APPLICATIONS OF PERSISTENT HOMOLOGY TO IDENTIFYING CLUSTERS IN GRAPHS

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Abstract. We study practical applications of persistent homology to identifying bridges in graphs. These graphs arise when analysing social networks, where bridges represent users who are members of multiple communities. In this paper, we outline several variations on an algorithm that utilises persistent homology and a metric on persistence diagrams, called the Wasserstein Distance, to identify cluster points. We also provide a mathematical justification for the efficacy of this algorithm and discuss ways in which it can be optimised to be applied to large data sets.

1. Introduction

Society is just beginning to see the effect that a group of dedicated diffusers of malicious information can have. Private and state agencies are using platforms such as Twitter to push their ideas, and the problem of identifying these information distributors is becoming more important. In this paper, we will demonstrate how techniques from the area of topological data analysis can be used to address this problem. Specifically, we will use ideas from persistent homology to identify bridges in graphs.

The field of topological data analysis (TDA) has been rising in prominence since the start of the 21st century. It utilises ideas from an area of mathematics called algebraic topology to draw inferences about large data sets by studying their structure when considered as a geometric object. As TDA becomes more widespread, various programming languages have added support. A full implementation of our algorithm in the language Julia can be found at [insert link here], making use of the package Eirene.

We will now give the important definitions, as well as state some important theorems without proof.

1.1. Graph Theory.

A graph is a tuple (V, E, μ) with V a set of vertices, E a set of edges and $\mu : V \cup E \to \mathbb{R}_{\geq 0} \cup \{\infty\}$ a weight function. An edge between vertices v_0 and v_1 will be denoted by (v_0, v_1). A graph is called *undirected* if $(v_0, v_1) = (v_1, v_0)$ for every edge. All the graphs considered in this paper will be undirected and will have both finite vertex and edge sets.

An important example of a weight function is the *shortest path* weight function, which can be computed using Djikstra's Algorithm. Fix a vertex v and for any other vertex w, define $\mu_v(w)$ to be the length of the shortest path from w to v. For an edge (v_0, v_1), we define $\mu_v((v_0, v_1)) = \max\{\mu_v(v_0), \mu_v(v_1)\}$.

The *path-component* of a vertex v is the subgraph of all vertices that can be reached from v. A graph is called *connected* if it only has one path-component. Notice that if v and w are in different path components then the distance between them under the shortest path weight function is ∞.

1.2. **Homology.** We will only give definitions for homology in the case of a graph, but recognise that these definitions can be generalised to any space. For a completely general definition of homology, see [1].

For a graph $X = (V, E, \mu)$, we define two groups $C_0(X)$ and $C_1(X)$ by

$$C_0(X) = \mathbb{Z}\{V\}$$
$$C_1(X) = \mathbb{Z}\{E\}$$

Here the notation $\mathbb{Z}\{V\}$ means that we take finite formal sums of elements in V with coefficients in $\mathbb{Z}$. For example, if $V = \{v_0, v_1, v_2\}$ then $5v_0 - v_1 + 2v_2$ is an element of $C_0(X)$. The notation $\mathbb{Z}\{E\}$ is entirely analagous. Elements of $C_0(X)$ are called 0-chains and elements of $C_1(X)$ are 1-chains.

We next define the boundary operator $d_1 : C_1(X) \to C_0(X)$. For an edge $e = (v_0, v_1)$, we set $d_1(e) = v_1 - v_0$ (considered as a formal sum in $C_0(X)$). For an arbitrary 1-chain, we can now define

$$d_1\left(\sum_i c_i e_i\right) = c_i \sum_i d_1(e_i)$$

Observe that we have defined d_1 on the basis E and extended it linearly to arbitrary 1-chains. This means that d_1 is a group homomorphism and so we can consider the subgroups $\ker(d_1)$ and $\operatorname{im}(d_1)$. The homology groups $H_0(X)$ and $H_1(X)$ are then given by

$$H_0(X) = C_0(X)/\operatorname{im}(d_1)$$
$$H_1(X) = \ker(d_1)$$

Intuitively, one can think of $H_n(X)$ as measuring the number of n-dimensional "holes" in X. This idea is illustrated by the following example.

