `g_overlap` = 0.1, clustering algorithm = DBSCAN with $\epsilon = 0.21$ and `MinPts` = 5. The cover was found in 16 iterations and consists of 17 intervals. Reference Mapper Parameters: number of intervals = 19, overlap = 0.4, and the same DBSCAN parameters.

4.2 Real-World Datasets

We next applied G -Mapper to three real-world datasets: *Passiflora* leaves, COVID-19 trends, and the CIFAR-10 image dataset. We explain these datasets in detail in Section 4.2.1, Section 4.2.2, and Section 4.2.3, respectively. Each data point is labeled by its morphotype, the state the data point was taken, and its image class in the *Passiflora* dataset, COVID-19 dataset, and CIFAR-10 image dataset, respectively. These datasets are of higher dimension than the synthetic datasets explored in the previous section. We visualize the nodes in the Mapper graphs as pie charts in order to represent the proportions of data points within the nodes belonging to different labels.

4.2.1 Passiflora Dataset

The *Passiflora* dataset [10] consists of 3,319 leaves from 40 different species of the *Passiflora* genus. Leaves of the *Passiflora* genus are of particular interest to biologists due to their remarkable diversity of shape. Each leaf in the dataset has 15 landmarks whose locations are 2-dimensional vectors expressed as x and y coordinates. Consequently, each leaf is represented as a 30-dimensional vector, and the correlation distance is used to measure the distance between leaf vectors. The correlation distance between two vectors is defined as $1 - r$, where r is the Pearson correlation coefficient. In this metric, leaf vectors with a high correlation will have a distance near zero.

The authors of [10] classified the 40 species into seven different morphotypes. For the classification, they performed principal component analysis (PCA) on the landmark dataset described in the previous paragraph and elliptical Fourier descriptors on the outline of the leaf. The first and second principal components are visualized in Figure 7a (given in [10, Figure 5] and [31, Figure 3C]). Because of the significant amount of overlap shown in the PCA plot, the authors also relied on their domain knowledge when assigning morphotypes. Mapper may help extend this process further to obtain better separation between morphotypes and extract hidden relationships between morphotypes. The Mapper algorithm has been utilized in [31] for this purpose.

In Figure 7b, we present the results of applying G -Mapper to the *Passiflora* dataset using the first principal component as the lens function. The G -Mapper graph has a strong linear backbone along the first principal component. The Mapper graph has multi-colored nodes with purple, brown, and red, meaning there is much overlap in the morphotypes, whereas it has single-colored nodes with orange, green, and pink, meaning the morphotypes are more distinct, as shown in the PCA plot. The reference Mapper graph shown in Figure 7c is generated based on parameters given in [31]. The G -Mapper graph is close to the reference Mapper graph in that it has a strong linear backbone and the coloring of nodes is similar.

However, these two Mapper graphs have different features originating from their constructions. The G -Mapper graph produces more edges between the multicolored purple, red, and green nodes compared to the reference Mapper graph. We suspect this is due to the greater density and overlap of morphotypes having a projection onto the first principal component range between 0-0.2. G -Mapper constructs more intervals in areas that are more dense whereas conventional Mapper constructs intervals in a uniform manner. In addition, the G -Mapper graph has more red nodes and fewer blue nodes than the reference Mapper graph since G -Mapper takes the distribution of the data into account.

