Visualizing the effects of a changing distance using continuous embeddings

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Abstract

Most ML methods, from clustering to nearest-neighbour classification, rely on a distance function to describe relationships between datapoints. For complex datasets it is often hard to avoid making some arbitrary choices when defining a distance function. To compare images, one must choose a spatial scale. To compare signals, one must choose a temporal scale. The right scale is hard to pin down and it is preferable when results do not depend too tightly on the exact value that one picked.

Topological data analysis seeks to address this issue by focusing on the notion of neighbourhood instead of that of distance. Here, we show that in some cases a simpler solution is available. One can check how strongly distance relationships depend on a hyperparameter using dimensionality reduction. We formulate a variant of dynamical multi-dimensional scaling (MDS), which embeds datapoints as timecurves. The resulting algorithm provides a simple and efficient way of visualizing changes and invariances in distance patterns as a hyperparameter is varied. We apply it to challenging brain connectivity datasets, which are difficult to average over subjects in a non-arbitrary way. We also show how the algorithm can be used to visualize the effects of changes in a weighted metric, when changing the relative weight of two groups of variables.

1 Introduction

The notion of distance is at the core of data analysis and machine learning: most methods need to know how similar two datapoints are. For complex data, distance or similarity can be arbitrary to some extent (Carlsson, 2009). It is, for example, often possible to describe signals on different temporal or spatial scales, and distance functions will give a certain scale more weight than another. Each datapoint might describe several features, and there is often no unique, optimal way to weigh the features when computing a distance measures: are two individuals more alike if they have similar eye colour or hair colour, or do we think the shape of the nose matters most?

There are ways around that problem. One is to select the distance function that is best adapted to the task at hand, for example the one that gives the best performance in classification (this is effectively what is done in kernel hyperparameter selection [Schölkopf and Smola, 2002]). Another is to give up on distance and rely instead on the weaker notion of neighbourhood ([Lum et al., 2013].

We argue here that a third option is available. One may simply study how the shape of the data evolves under a change in the distance metric. We suppose that a family of distance functions $d_\alpha(x, y)$ is defined by varying a hyperparameter $\alpha \in (0, 1)$. Suppose that for a given level of $\alpha$ the relative distances between datapoints are well described by representing the datapoints as points on the line. As we vary $\alpha$ the points will move, so that each point now describes a curve. Many scenarios are possible, and we sketch them in Figure 1. We may have full or partial invariance: patterns in the data that hold regardless of the value of the hyperparameter (Figure 1A). On
the other hand, the structure in the data may appear only for certain values of \( \alpha \) (Figure 1B and C), indicating that these values are more useful than others for characterizing the data. Analyzing the evolution of structures in the data might reveal interesting dependencies, for example, declustering (Figure 1C) or loss of information (Figure 1D).

Figure 1: Sketches of different effects on the data structure that emerge when varying a hyperparameter in a distance functions. A) Invariance: patterns hold independent of the hyperparameter. B/C) Structure emerges only for certain values of the hyperparameter. C) Declustering: clusters are lost with increasing hyperparameter. D) Information loss: Structure collapses with increasing hyperparameter.

To visualize the effects of varying the distance function we suggest to embed data into a space of smooth curves, forming what we call continuous embeddings: in continuous embeddings each datapoint is embedded as a smooth curve in \( \mathbb{R}^D \). We will show that this approach is quite general.