Example 1.1. The circle S^1 can be thought of as a graph with a single vertex v and a single edge $e = (v, v)$ which is a loop from v to itself. To compute d_1, we evaluate it on the basis element e to see that $d_1(e) = v - v = 0$. Thus d_1 is the zero map, so $\ker(d_1) = C_1(S^1) = \mathbb{Z}$ and $\operatorname{im}(d_1) = 0$. Therefore $H_0(S^1) = H_1(S^1) = \mathbb{Z}$. The single power of $\mathbb{Z}$ in $H_1(S^1)$ indicates that there is only one 1-dimensional "hole" in the circle which is exactly what one would expect. As we will see in the next theorem, the single $\mathbb{Z}$ in $H_0(X)$ shows that S^1 is connected.

A 0-dimensional hole is a gap between vertices that cannot be traversed, so one would hope for a relationship between the number of path-components and $H_0(X)$. Such a relationship is given by the following theorem.

Theorem 1.2. *Suppose X is a graph with m distinct path-components. Then $H_0(X) = \mathbb{Z}^m$.*

This gives us an easy method for computing $H_0(X)$ by simply counting path-components. There is one other relation, however, that will significantly simplify our calculations of homology.

The Euler characteristic χ is a well-known graph invariant defined as $\chi = |V| - |E|$. Using homology, it can be shown that:

Theorem 1.3. *The Euler characteristic of a graph X is also given by $\chi = \operatorname{rank}(H_0(X)) - \operatorname{rank}(H_1(X))$. Here rank is the function defined by $\operatorname{rank}(\mathbb{Z}^m) = m$.*

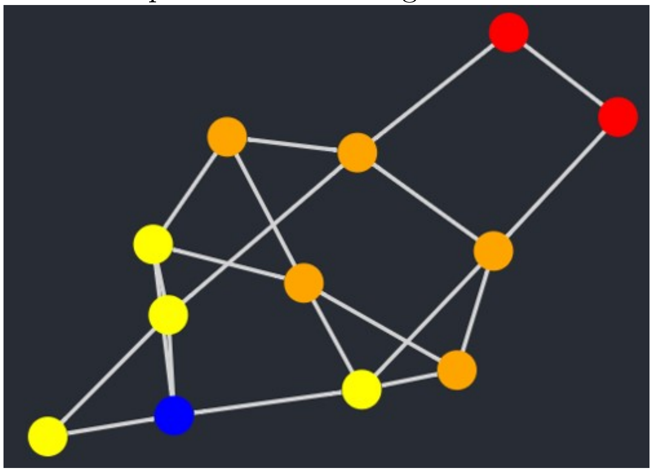
We already know how to compute rank($H_0(X)$): by Theorem 1.2, this is the number of path-components in X. Because $H_1(X)$ is the kernel of a group homomorphism between free abelian groups, it is always a free group (meaning there is no torsion) so its rank fully determines $H_1(X)$. Equating the two above expressions for χ and rearranging shows that $\text{rank}(H_1(X)) = m - |V| + |E|$ where m is the number of path-components in X. Thus the above two theorems give us a constant time method for computing homology.

1.3. **Persistent Homology.**

Building on homology is persistent homology. This is the idea that more information can be obtained from a graph by studying how $H_0(X)$ and $H_1(X)$ vary over time. To formalise this, we make use of filtrations. A filtration of a graph X is a finite nested sequence of subgraphs $X_0 \subseteq X_1 \subseteq X_2 \subseteq ... \subseteq X$. Essentially, a filtration is an inductive way to build the graph one stage at a time.

Using the shortest distance function defined earlier, we have a canonical way to obtain a filtration of X associated to each vertex v. We set X_0 to be the point v, X_1 to be the subgraph of vertices distance 1 away from v and so forth. In general, X_d is the subgraph of vertices distance d or less from v. Figure 1 below shows an example filtration of this sort, with v the blue vertex and the colour gradually increasing in intensity as we radiate outwards from v.

FIGURE 1. Example Filtration Using Shortest Path Function



Once we have a filtration, we can build what are called the persistence barcodes. There is a persistence barcode associated with each dimension n; the n-dimensional persistence barcode tracks the births and deaths of n-cycles (the elements of $H_n(X)$) as the filtration progresses. For example, because $H_0(X)$ measures path-components, the 0-dimensional barcode tracks the births and deaths of path-components. This means that if two disjoint path-components become connected by a bridge at some stage in a filtration, one of the 0-cycles will die at this stage. Because $H_1(X)$ measures 1-dimensional holes, one can think of the 1-dimensional persistence diagram as tracking the births and deaths of loops in X.