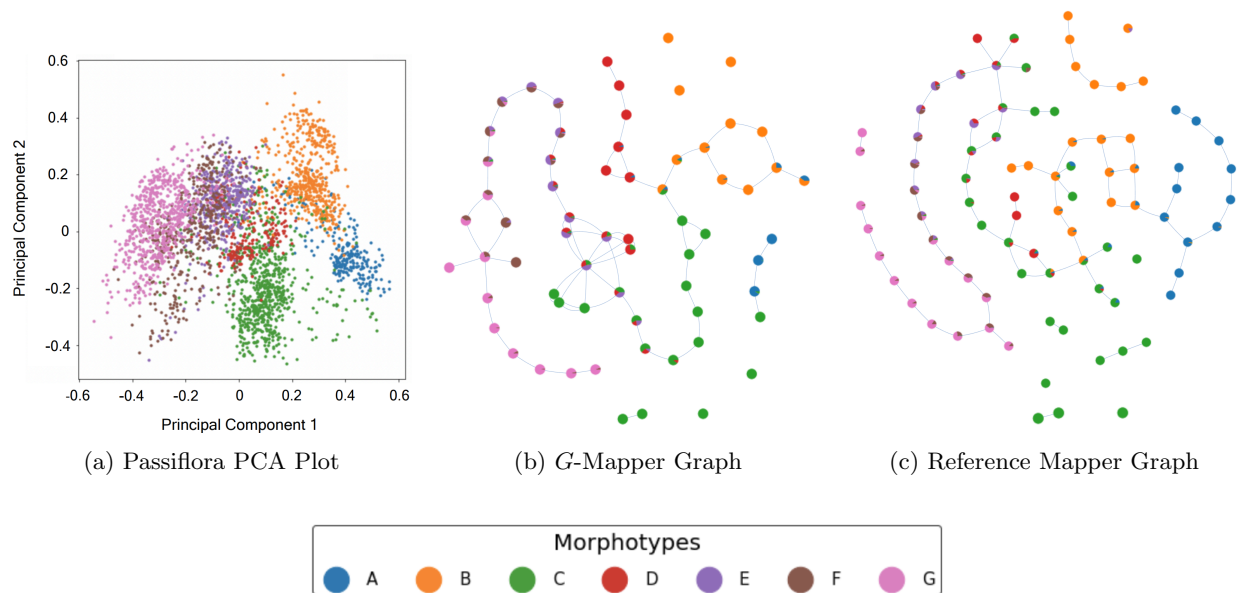


Figure 7: *Passiflora* Dataset. Lens Function: the first principal component normalized. G -Mapper Parameters: AD threshold = 2, $g_overlap$ = 0.1, clustering algorithm = DBSCAN with ϵ = 0.15, MinPts = 5, and distance = correlation distance, and search method = DFS. The open cover was found in 37 iterations and consists of 38 intervals. Reference Mapper Parameters: number of intervals = 40, overlap = 0.5, and the same DBSCAN parameters.

4.2.2 COVID-19 Dataset

COVID-19 data was collected in [13] and can be found in the data repository (<https://github.com/CSSEGISandData/COVID-19/>). In order to analyze COVID-19 state-wide trends, the authors of [45] selected 1,431 daily records of COVID-19 cases during 159 days between April 12, 2020 to September 18, 2020 for nine states (AZ, CA, FL, GA, IL, NC, NJ, NY, TX) from the dataset. These nine states were chosen since they had the largest number of confirmed cases. For each day, the dataset has the following 7 attributes: the numbers of confirmed cases, death cases, active cases, people tested, testing rate, mortality, and the numbers of cases per 100,000 people, where the number of active cases is defined by subtracting the number of death cases and recovered cases from the number of confirmed cases. Since the number of recovered cases is unavailable in some states, we simply estimate the number of active cases by the number of confirmed cases minus the number of death cases.

In Figure 8a, we present the results for applying G -Mapper to the COVID-19 dataset along with the parameters. The figure suggests that G -Mapper is able to identify COVID-19 trends according to each state and provides information concerning the relationships between them. The Mapper graph consists of three connected components: the main component, the pink component (NY), and the brown component (NJ), which suggests that NY and NJ have COVID-19 trends distinct from the other states. The purple branch (IL), orange branch (CA), green branch (FL), olive branch (TX), and gray branch (NC) appear sequentially in the main component. Two color nodes with blue (AZ) and red (GA) show up, which indicates that these two states share very similar COVID-19 trends at some point. These two states eventually bifurcate into a blue branch (AZ) and red branch (GA). We observe that the G -Mapper graph closely resembles the reference Mapper graph presented in Figure 8b since the features listed in this paragraph also appear in the reference Mapper graph.