Our implementation of continuous embeddings is based on MDS, one of the most widely-used tools for dimensionality reduction (Buja and Swayne, 2002; Buja et al., 2008). MDS, which builds on the pairwise relation between single data points, has an intuitive way of characterizing the structure in high-dimensional data. We use a continuous version of MDS (cMDS) by adding a smoothing penalty to the MDS cost function. Similar ideas have been used in the visualization of dynamic networks. A 2D embedding of a static graph is often constructed using MDS or similar methods (Kamada and Kawai, 1989; Gansner et al., 2005). In the dynamic context, where a graph is measured over time, it is important to preserve the so-called “mental map” when jumping from one timepoint to the next (Misue et al., 1995). This has been formalized as a regularization problem in Brandes and Wagner (1997). There have been three different approaches to the problem: aggregation, anchoring and linking. In aggregation methods, the graph is aggregated into an average graph which is then visualized with a static layout algorithm (Moody et al., 2005). Anchoring methods use auxiliary edges connecting nodes to stationary reference positions (Brandes and Wagner, 1997; Frishman and Tal, 2008). In linking, edges are created that connect instances of a single vertex over time. The resulting graph is then visualized using standard methods (Erten et al., 2004). Linking has been formulated in more rigorous ways in terms of regularized cost functions (Baur and Schank, 2008; Brandes and Mader, 2012; Xu et al., 2013) introduce an additional grouping penalty.

All these approaches visualize temporal developments and focus on 2D embeddings of graphs. We show that continuous embeddings can be applied to a wide variety of data. In particular, the continuous variable can be used to visualize artificial dynamics. This makes the method very general and is especially useful in the analysis of families of distance functions and their effects on data structure.

We present how continuous embeddings can be implemented using a straightforward iterative majorization approach, in which inner loops are nothing more than least squares regression with smoothing splines. We call the resulting algorithm cMDS, and illustrate the results of cMDS with three examples. We show that cMDS leads to novel forms of data visualization and enhances the analysis of various meta-effects in data, such as hierarchy levels in hierarchical clustering, weighting of different distance measures and consensus requirements across subjects. cMDS is especially well-suited to dynamic and interactive contexts (Cook and Swayne, 2007). We provide several examples of interactive, web-based visualizations based on cMDS.
2 Methods

We start by setting some notations and definitions. The original data or objects are denoted by \(s_1(\tau) \ldots s_N(\tau)\) and are defined in an arbitrary metric space, e.g. \(\mathbb{R}^D\). The parameter \(\tau\) measures a continuous dimension, e.g. time. We will see that other objects, such as images or networks, can be endowed with a continuous dimension, for example by examining them at different scales, so that scale plays the role of the continuous parameter. Another example is the one described in the introduction, where filter width is the continuous parameter. In practice, \(\tau\) will be sampled on a grid \(\tau_1 \ldots \tau_T\). With \(f(\tau_k)\) we refer to function values at all grid points while \(f(\tau_k)\) refers to a function value at a specific time. The objects are endowed with a distance function \(d(x, y)\). The appropriate distance function depends on the data-space and on the nature of the problem. Given a distance measure we can define a distance array \(D(\tau) \in \mathbb{R}^{T \times N \times N}\) where the entry \(d_{ij}(\tau_k)\) holds the distance between objects \(s_i\) and \(s_j\) at \(\tau_k\). We assume that the distances between datapoints give a good summary of the patterns in the data. The goal of cMDS will be to extract these patterns.

2.1 Objective

The objective of cMDS is to retrieve curves or manifolds in \(\mathbb{R}^d\), which we denote as \(x_1(\tau) \ldots x_N(\tau)\), such that evolution of the distances between the curves represents the evolution of the distances between the datapoints. The curves are represented as a configuration array \(X(\tau) \in \mathbb{R}^{T \times d \times N}\), and for a given time-point \(\tau_k\), \(X(\tau_k)\) is a \(d \times N\) matrix in which each column represents the coordinates of one curve at time \(\tau_k\). In \(\mathbb{R}^d\) we measure the distance between two curves at time \(\tau_k\) with the Euclidean distance. Thus, for each configuration, we have a distance array \(\tilde{D}(\tau) \in \mathbb{R}^{T \times N \times N}\) such that \(\tilde{d}_{ij}(\tau_k) = \|x_i(\tau_k) - x_j(\tau_k)\|_2\). These are the approximate distances given by our embedding, and the objective is to make the approximate distances as close as possible to the real distances. A natural expression of that objective is the following cost function, which quantifies the distortion of the embedding:

\[
\mathcal{L}(X(\tau), D(\tau)) = \sum_{i,j=1}^N \sum_{k=1}^T \left\| \tilde{D}(\tau_k) - D(\tau_k) \right\|^2
\]