One important feature which makes persistence diagrams so useful is that there is an associated metric, called the Wasserstein distance (in general this is only a pseudo-metric, but it will be a true metric for diagrams considered in this paper).

The Wasserstein distance between two persistence diagrams A and B is given by

$$W_{p,q}(A,B) = \inf_{\substack{\eta : A \to B \\ \text{a bijection}}} \left(\sum_{a \in A} |||a - \eta(a)|||_q^p \right)^{1/p}$$

The values p and q are arbitrary positive integers (also possibly ∞) but for computational efficiency we will always take $p = q = 2$.

1.4. **Bridges in Graphs.**

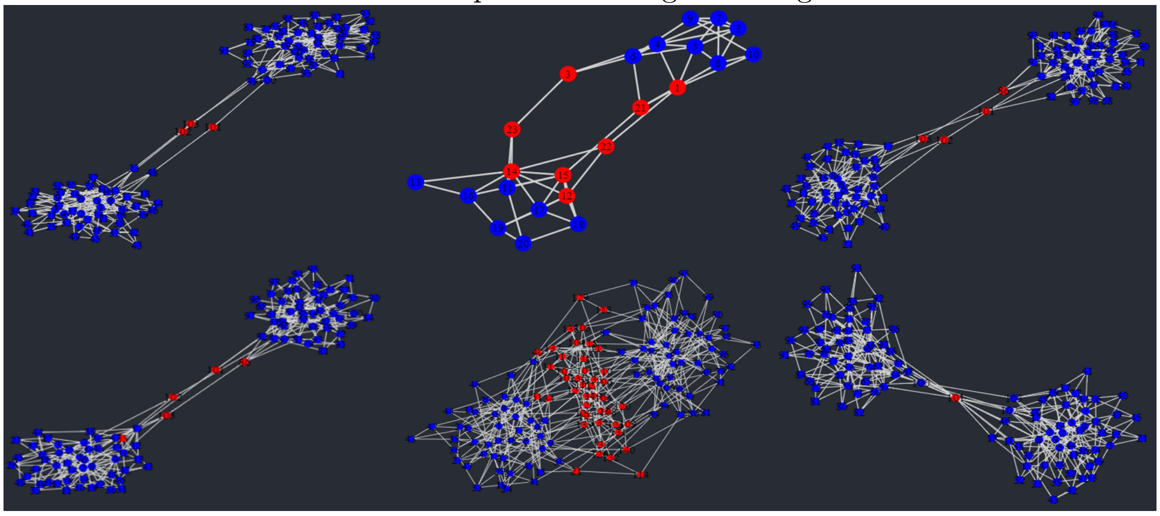
The purpose of this paper is to develop an algorithm that identifies bridges in graphs, so we must make clear what is meant by a bridge. This is difficult to do rigorously, but for intuition one should think of the following: a bridge between two clusters is a vertex which is connected to at least one vertex from each of the clusters.

It is important to emphasise that in our definition, a bridge is a vertex and not an edge as terminology sometimes varies across the field. We will not strictly adhere to the above definition of a bridge, but it is a useful starting point. As the reader sees example graphs, they will develop an understanding of what is meant by a bridge in a graph.

Conversely, a vertex which is not a bridge is called a cluster point and a collection of such cluster points is called a cluster. It is immediate that finding all bridges is equivalent to finding all cluster points and this will prove to be an easier problem.

Figure 2 depicts six example graphs with bridges and cluster points distinguished by colour. Throughout this paper, unless specified otherwise, we will take the convention that red vertices are bridges and blue vertices are cluster points.