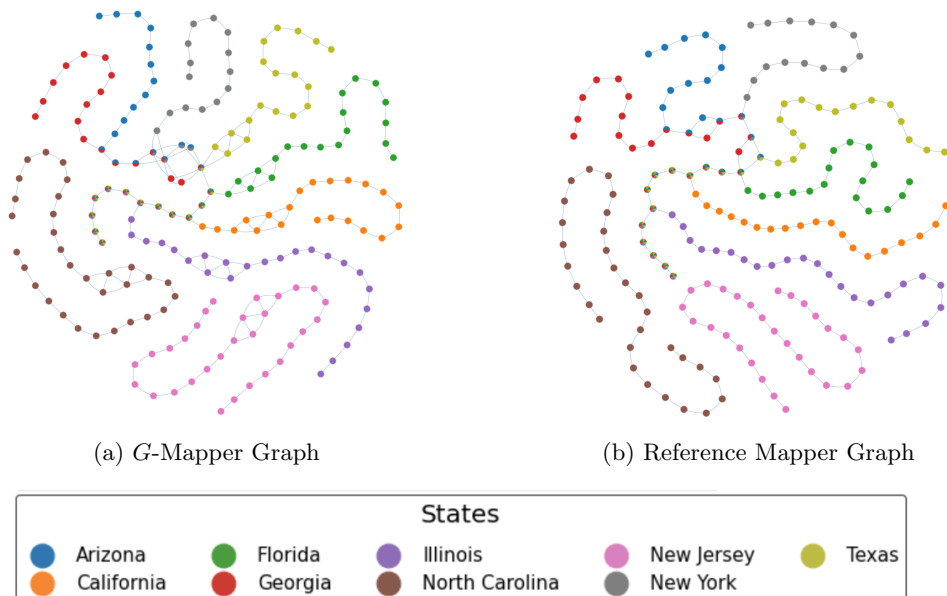


Figure 8: COVID-19 Dataset. Lens Function: the number of recorded days normalized. G -Mapper Parameters: AD threshold = 1.35, $g_{\text{overlap}} = 0.15$, clustering algorithm = DBSCAN with $\epsilon = 0.15$ and $MinPts = 5$, and search method = DFS. The open cover was found in 30 iterations and consists of 31 intervals. Reference Mapper Parameters: number of intervals = 30, overlap = 0.3, and the same DBSCAN parameters.

4.2.3 CIFAR-10 Dataset

The last real-world dataset we analyzed is a famous image dataset called CIFAR-10 [25]. The dataset consists of 60,000 images (50,000 training images and 10,000 test images) in 10 classes. The 10 different classes represent airplanes, automobiles, birds, cats, deer, dogs, frogs, horses, ships, and trucks. The raw dataset consists of 32×32 color images. The input data for applying the Mapper algorithm is obtained by learning the training images with the ResNet-18 neural network, passing the test images through the network, and collecting activation vectors from the last layer. Then 10,000 activation vectors are collected with 1,000 vectors per class, and each vector is 512-dimensional, which is tremendously higher than the previous two datasets.

The t-distributed stochastic neighbor embedding (t -SNE) algorithm is a well-known dimensionality reduction method [41]. A 2-dimensional t-SNE embedding of the collection of activation vectors is represented in Figure 9a. The plot shows that t-SNE separates the data points into the 10 different classes with some of the classes overlapping. In order to highlight relationships among the 10 classes, [32, 45, 8] utilized the Mapper algorithm.

Figure 9b and Figure 9c represent the G -Mapper graph and the reference Mapper graph for the dataset, respectively. Both Mapper graphs classify the data points into the 10 classes and detect three pairs of classes with some similarities. The three pairs are automobiles (orange points) and trucks (cyan points), cats (red points) and dogs (brown points), and airplanes (blue points) and birds (green points). The two classes in each of these three pairs are regarded as having similar features. Each pair has nodes containing data points in both classes, and it eventually bifurcates into two different branches with each branch representing a distinct class.