(1)

Because distances are invariant to rotations, translations and symmetries, the optimization problem based on this cost function is ill-defined. In addition we will require that each curve is continuous and smooth, which can be achieved by adding a suitable penalty function:

\[
\mathcal{C}(X(\tau), D(\tau)) = \mathcal{L}(X(\tau), D(\tau)) + \lambda \Omega(X(\tau))
\]

(2)

The function \(\Omega(X(\tau))\) should penalize functions that are not smooth, and we will see below that classical spline penalties [Ramsay and Silverman, 2002] are particularly convenient. For one-dimensional curves \(\Omega\) equals:

\[
\Omega (X(\tau)) = \sum_{i=1}^N \sum_{k=1}^T (\ddot{x}_i(\tau_k))^2
\]

(3)

Here, \(\ddot{x}\) denotes the second derivative with respect to \(\tau\). In practice we will approximate this with a discrete differential operator.

2.2 The optimization problem

2.2.1 Majorization-minimization for the classical MDS problem

Our algorithm builds on the standard MDS problem, for which [Agarwal et al., 2010] have developed an elegant framework. We review and reinterpret their approach and ultimately extend it to continuous embeddings. The cost function that is commonly used in metric MDS is

\[
\mathcal{L}(X, D) = \sum_{i,j} ((\|x_i - x_j\| - d_{ij})^2
\]

(4)
Minimizing this cost function with respect to $X$ is also known as *Kruskal-Shephard* scaling (Kruskal [1964]). Agarwal et al. (2010) take advantage of the fact that the objective function $\mathcal{L}$ is a sum over costs of single points $x_i$ to solve the problem iteratively. They suggest conditional optimization: optimization of a single point $x_i$ while all other points $x_j \neq i$ are fixed at the value of the most recent iteration.

To optimize a single point $x_i$, Agarwal et al. (2010) use an auxiliary function motivated by the geometry of the problem. The cost function for a single point $x_i$ is

$$f(x_i) = \sum_j (\|x_i - x_j\|_2 - d_{ij})^2$$

Agarwal et al. (2010) state that instead of optimizing this function, one can optimize the much simpler function

$$g(x_i) = \sum_j (\|x_i -  \hat{x}_j\|_2)^2,$$

where $\hat{x}_j$ are auxiliary points which we explain later in more detail. We interpret this approach as a majorization-minimization algorithm (De Leeuw and Heiser, 1977; Leeuw, 1994; Hunter and Lange, 2004) and prove the following prerequisite:

**Lemma.** $g(y)$ is a majorizing function for $f(y)$.

**Proof.** For each $(x_i)$, $f$ measures the difference between the original distance ($d_{ij}$) and the Euclidean distance between $x_i$ and $x_j$. A function that majorizes these terms ultimately also majorizes the sum. We thus argue with a single point $x_j$. Let $S_j$ denote the sphere of radius $r_j = d_{ij}$ centered at $x_j$. Consider another sphere, $S_\alpha$, also centered around $x_j$, but now with arbitrary radius $\alpha$. Since the cost function $f$ measures the distance to $S_j$, $S_\alpha$ is a level set of $f$:

$$f(y \mid y \in S_\alpha) = (\alpha - r_j)^2$$

This is the minimum distance between any two points on $S_j$ and $S_\alpha$. Thus, the squared distance between any point on $S_j$ and an arbitrary point $\hat{x}_j$ on $S_j$ is larger or equal to $(\alpha - r_j)^2$. These statements hold for any sphere centered at $x_j$. We thus know that the distance to $\hat{x}_j$ is an upper bound for the cost:

$$\|y - \hat{x}_j\|^2 \geq (\|y - x_j\|^2 - r_j)^2$$

The majorizing function $g$ should also be tight, that is, it should be equal to $f$ in the supporting point. This condition holds if we define the auxiliary point $\hat{x}_j$ to be the projection of $x_i$ on $S_j$. Then, the supporting point of the majorizing function is the point $x_i$. There is one case where this definition of $\hat{x}_j$ is ill-defined. If $x_j = x_i$, there are infinitely many possibilities for $\hat{x}_j$, namely the entire set $S_j$. In this situation, we define $\hat{x}_j$ to be randomly positioned on $S_j$. This does not violate the majorization/minimization principle.

