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Andreas Adolfsson, Margareta Ackerman, Naomi C. Brownstein

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**Highlights**

- The paper surveys and compares clusterability tests
- New clusterability tests are proposed
- Type I error and power of clusterability methods are reported for simulated data
- Clusterability tests are applied to well-known non-simulated data
- Provide guidelines to help users to select among clusterability tests

# To Cluster, or Not to Cluster: An Analysis of Clusterability Methods

Andreas Adolfsson<sup>a</sup>, Margareta Ackerman<sup>a,1</sup>, Naomi C. Brownstein<sup>b,1,\*</sup>

<sup>a</sup>*Department of Computer Engineering  
Santa Clara University  
500 El Camino Real  
Santa Clara, CA 95053*

<sup>b</sup>*Department of Behavioral Sciences and Social Medicine  
Florida State University  
1115 West Call Street  
Tallahassee, FL, 32306-4300*

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## Abstract

Clustering is an essential data mining tool that aims to discover inherent cluster structure in data. For most applications, applying clustering is only appropriate when cluster structure is present. As such, the study of clusterability, which evaluates whether data possesses such structure, is an integral part of cluster analysis. However, methods for evaluating clusterability vary radically, making it challenging to select a suitable measure. In this paper, we perform an extensive comparison of measures of clusterability and provide guidelines that clustering users can reference to select suitable measures for their applications.

*Keywords:* clusterability, cluster structure, cluster tendency, dimension reduction, multimodality tests

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## 1. Introduction

Clustering is an ubiquitous data analysis tool applied across diverse disciplines, such as bioinformatics, marketing, and image segmentation. Its wide utility is perhaps unsurprising, as its intuitive aim - to divide data into groups of similar items - applies at various stages of the data analysis process, from exploratory data analysis to collaborative filtering.

Despite its popularity, we have barely scratched the surface on fundamental questions about clustering. Issues as basic as the definition of clustering are being raised [1, 2]. Differences between clustering algorithms are studied to decide which should be used under different circumstances [3, 4, 5, 6]. Yet, perhaps an even more fundamental issue than algorithm selection is when clustering should, or should not, be applied.

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\*Corresponding author

*Email addresses:* aadolfsson@scu.edu (Andreas Adolfsson), mackerman@scu.edu (Margareta Ackerman), naomi.brownstein@med.fsu.edu (Naomi C. Brownstein)

<sup>1</sup>These authors contributed equally.

Cluster analysis may be utilized with either realistic or constructive aims [7]. The goal of realistic clustering is to uncover real groupings inherent in the data. For instance, phylogenetic analysis and other life science clustering applications look for real groupings in the data, and as such have realistic aims. By contrast, constructive clustering is relevant when clustering should take place irrespective of whether inherent cluster structure is present. Yet, even when the goal of clustering is constructive, for instance, while the application of cluster analysis to market segmentation may be primarily constructive, users may be interested in realistic groups when such are present in the data.

Clustering with realistic aims, which is our focus here, is only appropriate when cluster structure is present in the data. Otherwise, the results of any clustering technique become necessarily arbitrary and consequently potentially misleading. For concreteness, consider a data set generated from a single Gaussian distribution. Because the data contains only one cluster, further subdivision would be artificial. Most clustering algorithms (e.g.  $k$ -means with  $k \geq 2$ ) would find multiple clusters in this data, even though no multi-cluster structure is present. As such, the application of these data mining tools rely on the presence of inherent structure, rendering *notions of clusterability*, which aim to quantify the degree of cluster structure, integral to cluster analysis. Clusterability analysis should precede the application of clustering algorithms, as the success of any clustering method depends on the presence of underlying cluster structure.

To see how clusterability fits within the clustering process, consider the pipeline depicted in Figure 1.<sup>2</sup> The process begins with data preprocessing, often involving feature selection or extraction. Next, clusterability analysis determines whether the data possesses inherent cluster structure. If the data does not possess sufficient cluster structure to be meaningfully partitioned, then clustering may not be suitable for the given data, or the data may need to be reprocessed. Otherwise, if the data is found to be clusterable, a clustering algorithm may be selected or developed.<sup>3</sup> Finally, the solution is validated by applying clustering quality measures [2, 10], which may result in the selection of an alternate algorithm if a sufficiently high quality clustering has not been found.

Not unlike clustering algorithms, notions of clusterability, summarized in Section 2, disagree with each other in surprising ways [3]. An analysis by Ackerman and Ben-David [11] reveals that many notions of clusterability are pairwise distinct - despite the fact that they all attempt to evaluate the same characteristic. The plethora of clusterability methods presents a dilemma: how should one select a clusterability measure suited to their data?<sup>4</sup> Ben-David [12] approaches the problem from a theoretical standpoint, offering several properties that notions of clusterability should satisfy. In particular, he argues that clusterability notions need to be

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<sup>2</sup>A similar pipeline is presented in the famous survey of clustering algorithms by Xu and Wunsch [8], sans the second step. Figure 1 shows how clusterability fits within the clustering process.

<sup>3</sup>Note that multiple methods should be considered at this step, because different algorithms are apt at identifying different types of cluster structures [3, 9].

<sup>4</sup>The original “user’s dilemma” refers to the problem of selecting a clustering algorithm for a given task. Selecting a notion of clusterability is another dilemma that the clustering user faces, addressed in the current work.

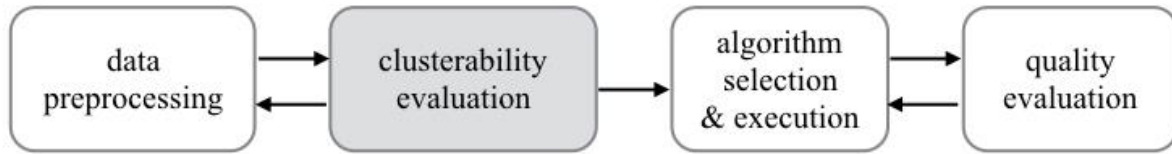


Figure 1: Clustering pipeline. This figure shows the feedback pathways in cluster analysis and the role of clusterability in this process.

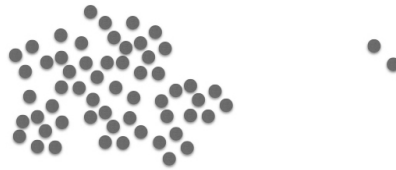


Figure 2: Data with ambiguous cluster structure. Outliers can be ignored or considered a small cluster. Whether or not this data is considered clusterable depends on the needs of the given application.

computationally efficient and effective; see section 2.1 for details.

The effectiveness requirement is complicated by the inherent ambiguity of cluster analysis. Whether an algorithm is effective for a given application depends on the needs of that applications [3]. Similarly, the needs of the application at hand may dictate whether the given data is clusterable. For example, allowing small clusters can change how we evaluate the clusterability of the data in Figure 2; If small clusters are appropriate for the given application, then the data would be clusterable, whereas otherwise it would be unclusterable. Distant elements are typically considered important when clustering phylogenetic data, whereas outliers are often ignored when clustering is applied to market segmentation; a detailed discussion is provided elsewhere [6]. Such considerations make room for multiple legitimate clusterability measures, and create the need for guidelines that would help a user determine which notion to choose for their data.

In this paper, we perform an extensive empirical statistical analysis of clusterability measures. We not only identify effective notions, but also discover important differences amongst them that can enable a clustering user to make informed decisions when selecting a clusterability technique.

We begin by formalizing clusterability and presenting several properties that notions of clusterability should satisfy. This enables us to identify promising clusterability measures, which we overview in Section 2. We then present our extensive simulations, which allow us to discern between approaches to clusterability and determine which are more appropriate under different circumstances. Next, we apply these measures of clusterability to real data. We conclude with a summary of our findings and recommendations.

## 2. Measures of Clusterability

A plethora for measures of clusterability have been proposed in the literature. We begin by formalizing clusterability and propose several requirements. This formal framework enables us to focus our analysis on the most promising measures. An extensive statistical analysis of these measures is performed in Section 3.

### 2.1. Requirements of Clusterability Measures

While the aim of clustering - to group similar items - is both intuitive and highly applicable, formalizing clustering has proven to be a difficult task. Despite extensive research in the field, clustering remains ill-defined [2]. In particular, we do not have a formal definition of clusterability (or even a formal definition of clustering<sup>5</sup>). Recently, Ben-David [12] began tackling the challenge of formalizing clusterability by proposing several interesting properties. In this section, we distill several properties that will help sift through the plethora of clusterability measures to identify those that are most likely to be useful in practice. Two of our properties, the first and third, are based on Ben-David's requirements.