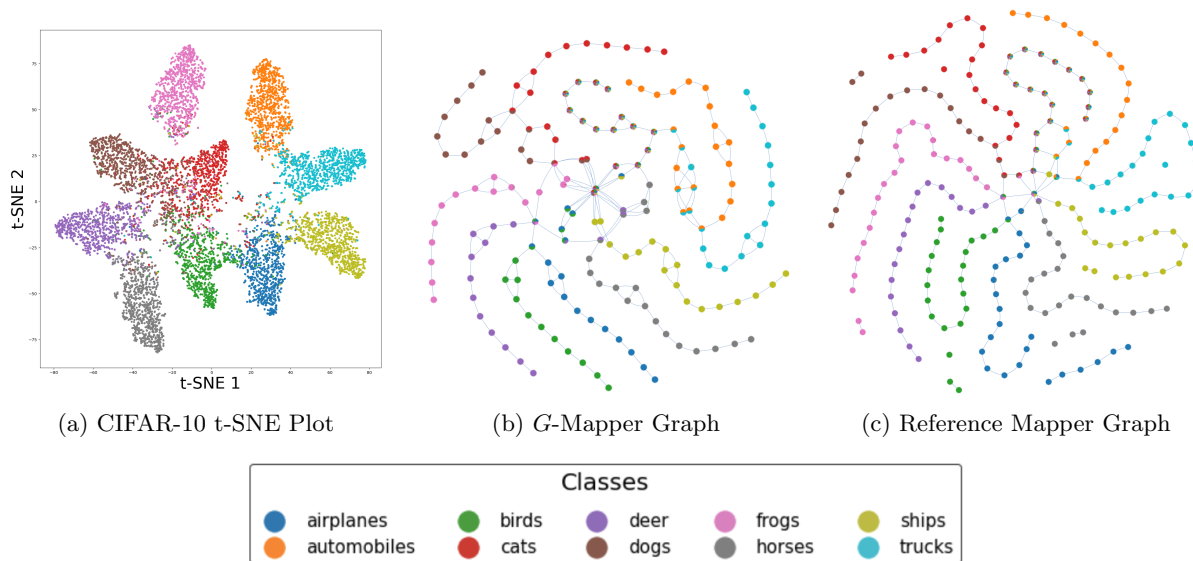


Figure 9: *CIFAR-10* Dataset. Lens Function: the L_2 norm of each activation vector. G -Mapper Parameters: AD threshold = 9, $g_{\text{overlap}} = 0.2$, clustering algorithm = DBSCAN with $\epsilon = 2$ and $\text{MinPts} = 5$, and search method = DFS. The open cover was found in 32 iterations and consists of 33 intervals. Reference Mapper Parameters: number of intervals = 70, overlap = 0.35, and the same DBSCAN parameters.

4.3 Comparison to Other Methods

We compare the G -Mapper algorithm to other state-of-the-art techniques on the same synthetic and real-world datasets as above. We analyze how Mapper graphs generated by another iterative algorithm, the Multipass BIC algorithm, are different from G -Mapper graphs. In addition, we produce Mapper graphs from F -Mapper and the balanced cover strategy utilizing the number of cover intervals estimated by G -Mapper as an input parameter. We refer the reader to [8, Sect. VI-A] for a discussion and analysis of the performance of the statistical cover strategy. Throughout this section, we maintain the same DBSCAN parameters as used in G -Mapper for each dataset.

4.3.1 Multipass BIC

The Multipass BIC algorithm repeatedly splits intervals uniformly from some initialized coarse cover based on information criteria. The main parameters that need to be specified for this algorithm include the initial number of intervals used before splitting and the amount of overlap between consecutive intervals in the cover. There is also a threshold parameter δ for deciding when to split, but this is often set to zero meaning that a split is performed as long as the information criterion statistic improves. We set $\delta = 0$, use the BIC statistic, and use the DFS method. We tried to follow the parameters specified in [8], but we had to adjust overlap parameters due to an error in the Multipass AIC/BIC code. Mapper graphs built by the code failed to create edges between nodes generated from non-consecutive intervals even though they shared data points.

Figure 10 shows that the Multipass BIC algorithm provides a simplified representation of the datasets although the algorithm does not thoroughly capture the essence of each dataset. For the two circles dataset, the inner circle does not appear while the outer circle consists of numerous nodes. For the human dataset, the two arms in the output graph are much shorter than the two legs. Several flares are missing from the Klein bottle output graph. Additionally, we see in the Klein bottle dataset that starting from the numbers of intervals less than the input, 4, used for generating Figure 10c does not lead to splitting intervals. This experiment indicates that choosing the initial number of intervals is a crucial task, which is not required in the G -Mapper algorithm.

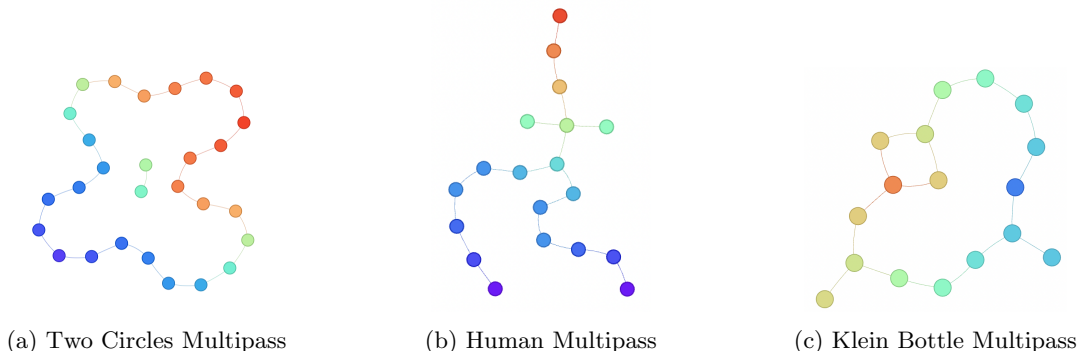


Figure 10: Results of using the Multipass BIC Algorithm on the Synthetic Dataset. Figure 10a Two Circles: number of initial intervals = 2 and overlap = 0.2. Figure 10b Human: number of initial intervals = 2 and overlap = 0.2. Figure 10c Klein Bottle: number of initial intervals = 4, and overlap = 0.4. The numbers of resulting intervals are 14, 10, and 8, respectively.

