

# A Tool for Visualizing and Analyzing High-Dimensional Clustering Performance

Justin Lin\* and Julia Fukuyama†

## Abstract

Technological advances have spurred an increase in data complexity and dimensionality. We are now in an era in which data sets containing thousands of features are commonplace. To digest and analyze such high-dimensional data, dimension reduction techniques have been developed and advanced along with computational power. Of these techniques, nonlinear methods are most commonly employed when working with high-dimensional data because of their ability to construct visual two-dimensional representations of high-dimensional data. These methods unevenly stretch and shrink space in a way that represents the data’s structure in a fewer number of dimensions. However, attempting to capture high-dimensional structures in a significantly lower number of dimensions requires drastic manipulation of space. As such, nonlinear dimension reduction methods are known to occasionally capture false structures, especially in noisy settings. In efforts to deal with this phenomenon, we developed an interactive tool that enables researchers to better understand and diagnose their dimension reduction results. It uses various analytical plots to provide a multi-faceted perspective on captured structures in the data to determine if they’re faithful to the original data or remnants of the dimension reduction process. The tool is available in an R package named *insert name here*.

## 1 Introduction

The potency of nonlinear dimension reduction methods lies in their flexibility, allowing them to model complex data structures. That same flexibility, however, makes them difficult to use and interpret. Each method requires a slew of hyperparameters that need to be calibrated, and even when adequately calibrated, these methods require a trained eye to interpret. For example, the two most popular nonlinear dimension reduction methods, t-SNE and UMAP, are known to generate unintuitive results ([5], [15]). The results often cluster, even when no clusters exist in the data. Moreover, cluster sizes and inter-cluster distances can be unreliable. We’ve developed an interactive tool that researchers may use to conduct a post-hoc analysis when applying high-dimensional clustering. The main goal of the tool is provide an additional perspective on inter-cluster relationships, making it easier to distinguish structures faithful to the signal from the noise.

## 2 Methods

### 2.1 The Minimum Spanning Tree

Graphs have been applied to many multivariate statistical problems. The authors of [14] introduced the minimal ascending path spanning tree as a way to test for multimodality. The Friedman-Rafsky test [8], along with its modern variations [2, 3, 4], use the minimum spanning tree (MST) to construct a multivariate two-sample test. Single-linkage clustering [7] and runt pruning [11] are both intimately related with the MST. In the context of dimension reduction, IsoMap [12] makes use of neighborhood graphs, [9] introduces the maximum information spanning tree, and [13] uses the MST. These methods, which fall under the category of manifold learning, use graphs to model high-dimensional data assumed to be drawn uniformly from a non-linear manifold. An accurate low-dimensional representation can then be constructed from these graphs. It’s apparent that graphs are useful for modeling high-dimensional

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\*Department of Mathematics, Indiana University

†Department of Statistics, Indiana University

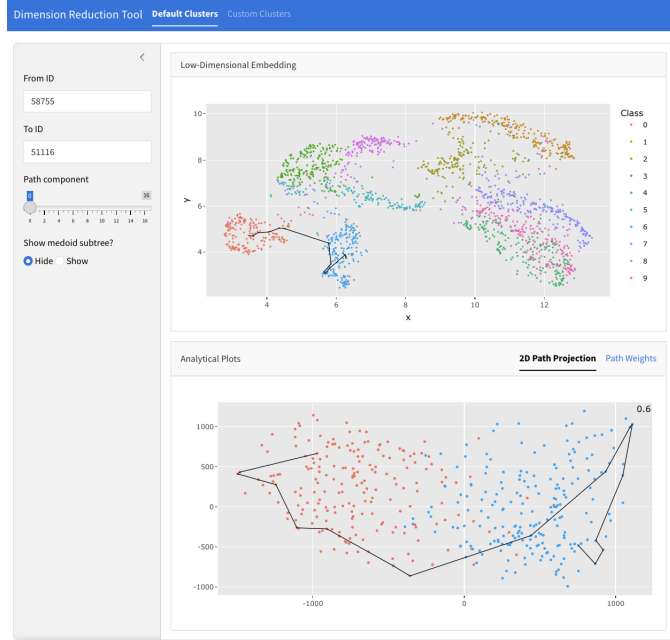


Figure 1: Dashboard

data, especially when it comes to dimension reduction and cluster analysis. Our tool uses the MST to analyze the reliability of visualizations produced by nonlinear dimension reduction methods.