A *measure of clusterability* is a function that takes in a data set and outputs a number quantifying its degree of inherent cluster structure.<sup>6</sup> Naturally, additional requirements are necessary, as functions (e.g. constant functions that declare all data sets to be clusterable) can easily contradict our intuition about how a measure of clusterability should behave. To this end, we propose several properties. We rely on these properties to select clusterability measures for our analysis in Section 3.

- **Efficiency:** *For practical utility, a measure of clusterability should be efficiently computed.* Without being overly restrictive, we require that the measures be computable in low polynomial time. In particular, this eliminates measures that are NP-hard to compute. This requirement relates to Ben-David's third requirement [12].
- **Algorithm Independence:** *The clusterability measure should not be based on a specific clustering algorithm or objective function.* Notions of clusterability that are based on a specific algorithm ask a different question than ours; While we ask whether data is clusterable, algorithm-specific notions aim to discover if the data can be clustered using a particular method.
- **Effectiveness:** *The measure of clusterability should be highly accurate in identifying data as clusterable or unclusterable.* As discussed in section 1, the inherent ambiguity of clustering necessitates flexibility on what it means to be "clusterable." Yet, there are many clear examples of both clusterable and unclusterable data, such as, for instance, a single Guassian (unclusterable) or two well-separated Guassians (clusterable). This property is related to the first requirement in Ben-David's paper [12].

<sup>5</sup>While axioms and properties have been proposed, e.g. [1, 2, 3], we do not yet have a formal definition of clustering, clustering functions, or clusterability.

<sup>6</sup>Outputs may be real values, binary indicators ("clusterable" or "unclusterable"), or probability measures.

The first requirement is that measures be efficient in practice. We address this requirement in section 5.1. They should certainly be computable in polynomial time and run in reasonable time on large data sets. Our second requirement concerns the role of clusterability in the clustering pipeline in Figure 1. Since different clustering algorithms are adept at identifying distinct types of cluster structure [13, 9], centering a measure of clusterability on a specific algorithm restricts it from identifying structure that the underlying algorithm cannot capture.

Finally, the third and most challenging requirement, the identification of methods that satisfy effectiveness, is the focus of our work. We first collect a body of existing measures and propose additional measures that satisfy the first two requirements. Next, we empirically compare the performance of these methods on a large number of real and simulated data sets. Our data includes many examples that leave no room for ambiguity, allowing us to determine which clusterability measures are effective. Differences in their behavior on more ambiguous data allow us to identify guidelines that can be used to help clustering practitioners select suitable notions of clusterability for their tasks. The combination of extensive simulations and analysis on real data allows us to gain insight into different approaches to clusterability evaluation, compare their effectiveness and fit for distinct clustering scenarios.

## 2.2. Effective Approaches to Clusterability Evaluation

A large, practical class of clusterability notions rely on one or more of the following: dimensionality reduction and statistical tests of multimodality. The reduced data informs the clusterability of the original data, as shown in Figure 3. When data is generated from a single bivariate normal distribution, the original data forms one cluster, and the pairwise distance and first principal component distributions are unimodal. By contrast, when the data is generated from multiple clusters, the pairwise distances and first principal component distributions are multimodal. It is important to note that the modes of the reduced data need not correspond with the clusters. For example, the distribution of pairwise distances generated from three clusters, depicted in Figure 3h, has only two modes, corresponding to the smaller within-cluster and larger between-cluster distances.

In the following two subsections, we briefly review data reduction methods and multimodality tests, before delving into clusterability methods.

### 2.2.1. Data reduction methods

Data sets often contain a large number of features, which may even outnumber the observations. Due to the computational and theoretical challenges associated with high dimensional data, reducing the dimension while maintaining the structure of the original data is desirable. If dimensions are measured on different scales, then the data may be centered about its mean or scaled to have unit variance, as recommended in [14]. Specific techniques to reduce data to one dimension are now discussed in greater detail.

One famous data reduction method is principal component analysis (PCA), which projects the data onto independent dimensions that explain the original variance [15]. There are natural connections between PCA and clustering. In fact, the principal components (PC) correspond to the  $k$ -means cluster membership indicators [16, 17]. PCA has been recommended to visually inspect for grouping structure [18]. While multiple components are often retained,

the first PC, by definition, explains most of the variation in the data [19, 20]. PCA is less prone than other data-reduction methods to the curse of dimensionality but is not well suited to non-linear structures [19], for which principal curves [21, 22], which produce a non-linear transformation of the data, may be more appropriate.

The set of dissimilarities between pairs of points in a data set forms another one-dimensional summary. Distances, which can be calculated using a variety of metrics, are often used as inputs to clustering algorithms, can be calculated for any data set, and have been shown to preserve structural features, such as correlation [23]. Yet, distances are sensitive to the curse of dimensionality, potentially yielding misleading results for data with many features. Also, the use of pairwise distances increases the sample size of the summary to nearly the square of the original size, rendering this approach impractical for datasets with a large number of observations.

### 2.2.2. Multimodality tests

Intuitively, if a data set contains multiple clusters, then there should be some separation between the clusters. For example, a histogram of pairwise distances should show a group of small distances, representing those within clusters, and a group of large between-cluster distances. On the other hand, homogeneous data should not show such a separation. See Figure 3 for an illustration.

A statistical test of multimodality can formally determine if the set of distances for a given dataset has multiple modes, indicating that there are multiple clusters. Likewise, tests on data reduced by other methods help detect cluster structure. Multimodality tests [24] are used for other clustering purposes, such cluster splitting, merging, and validation [25, 26, 27, 28, 29].

Multimodality tests initially assume that data is generated from a unimodal distribution (the null hypothesis), but may refute that assumption based on the data. The  $p$ -value is the probability of observing the given input or a more extremely multimodal input under the null hypothesis. If only a single mode is present, then the  $p$ -value should be large, indicating that the underlying data is deemed unclusterable. By contrast, small  $p$ -values make us question the original assumption of unimodality and instead conclude that multiple modes (and multiple clusters) are present in the population from which the data was generated.

Two multimodality tests are widely used and available in standard software. The dip test computes a statistic called the dip, defined as the maximum distance between the empirical distribution and the closest uniform distribution. Details on the dip statistic and the algorithm used to implement it are described elsewhere [30, 31, 32]. The dip test rejects the assumption of unimodality if the dip is sufficiently large, indicating that the data is sufficiently different from the closest uniform distribution. Another popular test by Silverman [33] rejects the unimodality assumption if the kernel density estimate requires a sufficiently large bandwidth to produce an empirical distribution based on one Gaussian component rather than a Gaussian mixture. In particular, the critical bandwidth  $h_{crit}$ , is defined by Equation 1

$$h_{crit} = \inf\{h : \hat{f}(\cdot, h) \text{ has at most one mode}\} \quad (1)$$