Figure 11 represents the Mapper graphs generated by applying the algorithm to the real-world datasets. For the Passiflora dataset, the algorithm does not split the intervals for the pink and purple data points effectively while it splits intervals for blue data points unduly. The Mapper graph for the COVID-19 dataset has similar features to the G -Mapper graph even though it has a lot more nodes than the G -Mapper graph. The Mapper graph for the CIFAR-10 dataset separates the 10 different classes, but it does not capture relationships between the classes. In addition, the algorithm splits specific intervals interminably since the data is very high-dimensional, and hence we had to limit the minimum length of intervals.

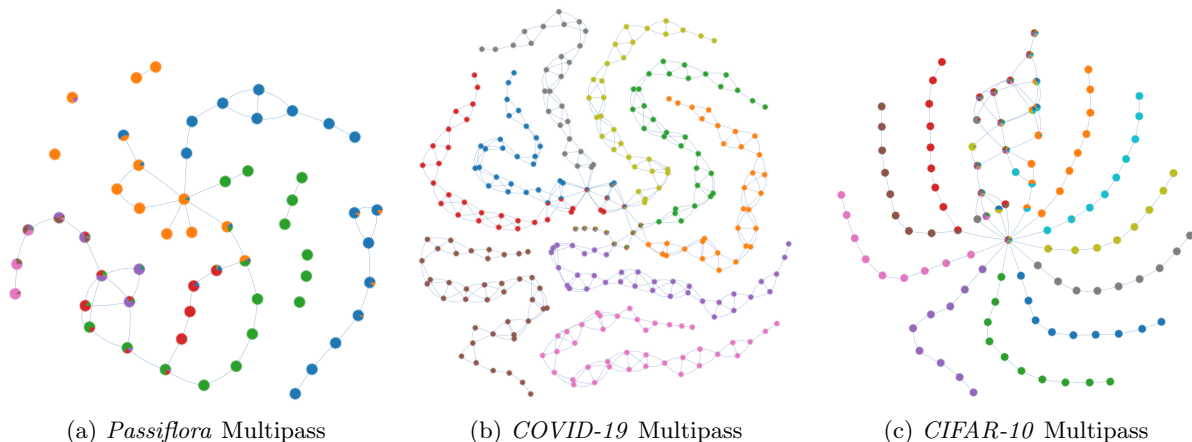


Figure 11: Results of using the Multipass BIC Algorithm on the Real-World Datasets. Figure 11a Passiflora dataset: number of initial intervals = 2 and overlap = 0.2. Figure 11b COVID-19 dataset: the number of initial intervals = 2 and overlap = 0.5. Figure 11c CIFAR-10 dataset: number of initial intervals = 2 and overlap = 0.2. The numbers of resulting intervals are 28, 40, and 22, respectively.

4.3.2 *F*-Mapper

The *F*-Mapper algorithm finds open intervals based on the Fuzzy *C*-means clustering. For the Mapper construction, Fuzzy *C*-means is applied to cluster the image $f(X)$ of the data points X under a lens function f . For each $p \in f(X)$, the clustering method provides a probability that p belongs to each cluster. To construct intervals from this clustering, the user needs to specify a probability threshold τ . If the probability that p belongs to a specific cluster exceeds τ , then it is declared to be part of the interval containing p .

F-Mapper requires the user to specify parameters, including the number of clusters, a threshold value, an exponent value for determining how “fuzzy” to make the clusters, and an error or convergence parameter. In [5], an exponent value of 2 and an error of 0.005 were used for all their examples. The threshold value can be viewed as an overlap parameter. As mentioned before, the number of clusters is difficult to know a priori and is the parameter we are trying to estimate with *G*-Mapper.

As an input parameter for the *F*-Mapper algorithm, we picked the number of intervals obtained from *G*-Mapper and applied the algorithm to each dataset. For its implementation, we used the Python package SciKit-Fuzzy 0.4.2 to implement *F*-Mapper. The results and parameters for *F*-Mapper are given in Figure 12 and Figure 13. These figures illustrate that *F*-Mapper with our selective inputs produces Mapper graphs that are almost identical to the reference Mapper Graphs. These examples suggest that *G*-Mapper could be a useful tool to determine the number of intervals as its input parameter for *F*-Mapper.

