Cluster-based dual evolution for multivariate systems

Nick James\textsuperscript{1} and Max Menzies\textsuperscript{2}

\textsuperscript{1}\textit{School of Mathematics and Statistics, University of Sydney, NSW, Australia}
\textsuperscript{2}\textit{Yau Mathematical Sciences Center, Tsinghua University, Beijing, China}

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This paper proposes a cluster-based method to analyse multivariate systems that change over time. We apply this method to analyse the evolution of COVID-19 cases and deaths, partitioning data points into an appropriate number of clusters on each day to track both the total number of clusters and their changing constituency over time. This method can be used to track the trajectory of both the entire system as well as individual countries relative to the system. Applying our analysis to cases and deaths independently reveals a close relationship between the evolution of these two systems. With this in mind, we also develop a method to analyse the similarity and anomalies between two related multivariate systems in conjunction, allowing us to identify anomalous countries in the progression of cases to deaths.

The primary focus of this work is the analysis of the number of cases and deaths due to COVID-19 on a country by country basis. Reporting these numbers on a daily basis provides us with two related multivariate systems that evolve over time. We develop a new method with three goals in mind: first, we analyse each system individually and observe a close relationship; second, we analyse the two systems in conjunction to further understand their similarity; third, we determine anomalous countries relative to cases and deaths. Our methodology is flexible and not limited to this particular application.

I. INTRODUCTION

The evolutionary nature of multivariate systems over time is commonly studied in physics, engineering, biology and other fields. There are numerous approaches to the analysis of such evolving systems. In epidemiology, researchers have frequently studied evolving systems with explicit parametric models\textsuperscript{[1]} such as exponential or power-law models\textsuperscript{[2]}. In the wider field of \textit{time series analysis}, researchers have developed various nonparametric techniques to analyse systems of time series such as distance analysis\textsuperscript{[3,4]} and distance correlation\textsuperscript{[5,6]}. Network models\textsuperscript{[7] have recently been implemented to model the COVID-19 pandemic, among other analyses.\textsuperscript{[8]} Each of these methods has a component of analysing each individual time series separately and analysing the system as a whole.

In this paper, we analyse both the overall properties of a multivariate system and the trends of individual elements through the lens of \textit{cluster analysis}. Clustering algorithms seek to group elements of a data set according to their proximity. Common clustering algorithms are K-mean\textsuperscript{[9]} and spectral clustering\textsuperscript{[10]}, which partition elements into discrete sets, and hierarchical clustering\textsuperscript{[11,12]} which does not specify a precise number of clusters. The first two methods usually proceed with the number of clusters \(k\) chosen \textit{a priori}. It is a subtle question of how to select this \(k\) - we draw upon several methods to do so.

We apply our methodology to analyse the COVID-19 pandemic. First observed in late 2019, this disease has spread around the world, impacting each country differently. Studying the evolving numbers of cases and deaths by country gives two related multivariate systems that grow over time. The changing cluster membership of individual countries tracks their numbers relative to the rest of the system, while the number of clusters tracks the spread of the system in its entirety. After smoothing out the number of clusters, we notice a close relationship between the evolution in the number of clusters relative to cases and deaths. Having shown broad similarity between the two systems, we then seek to identify countries that are anomalous in this correspondence. Such countries have anomalous relationships between their case and death counts. While many explanations for these anomalies abound, including discrepancy in testing in different countries at different times, our focus is on the identification of trends and anomalies in a mathematical analysis. Our methodology is flexible and can build off any desired clustering algorithm that may be appropriate for the particular context.

This paper is structured as follows. In the proceeding three sections, we introduce portions of our methodology and present our results. Section \textbf{II} analyses the multivariate systems of cases and deaths individually. Section \textbf{III} compares the two systems in conjunction, determining suitable offsets for the spread of the systems and the cluster memberships. Section \textbf{IV} analyses anomalous countries in this relationship. We conclude in Section \textbf{V}. Existing theory that we draw upon is summarised in Appendix \textit{A}.