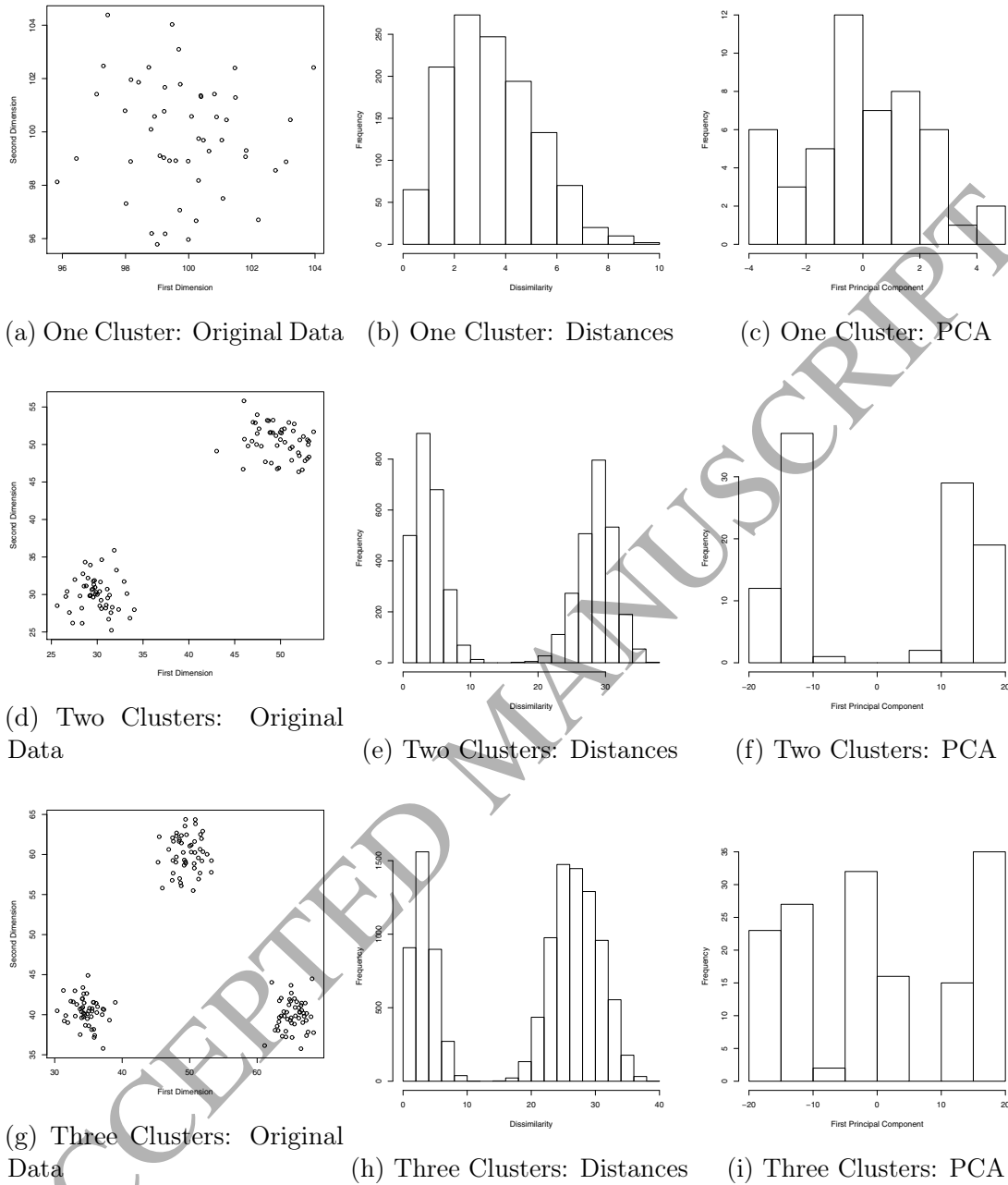


Figure 3: An illustration of dimension reduction for clusterability evaluation. The left column, Figures 3a, 3d and 3g, depicts data generated from one, two, or three Gaussian clusters using the same parameters as in Table 2 (row 1) and Table 4 (rows 11 and 16). The middle column, Figures 3b, 3e and 3h, includes histograms of the pairwise dissimilarities of the data. The right column, Figures 3c, 3f and 3i, includes histograms of the first principal component of the data. Distributions of reduced data contained a sole mode for data generated from a single cluster and multiple modes for data generated from multiple clusters.

where

$$\hat{f}(t, h) = n^{-1} h^{-1} \sum_{i=1}^n K(h^{-1}(t - X_i)), \quad (2)$$

$X_1, \dots, X_n$  denotes the observed data, and  $K$  is the density of the standard normal distribution.

One may be tempted to forgo dimension reduction, apply a multimodality test, and conclude that the data is clusterable if the data set rejects the null hypothesis for unimodality [34]. Unfortunately, the asymptotic behavior of these multimodality tests is unknown when the data is multi-dimensional [34, 35, 20, 36]. These severe limitations render these methods unpredictable for real data sets, most of which have multiple, if not high dimensions, unless the user first reduces the data to one dimension.

### 2.3. Clusterability via Multimodality

We now introduce previous notions of clusterability and several new notions. For these notions, if the user fails to reject the null hypothesis of unimodality of the reduced data, then the data does not have clear evidence of cluster structure *and should not be clustered*.

The majority of this section describes the idea behind each clusterability methods and how it was implemented. All methods described in this paper were implemented using readily available functions in *R* statistical software version 3.3.2 [37]. Details are found in Subsections 2.3.1-2.5.3.

Runtime analysis is presented in Section 5. This section concludes with a brief summary of notions of clusterability that are not well-suited to the goals of the current analysis.

#### 2.3.1. Dip Test on Pairwise Distances (Dip-dist)

Dip-dist [25] tests for clusters in the set of dissimilarities using the Dip test [30]. The lengths of the pairwise distances are sufficient for clusterability analysis without needing to consider how the distances are arranged to form the data. Multiple modes in the distance distribution suggest the presence of multiple clusters. The implementation of the dip test is detailed by Hartigan [31]. In brief, the (one-dimensional) set of pairwise Euclidean distances is calculated, sorted, and used as inputs to the Dip test. We utilized the *dist()* function within *R* [37] and the *dip.test()* function within the *dip.test* package [32].

#### 2.3.2. Silverman Test on Principal Curve (PC Silv.)

One method proposes to use Silverman's test for multimodality of the principal curve proposed by Ahmed [38]. The first dimension of the principal curve is extracted and Silverman's test is used to determine if that dimension is unimodal or multimodal. A multimodal principal curve suggests that the original, higher dimensional data exhibits cluster structure. The implementation of Silverman's test was based on the *silvermantest* package in *R* [39], which includes the calibration recommended by Hall and York [40]. Corrections for both Silverman's original test and the dip test have been proposed [40, 41], but only the correction for Silverman is available in standard software, such as *R*. Principal curves were created using the *princurve* package [42].

### 2.3.3. Silverman Test on Principal Component (PCA Silv.)

A linear alternative to the principal curve is to extract the first principal component, also suggested by Ahmed [38], which explains the maximum variation in the data. The Silverman test [33, 39, 40] is then applied to this first principal component. The implementation in the paper performs PCA using the singular value decomposition of the centered data, and then the rotated variables are extracted. Computationally, the program calls the *prcomp()* function, available in the *stats* package in *R* [37]. A multimodal first principal component suggests that the original data is clusterable.

### 2.3.4. Classic Methods

While it is known that multimodality tests may be problematic in higher dimensions, we include these methods in our comparisons for completeness. That is, Classic Silverman (Cl. Silverman) and Classic Dip (Cl. Dip) conduct, respectively, Silverman's and the Dip test of multimodality on the original, multi-dimensional data.

### 2.4. Clusterability via Spatial Randomness

Another method [43, 44], a test of spatial randomness, tells us if a feature is distributed non-randomly across the data set. Hopkins (Hop.) compares the distances between a sample of data points and their nearest neighbors to the distances from a sample of pseudo points – with each feature randomly selected from the full data set – and their nearest neighbors. If the data are not distributed in clusters, then both sets of distances should be similar on average. Clusterability can be inferred by comparing to a threshold calculated based on the distribution of the Hopkins statistic. Under the null hypothesis that the data is unclusterable, the test statistic follows a beta distribution with both parameters equal to the number of points selected to sample  $n$  [43, 44]. Thus, Hopkins' statistic should be compared to a Beta quantile  $q_\alpha(n, n)$ . The Beta quantile  $q_\alpha(n, n)$  is defined as the value such that, assuming the data was generated without clusters, the chance of concluding that the data is clustered, i.e.  $P(H < q_\alpha(n, n))$  is  $100\alpha\%$ . We use a one-sided test, because if the data were more spatially random than expected by chance, it would still be considered unclusterable. Yet, the choice of  $n$  requires caution. According to Lawson and Jures [44], “if too few points are chosen, then the nearest-neighbor distances chosen will not be representative of the entire distribution of distances.” If too many points are chosen, [45] warn that the “assumptions about the Beta distribution will be invalid.” Previous authors recommend sampling 5 – 10% of the data [44, 46]. In this paper, we use a 10% sampling rate. In this manuscript, Hopkins was implemented using the *hopkins()* function in the *clustertend* package [47].

### 2.5. New Clusterability Methods

This section describes our new proposed approaches for evaluating clusterability. Since both the dip and Silverman's test are valid multimodality tests, we propose to use both on each reduced version of the data. To our knowledge, the following methods below have not been previously proposed.

### 2.5.1. Silverman's test on dissimilarities (*Silv.-dist*)

Rather than using the dip test on the set of pairwise Euclidean distances [25], we propose to use Silverman's test, with the necessary correction [40].

### 2.5.2. Dip test on principal component (*PCA Dip*)

Instead of using Silverman's test of whether the first principal component is multimodal, this method uses the dip test.

### 2.5.3. Dip test on principal curve (*PC Dip*)

The dip test classifies the modality of the principal curve.

## 2.6. Other Clusterability Methods

Some notions of clusterability in the literature have been omitted from our study, as they are either impractical or otherwise unsuited to our goals. The effectiveness requirement allowed us to eliminate several notions of clusterability. For example, worst pair ratio [48] identifies data as clusterable if and only if there is a  $k$ -clustering where the minimum between-cluster distance is greater than the maximum in-cluster distance. Despite the simplicity and elegance of this notions, it identifies many clearly clusterable data sets as unclusterable (for example, three Gaussian distribute clusters positioned closer to each other, so that the separation between them is smaller than the radius of the clusters), and as such fails the effectiveness condition.