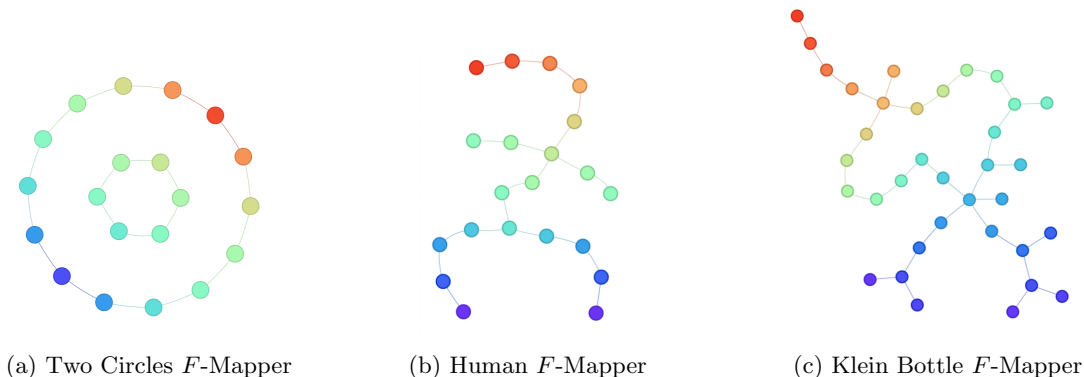


Figure 12: Results of using the *F*-Mapper Algorithm on the Synthetic Datasets. The numbers of clusters used for Figure 12a, Figure 12b, and Figure 12c are 8, 12, and 17, respectively.

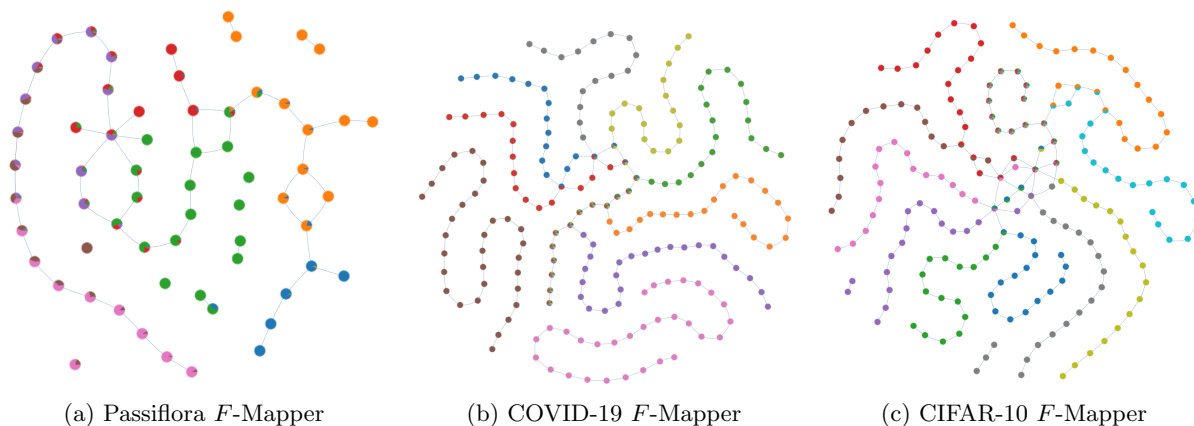


Figure 13: Results of using the *F*-Mapper Algorithm on the Real-World Datasets. Figure 13a Passiflora dataset: number of intervals = 38. Figure 13b COVID-19 dataset: number of intervals = 31. Figure 13c CIFAR-10 dataset: number of intervals = 33.

4.3.3 Balanced Cover

The balanced cover strategy forms open intervals so that each interval contains the same number of points. To apply the method, the user must specify the number of intervals. When we choose the number of intervals found using *G-Mapper* as the input for the balanced cover method as done in *F-Mapper*, it does not always generate the desired Mapper graph because of differences in constructing covers. Hence, we start from the number of intervals obtained by *G-Mapper* and adjust this number in order to decide the optimal input number of intervals for the balanced cover strategy.