With $g(y)$ as a simple quadratic majorizing function, the optimization is straightforward. Since the auxiliary points depend on the current configuration, we iteratively optimize $x_{\alpha}$, compute the auxiliary points, again optimize, etc. The auxiliary points are computed based on the current $x_i^{(m)}$. The point which minimizes $g(y)$ is the centroid of the auxiliary points $\hat{x}_j$.

### 2.2.2 Extension to cMDS

We have shown that the algorithm by Agarwal et al. (2010) can be interpreted as a majorization-minimization algorithm. In the case of continuous embeddings we have to optimize the set of curves $X(\tau)$. With cMDS, we not only minimize the distortion at each timestep. Additionally, we enforce smooth functions $x(\tau)$ by including a penalty function $\Omega$. The cost function for this optimization problem (2) can be discretized as:

$$\mathcal{L}(X(\tau), D(\tau)) = \mathcal{L}(X(\tau), D(\tau)) + \lambda \Omega(X(\tau))$$

$$= \sum_{k=1}^{T} \sum_{i,j=1}^{N} (\|x_i(\tau_k) - x_j(\tau_k)\|_2 - d_{ij}(\tau_k))^2$$

$$+ \lambda \sum_{i} x_i^T(\tau) (\Delta^2)^T \Delta^2 x_i(\tau)$$

where $\Delta$ denotes the discrete first order differential operator.
The parameter $\lambda$ controls how strongly the roughness of the curves is penalized. For $\lambda = 0$, we recover the classical cost function of MDS, with the extension that we have $T$ separate MDS problems, one for each time step. For $\lambda \to \infty$ the resulting curves are straight lines, independent of the original data. This parameter is easy to set by visual inspection. It should simply be large enough to result in fairly smooth curves, while keeping the distortion reasonably small. A reasonable strategy for setting $\lambda$ automatically is then to maximize $\lambda$, under a constraint on the quality of the embedding. The quality of the embedding can be measured in various ways (Kaski and Peltonen 2011; Mokbel et al. 2013). Similarly to the point set embedding, the cost function $C$ in cMDS is a sum over costs $f$ for single curves:

$$f(x_i(\tau)) = \sum_k \sum_j \left(\|x_i(\tau_k) - x_j(\tau_k)\|_2^2 - d_{ij}(\tau_k)\right)^2 + \lambda x^T(\tau) M x_i(\tau)$$

where $M = (\Delta^2)^T \Delta^2$. Note that the penalty term in $f$ is independent of the transition to the auxiliary points $\hat{x}_j(\tau)$. We can thus simply add the penalty to $g$ and have that the proof of $g$ being an upper bound is still valid. The penalty term is quadratic in $x_i$. Thus, the minimization of $g$ can be done analytically also in the continuous case. This qualifies $g$ as a suitable majorizing function.

The complete definition of the majorizing function in cMDS is

$$g(y(\tau), x_i(\tau)) = \sum_k \sum_j \|y(\tau_k) - \hat{x}_j(\tau_k)\|^2 + \lambda y^T(\tau) M y(\tau)$$

s.t. project ($x_i(\tau), S_j(\tau)$) = $\hat{x}_j(\tau)$ $\forall j \neq i$

At this point, we can minimize the local cost function $f$ by means of a majorization-minimization algorithm. Together with the iteration over the curves $x_i(\tau)$ we have everything we need for the cMDS algorithm (see Algorithm 1). The complexity of the algorithm is $O(dTN^2)$ per iteration, since its function MM has complexity $O(dTN)$, but the complexity of computation of the cost function is $O(dTN^2)$.

