Recursive Shortest Path Algorithm with Application to Density-integration of Weighted Graphs

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Abstract

Graph theory is increasingly commonly utilised in genetics, proteomics and neuroimaging. In such fields, the data of interest generally constitute weighted graphs. Analysis of such weighted graphs often require the integration of topological metrics with respect to the density of the graph. Here, density refers to the proportion of the number of edges present in that graph. When topological metrics based on shortest paths are of interest, such density-integration usually necessitates the iterative application of Dijkstra’s algorithm in order to compute the shortest path matrix at each density level. In this short note, we describe a recursive shortest path algorithm based on single edge updating, which replaces the need for the iterative use of Dijkstra’s algorithm. Our proposed procedure is based on pairs of breadth-first searches around each of the vertices incident to the edge added at each recursion. An algorithmic analysis of the proposed technique is provided. When the graph of interest is coded as an adjacency list, our algorithm can be shown to be more efficient than an iterative use of Dijkstra’s algorithm.

Introduction

The last ten years has seen a surge of interest in graph theory among biologists, physicists and other natural scientists. This was primarily stimulated by the seminal papers of Watts and Strogatz (1998) and Barabasi and Albert (1999). In particular, a wide range of different data types are now analyzed through systematic calculations of various topological measures, such as the characteristic path length or clustering coefficient. In systems biology and neuroscience, subject-specific networks can be constructed in order to compare several populations of networks for testing putative differences between groups of subjects (see Bullmore and Sporns, 2009, for a review). (For convenience, the terms network and graph will here be used interchangeably, as this reflects some of the recent developments in the literature.) Such biological networks, however, tend to be weighted undirected graphs, which generally correspond to some standardized covariance matrices between a set of regions of interest. By contrast, most of the topological measures introduced by Watts and Strogatz (1998) and Barabasi and Albert (1999) pertain to unweighted networks.

There is currently no general consensus on how to compute or compare the topology of weighted graphs. This is a particularly arduous problem, since it requires the use of real-valued mathematical tools on objects, which are essentially discrete. One of the possible solutions to this conundrum has been advanced by He et al. (2009), who suggested integrating the topological measures of interest with respect to the density of the network (see also Achard and Bullmore, 2007, Ginestet and Simmons, 2011). The density of a network is here defined as the proportion of the number of edges in a given graph. Such integration, however, is computationally expensive, and its complexity grows quadratically with the number of nodes. A Monte Carlo scheme has been proposed in the literature to address this issue and approximate the value of such an integral (Ginestet et al., Submitted). Such Monte Carlo methods, however, also necessitates large number of simulations in order to reduce the variability of the resulting estimates.

Most of the topological metrics of interest to researchers in neuroscience and systems biology tend to involve the computation of the matrix of shortest paths, denoted $D$. This includes, for instance, the global and local efficiency measures proposed by Latora and Marchiori (2001) (see also Latora and Marchiori, 2003). The computation of $D$ for a given network can be done
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efficiently using the celebrated Dijkstra’s algorithm (Dijkstra, 1959). However, when considering weighted networks, Dijkstra’s algorithm may need to be invoked as many times as the number of edges in the graph of interest. In this short note, we address this specific problem by proposing a recursive shortest path algorithm based on applying single edge updates to $D$. In this setup, we only work with the shortest path matrix and compute the value of the desired topological metric at every density level. Taken together, we therefore provide an efficient algorithm for the density-integration of the topological functions of weighted networks.

**Density-integration of Topological Metrics**

In this paper, our main focus will be on undirected weighted graphs, containing no graph loops or multiple edges. However, since we also need to refer to unweighted graphs, we introduce the following notation. A graph $G$ is here defined as a triple $(V, E, W)$, where $V(G)$ is the standard vertex set, $E(G)$ is the edge set and $W(G)$ is a multiset of real-valued weights. Our convention generalizes to directed graphs. In addition, this also includes undirected unweighted (simple) graphs as special cases, for which the elements of $W$ belong to $\{0, 1\}$. Such a setup may, for instance, apply to the consideration of correlation matrices or other matrices of similarity measures with real-valued entries. In addition, we will make use of the following notation,

$$N_V := |V(G)|, \quad N_E := |E(G)|, \quad \text{and} \quad N_I := \frac{N_V(N_V - 1)}{2},$$

where := signifies that the left-hand side is defined as the right-hand side. We define $N_I$ as the number of shortest paths in $G$. Naturally, $N_I$ here takes this value because $G$ is undirected. For a directed network, $N_I$ would be $N_V(N_V - 1)$. For convenience, we will interchangeably use the following two sets of indices to label the elements of $W$,

$$W(G) = \{w_{v_1v_2}, \ldots, w_{ij}, \ldots, w_{N_V-1,N_V}\} = \{w_1, \ldots, w_e, \ldots, w_{N_E}\}. \quad (1)$$

Albeit we will here restrict our attention to undirected graphs, an extension of our proposed technique to directed networks will be discussed in the conclusion.