Figure 2. Graphs with Bridges Distinguished



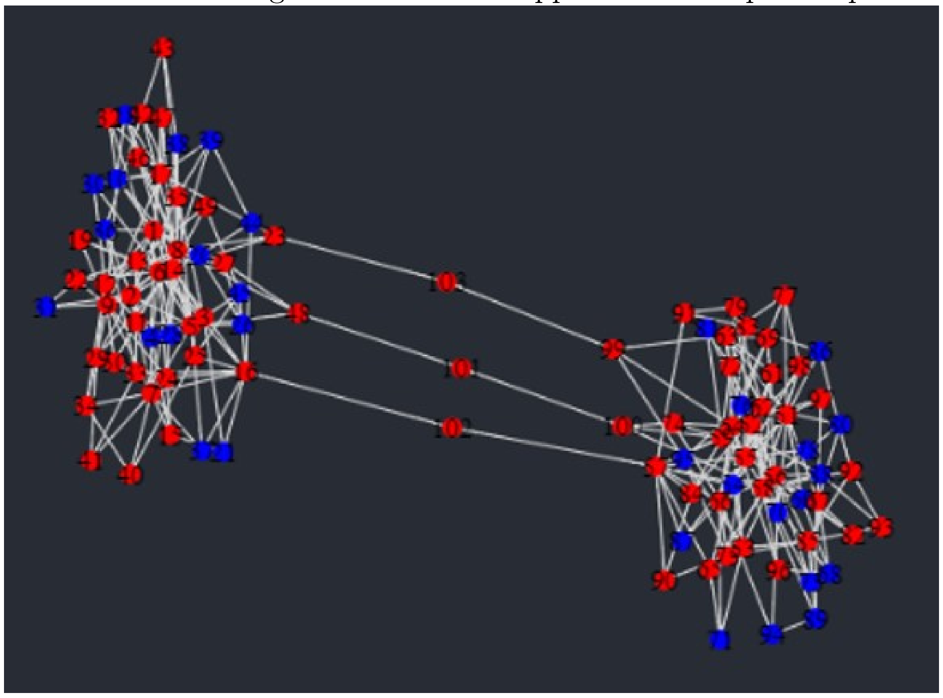
2. The Algorithm

Here we will describe the development of the algorithm. Before we do, however, we make the following observation. A vertex v being a bridge is a local property in the sense that it only depends on the path-component of v. This means that we may assume without loss of generality that the graph X is connected by simply running the algorithm on each path-component of X separately. This is the first instance of parallelizability in the algorithm, since the existence of bridges in one path-component does not in any way affect bridges in other path-components.

2.1. **Early Attempts.**

Continuing with this idea of locality, we describe our initial test for bridges which we shall call the "neighbourhood test". The key point is that a vertex v should be a bridge only if it is a bridge once we restrict to some small neighbourhood. This is because vertices far from v should not affect the behaviour of v. Having restricted to a suitably small neighbourhood, we can now use more classical tests for bridges such as checking if removing v disconnects the graph. As a first choice of small neighbourhood, consider the subgraph of vertices all directly adjacent to v. Figure 3 shows the neighbourhood test (with this choice of neighbourhood) applied to a typical graph.

Figure 3. Neighbourhood Test Applied to Example Graph

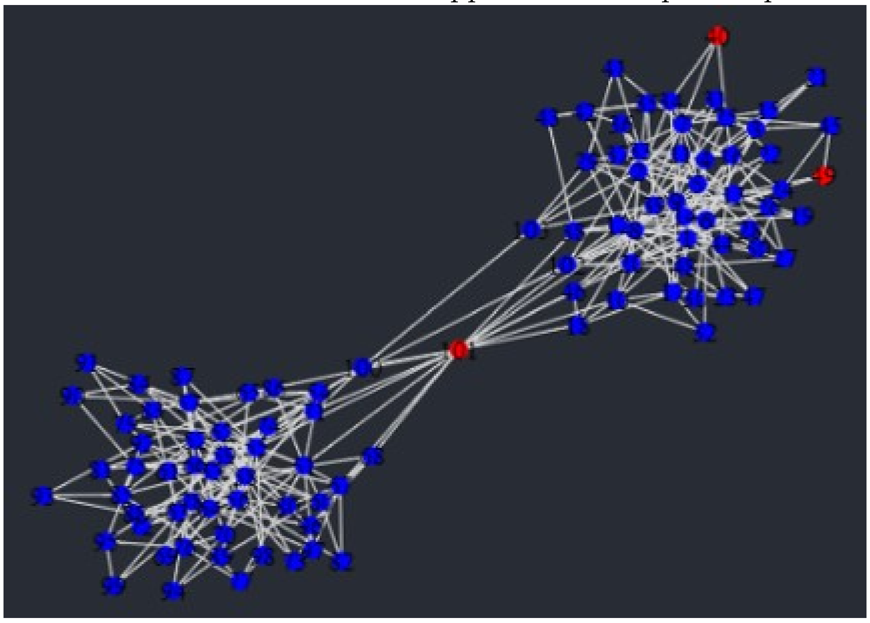


While it is better to have false positives than to eliminate bridges, the neighbourhood test incorrectly identified a large number of cluster points as bridges. This problem can be resolved by taking a larger neighbourhood around each vertex, since removing v from a larger neighbourhood is less likely to disconnect the graph. However, this method often eliminates parallel bridges such as those shown in Figure 3 because the parallel bridges are included in larger neighbourhoods, so removing v no longer disconnects the graph.