**Function 1** cMDS$D(\tau), X_0(\tau), \lambda, M, \delta$

repeat
\$\epsilon \leftarrow C(D(\tau), X(\tau))$
for $i = 1 : N$ do
\$x_i(\tau) \leftarrow \text{MM}(D(\tau), X(\tau), i, \text{params})$
end for
until ($\epsilon - C(D(\tau), X(\tau)) > \delta$)
\$\epsilon \leftarrow [C(D(\tau), X(\tau)), L(D(\tau), X(\tau)), \Omega(D(\tau), X(\tau))]$
return $X(\tau), \epsilon$

**Function 2** MM$D(\tau), X(\tau), i, \text{params}$

repeat
\$\epsilon \leftarrow f(D(\tau), X(\tau), i, \text{params})$
\$\hat{x}(\tau) \leftarrow$
\$X(\tau) \leftarrow \text{MINIMIZE}(X(\tau), \hat{x}(\tau), i, \text{params})$
until ($\epsilon - f(D(\tau), X(\tau), i, \text{params}) > \delta$)
return $X(\tau)$

### 2.3 Initialization

The cMDS algorithm needs to be seeded with a starting configuration. The optimization works with a random initialization, but performance can be improved with a more structured approach.
Figure 2: Effects of changes in a weighted metric. Economic and demographic distance measures are weighted according to $D(\alpha) = \alpha \cdot D_E + (1 - \alpha) \cdot D_D$. Thus, the first panel represents an embedding that is solely based on the demographic metric, while the last one is based on the economic one. In between are samples of different weights, denoted by $\alpha$. The red labels depict an example of a neighborhood relation between the Netherlands (NLD) and Finland (FIN) that is invariant with respect to $\alpha$, while the green ones, Bulgaria (BGR) and Estland (EST) are an example of a strong dependency on $\alpha$. 
Figure 3: Embedding of regional networks acquired by DTI and tractography (Hagmann et al., 2008). The different panels correspond to different threshold levels $\alpha$ when building consensus networks. The superior frontal cortex (SF) and paracentral lobule (PARC) are stable regions in the core and at the periphery of the network. On the contrary, the parahippocampal cortex (PARH) and the fusiform gyrus (FUS) change their role in the network.
One possibility is to perform classical scaling (Kruskal, 1964; Torgerson, 1952) for each timestep. In this case, we run into the problem that MDS configurations are invariant with respect to translation and rotation, since these operations do not affect distances. Classical scaling yields configurations with zero mean, which solves the problem of translation invariance. But the rotation invariance remains. To solve this, we can initialize cMDS with an aggregated solution. To obtain this solution we average each curve \( x_i(\tau) \) over time and then perform classical scaling on \( \bar{X} \).

3 Examples

In the following examples we show how cMDS can be used to analyze the effect of hyperparameters of distance functions on the data. In the first example, we used a weighted metric: distances evolve according to the relative weight given to some of the dimensions. In the second example, the distance function in a network varies according to a thresholding rule. In the third, we derive a multiscale representation of data using hierarchical clustering, and visualize changes in distance over scale.

3.1 Economic and demographic descriptors of EU countries

For this example we use economic and demographic descriptors of the 27 EU countries. The data are publicly available from the gapminder website. As economic variables we use income per capita (2008), CO\(_2\) emissions per capita (2008) and number of granted patents per capita (2002). Demographic variables are total fertility rate, life expectancy at birth and the fraction of urban population. We scale all variables logarithmically. We then build two distance matrices, one solely based on economic variables, \( D_E \), the other on demographic variables, \( D_D \). Now, we put different weights on both variable groups and have a continuous range with one extreme only considering demographic variables and the other extreme only considering economic ones:

\[
D(\alpha) = \alpha \cdot D_E + (1 - \alpha) \cdot D_D
\]