Other elegant clusterability measures that have been useful in theoretical analysis are omitted from our study since they are either NP-hard to compute [11] or too strict for practical application due to their high sensitivity to noise and outliers. Since we seek notions that are efficient, and applicable in practice, we had to omit all such measures from our analysis. Notions based on specific algorithms or objective functions [11, 49, 50, 51, 26, 52], are omitted from our analysis, which seeks to identify the presence of any cluster structure, not only that which can be discovered by a specific clustering technique. Approaches to clusterability, such as [53], relying on subjective judgment rather than a quantifiable measure, are also omitted.

## 3. Simulations

Our analysis of clusterability measures begins with extensive simulations. The purpose of the simulations is twofold. First, simulations allows us to perform basic tests to ensure that clusterability measures behave reasonable on clearly clusterable data and clearly unclusterable data. If we discover, for instance, that a measure fails to identify data generated from two well-separated Gaussian distributions as clusterable, then the measure fails our effectiveness requirement. Similarly, failure to identify data generated from a single Gaussian distribution as unclusterable would preclude the application of a measure in practice, as it would contradict basic intuition about what it means to be clusterable.

The other major goal achieved by simulations is identifying under what conditions different measures are most appropriate. In addition to testing clear cut cases, we also include

simulations with noise, varied number of cluster sizes and diameters, outliers, etc, to check for robustness of clusterability methods. For example, in some contexts, the inclusion of a single distant outlier in otherwise unclusterable data may indicate the formation of a second cluster. Yet, for other applications, the outlier is best ignored. Our simulations let us identify which clusterability technique allows for small clusters, and which exhibit outlier robustness. This information can then be used by clustering users to make informed choices when selecting a clusterability approach for their data.

One of the main approaches to the study of clustering involves the analysis of common statistical distributions (see, for example, [54, 55, 56]). Our extensive simulations evaluate each approach to clusterability using all clusterability tests in Sections 2.3-2.5. The simulations include 31 types of data sets, each generated with the same parameters 1000 times, for a total of 31,000 simulations. Simulations consist of clusters generated from one or more Gaussian or t-distributions, sometimes with a small number of outliers, and chaining data with one or more lines or circles. Simulations were performed in *R* version 3.3.2 [37]. Code is found at the following link: <http://www.mayaackerman.info/clusterability.R>. Further details for each simulation scenario are included in Section 3.1.

Tables 2 through 5 include the the percentage of data sets on which the test yielded a  $p$ -value less than 0.05, indicating that the tests rejected the null hypothesis of unimodality at the traditionally used 5% significance level. *High values in Tables 2-5 indicate clusterable data, while low values indicate poor clusterability.* For unambiguously unclusterable data sets, the proportion of rejections corresponds to type I error, the rate of erroneously classifying data sets generated without clusters as clusterable. Type I error greatly exceeding 5% indicates that the method is invalid and produces excessive false positives.

For unambiguously clusterable data sets, the proportion of rejections corresponds to the statistical power, or ability of the test to correctly classify clusterable sets as having cluster structure. Higher power is desirable. Yet, results are complicated by the ambiguous nature of clustering. When a small number of outlying points are present, the decision to classify the data as clusterable depends on whether outliers should be considered as small clusters.

### 3.1. Simulation Details

Table 1 summarizes the parameters used in the simulations. Unless otherwise specified, observations have independent and identically distributed dimensions with the given parameters.  $N(\mu, \sigma)$  denotes data generated from independent Gaussian distributions in each dimension with mean  $\mu$  and standard deviation  $\sigma$ . For example, lines 3 and 4 each include data generated from a single Gaussian cluster in 10 and 50 dimensions, respectively, each with mean and standard deviation equal to 2.  $T_d(\lambda)$  denotes data generated independently in each dimension from a  $T$  distribution with  $d$  degrees of freedom and non-centrality parameter  $\lambda$ . In lines 22-24, each scenario was generated from two 2-dimensional non-central  $T$  distributed clusters with either 5, 10, or 15 degrees of freedom and non-centrality parameters of 50 and 150.  $U(a, b)$  means that data independently generated in each dimension from a uniform distribution with density equally distributed between  $a$  and  $b$ .

When dimensions are non-identical, each dimension is specified as needed. For example,  $N((\mu_1, \mu_2, \dots, \mu_d), \sigma)$  denotes data generated from a  $d$ -dimensional Gaussian distribution

Row	Clusters	Dim	Distribution(s)	Clust size	Total
1	1	2	$N(100, 2)$	50	50
2	1	3	$N(100, 2)$	50	50
3	1	10	$N(2, 2)$	50	50
4	1	50	$N(2, 2)$	100	100
5	1 +1 outlier	2	$N(50, 2)$ $N(\mu, 2) : \mu \sim U(60, 65)$	50 1	51
6	1 +1 outlier	2	$N(50, 2)$ $N(\mu, 2) : \mu \sim U(60, 65)$	250 1	251
7	1 +3 outliers	2	$N(50, 2)$ , $N(\mu, 2) : \mu \sim U((40, 55), (45, 60))$ $N(\mu, 2) : \mu \sim U((65, 65), (70, 70))$ $N(\mu, 2) : \mu \sim U((65, 45), (70, 50))$	50 1 1 1	53
8	1	2	$T_5(100)$	100	100
9	1	2	$T_{10}(100)$	100	100
10	1	2	$T_{15}(100)$	100	100
11	2	2	$N(30, 2), N(50, 2)$	50	100
12	3	2	$N((30, 20), 2), N((40, 20), 2), N((35, 30), 2)$	50	150
13	3 +noise	2	$N((30, 40), 2), N((70, 40), 2), N((50, 80), 2)$ $N(50, 20)$	50 80	230
14	3	2	$N((30, 20), 1), N((40, 20), 3), N((35, 30), 5)$	50	150
15	3	2	$N((35, 40), 2), N((65, 40), 2), N((50, 60), 2)$	100,66,33	199
16	3	2	$N((35, 40), 2), N((65, 40), 2), N((50, 60), 2)$	50	150
17	3	2	$N(20, 2), N(40, 2), N(60, 2)$	50	150
18	2	10	$N(10, 2), N(20, 2)$	50	100
19	4	10	$N(10, 2), N(20, 2), N(60, 2), N(80, 2)$	50	200
20	2	50	$N(5, 2), N(10, 2)$	100	200
21	2	50	$N(3, 2), N(6, 2)$	100	200
22	2	2	$T_5(50), T_5(150)$	100	200
23	2	2	$T_{10}(50), T_{10}(150)$	100	200
24	2	2	$T_{15}(50), T_{15}(150)$	100	200
25	1	2	unit circle	50	50
26	2	2	2 concentric circles (radii: 1,2)	50	100
27	3	2	3 concentric circles (radii: 1,2,3)	50	150
28	5	2	5 concentric circles (radii: 1,2,3,4,5)	50	250
29	1	2	1 line ( $x = 50, y \sim N(50, 25)$ )	100	100
30	2	2	2 lines ( $x_1 = 30, x_2 = 55, y \sim N(50, 25)$ )	100	200
31	2	2	circle (radii: 3) at origin line ( $x = 5, y \sim N(0, 2)$ )	100 100	200

Table 1: Parameters Used in Simulations. Simulations include clusters with Gaussian, T, and uniform distributions, separate outlying points, as well as parallel lines and circles. Dimensions are generated independently and identically unless specified otherwise. Notation is described in Section 3.1.

with means located at  $\mu_i$  for independent dimensions  $i = 1, 2, \dots, d$  and standard deviation  $\sigma$  in each dimension. In particular, in line 12, data was generated from three two-dimensional Gaussian distributions, each with standard deviation 2 in each independent dimension, and centers at (30, 20), (40, 20), and (35, 30).

In some cases, additional points are added to represent outliers and noise. Line 13 describes data generated from three two-dimensional Gaussian distributions, similar to line 12 but with means at (30, 40), (70, 40), and (50, 80), and a fourth, much wider, Gaussian distribution with mean 50 and standard deviation 20 in both dimensions. The outliers in lines 5-7 include between one and three additional Gaussian observations generated with high probability to be far apart from the rest of the data. In particular, while all two-dimensional data in line 5 is generated from a Gaussian distribution with standard deviation 2 in each dimension, the main cluster of 50 points was generated from a mean at (50, 50), and the remaining point was generated with mean in each dimension randomly selected from a uniform distribution bounded by 60 and 65.