II. INDIVIDUAL ANALYSIS OF COVID-19 SYSTEMS: CASES AND DEATHS

A. Time-varying cluster analysis methodology

The most general setup of our methodology is as follows. Let \(x^{(i)}_t\) be a collection of \(n\) time series over a time interval of length \(T\), with \(i = 1, \ldots, n\) and \(t = 1, \ldots, T\). Assume each data point \(x^{(i)}_t\) is an element of a common normed space \(\mathcal{X}\). Slightly different procedures apply if \(\mathcal{X}\) is one-dimensional, namely \(\mathbb{R}\), or higher-dimensional.

In this paper, the two systems we present are the cumulative number of daily cases and deaths on a country by country basis. Our data spans 31/12/2019 to 30/4/2020, a period of \(T = 122\) days across \(n = 208\) countries. Ordering the countries by alphabetical order yields daily counts of cases and deaths.
We use this value with this value. \( k \) we compute the average for clarity. At each point, associate a standard and Gaussian centricity matrices \( x \) matrices. Let \( B \). Matrix analysis of system

Given the exponential nature of the data, we choose a logarithmic difference as our metric. First, we do some data pre-processing: any entry in the data that is empty or 0 - before any cases are detected - we replace with a 1, so that the log of that number is defined. Then we define a distance on case and death counts by \( d(x, y) = |\log(x) - \log(y)| \). Effectively, this pulls back the standard metric on \( \mathbb{R} \) under the homeomorphism \( \log : \mathbb{R}^+ \to \mathbb{R} \) and makes the positive real numbers a one-dimensional normed space.

The goal is to partition the data points \( x_1^{(t)}, \ldots, x_n^{(t)} \) into \( k_t \) clusters at every time \( t \) by applying appropriate clustering algorithms to the data at that time. An overview of such algorithms is provided in \[\text{Appendix A}\] We wish to care fully choose the number of clusters in such a way that provides us meaningful inference on how the system changes. A wildly varying number of clusters \( k_t \) would obscure inference on individual countries’ cluster memberships changing with time. Thus, we combine several methods of choosing \( k_t \) to reduce the bias in our estimator and perform additional exponential smoothing to yield a suitably changing number with time. In our experiments, we use six methods outlined in \[\text{Appendix A}\]. These have been chosen after experimentation and consultation with the literature, but our method is flexible and could use any combination of methods. Given cluster numbers \( k_1^{(t)}, \ldots, k_6^{(t)} \) offered by these methods, we compute the average \( k^{(t)}_{av} = \frac{1}{n} \sum_{i=1}^{n} k_i^{(t)} \). Note this is not necessarily an integer; we do not compute clusters directly with this value.

In our implementation, this average value \( k^{(t)}_{av} \) exhibits itself as approximately locally stationary. Thus, we apply exponential smoothing to \( k^{(t)}_{av} \) to produce a smoothed integer value \( \hat{k}_t \). We use this value \( \hat{k}_t \) at each \( t \) to obtain a clustering at that point. In this paper, data is real-valued, so we cluster according to the optimal K-means algorithm\[\text{13}\] and sort the clusters according to the order on \( \mathbb{R} \). Similar choices of \( \hat{k}_t \) exist when performing standard K-means or spectral clustering on higher-dimensional data.

### B. Matrix analysis of system

Record the results of this analysis in several sequences of matrices. Let \( D^{(t)} \) be the \( n \times n \) matrix of distances between \( x_i^{(t)} \) at times \( t \). Form two different affinity matrices and adjacency matrices at every \( t \). These definitions are motivated by standard constructions in \[\text{Appendix A}\], but our notation differs for clarity. At each point, associate a standard and Gaussian affinity matrix:

\[
\text{Aff}^{(t)}_{ij} = 1 - \frac{D_{ij}^{(t)}}{\max D^{(t)}},
\]

\[
G^{(t)}_{ij} = \exp\left(\frac{-m^2(D_{ij}^{(t)})^2}{2(\max D^{(t)})^2}\right)
\]