One possible solution to this is to make the radius of the neighbourhood around each vertex dependent on v. This means that smaller radii can be chosen for parallel bridges to avoid the above problem. However, there is no obvious way to choose a meaningful radius (doing so is almost identifying whether a vertex is a bridge or a cluster point). Instead, we introduce a generalisation of the neighbourhood test called the annulus test.

Define the closed annulus $\Delta(v, a, b) = \{w \in V \mid a \leq \mu_v(w) \leq b\}$. Rather than choosing a radius dependent on v for use in the neighbourhood test, we will check if $\Delta(v, a, b)$ is disconnected for sufficiently many a and b. Since the neighbourhood test applied to the neighbourhood of radius r about v is simply checking if $\Delta(v, 1, r)$ is disconnected, the annulus test is a true generalisation. Figure 4 shows the results of the annulus test applied to an example graph.

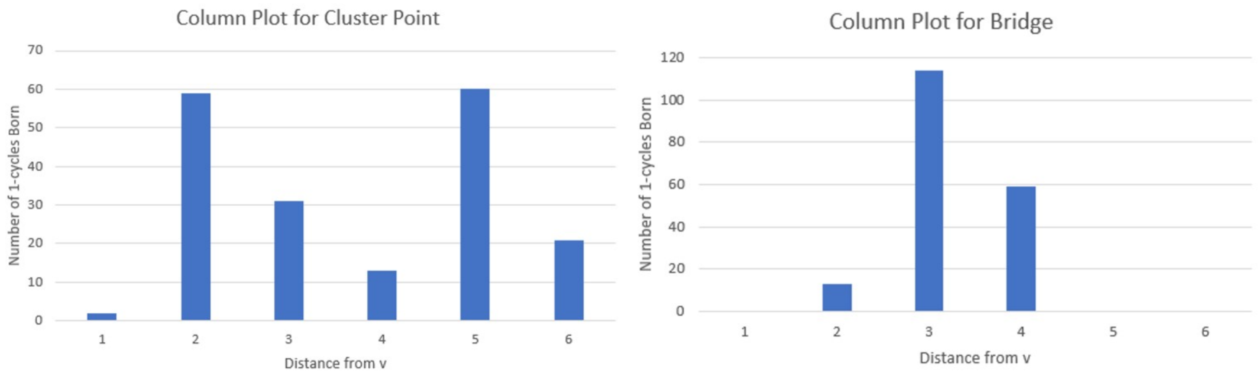
Figure 4. Annulus Test Applied to Example Graph



While the annulus test was noticeably more accurate than the neighbourhood test, it still incorrectly identified some cluster points as bridges (such as those in the upper right of Figure 4). This was surprising because, in general, the vertices which were classified incorrectly clearly belonged to clusters. To rectify this problem, the key observation was that the annulus test was not marking bridges as cluster points (it was only giving false positives). This meant that we could simply add further tests, now with the additional information of which nearby vertices were cluster points.

By considering graphs such as Figure 4, one might hope to find a meaningful way to say that two nearby vertices "look similar" so that if one has been identified as a cluster point then the other should be too. Persistent homology provides such a method by considering the persistence barcodes generated by the shortest path filtration. In a cluster, there are a large number of 1-cycles being born in quick succession because there is a high density of edges forming loops. For a bridge, though, there is an initial lull before a large number of births. Figure 5 shows column plots for the number of 1-cycles born each time the filtration progresses one step further from v. The left diagram corresponds to a typical cluster point and the right to a bridge.

FIGURE 5. Column Plots for Number of 1-cycles Born vs. Distance from v



The Wasserstein distance allows us to compare the 1-dimensional persistence diagrams to find cluster points that may have been misidentified in our initial search for bridges. This is a significant simplification because it reduces our search to an extremal problem: we need only identify the vertices which are the most densely clustered (which one would hope to be easier) and then use the Wasserstein distance to identify those neighbours which are also cluster points.