A subset of simulations, shown in lines 25-31 of Table 1 include data generated with chaining structure, including one or more circles or lines. The circles were all centered at the origin (0,0), and the radius of each was an integer between 1 and 5. The lines were each vertical, with constant x-coordinates (denoted in the table by  $x = c$ ) and y-coordinate generated from a univariate Gaussian distribution. Line 31, which includes both a circle and a lines exemplifies this notation. The circle, centered at (0,0) has a radius of 3, and the line, located to the right of the circle at  $x = 5$ , has points vertically generated from a Gaussian distribution with mean 0 and standard deviation 2.

### 3.2. Type I error: Results for Unclusterable Data

Principal curve methods were invalid, concluding that single-cluster data sets were clusterable at a much higher rate than 5%. Hopkins, PCA-Silverman and classic Silverman have type I error around 5% as expected in two dimensions.<sup>7</sup> Hopkins (in multiple dimensions) and distance based methods have excessively low type 1 error of less than 1%, indicating that they may be overly conservative. All methods except principal curves have low false positive rates for single Gaussian clusters.

### 3.3. Performance with Outliers and Small Clusters

When outlying points are introduced to otherwise unclusterable data, one could argue either for or against clusterability. Methods vary in their conclusions: Dip-based methods

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<sup>7</sup>For valid methods, values in Table 1 should be below or reasonably close to 0.05. If the true false positive rate is 5%, then we would expect with 95% confidence that the observed value should be below  $0.05 + 1.96 * \sqrt{0.05 * 0.95/1000} \approx 0.064$ . Based on this threshold, PCA Silverman has slightly inflated type I error in 50 dimensions, and Classic Silverman has inflated type I error in 3 dimensions. However, because we would expect 5% of the results for unclusterable data sets to exceed this value, it is not unusual to see 2 results with slightly inflated type I error rates. In fact, if we adjust for the total number of comparisons for unclusterable data, then the false positive rates would be compared to a different threshold (0.072) and would not be considered excessive.

	Data	Dip Dist	Silv Dist	Hop	Cl. Dip	Cl. Silv	PCA Dip	PCA Silv	PC Dip	PC Silv
1.	1 cluster 2D	0.000	0.042	0.057	0.001	0.055	0.001	0.053	0.179	0.346
2.	1 cluster 3D	0.000	0.042	0.012	0.000	0.068	0.002	0.062	0.213	0.444
3.	1 cluster 10D	0.000	0.035	0.000	0.000	0.055	0.003	0.057	0.235	0.585
4.	1 cluster 50D	0.000	0.033	0.000	0.000	0.052	0.002	0.064	0.220	0.764

Table 2: Results of Simulations for Data Generated from A Single Cluster. Proportion of data sets considered clusterable out of the 1000 data sets for each type. Entries are interpreted as type I error, which should not greatly exceed 5%. Strike-through denotes entries that have excessive Type I error. Methods had reasonably low false positive rates, with the exception of those using principal curves.

	Data	Dip Dist	Silv Dist	Hop	Cl. Dip	Cl. Silv	PCA Dip	PCA Silv	PC Dip	PC Silv
5.	1 cluster 2D with outlier	0.000	0.987	0.858	0.000	0.890	0.005	0.998	0.136	0.984
6.	1 large cluster 2D with outlier	0.000	0.975	1.000	0.000	0.911	0.001	0.989	0.331	0.980
7.	1 cluster 2D with 3 outliers	0.101	0.976	0.815	0.000	0.954	0.003	0.942	0.016	0.935
8.	1 T-dist cluster with df=5	0.007	0.573	0.852	0.000	0.440	0.000	0.463	0.070	0.490
9.	1 T-dist cluster with df=10	0.000	0.214	0.657	0.000	0.240	0.000	0.282	0.095	0.348
10.	1 T-dist cluster with df=15	0.000	0.117	0.579	0.002	0.209	0.000	0.220	0.098	0.344

Table 3: Results of Simulations Generated from Data with Outliers. Proportion of data sets considered clusterable out of the 1000 data sets of each type. Methods differed in their conclusions on such data sets, reflecting the ambiguous nature of clustering for data with outliers. Methods using Hopkins or Silverman tended to consider outliers as separate clusters, while dip-based methods tended to be robust to outliers.

classify the data as unclusterable, while the Hopkins statistic and Silverman-based methods classify such data as clusterable, identifying the outliers as separate clusters. Dip-based methods consider the data clusterable less than 10% of the time, even for t-distributions with 5 degrees of freedom, when multiple outliers are likely; Hopkins and Silverman-based methods frequently conclude that the data is clusterable, ranging from 44% to 85% of the time. As expected, the proportion decreases as the degrees of freedom increases and the distribution converges to Gaussian. *Where the dip test is robust to outliers, Silverman's test and the Hopkins statistic allow for small clusters.* This finding reflects the inherent ambiguity of clustering; for some applications, small clusters are acceptable, while for others, robustness to outliers is desired. In fact, clustering algorithms display the same phenomenon: some tend to identify small clusters, while others effectively view such data as outliers [13].



	Data	Dip Dist	Silv Dist	Hop	Cl. Dip	Cl. Silv	PCA Dip	PCA Silv	PC Dip	PC Silv
11.	2 separated clusters 2D	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
12.	3 close clusters 2D	0.996	1.000	0.789	1.000	1.000	0.801	0.974	0.757	0.826
13.	3 noisy clusters 2D	1.000	0.996	0.989	0.999	0.995	1.000	0.999	1.000	0.983
14.	3 clusters 2D, varied radii	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
15.	3 clusters 2D, varied density	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
16.	3 separated clusters 2D	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
17.	3 separated clusters 3D	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
18.	2 separated clusters 10D	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
19.	4 separated clusters 10D	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.884
20.	2 close clusters 50D	1.000	1.000	1.000	0.691	0.999	1.000	1.000	1.000	1.000
21.	2 partially overlapping 50D	1.000	1.000	<b>0.445</b>	<b>0.000</b>	<b>0.041</b>	1.000	1.000	0.995	0.997
22.	2 T-dist cluster with df=5	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
23.	2 T-dist cluster with df=10	1.000	1.000	0.999	1.000	0.998	1.000	1.000	1.000	0.999
24.	2 T-dist cluster with df=15	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Table 4: Results of Simulations Generated with Multiple Clusters. Proportion of data sets considered clusterable out of the 1000 data sets of each type. These numbers correspond to statistical power to detect the cluster structure. Numbers in bold denote methods with much lower power than others. In particular, Hopkins and especially classic multimodality tests lose power in high dimensions. All other methods had reasonably high power for these simulations.

	Data	Dip Dist	Silv Dist	Hop	Cl. Dip	Cl. Silv	PCA Dip	PCA Silv	PC Dip	PC Silv
25.	Single Circle	0.010	<del>0.309</del>	<del>0.837</del>	<del>0.951</del>	0.945	0.909	0.988	0.626	0.775
26.	2 concentric circles	1.000	1.000	0.873	0.533	0.751	0.322	0.472	0.619	0.802
27.	3 concentric circles	1.000	1.000	0.894	0.167	0.486	0.079	0.193	<del>0.607</del>	0.774
28.	5 concentric circles	1.000	1.000	1.000	0.364	0.394	0.159	0.364	0.726	0.895
29.	Single Line	0.004	0.049	<del>0.378</del>	0.000	<del>0.112</del>	0.000	0.055	<del>0.642</del>	N/A
30.	2 parallel lines	1.000	0.889	1.000	1.000	0.996	0.000	0.055	0.997	0.989
31.	Line and Circle	0.998	0.999	1.000	1.000	0.958	<del>0.209</del>	0.894	0.876	0.982

Table 5: Results of Simulations for Chaining Data. Proportion of data sets considered clusterable out of the 1000 data sets of each type. Results correspond to type I error for data sets with a single cluster circle or line and statistical power for data sets with multiple circles and/or lines. Strike-through denotes entries that have excessive Type I error. Looking at the columns shows that the only method that had type I error controlled, and thus the only valid method for chaining data, is Dip-Dist. Principal curves, which are non-linear reductions, failed to converge for linear data.

Data	n	d	Dip Dist	Silv Dist	Hop	Cl. Dip	Cl. Silv	PCA Dip	PCA Silv	PC Dip	PC Silv
Faithful	272	2	0.0000	0.0000	1.00	0.0000	0.0000	0.0017	0.0000	0.0000	0.0000
Iris	150	4	0.0000	0.0000	1.00	0.0014	0.0010	0.0000	0.0000	0.0164	0.0022
Rivers	141	1	0.2772	0.0000	0.92	0.9922	0.0192	0.9922	0.0334	0.9922	0.0291
Swiss	47	6	0.0000	0.0000	0.41	0.1386	0.0000	0.0001	0.0000	0.0000	0.0010

Table 6: Results of Clusterability Tests for Non-Simulated Data with Previously Known or Visually Ambiguous Cluster Structure. This table presents the  $p$ -values, rounded to the nearest ten-thousandth, for the each clusterability test on real data sets from the R Datasets package. Recall that  $p < 0.05$  signals clusterable data and  $p \geq 0.05$  signals that data is unclusterable at the 5% significance level. The Hopkins value presented is the proportion of the time out of 100 runs that the Hopkins statistic was below the appropriate beta quantile. For the Hopkins results, high values indicate clusterability. The top two rows illustrate famous datasets known to possess multiple large clusters. The bottom two rows include datasets with a small number of outliers. The letter “n” refers to the number of observations in the dataset, and “d” the number of dimensions, or features.