where \( \alpha \) is between 0 and 1. We sample this continuum at \( N \) different values of \( \alpha \) and thus get a distance array in \( R^{N \times 27 \times 27} \). For this example, a 1D embedding is not sufficient to capture relevant trends in the data. Thus, we give snapshots of the 2D results in Figure 2. In this case, an interactive presentation of the results is much easier to read and thus an advantageous choice. An interactive visualization is viewable here. The 2D embedding shows that the changes in weighting have significantly different effects on the individual neighborhood relations. For example, some demographically very similar countries start diverging when economic variables are taken into account and end up far apart under the economic distance metric (e.g. Bulgaria and Estonia). Other countries stay similar, invariant of the weighting of different distances (e.g. Finland and the Netherlands). These patterns are lost when deciding a distance measure a priori. Using cMDS to visualize the effects of the hyperparameter makes them easier to discover and understand, especially using an interactive context.

3.2 Diffusion Tensor Imaging

Brain regions are linked by white matter tracts, forming a network called the Connectome (Sporns et al., 2005). Diffusion Tensor Imaging (DTI) is a form of magnetic resonance imaging that can be used to find connections between brain regions (using tractography, (Hagmann et al., 2003)). Here we use data obtained by Hagmann et al. (2008), available here. DTI produces noisy results, and connectivity must often be averaged over individual subjects. There is by necessity some arbitrariness in the averaging, and we show here how cMDS can be used to visualize changes in network structure as the averaging criterion is varied. In the original data, the brain is segmented into 998 regions of interests that cover about 1.5 cm\(^2\) each and belong to one of 66 anatomical regions (33 per hemisphere). Here, we do not work with the full network, but rather with regionally aggregated data. That is, the data are adjacency matrices in \( R^{66 \times 66} \), where \( A_{ij}^{(s)} \) is a binary indicator of a connection between regions \( i \) and \( j \) for subject \( s \). Connections are measured for five different subjects, and because of the relatively high noise in the data some form of averaging (over subjects) may be useful. One approach is to produce a consensus network out of the individual networks, with the rule that a link is introduced in the 50%
consensus network if and only if it is present in at least 50% of the individual networks. Thus, we look at the average adjacency matrix $\bar{A}$, where $\bar{A}_{ij} = (1/N) \sum_s A^{(s)}_{ij}$ and threshold it at different levels to produce the different consensus networks. We use the threshold level $\alpha$ as the continuous parameter in cMDS, such that $\bar{A}_{ij}(\alpha) = \bar{A}_{ij} > \alpha$. If we take the shortest-path distance on the graph that is defined by $\bar{A}(\alpha)$ as the distance measure between two regions, then changing the threshold level is exactly the same as changing the distance measure, as some links will start disappearing with higher threshold values. We can therefore apply cMDS to visualize the changes in network structure as the averaging rule is changed. For this example, we implement a weighted version of the algorithm, to mirror the standard Kamada-Kawai layout methods (Kamada and Kawai, 1989). The results are shown in Figure 3 for regions in the left hemisphere. A first (and unsurprising) result is that the network density decreases significantly with the threshold level. That is, as we start requiring higher levels of consistency among the subjects, a lot of connections are rejected.

Results show that some regions are very stable: for example, the superior frontal cortex (SF) stays at the core of the network, while the paracentral lobule (PARC) remains at the periphery regardless of the threshold. Other regions move a lot. The parahippocampal cortex (PARH) starts out in the periphery, then moves to the core and to the periphery again. The fusiform gyrus (FUS) moves from the core of the network to the periphery. Since core-periphery relationships are central to the interpretation of connectome data, it is crucial to know which regions can be reliably called peripheral and others central (Hagmann et al., 2008). cMDS provides that at a glance.