The denominator in the Gaussian is chosen to appropriately normalise \( G \), which is essential for subsequent analysis. We will vary \( m = 1, 2, 3 \) in experiments so the matrix elements mimic Gaussian spreads over 1, 2, 3 standard deviations respectively. Associate an adjacency matrix defined by

\[
\text{Adj}^{(t)}_{ij} = \begin{cases} 
1 & x_i^{(t)} \text{ and } x_j^{(t)} \text{ are in the same cluster} \\
0, & \text{else}
\end{cases}
\]

Finally, we can analyse the change in cluster memberships over time via the adjacency matrices. For a \( n \times n \) matrix \( A \), define its Frobenius norm by \( ||A|| = \left( \sum_{i,j=1}^{n} \left| a_{ij} \right|^2 \right)^{\frac{1}{2}} \). With this norm we can perform hierarchical clustering on the entire collection of adjacency matrices. Given points in time \( s, t \in [1, \ldots, T] \), we can consider the difference between the two cluster structures by defining \( d(s, t) = ||\text{Adj}^{(t)} - \text{Adj}^{(s)}|| \) and performing hierarchical clustering on these distances. We term the resulting \( T \times T \) dendrogram a cluster evolution dendrogram. This groups moments in time according to similarity in the cluster structure at each time.

### C. Results for system of cases

In this section, we implement an optimal K-means clustering algorithm on daily counts of cases. Experiments using K-means and spectral clustering on 3-day rolling counts of cases produce similar results. Our analysis confirms known phenomenology regarding the spread of COVID-19 cases. The smoothed number of clusters \( \hat{k}_t \) ranges between \( \{2, \ldots, 17\} \) and is depicted in Figure 2a. Until the end of January, there are only two clusters, with China being the only country severely impacted by the virus. Soon after, the virus spread around the world, with reported numbers changing day by day. During this time, the number of clusters increases rapidly towards a peak in early March. Italy is the first country to join the most severely impacted cluster, with the United States, Spain, France, Germany, Iran and the United Kingdom all joining by late March. Subsequently, cluster numbers slowly decline until the end of our analysis window and appear to stabilise. Indeed, the ranking of worst affected countries has largely stabilised in April, producing more consistent clustering results. Figure 3a tracks the changing cluster membership of severely impacted countries. Using the ordered cluster membership, we track each country’s severity relative to the rest of the world. We compute the cluster evolution dendrogram defined in Section II B for the daily cases to study the evolutionary nature of the cluster structure. This clusters the different adjacency matrices, which encode the cluster structure, at different times. We exp-
exclude the first 50 points of time, in which the cluster structure and associated adjacency matrices are all identical, with only China in its own cluster. This is displayed in Figure 1a.

D. Results for system of deaths

In this section, we implement an optimal K-means clustering algorithm on daily counts of deaths. The smoothed number of clusters $\hat{k}_t$ ranges between $\{1, \ldots, 17\}$ and is depicted in Figure 2a. The trajectory for number of death clusters follows a similar pattern to that of cases, with a lag of approximately one month. Like COVID-19 cases, our analysis highlights the key takeaways in severely impacted countries. Although we have highlighted a one-month offset in the general evolution of COVID-19 cases and deaths, there are dissimilarities regarding the membership of the worst affected cluster. In mid-March, China moves out of the worst cluster, into the second death cluster, demonstrating its relative success in responding to the pandemic. On the other hand, the United States, Spain, Italy, France and the United Kingdom have recently moved into this worst cluster. Upon examining the cluster constituencies after accounting for lag, we may yield insights into countries that have most and least effectively managed the progression from cases to deaths. Our method confirms that China has managed potential COVID-19 deaths relatively effectively, while Italy, Spain, the United Kingdom and the United States have been ineffective. Figure 3b tracks the changing cluster membership of severely impacted countries. Again, we compute the cluster evolution dendrogram defined in Section II B for the daily death numbers. We exclude the first 66 points of time, in which the cluster structure and associated adjacency matrices are all identical. This is displayed in Figure 1b. Once again, we see a strong similarity between cases and deaths in Figures 1a and 1b. These demonstrate near-identical hierarchical clustering results for the two systems. Both systems identify two distinct clusters. The visual depiction highlights two meaningful sub-clusters within the larger cluster: one highly prominent cluster with a high degree of similarity, and a smaller cluster with less pronounced similarity.