Data	n	d	Dip Dist	Silv Dist	Hop	Cl. Dip	Cl. Silv	PCA Dip	PCA Silv	PC Dip	PC Silv
Attitude	30	7	0.9040	0.9598	0.00	0.9113	0.9150	0.6846	0.1534	0.1823	0.2174
Cars	50	2	0.6604	0.9931	0.19	0.8613	0.3396	0.8320	0.4213	0.7680	0.5866
Trees	31	3	0.3460	0.2900	0.18	<b>0.0001</b>	<b>0.0000</b>	0.8414	0.3675	0.6717	0.2282
Ratings	43	12	0.9938	0.7313	0.69	<b>0.0014</b>	<b>0.0187</b>	0.8550	0.1412	0.4501	<b>0.0000</b>
Arrests	50	4	0.9394	0.1887	0.01	0.6261	<b>0.0171</b>	0.5545	0.1286	<b>0.0045</b>	<b>0.0000</b>

Table 7: Results of Clusterability Tests for Non-Simulated Data Lacking Known Cluster Structure. This table presents the  $p$ -values, rounded to the nearest ten-thousandth, for the each clusterability test on real data sets from the R Datasets package. The Hopkins value presented is the proportion of the time out of 100 runs that the Hopkins statistic was below the appropriate beta quantile. For the Hopkins results, high values indicate clusterability. Recall that  $p < 0.05$  signals clusterable data (entries are in **bold**) and  $p \geq 0.05$  signals that data is unclusterable at the 5% significance level. Notably, the only bold entries are from methods that performed poorly in simulations.

### 3.4. Power: Results for Clusterable Data

When clusters were well-separated, all methods approached or reached 100% power, even in the presence of noise. When two fifty-dimensional clusters were close to each other as in row (20), all methods have nearly perfect power except for Classic Dip with around 70% power. For partially overlapping 50D clusters, e.g. row (21), the power of the Hopkins test drops to 32% and both classic methods drop below 5%. *This indicates that classical methods perform poorly in high dimensions for overlapping clusters.* By contrast, utilizing either PCA or pairwise distances, both Dip and Silverman tests maintain near perfect power to detect the presence of close or overlapping high dimensional clusters. We also examine two-dimensional data generated from independent t-distributions with 5, 10, and 15 degrees of freedom. All methods have nearly 100% power to detect the t-distributed clusters. Most methods had high power to detect three or four clusters, except that power for PCA dip and the Hopkins statistic dropped when the separation between clusters decreased. Specifically, classic, distance-based methods, and PCA-based methods considered all or nearly all (95+%) datasets as clusterable.

### 3.5. Results for Data with Chaining Structure

Finally, we examine data with chaining structure, including a single line, two parallel lines, one, two, three, and five concentric circles, and both a line and a circle. For data arranged in one line, classic dip, PCA methods and distance methods did not conclude that the data had multiple clusters. Hopkins classified the line as clusterable nearly 40% of the time, and classic Silverman concluded the data had structure over 10% of the time. Surprisingly, all methods except dist-dip considered a single circle as clusterable. Distance Silverman concluded that the single circle had cluster structure about 30% of the time, while PCA, classical methods, and Hopkins concluded the same over 85% of the time. Principal curve methods nearly always failed to converge for data comprising a single line. *Thus, dip-dist may be the only valid method for chaining data.*

While both classic and PCA methods have relatively low power to detect the inherent structure of multiple groups of chaining data, distance-based methods and Hopkins continue to detect the clusters. Multiple parallel lines, depicted in row 18, are considered clusterable by distance based methods and reasonably well (87% power) by Hopkins. PCA based methods have less than 6% power, failing to detect the separate lines most of the time. Distance based methods have 100% power and Hopkins has nearly 90% power to detect distinct circles, while PCA and classic methods have reduced power for 2 or 3 circles. Curiously, power for PCA methods did not change monotonically with the number of circles. Power was highest for two circles, lowest for three circles, and in between for five circles. However, strange behavior for PCA based methods is likely due to fact that PCA forms linear projections, which may not be appropriate for clearly non-linear data, such as circles.

All methods had high power ( $\geq 89\%$ ) to detect cluster structure in data consisting of one circle and one line except PCA dip, which only concluded the data was clusterable 20% of the time. *In sum, dip-dist was the most effective method for chaining data, retaining high power to detect clustered chaining data and being the only method that didn't excessively conclude that data generated to lack groups was clusterable.*

#### 4. Results on Non-Simulated Data

In this section, we apply our methods of clusterability evaluation to non-simulated data sets from the *R datasets* package, a collection of datasets from prior studies.<sup>8</sup> The datasets we present were selected among data sets of standard structure (e.g. time series were not considered) to ensure sufficient sample size and varied dimension. For the sake of completeness, we include all tests, but the reader should recall based on Section 3 that some tests may be inappropriate under various conditions (e.g. principal curve methods due to their inflated false positive rates and classic tests for data with multiple dimensions). References for all data sets [57, 58, 59, 60, 61, 62, 63, 64, 65, 66] were examined for evidence of previously known cluster structure. Data sets were also visually inspected for clear outliers, which could indicate ambiguous structure. Figures in an accompanying article depict two-dimensional projections of each dataset and histograms of the data reduced by distances and PCA, respectively. All methods were implemented using *R* functions as described in section 2.3.

Overall, results of the clusterability tests were consistent with expectations based on the references and simulations, detailed in Section 3. Methods agreed in capturing clear structure in famous data sets and differed in their treatment of data with ambiguous structure, showing similar response to outliers as in the simulations. (The use of Silverman's tests corresponded to considering outliers as separate clusters, while the use of the dip test corresponded to considering outliers as noise.) Similarly, methods generally failed to declare cluster structure in data sets with no prior evidence of clusters, with a few exceptions. For example, the finding for classic methods to deem some multidimensional data sets as clusterable when no prior evidence could be found to confirm the existence of clusters was consistent with

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<sup>8</sup>Due to the use of sampling in Hopkins' method, we run the method 100 times for each dataset and report the proportion of *p*-values less than 0.05.

prior knowledge that the methods have unknown asymptotic behavior. Principal curve methods both considered as clusterable some data sets that lacked known evidence of cluster structure and failed to converge on a famous highly linear data set, paralleling its problems in simulations with convergence and excessive false positives. Specific results for each dataset follow.

Two famous data sets that were known *a priori* to have cluster structure were considered clusterable under all methods. First, the *iris* data set [57] is known to have three clusters corresponding to three species of iris flowers. Second, the *faithful* data set [58, 59], which captures eruption duration and waiting time for the Old Faithful geyser, has previously been shown to have two groups [60]. All of the tests conclude that both data sets are clusterable, agreeing with previous knowledge.

Paralleling our simulations, we find that methods relying on the Hopkins statistics or the Silverman tests may be preferred when small clusters are of interest, while techniques using the Dip test may be desired when the application calls for robustness to outliers. The one-dimensional *rivers* data set [61], which contains the lengths, in miles, of 141 major North American rivers, exhibits inherent cluster structure *if we allow small clusters*. Hopkins method and all methods that use Silverman indicate that the data is clusterable ( $p < 0.05$ ), while all dip-based methods fail to reject the null hypothesis of lack of structure. Similarly, *swiss* [62], consisting of 6 measures of socio-economic status and fertility for 47 French-speaking nineteenth-century Swiss provinces, illuminated logically pre-existing structure. While Classic Dip considers the data as unclusterable, and Hopkins considers the data as clusterable 40% of the time, all other tests detect clusters. Results support literature that economic indicators between and within countries may fall into clusters, including a richer cluster much smaller than the others [67, 68].