There is one problem with this approach, which is that highly symmetric graphs can generate similar persistence barcodes for vertices which are quite far apart. There are cases where the persistence diagrams corresponding to vertices can be very close under the Wasserstein distance even though the vertices themselves are separated in the graph. Worse, it has happened that two such vertices were identified when one lay at the edge of a cluster and the other was clearly a bridge. To address this, we only compare the persistence barcodes of vertices which are within a certain distance of one another. This has the added effect of reducing the number of Wasserstein distance calculations needed, which can be quite costly (see Discussion).

2.2. **Identifying Initial Cluster Points.** We now turn to the problem of finding vertices at the centres of clusters. The annulus test offers a partial solution but, in some cases, fails to identify any vertices if the cluster is densely connected (so that removing v does not disconnect the neighbourhood). To motivate the following method, we return to the previous discussion about the times at which large numbers of 1-cycles are born. From Figure 5, one would expect the vertices at the centres of clusters to be those which have a large portion of the 1-cycles born early in the shortest path filtration.

It is easy to compute the number of 1-cycles born at each stage of the filtration using the Euler characteristic method outlined earlier. We then mark vertices for which a large number of births occur sufficiently early as being cluster points. It is worth noting that, currently, "sufficiently early" is taken to mean that the largest portion of 1-cycles is born less than some fraction q of the way through the filtration. This test is implemented in such a way that q is taken to be as small as possible, meaning we start with the value $q = 0.05$ and increment q by 0.05 until any initial cluster points are found. We then fix q and stop searching for initial cluster points.

Figure 6. Example of Using 1-cycle Birth Times to Identify Cluster Points

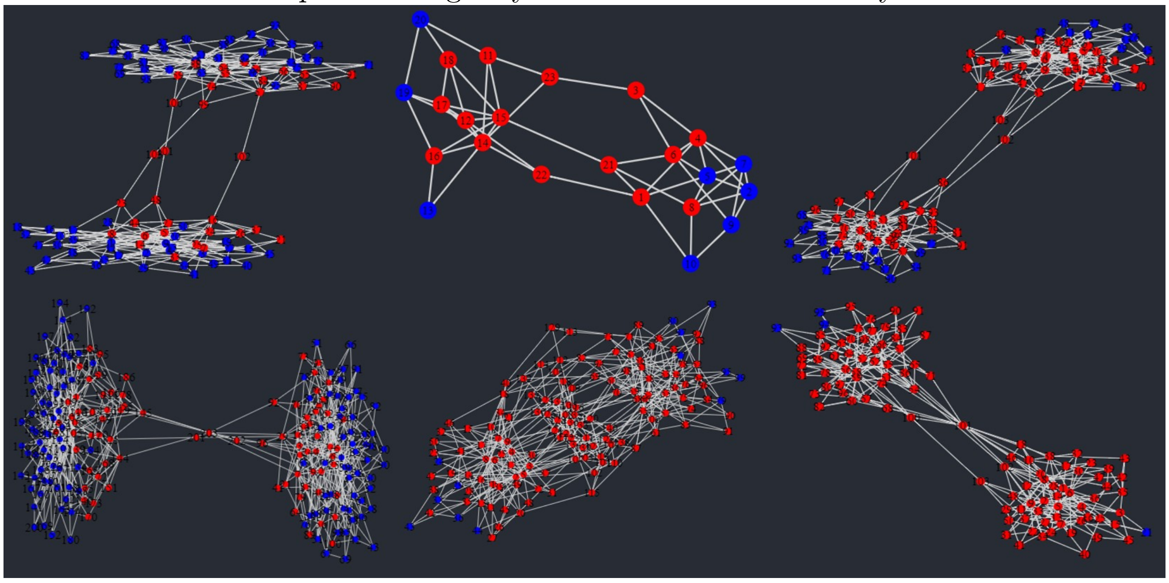


Figure 6 shows this method applied to various example graphs. In general, it will identify more vertices in densely connected clusters than in sparse clusters (compare the fourth and fifth graphs in Figure 6) simply because there are more 1-cycles in a densely connected cluster. The choice of q discussed above gives us an easy solution to the extremal problem but it has some drawbacks that should be discussed:

- The fewer initial cluster points are identified, the more Wasserstein distance computations need to be made and this is by far the most computationally expensive part of the algorithm.
- Suppose we have two distinct clusters, one densely connected and the other sparse. Because this test stops as soon as any cluster points have been identified, it is possible for cluster points in the dense cluster to be identified for small values of q while no cluster points are identified in the sparse one. This means that we have no vertex to compare the rest of the sparse cluster against, so we could fail to identify an entire cluster.