III. SYSTEM OFFSET ANALYSIS

In this section, we describe further analysis on two related multivariate systems $x_i(t)$ and $y_i(t)$ valued in a common normed space $\mathcal{X}$. We wish to determine relations between the two, and individual constituents of the system that are anomalous in this comparison. In particular, with our primary application of COVID-19 cases and deaths in mind, we wish to examine similarity up to an offset in time. We perform several analyses to identify an optimal time offset to measure similarity; in the next section we can subsequently study anomalous individual countries.

First, we have already observed a clear offset in the evolution of $\hat{k}_t$ for the systems of cases and deaths, and wish to determine it precisely. We define the system evolution offset with respect to the changing number of clusters as follows: Let $f(t) = \hat{k}_X(t)$ and $g(t) = \hat{k}_Y(t)$ be the smoothed number of clusters for each system. Given an offset $\tau$, define the translated function $f_\tau(t) = f(t + \tau)$. The system evolution offset is defined as the $\tau$ that minimises

$$||f_\tau - g||_1$$

For our application, this offset is $\tau = 32$, confirming the one-month offset observation in Figure 2a.

Next, we define the cluster consistency offset. This identifies for which offset in time is the cluster partition of the two systems most similar. This is not necessarily the same as the offset relative to the number of clusters. We seek to minimise the discrepancy between adjacency matrices $\text{Adj}_X$ and $\text{Adj}_Y$ of the two systems. Thus, we choose an offset $\tau$ that minimises

$$\frac{1}{T - |\tau|} \sum_{1 \leq s \leq T - \tau} ||\text{Adj}_X^{(s)} - \text{Adj}_Y^{(s)}||$$

Note that we normalise by the number of terms in this sum,
Cluster-based dual evolution for multivariate systems

FIG. 2: Evolution of the number of cases and deaths over time. The system evolution offset, defined in Section III, is \( \tau = 32 \). After translation and truncation, Figure 2b shows significant similarity between the two systems.

which varies with \( \tau \), for an appropriate comparison. When \( \tau > 0 \) we can rewrite this

\[
\frac{1}{T - \tau} \sum_{i=1}^{T-\tau} ||\text{Adj}_X^{(r)} - \text{Adj}_Y^{(r+\tau)}||
\]

We can also do the same for the offset in the standard or Gaussian affinity matrices \( \text{Aff} \) and \( G \). Note all these matrices are normalised, so a comparison of their values is appropriate. We choose the normalisation parameter of the Gaussian affinity matrix in Equation (2) for this purpose.

Results are displayed in Table I, with the minimal adjacency matrix offset determined in Figure 3. To illustrate the flexibility of the method, we choose different start dates for our offset analysis. The first 30 days carry some triviality in the cluster structure, with very few cases observed outside China, so it may be desirable to exclude them from the analysis. Fortunately, the optimal offset differs only slightly with different start dates.

FIG. 3: Heat maps display countries’ changing cluster membership. Darker and brighter colours denote membership in worse and less affected clusters respectively. Cluster membership depicts severity relative to the system.