The remaining data sets lacked previously known structure. Most tests of clusterability that weren't known or shown to be questionable in simulations provided little or no evidence of clusters. Methods based on distances or PCA concluded that *cars* [63], *attitude* [64], *USArrests* [61], *trees* [65], and *USJudgeRatings* [66], were unclusterable. Hopkins' method agreed for *attitude* and *USArrests*. Most methods (principal curve and classic) that concluded that any of these remaining data sets, without known structure, were clusterable also exhibited questionable behavior on our simulations in section 3. Classic methods may be unreliable in multiple dimensions (see section 2.2.1), and principal curve methods had high false positive rates in our simulations. Classic Silverman and principal curve methods declared the *USArrests* [61] and *USJudgeRatings* [66] data sets clusterable. Curiously, Hopkins considered *USJudgeRatings* clusterable nearly 70% of the time, *trees* clusterable 18% of the time, and *cars* 19% of the time.

Overall, the methods with the most reasonable results include distance dip, distance Silverman, PCA dip, and PCA Silverman. Although classic Dip and Silverman methods appear to produce reasonable conclusions in some famous data sets such as *iris*, they have produced counterintuitive results when classifying other real data, such as *USJudgeRatings* and *USArrests*. This finding, which supports theory on the unpredictability of these tests in multiple dimensions, reflects the importance and value of carefully utilizing dimensionality

reduction in clusterability evaluation.

## 5. Runtime

In this section, we discuss the runtime of the clusterability methods studied in this paper. The computational complexity of the methods is addressed in Subsection 5.1. We report on the average observed times to complete the simulations in Subsection 5.2, as well as the elapsed time to apply each method to the non-simulated data in Subsection 5.3.

### 5.1. Quantifying Efficiency

There are significant differences in the computational complexity of clusterability techniques that render some of them impractical when the number of elements ( $n$ ) or the dimension ( $d$ ) is large. Classic Dip is linear in  $n$  [20]. Hopkins, Classic Silverman, and Dip-Dist have quadratic running time in  $n$ . The dimensionality of the data impacts the running time of PCA-based approaches, with PCA dip having asymptotic running time of  $O(nd^2 + d^3)$  [69]. Silverman-dist is bounded by a quartic function in  $n$ . Finally, PCA Silverman has complexity of  $O(n^2 + d^2n + d^3)$ .<sup>9</sup>

### 5.2. Simulation times

The average runtime of one execution of each clusterability method on each dataset is provided in Tables 8 and 9. Methods utilizing the Silverman critical bandwidth test are slower than the corresponding methods relying on the dip test, which lasted less than one hundredth of a second. As such, Dip-dist is much faster than Silv-dist, and PCA Dip is much faster than PCA Silv. The runtime of Hopkins' method generally fell in between the runtime of methods that utilize the dip test and methods that utilize the Silverman test, averaging between approximately 0.01s and 0.3s.

For all simulations, the use of Silverman's test on the pairwise distances was slower than all other methods by one to three orders of magnitude, requiring between nearly 1s and over 8.5s. This occurs due to the quadratic number of operations required for processing all pairwise distances, followed by the Silverman test, as discussed in Subsection 5.1.

### 5.3. Runtime for non-simulated data

The relative runtime for non-simulated data was comparable to that of the simulations, and confirmed expectations based on the methods' computational complexity. Hopkins is slower than dist-dip and PCA dip but faster than Silverman methods. PCA dip is similar to distance dip, both of which ran in one to three thousandths of a second. Reducing the data using PCA and then testing with the Silverman critical bandwidth test took about seven-tenths to eight-tenths of a second on non-simulated data. By contrast, running Silverman's test on the set of pairwise distances takes much longer, nearly ten seconds for the largest dataset, *faithful*, compared to about three seconds for the two datasets that are about half of the size.

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<sup>9</sup>As shown in [69], PCA Silverman needs  $O(nd^2 + d^3)$  operations to calculate the principal component. Then it performs Silverman's test, which is bounded by  $O(n^2)$ . Therefore, the total complexity is  $O(n^2 + d^2n + d^3)$ .

	<b>Data</b>	<b>Dip Dist</b>	<b>Silv Dist</b>	<b>Hop</b>	<b>Cl. Dip</b>	<b>Cl. Silv</b>	<b>PCA Dip</b>	<b>PCA Silv</b>	<b>PC Dip</b>	<b>PC Silv</b>
1.	1 cluster 2D	0.0016	0.9885	0.0130	0.0017	0.7333	0.0016	0.7221	0.0212	0.7445
2.	1 cluster 3D	0.0016	0.9817	0.0128	0.0014	0.7476	0.0016	0.7227	0.0295	0.746
3.	1 cluster 10D	0.0016	0.9755	0.0132	0.0014	0.8213	0.0017	0.7249	0.0742	0.7871
4.	1 cluster 50D	0.0032	1.8049	0.0578	0.0018	1.8045	0.0037	0.7415	0.3119	0.728
5.	1 cluster 2D with outlier	0.0016	1.0028	0.0146	0.0013	0.7429	0.0016	0.7295	0.0240	0.7444
6.	1 large cluster 2D with outlier	0.0062	8.5395	0.3186	0.0014	0.8264	0.0016	0.7738	0.0834	0.8509
7.	1 cluster 2D with 3 outliers	0.0016	1.0331	0.0141	0.0013	0.7443	0.0016	0.7363	0.0249	0.7551
8.	1 T-dist cluster with df=5	0.0021	1.8717	0.0505	0.0013	0.7908	0.0016	0.7692	0.0270	0.7937
9.	1 T-dist cluster with df=10	0.0021	1.8487	0.0509	0.0013	0.7835	0.0016	0.7605	0.0270	0.7832
10.	1 T-dist cluster with df=15	0.0021	1.8402	0.0508	0.0013	0.7820	0.0016	0.7564	0.0273	0.7828
11.	2 separated clusters 2D	0.0020	1.8538	0.0506	0.0013	0.7762	0.0016	0.7487	0.0329	0.7846
12.	3 close clusters 2D	0.0030	3.3283	0.1132	0.0013	0.7880	0.0016	0.7530	0.0267	0.7728
13.	3 noisy clusters 2D	0.0054	7.2108	0.2673	0.0014	0.8380	0.0016	0.7840	0.0479	0.8285
14.	3 clusters 2D, varied radii	0.0031	3.3522	0.1133	0.0013	0.7960	0.0016	0.7667	0.0299	0.7937
15.	3 clusters 2D, varied density	0.0042	5.4950	0.1899	0.0014	0.8100	0.0016	0.7769	0.0307	0.8064
16.	3 separated clusters 2D	0.0030	3.3443	0.1139	0.0013	0.7896	0.0016	0.7587	0.0225	0.7802
17.	3 separated clusters 3D	0.0030	3.3533	0.1140	0.0014	0.8297	0.0016	0.7662	0.0324	0.7944
18.	2 separated clusters 10D	0.0023	1.8576	0.0528	0.0014	0.9477	0.0017	0.7561	0.1042	0.8567
19.	4 separated clusters 10D	0.0048	5.5649	0.2122	0.0015	1.1694	0.0018	0.7929	0.0441	0.8227
20.	2 close clusters 50D	0.0086	5.5515	0.2382	0.0024	3.0199	0.0046	0.7871	0.5654	1.3229
21.	2 partially over- lapping 50D	0.0087	5.5314	0.2369	0.0025	2.9757	0.0046	0.7752	0.5429	1.2955
22.	2 T-dist clust. with df=5	0.0042	5.5759	0.2007	0.0013	0.8323	0.0016	0.7985	0.0450	0.8346
23.	2 T-dist clust. with df=10	0.0043	5.5694	0.2012	0.0013	0.8359	0.0016	0.7890	0.0423	0.8352
24.	2 T-dist clust. with df=15	0.0042	5.5745	0.2019	0.0013	0.8381	0.0016	0.7952	0.0489	0.8363

Table 8: Average runtime in seconds of all methods for each simulated dataset over 1000 computations.

	<b>Data</b>	<b>Dip Dist</b>	<b>Silv Dist</b>	<b>Hop</b>	<b>Cl. Dip</b>	<b>Cl. Silv</b>	<b>PCA Dip</b>	<b>PCA Silv</b>	<b>PC Dip</b>	<b>PC Silv</b>
25.	Single Circle	0.0016	0.7516	0.0026	0.0013	0.6916	0.0017	0.6822	0.0183	0.6994
26.	2 concentric circles	0.0022	1.8257	0.0510	0.0013	0.7524	0.0016	0.7274	0.0399	0.7653
27.	3 concentric circles	0.0029	3.3041	0.1129	0.0013	0.7760	0.0016	0.7431	0.0503	0.7869
28.	5 concentric circles	0.0062	8.4360	0.3162	0.0014	0.8157	0.0017	0.7628	0.0736	0.8357
29.	Single line	0.0025	2.0360	0.0595	0.0017	0.8681	0.0019	0.8393	0.1624	0.1608
30.	2 parallel lines	0.0044	5.5498	0.2024	0.0013	0.8232	0.0016	0.7801	0.0687	0.8394
31.	Line and circle	0.0022	1.8136	0.0524	0.0016	0.7590	0.0018	0.7417	0.0544	0.7971

Table 9: Average run time in seconds of all methods for each simulated dataset with chaining structure over 1000 computations.