In Figure 14 and Figure 15, we present Mapper graphs generated by applying the balanced cover strategy to the synthetic and real-world datasets along with the parameters used. For the synthetic datasets, we chose the number of intervals found using the *G-Mapper* algorithm except for the human dataset. For that dataset, *G-Mapper* found 12 intervals but this number results in a disconnected Mapper graph for the Balanced strategy so we opted for 13 intervals instead. For the real-world datasets, we selected the number of intervals derived from *G-Mapper* except for the CIFAR-10 dataset. For that dataset, *G-Mapper* found 33 intervals but this number failed to capture the relationship between airplanes (blue points) and birds (green points) for the Balanced strategy so we decided to use 29 intervals instead. Figure 14 and Figure 15 indicate that the balanced cover strategy can generate Mapper graphs similar to both *G-Mapper* graphs and the reference Mapper graphs although they are not almost identical as in *F-Mapper*.

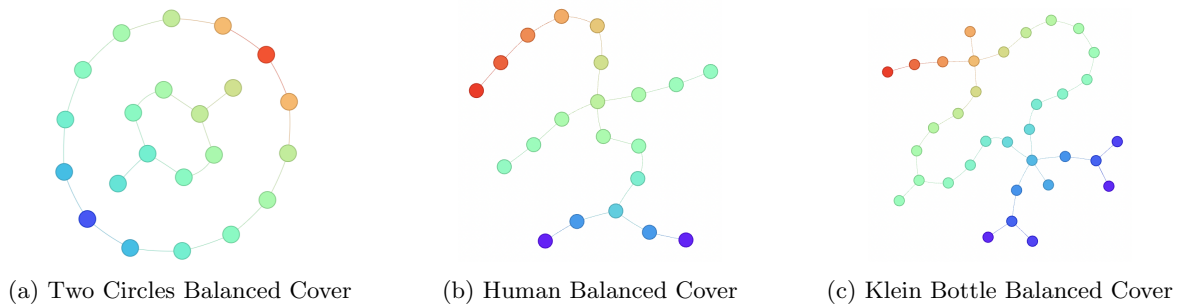


Figure 14: Results of using the Balanced Cover Strategy on the Synthetic Datasets. The numbers of intervals used for Figure 14a, Figure 14b, and Figure 14c are 8, 13, and 17, respectively.

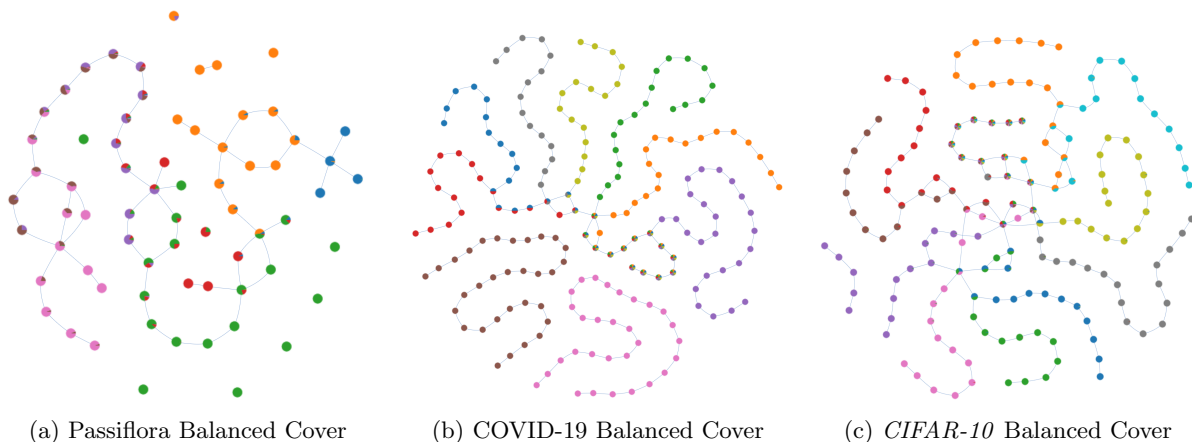


Figure 15: Results of using the Balanced Cover Strategy on the Real-World Dataset. Figure 15a *Passiflora* dataset: number of intervals = 38. Figure 15b COVID-19 dataset: number of intervals = 31. Figure 15c *CIFAR-10* dataset: number of intervals = 29.

4.3.4 Runtime Analysis

In Table 1, we provide the runtimes of generating covers of Mapper construction algorithms in seconds for G -Mapper, Multipass BIC, F -Mapper, and the balanced cover strategy. All the algorithms are executed on a 5 GHz, 8-core laptop with 8 GB of RAM. The times in Table 1 are averaged over five trials and the sizes and the dimensions of the datasets are also listed in the table.