FIG. 4: Optimal cluster consistency offset between adjacency matrices of cases and deaths.
TABLE I: Cluster consistency offset for adjacency and affinity matrices. The parameter $m$ is defined in Equation 1.

| Start date   | Gaussian $m = 1$ | Gaussian $m = 2$ | Gaussian $m = 3$ | Adj | Aff |
|--------------|-----------------|-----------------|-----------------|-----|-----|
| 31/12/2019   | 16              | 16              | 16              | 20  | 16  |
| 13/1/2020    | 12              | 13              | 14              | 20  | 15  |
| 21/1/2020    | 12              | 13              | 14              | 19  | 15  |
| 31/1/2020    | 12              | 13              | 14              | 19  | 15  |

Note that the optimal cluster consistency offset is overwhelmingly around 16. This confirms known medical findings indicating time from diagnosis to death has generally been around 17 days. This is quite different from the system evolution offset of 32 days. While the cluster consistency offset seeks to align the similarity of case and death counts among individual countries, the system evolution offset seeks to quantify the spread of the whole system.

One explanation for the system evolution offset being longer is that there is an additional delay between cluster membership changes with respect to cases and deaths that can be attributed to stresses on a country’s healthcare system. First, the number of cases may increase significantly, placing a country into a different cluster relative to cases. This has an effect on the healthcare system, which subsequently leads to a greater impact in death counts. That is, the progression from elevation in cases cluster to deaths cluster is not necessarily just due to individual progressions from cases to deaths, but intermediate developments like stresses on hospitals. Perhaps the initial wave of patients can be treated with ventilators but these may quickly run out, causing more deaths from later instances of cases. Regardless, it is an interesting observation that the clear offset of 32 days in the number of clusters does not minimise the offset in affinity or adjacency matrix norm differences.

IV. ANOMALY ANALYSIS

Having identified a suitable $\tau$ such that two multivariate systems exhibit similarity up to this offset, one can then compare affinity matrices to identify individual elements which are anomalous between the two systems. To do so, we compute consistency matrices that measure the consistency between the two systems, up to an offset. Using the standard affinity matrices $\text{Aff}$, the consistency matrices are defined as $\text{Con}^{(t)} = |\text{Aff}^{(t)} - \text{Aff}^{(t+\tau)}|$. At each slice in time, we can apply hierarchical clustering. The sequence of hierarchical clusters highlights the emergence and disappearance of specific anomalies and quantifies the total amount of anomalous behaviour across the system. We can also identify the most anomalous elements at any point in time. By computing $c^{(t)}_{ij} = \sum_{j=1}^{n} c^{(t)}_{ij}$, we may assign an anomaly score to a particular element relative to its consistency between two multivariate systems. We also compute a lag-adjusted death rate for each country, defined by

$$ DR^{(t)}_{\text{lag}} = \frac{y^{(t)}}{x^{(t-\tau)} - x^{(t-\tau - \tau)}} \forall t \in \{\tau + 1, \ldots, T\} $$

These ratios may be orders of magnitude higher than standard reported death rates, and are no longer bound between 0 and 1. This measure provides insight into the rate of spread, and how well a country has managed the total number of deaths, conditional on a given number of cases $\tau$ days prior.

In Table II, we depict the results of ordering the 10 most anomalous countries from 28/1/2020 - 27/4/2020. In Figure 5, we display the affinity matrices for cases and deaths and the consistency matrix for 27/4/2020, with an offset of $\tau = 16$ from Table II. We only analyse countries that had at least 5000 cases as of 30/4/2020. Anomalies may signify either disproportionately high or low number of deaths relative to the number of cases.

This analysis confirms known phenomenology and offers several insights. Early in the global spread of COVID-19, Iran and Italy were internationally known as countries that were struggling to contain the number of deaths. Both Table II and consistency matrices identify both as anomalous on 27/2/2020 and 8/3/2020, reflecting their sharp rise in deaths even before other severely impacted countries. On the other hand, Singapore is identified as anomalous during this period due to its relatively small number of deaths. As at 7/3/2020, Singapore had 130 COVID-19 cases and 0 deaths.