<b>Data</b>	<b>n</b>	<b>d</b>	<b>Dip Dist</b>	<b>Silv Dist</b>	<b>Hop</b>	<b>Cl. Dip</b>	<b>Cl. Silv</b>	<b>PCA Dip</b>	<b>PCA Silv</b>	<b>PC Dip</b>	<b>PC Silv</b>
Faithful	272	2	0.0113	9.8536	0.3696	0.0020	0.8126	0.0015	0.7910	0.4809	1.2679
Iris	150	4	0.0030	3.2233	0.1136	0.0015	0.8166	0.0020	0.7305	0.0270	0.7530
Rivers	141	1	0.0030	3.0371	0.0970	0.0010	0.7530	0.0015	0.8021	0.1386	0.9036
Swiss	47	6	0.0020	0.9872	0.0099	0.0015	0.8286	0.0015	0.7285	0.0605	0.8351
Attitude	30	7	0.0015	0.8063	0.0048	0.0015	0.7770	0.0015	0.7410	0.0555	0.7475
Cars	50	2	0.0015	0.9537	0.0126	0.0010	0.7270	0.0020	0.7856	0.0070	0.7435
Trees	31	3	0.0010	0.7906	0.0049	0.0010	0.7780	0.0015	0.7350	0.0110	0.6890
Ratings	43	12	0.0015	0.9156	0.0093	0.0010	0.8071	0.0015	0.7090	0.0405	0.7846
Arrests	50	4	0.0015	1.0182	0.0129	0.0015	0.7921	0.0015	0.7595	0.0085	0.7565

Table 10: Runtime in seconds of each method on each non-simulated dataset. Recorded time for Hopkins is the average of 100 runs. The numbers of observations and number of features of the data are denoted by  $n$  and  $d$ .



## 6. Discussion

Though many approaches to clusterability evaluation have been previously proposed, they vary radically and often result in different conclusions. Here, we perform an extensive analysis of a variety of clusterability methods, identifying which are most effective as well as when certain measures are better suited than others based on the needs of the application at hand. While other notions of clusterability may also warrant investigation, our paper is the most comprehensive study to date. We compare several approaches, which apply either spatial randomness tests to the original data or multimodality tests to one-dimensional reductions of the data. Extensive simulations allow us to identify effective approaches, as well as differentiate amongst them. Notably, experiments on real data sets parallel the conclusions of our simulations. Our findings indicate that spatial randomness tests and multimodality tests on one-dimensional reductions are frequently effective at classifying data sets by their level of clusterability. Both clusterable and unclusterable data sets were identified as such in most simulations.

Methods perform differently according to dimension, treatment of outliers, and shape and separability of clusters. Distance-based methods perform well in most scenarios. PCA methods detect structure in data with two or three clusters and does not detect spurious clusters in data with a single cluster. However, in low dimensions, PCA power is lower than for distance-based methods, and PCA performs poorly for non-linear data. Outliers are treated as clusters by all variations of Silverman and the Hopkins statistic. The Hopkins statistic loses signal when clusters touch or overlap. Classical methods are inappropriate in multiple dimensions and for chaining data. Finally, principal curve methods were highly problematic on both simulated and non-simulated data sets. Even on the famous, well-defined data set *faithful*, the principal curve failed to converge after 1000 iterations. Principal curve methods also had excessive false positives on simulated data generated from a single distribution.

We summarize several qualitative criteria that can be used to select a suitable clusterability measure for a given application. Quantitative comparison based on the efficiency of these methods could also be integrated, particularly when data is large in number of observations or dimensions or both. See Section 5 for a comparison of the methods considered in this analysis based on their computational complexity and empirical runtime on simulated and non-simulated data.

- **False Positives:** Methods proclaiming to discover cluster structure when none is present have excessive false positives (Type I error) and are considered statistically invalid. Reducing data using the principle curve consistently yielded inflated Type I error rates and is not recommended.
- **Outliers/Small Clusters:** Clusterability measures vary in their treatment of sparse distant points. Hopkins and Silverman-based methods treat the points as small clusters; Dip-based methods exhibit outlier robustness.
- **Chaining Data:** Dip-dist was the only method that consistently performed well on chaining-type data, identifying both clusterable and unclusterable structures of these types.

- **High Dimensionality:** We tested data sets on up to 50 dimensions. In our experiments, PCA dip, PCA Silverman, and Dip-dist did well and were reasonably efficient, suggesting that these methods may be better suited to high dimensional data than the other techniques considered in this analysis.

While our results suggest that some of the methods considered here work well for data of reasonably high dimension, for very high dimensional data (particularly when the number of dimensions is much greater than the number of elements), additional investigation is desirable. It is possible that simply modifying the data reduction method, such as by using Sparse PCA [70], may be sufficient. These avenues of investigation are left for future work. However, we would expect that Dist-dip would be the most efficient method, followed by Hopkins, for such data based on the theoretical complexity discussed in Subsection 5.1.

The choice of dimension reduction method should be made carefully. For example, if applicable, an appropriate distance metric is crucial for proper analysis in both cluster analysis and clusterability evaluation. For the purpose of this paper, we focus on Euclidian distance, which is the most common metric. Investigation of other metrics, while a popular topic of recent interest [71], is left for future research. Similarly, if the data is known to be highly non-linear, then the user may not wish to use PCA. Other data reduction methods for non-linear data will be explored in future work.

## 7. Conclusions

The application of clustering algorithms presupposes the existence of cluster structure. Clustering techniques tend to produce some partition for any given data set, which can lead to invalid conclusions when the data is unclusterable. Consequently, we advocate for the integration of clusterability into cluster analysis, allowing users to determine whether clustering is appropriate for the given data before proceeding with further processing.

A succinct, practical summary of our results is shown in the table below. The table includes only methods that were found to be effective in our simulations, and allows users to select from amongst these methods on the basis of three simple metrics: whether small clusters should be treated as outlier (do we want an outlier robust measure, or one that allows for small clusters?), whether the target clustering may consists of clusters with chaining structure, or is high dimensional (up to 50 dimensions). The following table focuses on qualitative analysis, see Section 5 for runtime analysis.

	Outliers/Small Clusters	Chaining Data	High Dimensional
PCA dip	small clusters	x	✓
PCA Silverman	small clusters	x	✓
Dist dip	outlier robust	✓	✓
Dist Silverman	outlier robust	x	x
Hopkins	small clusters	x	x

Please see Section 6 for a thorough discussion.

We look forward to the widespread application of clusterability tests as part of the clustering process. As of the writing of the present manuscript, implementation of the clusterability methods described in this paper is in progress. To this end, two macros were written to conduct multimodality tests in *SAS*, as the procedures were previously unavailable in *SAS* [72]. Software development is in progress to facilitate user-friendly applications of the clusterability methods in common statistical software *SAS* and *R*. Documentation of these clusterability algorithms is also in development and will be published in future manuscripts.

We close with the following quote to remind of the importance of testing for clusterability before proceeding with further – potentially unnecessary – cluster analysis tasks.

“There is nothing so useless as doing efficiently that which should not be done at all.” -Peter F. Drucker

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**Andreas Adolfsson**, MS is a doctoral student at Santa Clara University in the Department of Computer Engineering. He completed his bachelors and master's degrees in computer science at Florida State University, where he worked as an intern in robotics.

**Margareta Ackerman**, Ph.D is an Assistant Professor at the Department of Computer Engineering at Santa Clara University, specializing in machine learning, spanning from theoretical foundations to applications in big data and computational creativity. She received her PhD from the University of Waterloo and was a Postdoctoral Fellow at Caltech and UC San Diego. Her work is funded by the Office of Naval Research and she has received extensive support from the Natural Sciences and Engineering Research Council of Canada.

**Naomi Brownstein**, Ph.D is an Assistant Professor in the Department of Behavioral Sciences and Social Medicine and the sole faculty level biostatistician in the College of Medicine at Florida State University. She conducts research on statistical methodology related to clusterability and survival analysis, as well as a plethora of applications in medicine and public health. After completing her master's degree and doctorate in biostatistics at the University of North Carolina at Chapel Hill, she worked as a Postdoctoral Associate at the National High Magnetic Field Lab before coming to the FSU College of Medicine in 2015. Naomi has received financial support from the National Science Foundation, the National Institute of Environmental Health Sciences, and the Substance Abuse and Mental Health Services Administration.