Both of these issues can be resolved by using a larger value of q. However, there is no longer an obvious way to make q dependent on the graph. This problem is still unresolved, but the scenario in the second point above happens very infrequently.

Soon we will see how this test performs on graphs with more than two clusters. Before this, though, let us compare it to a more classical method for clustering to see how it performs. We define the Laplacian matrix L for a graph by the formula

$$L_{i,j} = \begin{cases} \deg(v_i) & \text{if } i = j \\ -1 & \text{if } v_i \text{ is adjacent to } v_j \\ 0 & \text{otherwise} \end{cases}$$

The matrix L is symmetric and positive-semidefinite, so its eigenvalues are all real and non-negative. An easy result is that the multiplicity of the eigenvalue $\lambda = 0$ is exactly the number of path-components in X. By our assumption that X is connected, this means that $\lambda = 0$ always has multiplicity 1.

The smallest non-zero eigenvalue of L is called the spectral gap. By the above, the spectral gap will always be the second eigenvalue when they are ordered. The associated eigenvector is called the Fiedler vector and it gives us a method for partitioning X into two connected clusters which we will now describe. Let s denote the spectral gap and f denote the Fiedler vector, so $Lf = sf$. Because eigenvectors are only defined up to scaling by a non-zero constant, we will have to check that any information we deduce from f is invariant under scaling.

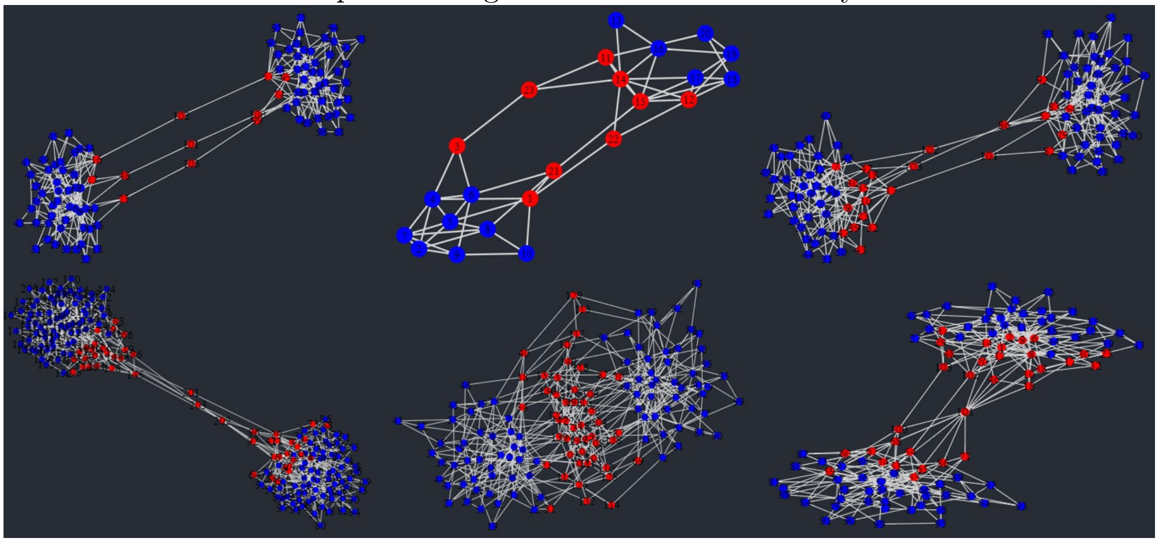
For each vertex v_i, the sign of the i^{th} entry of f tells us which of the two clusters v_i should belong to. That is, if the signs of f_i and f_j are different then v_i and v_j belong to different clusters. This property is clearly preserved under scaling because, although scaling by a negative constant value may change the sign of the entry, it will always preserve the property of having different signs.