A similar trend continues until late March, during which Spain and Italy are identified as the most consistently anomalous countries due to their high death rates. The respective lag-adjusted death rates for Spain and Italy are 227% and 73.3% respectively. Indeed, the number of deaths in Spain on 28/3/2020, was more than 2 times greater than the number of cases 16 days earlier. This confirms the severity of the COVID-19 pandemic: Spain and Italy suffered a massive number of deaths within a short window. As of late March, Singapore was still identified as anomalous due to the relatively small number of deaths. Towards the end of our analysis window, Qatar and Australia are also identified as anomalous with strikingly low death rates, while the UK and Bangladesh are identified as anomalous due to high death rates. The lag-adjusted death rates for Qatar, and Australia as at 27/4/2020 are 0.42%, and 1.33% respectively. The lag-adjusted death rates for the UK and Bangladesh are 34.2%, and 34.1% respectively.

V. CONCLUSION

Our methodology identifies a close relationship in the spread of cases and deaths due to COVID-19 across various countries, with the number of clusters pertaining to these two phenomena exhibiting remarkably similar behaviour up to an offset. The clustering and analysis of affinity and adjacency matrices provides us with an alternative means of computing a suitable offset between these multivariate systems.

With such an offset under consideration, our anomalous matrix walls are able to reconcile previously disparate analyses.
Cluster-based dual evolution for multivariate systems

(a) Cases affinity matrix  (b) Deaths affinity matrix  (c) Consistency matrix

FIG. 5: Cases affinity matrix, deaths affinity matrix and consistency matrix with $\tau = 16$ at 27/4/2020. The more prominent the respective row and column in the consistency matrix, the more anomalous the country. The three most prominent anomalies in Figure 5c are Qatar, Singapore and Bangladesh.

TABLE II: 10 most anomalous countries at various times, as defined in Section IV. AE: United Arab Emirates, AT: Austria, AU: Australia, BD: Bangladesh, BY: Belarus, CA: Canada, CN: China, DE: Germany, DO: Dominican Republic, ES: Spain, FR: France, ID: Indonesia, IE: Ireland, IL: Israel, IN: India, IR: Iran, IT: Italy, JP: Japan, KR: South Korea, MY: Malaysia, NL: Netherlands, NO: Norway, QA: Qatar, SG: Singapore, SW: Sweden, TR: Turkey, UA: Ukraine, UK: United Kingdom, US: United States, ZA: South Africa.

| Date     | A1 | A2 | A3 | A4 | A5 | A6 | A7 | A8 | A9 | A10 |
|----------|----|----|----|----|----|----|----|----|----|-----|
| 28/1/2020| US | UK | IT | IL | IE | IR | ID | IN | DE | FR  |
| 7/2/2020  | US | DO | IT | IL | IE | IR | ID | IN | DE | FR  |
| 17/2/2020 | SG | JP | KR | AU | MY | US | DE | FR | AE | CA  |
| 27/2/2020 | IR | SG | MY | IT | AU | US | DE | UK | AE | CA  |
| 8/3/2020  | IT | IR | SG | MY | DE | AE | CA | JP | ES | US  |
| 18/3/2020 | ES | SG | IT | IR | AE | UK | NL | FR | US | KR  |
| 28/3/2020 | QA | ES | TR | UK | SG | KR | AE | BY | US | IT  |
| 7/4/2020  | QA | SG | KR | UK | CN | UA | NO | ZA | AU | TR  |
| 17/4/2020 | BD | QA | SG | UK | AU | KR | BE | ZA | AT | FR  |
| 27/4/2020 | QA | SG | BD | ME | AU | UK | SW | BE | DE | IL  |

- identifying anomalies over time relative to cases and deaths.
This provides a framework for sequential anomaly analysis, wherein two phenomena are evolving over time and anomalies may emerge and disappear sequentially. This methodology is flexible: different metrics between data, clustering methods and means of learning offset in data could all be used to study related time-varying multivariate systems and identify similarity and anomalies that evolve over time.

DATA AVAILABILITY

The data that support the findings of this study are openly available at Ref. [15].

Appendix A: Existing cluster theory

General clustering frameworks used in our methodology and experiments are described below. In our most general setup, $x_1, \ldots, x_n$ are elements of a normed space $\mathcal{X}$.