3.3 Hierarchical clustering

We mentioned in the introduction that distance is often computed relative to a certain scale. For spatial or temporal data scale corresponds to a concrete spatial or temporal window, but there are other ways to obtain a multiscale representation. Hierarchical clustering (Kaufman and Rousseeuw, 1990; Hastie et al., 2009) is such a technique. We focus here on agglomerative clustering, where the algorithm starts with each observation in one cluster. At each level, the algorithm merges the two closest clusters until only one cluster remains. Thus, there are $N - 1$ levels in the hierarchy, which gives a view of the data going from the roughest to the most detailed level. cMDS provides an interesting visualization of the results.

We first define a distance function at each level of the hierarchy. For each level, we build the distance matrix for the $N$ datapoints as follows: if two datapoints are in the same cluster we assign a very small positive distance, otherwise we assign the distance between the respective cluster centers. Here, we use the publicly available USArrests dataset from the R datasets package. It contains data on murder arrests, assault arrests, rape arrests and urban population for the different US states in 1973. We picked this dataset because it is used as an example for the R hclust function. We use cMDS to embed these data (Figure 4). The result is a tree structure with the property that, at each level of the tree, distances between branches are representative of distances between clusters. This enables an immediate understanding of the hierarchical clustering results. We also developed an interactive visualization based on a 2D embedding, which better captures the potential of cMDS for such applications. We invite readers to have a look at these results (online here).

4 Discussion

We have introduced an easy to implement and flexible version of continuous (or dynamic) multi-dimensional scaling, namely cMDS. We have applied cMDS to three different data sets. With the first example on EU data we showed the effects of changing a weighted metric, putting different weights on two feature classes. Visualization revealed countries whose neighborhood relations are invariant to the change in weights as well as countries whose relative position strongly depends on the weights. In a brain connectivity example, where averaging over subjects is not straightforward, we found that the shape of the network changes according to the averaging rule. With cMDS, identifying stable and unstable regions turned out to be straightforward. Finally, we showed how hierarchical clustering can be thought of as a multiscale representation of data, and we used cMDS to visualize how the structure of the data changes across scale.
Figure 4: Embedding of an hierarchical clustering results for the USArrests data set which is publicly available as part of the R datasets package. We selected a sample of 17 states. We ran hierarchical clustering using the centroid of clusters for agglomeration. Then, we built the distance matrix for each level: two datapoints are assigned a small positive distance if they are in the same cluster and the distance between cluster centers otherwise. The cMDS result is a visualization of the tree structure. At each level, the distances between branches represents the distances between cluster centers.

In the connectivity example, we used Kamada-Kawai weighting instead of standard MDS cost. cMDS is easily adapted to different weighting approaches, such as local MDS (Chen and Buja, 2009), or asymmetrical cost functions. Note that ISOMAP (Tenenbaum et al., 2000) can be used as well. ISOMAP uses a particular form of MDS for manifold learning. cMDS can be extended in the same way to characterize changes in manifold structure induced by a change in metric.

We have only considered small datasets here, for which cMDS is very fast (with a runtime of a few seconds). As other MDS methods, cMDS has $O(n^3)$ scaling in its naive version. Runtime remains reasonable with a few hundred datapoints, and straightforward extensions for larger datasets are possible. One idea is to embed a subset of landmark points, as in landmark MDS (Silva and Tenenbaum, 2003). Another is to use sparse weighting matrices, tying each datapoint to a random subset of neighbours.

By visual inspection, cMDS immediately reveals qualitative structures in the neighborhood dynamics for various datasets. Furthermore, quantitative analyses are possible. For example, performing clustering on cMDS output can yield results that are robust to changes in the distance measure. We leave these extensions to future work.

5 Conclusion

We have argued that continuous MDS techniques provide a tool to visualize the dynamics that (so far) arbitrary choices in distance functions introduce in data. cMDS can deal with numerous sources of arbitrariness in the distance metric, examples of which are varying scale or weighting. We have shown that interesting and impor-
tant dynamics, such as invariance and declustering, are readily revealed by cMDS. Finally, we have provided a cMDS algorithm that is straightforward to implement, use and extend.

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