Building on this, the magnitude of f_i directly relates to how close to the centre of a cluster v_i is. To account for scaling, we identify those vertices for which $|f_i|$ is greater than the mean as being initial cluster points. To show that this is invariant under scaling, suppose that X has n vertices and that $|f_i| > \frac{\sum_j |f_j|}{n}$. Then

$$\begin{aligned} |(cf)_i| &= |c| \cdot |f_i| \\ &> |c| \cdot \frac{\sum_j |f_j|}{n} \\ &= \frac{\sum_j |c| \cdot |f_j|}{n} \\ &= \frac{\sum_j |(cf)_j|}{n} \end{aligned}$$

Thus this property is well-defined under scaling. To determine if our test using 1-cycle birth times produces reasonable results, let us compare it to the vertices identified by the Fiedler vector. Figure 7 shows the results of using the Fiedler vector applied to the same graphs as in Figure 6.

FIGURE 7. Example of Using Fiedler Vector to Identify Cluster Points



In general, the Fiedler vector produces as many or more initial cluster points, as illustrated by comparing Figures 6 and 7. In fact, not once across twenty test graphs did the 1-cycle test identify a vertex as a cluster point that the Fiedler vector did not. Unfortunately, there is no generalisation of the Fiedler vector for graphs with more than two clusters; it is a special feature of *bipartitioning* a graph. However, that the 1-cycle test and the Fiedler vector agree in the two cluster case supports the accuracy of this method.

2.3. **Graphs with More than Two Clusters.**

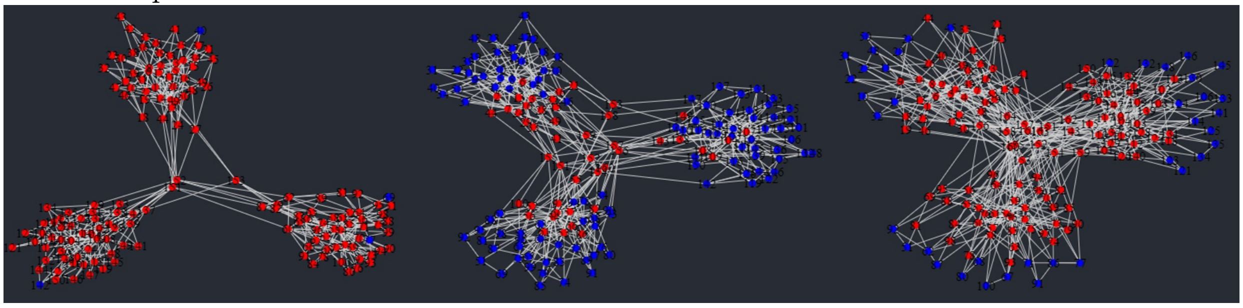
We will now study how the algorithm performs on graphs with more than two clusters. Everything we have done thus far still holds in the general case and any assumptions (such as the connectedness of X) are still reasonable, for the same reasons as before.

The only real complication that arises with graphs with more than two clusters is that there are more opportunities for variation in the density of the clusters. This can cause the problem that, for a poor choice of q, we fail to identify any initial cluster points in some sparse cluster. We do not have a solution to this as of yet, so we will restrict ourselves to the class of graphs with clusters of similar densities. This is still the majority of graphs used to model social networks since communities tend to be densely connected.

As a partial solution if this problem occurs, a user could manually identify some small set of initial cluster points and then proceed to use the Wasserstein distance to find the rest of the cluster.

Figure 8 shows the results of applying the 1-cycle birth test to graphs with more than two clusters. The results are in keeping with the two cluster case and this pattern continues on graphs with more clusters.

Figure 8. Initial Cluster Points Identified by 1-cycle Birth Test on Graphs with More Than Two Clusters



If one does not wish to work with graphs with more than two clusters, it is theoretically possible to reduce to the two cluster case (we have not implemented this) in the following way: we identify a set of initial cluster points and designate some neighbourhoods of these points as being potential clusters. We then choose any two of these potential clusters (if there are k potential clusters then there are $\binom{k}{2} = \frac{k(k-1)}{2}$ possible combinations) and include any vertices that lie between them as potential bridges. This gives rise to a connected subgraph which has at most two clusters, so we can run the algorithm from the two cluster case (or perhaps use the Fiedler vector). We will not explore this approach as it would be more time-consuming than running the algorithm on the entire graph. Additionally, it still suffers from the problem of needing to identify initial cluster points to find the potential clusters.

3. Discussion

References

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