Hierarchical clustering is an iterative clustering technique that does not specify discrete groupings of elements. Rather, it seeks to build a hierarchy of similarity between elements. Hierarchical clustering is either agglomerative, where each element $x_i$ begins in its own cluster and branches between them are successively built, or divisive, where all elements begin in one cluster and are successively split. The results of hierarchical clustering are commonly displayed in dendrograms. For further details, see [11] and [12]. We implement agglomerative clustering.

K-means clustering seeks to minimise an appropriate sum of square distances. With $k$ chosen a priori, we investigate all possible partitions (disjoint unions) $C_1 \cup C_2 \cup \cdots \cup C_k$ of $\{x_1, \ldots, x_n\}$. Let $z_j$ be the centroid (average) of the subset $C_j$. One seeks to minimise the sum of square distances within each cluster to its centroid.
\[
\sum_{j=1}^{k} \sum_{x \in C_j} ||x - z_j||^2
\]

For a normed space with dimension at least 2, it is NP-hard to find the global minimum of this problem. The K-means algorithm due to Lloyd is an iterative algorithm that converges quickly and suitably to a locally optimal solution. It is usually sufficient for applications.

On the other hand, the K-means optimisation problem is efficiently solvable in the one-dimensional case. That is, when \( x_i \) are real numbers, they are equipped with an ordering, which considerably simplifies the problem. To cluster \( n \) elements of \( \mathbb{X} = \mathbb{R} \) into \( k \) clusters requires one to order the elements and then determine \( k - 1 \) breaks in the ordering. This is far less computationally intensive than the higher-dimensional analogue. Wang et al. implement a dynamic programming algorithm that guarantees optimal clustering in one dimension, choosing \( k \) a priori.

Spectral clustering is a technique that performs K-means clustering on the eigenvalue spectrum of a judiciously chosen matrix. Given \( x_1, \ldots, x_n \) one forms the \( n \times n \) distance matrix \( D \) consisting of all pairwise distances between elements. With one of several transformations, one associates an affinity matrix \( A \). The two most common transformations are as follows:

\[
A_{ij} = 1 - \frac{D_{ij}}{\text{max}D}, \quad \text{or}
\]

\[
A_{ij} = \exp \left( \frac{-D_{ij}^2}{2\sigma^2} \right), \quad \text{where} \ \sigma \ \text{is a parameter}
\]

Next, let \( E \) be the diagonal degree matrix associated to \( A \), that is, \( E_{ii} = \sum_j A_{ij} \). Form the Laplacian matrix \( L = E - A \) and its normalisation \( L_{\text{sym}} = E^{-1/2}AE^{-1/2} \). \( L_{\text{sym}} \) is a positive semi-definite matrix with eigenvalues \( 0 = \lambda_1 \leq \cdots \leq \lambda_n \). Spectral clustering proceeds by applying K-means clustering to the eigenvectors of \( L_{\text{sym}} \). A fixed choice of \( k \) is required.

### Choice of number of clusters

In hierarchical clustering, choosing the number \( k \) of clusters is not required, or even applicable. In spectral clustering, there is a standard choice of \( k \). One chooses \( k \) that maximises the eigengap \( \lambda_{k+1} - \lambda_k \) as defined above.

On the other hand, how to best choose the number of clusters \( k \) for the K-means algorithm is a difficult problem. Different methods for estimating \( k \) may produce considerably differing results. In this paper, we draw upon six methods to determine the appropriate number of clusters before implementing K-means, in both the one and higher-dimensional cases. These methods are well-known: Pbiserial index, silhouette score, KL index, C index, McClain-Rao index and Dunn index. We have chosen these methods based upon consultation with the literature and our own experiments. However, our methodology is flexible, and any combination of existing methods may be used. For one-dimensional data, it is often regarded as unsuitable to use higher-dimensional K-means or spectral clustering, as optimal alternatives exist. Since we study one-dimensional data in this paper, it is necessary to use these methods to choose the number \( k \) before implementation of the optimal K-means.

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