To construct the MST from a data set, start with a set of vertices, one for each point in the data set. When an edge is added between two vertices, its assigned a weight equal to the dissimilarity between the pair of points corresponding to the two vertices. The edges of the MST are selected from all possible edges so that the sum of edge weights is minimized and there exists a path between any two vertices. We’ve opted for the MST for a couple of key properties. Firstly, the MST and shortest paths along it are quick to compute. Secondly, the MST contains a unique path between any two vertices, providing inter-point distances between all pairs of points. Lastly, it provides a good summary of the data’s structure. It contains as a subgraph the nearest-neighbor graph, and any edge deletion in the MST partitions the vertices into two sets for which the deleted edge is the shortest distance between them [8].

## 2.2 The Inputs

The interactive tool takes as input a dissimilarity matrix  $D \in \mathbb{R}^{n \times n}$  representing the dissimilarities between the  $n$  high-dimensional points, a two-dimensional embedding  $X \in \mathbb{R}^{n \times 2}$ , and a clustering  $\mathcal{C} \in \{1, \dots, k\}^n$  where  $k$  is the number of classes. Optionally, it also takes a set of ID’s to denote the points.

The dissimilarity matrix must be a symmetric matrix with 0’s along the diagonal. The entry  $D_{ij} = D_{ji}$  should represent the dissimilarity or distance between points  $i$  and  $j$ . The chosen dissimilarity measure should be appropriate for the type of data. For example, the  $L_1$  norm and even fractional  $L_p$  distance measures have been suggested for high-dimensional numerical data [1], Jaccard and cosine metrics are popular when working with text data [10], and a variety of Image Distance Functions (IDFs) have been suggested for image data [6]. From this dissimilarity matrix, the MST is calculated.

## 2.3 The Dashboard

The dashboard contains two main panels, as well as a side panel include adjustable settings. The first main panel depicts the low-dimensional embedding colored according to the provided clustering. The second main panel contains analytical plots. When supplied with a pair of points via “From ID” and “To ID”, the MST path is calculated between the high-dimensional points and corresponding path in low-dimension is drawn upon the low-dimensional embedding (Figure 1). The first analytical plot depicts a PCA projection of the high-dimensional path along with the clusters the two endpoints belong to. The PCA transform is calculated using only the points along the path then applied to the rest of the points.

The second analytical plot contains a bar plot of path weights. The user may cycle through the segments along the path using the “Path component” slider in the side panel. The corresponding segment will be highlighted in both the low-dimensional embedding and the 2D path projection. The corresponding path weight will also be highlighted in the plot of path weights.

To get a holistic view of the data’s structure, the user may view the medoid subtree by selecting “Show” in the side panel. The medoid subtree is the minimal subtree of the MST containing the medoid of each class. The medoid subtree represents the global arrangement of clusters.

Along the top bar, the user may also navigate to the next page named “Custom Clusters”. This page contains the same plots, but the user may instead define their own clusters of interest. To define a cluster, the user may select a subset of points by clicking and dragging along the low-dimensional embedding plot. Once the points are selected, the user can save the selected points by clicking “Submit Group 1”. The user must then repeat the process with the second cluster of interest and click “Submit Group 2”. Once both clusters have been submitted, the path between the (high-dimensional) medoids of the selected clusters will be portrayed. The 2D path projection will contain the points along the path along with the selected points.

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