The G -Mapper algorithm computes a cover faster than the Multipass BIC strategy on all datasets, and is significantly faster for four of the datasets. These four datasets are high-dimensional or have big sizes. The AD statistic is a splitting criterion in G -Mapper and is evaluated on an individual interval. On the other hand, deciding to split an interval for Multipass BIC involves (1) performing a soft clustering on the pre-image of two intervals, if the interval is split for constructing nodes of a Mapper graph, (2) performing a hard clustering on the same set using the previous clustering result, and (3) computing the BIC of the hard clustering. We observe that the first step is the most time-consuming part of the above three steps, dominating the time required for computing the AD statistic in G -Mapper.

G -Mapper performs faster than F -Mapper for all datasets, and runs significantly faster for the three datasets that are high-dimensional or have big sizes. Hence, utilizing the number of cover intervals generated by G -Mapper as an input parameter for F -Mapper is more effective in regards to runtime than applying F -mapper multiple times while varying the number of cover intervals. Since the balanced cover strategy only considers the number of data points in each interval, it computes an open cover much faster than the other methods.

Dataset	Size	Dim	G -Mapper	Multipass BIC	F -Mapper	Balanced
Two Circles	5000	2	0.170	1.959	0.202	0.000177
Human	4706	3	0.182	1.448	0.294	0.000211
Klein Bottle	15875	5	0.414	36.095	8.109	0.000155
Passiflora	3319	30	0.197	6.798	2.492	0.000173
COVID-19	1431	7	0.114	2.151	0.338	0.000147
CIFAR-10	10000	512	0.350	60.849	8.012	0.000133

Table 1: Size, dimension, and runtime in seconds of each dataset for each algorithm.

5 Discussion and Conclusion

We have proposed G -Mapper, a novel method for optimizing the cover parameter of a Mapper graph that is motivated by G -means clustering. G -Mapper involves an iterative procedure of splitting cover elements using statistical tests and Gaussian Mixture Models (GMMs). The Multipass AIC/BIC algorithm is based on X -means clustering and iteratively splits intervals according to information criteria. These two methods aim to select an optimal number of intervals. Another Mapper construction algorithm, F -Mapper, relies on Fuzzy C -means clustering. In contrast to the previous two algorithms, F -Mapper requires choosing the number of intervals in advance. To address this issue, we suggest utilizing the number of intervals generated by G -Mapper as an input for F -Mapper, and show that it is effective in our examples (see Section 4.3.2).

Our experiments (given in Section 4.1 and Section 4.2) for synthetic and real-world datasets reveal that G -Mapper is able to generate Mapper graphs that illustrate key features of the given data. G -Mapper works well even on non-spherical datasets and high-dimensional datasets as does G -means. We found that the G -Mapper algorithm extracts essential parts that are not uncovered by the Multipass BIC algorithm based on information criteria (see Section 4.3.1). In addition, the runtime comparison (given in Section 4.3.4) shows that G -Mapper considerably outperforms Multipass BIC. The running time of G -Mapper hardly depends on the dimension and the size of a given dataset while Multipass BIC is overwhelmingly influenced by these factors.

The G -Mapper method makes use of a GMM for splitting an interval into two overlapping intervals, which provides an elaborate splitting of intervals. Also, this approach enables G -Mapper to start from the whole target space without choosing the initial number of intervals. In contrast, regardless of the distribution of a given dataset, the conventional Mapper employs uniform covers, and the Multipass AIC/BIC uniformly splits intervals and requires initialization of a cover. We utilize the means and the variances derived from the GMM for designing two overlapping intervals (refer to Section 3.1). Considering the weight of each mixture component would give a more specified splitting.

Various clustering algorithms other than G -means, X -means, and Fuzzy C -means may also be suitable to optimize covers in the Mapper construction. Spectral clustering [43] uses the connectivity of data points instead of compactness like k -means, and its fuzzy versions can be found in [35, 44]. Agglomerative clustering [23, 22] is a hierarchical algorithm that recursively merges the closest pairs of clusters, and its fuzzy version was established in [24]. A recent clustering algorithm [2] introduces a novel technique, partitioned local depth cohesion, interpreted as cohesion, but its soft clustering version has not been developed.

We compared different methods for selecting a cover using qualitative methods and runtimes. We leave making more quantitative comparisons between the Mapper outputs of the different methods as future work. A co-optimal transport metric between hypergraphs is proposed in [11]. Since Mapper graphs can be viewed as hypergraphs, the metric is suitable for comparing different Mapper graph outputs from each cover selection method as it was utilized in [33, 46].

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