A range of topological metrics necessitating the computation of the shortest path matrix have been proposed in the literature. Two popular choices of topological measures are the global and local efficiency measures introduced by Latora and Marchiori (2001). Both of these quantities can be derived from the general definition of the efficiency, $E(\cdot)$, of a simple graph $G = (V, E, W)$, which is defined as follows,

$$E(G) := \frac{1}{N_I} \sum_{i<j} d_{ij}^{-1}, \quad (2)$$

where summation over $i < j$ implies the consideration of all the elements of the following set, $\{i < j : i, j = 1, \ldots, N_V\}$, and with $d_{ij}$ denoting the length of the shortest path between vertices $v_i$ and $v_j$ in $G$. According to Latora and Marchiori (2001), the global and local efficiencies of an
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unweighted undirected graph are respectively defined as follows,

\[ E^{\text{Glo}}(G) := E(G), \quad \text{and} \quad E^{\text{Loc}}(G) := \frac{1}{N^\ell} \sum_{i=1}^{N^\ell} E(G_i), \]  

(3)

where \( G_i \subseteq G \) for every \( i = 1, \ldots, N^\ell \), such that each \( G_i \) is the subgraph of all the neighbors of the \( i^{\text{th}} \) node. That is, \( V(G_i) = \{ v_j \in G_i : v_jv_i \in E(G) \} \).

The computation of the efficiency or any other topological function of \( G \), which we will denote by \( T(G) \) is ill-defined for a weighted graph \( G = (V, E, W) \). In such a case, one may resort to integrating the topological measure of interest with respect to all the possible densitys of the graph under scrutiny, where the density of an unweighted undirected graph is defined as follows,

\[ K(G) := \frac{N_E}{N_I}. \]  

(4)

Now, integrating a topological function with respect to the different densitys of \( G \) can be expressed as

\[ \overline{T}(G) := \int_{\Omega_K} T(\gamma(G,k)) dk, \]  

(5)

where the function \( \gamma(G,k) \) in equation (5) is a density-thresholding function, which takes a weighted network as well as a specific level of density and returns an unweighted network with density \( k \). Here, density is treated as a discrete random variable, \( K \), with realizations in lower case. As \( K \) is discrete, it only takes a countably finite number of values, which is the following set,

\[ \Omega_K := \left\{ 1 - \frac{1}{N_I}, \frac{2}{N_I}, \ldots, \frac{N_I - 2}{N_I}, \frac{N_I - 1}{N_I}, 1.0 \right\} =: \mathbf{k}, \]  

(6)

where \( |\Omega_K| = N_I \). It will also be useful to label the elements of \( \mathbf{k} \) with the following indices \( t = 1, \ldots, N_I \). Therefore, equation (5) can be re-written as follows,

\[ \overline{T}(G) = \frac{1}{N_I} \sum_{t=1}^{N_I} T(\gamma(G, k_t)). \]  

(7)

If the topological metric of interest involves the computation of the matrix of shortest paths, \( D \) for every thresholding of \( G \), such an integration would necessitate invoking Dijkstra’s algorithm or an equivalent method \( N_I \) times. In the next section, we propose an alternative to this computationally expensive integration by directly updating \( D \) instead of updating the underlying adjacency matrix, \( A \), for every new density.

**Recursive Shortest Path Algorithm for Density-integration**

Our strategy for bypassing the need to invoke a shortest path algorithm at every density level consists of three stages: (i) we compute the ranks of the entries of the weight matrix, (ii) we update the shortest path matrix by successively adding edges in the order corresponding to the ranks obtained in the first stage, and finally (iii) we collect the values of the topological metric of interest for every shortest path matrix and return the mean value of that topological metric. We
describe these three stages, in turn.

Firstly, we compute the ranks for the weighted network of interest \( G = (V, E, W) \) as follows,

\[
R_{ij}(W) := \sum_{u>v} I_{\{w_{ij} \geq w_{uv}\}},
\]

where \( I\{\cdot\} \) is the indicator function returning 1 if the argument is true and 0 otherwise. We will assume that are no ties in the values of \( W \). In practice, the presence of ties can be resolved by randomization.

Secondly, we extract each edge in the order provided by the ranks. That is, running over the ranks \( k_t \), where \( t = 1, \ldots, N_I \), we have the following \( N_I \) ordered pairs:

\[
\{v_1, v_2\}_t := \text{argmax}_{\{i,j\}} I\{P_{ij}(W) = k_t\}.
\]

It then suffices to update \( D \) using each of these pairs recursively, as follows,

\[
D_t = \text{edgeUpdate}(D_{t-1}, \{v_1, v_2\}_t).
\]

For each \( D_t \), we can now collect the topological measure based on this particular shortest path matrix, \( T(D_t) \). Finally, it remains to compute the mean value of these collected topological measures in order to obtain the desired density-integrated metric of the graph of interest. That is,

\[
\bar{T}(G) = \frac{1}{N_t} \sum_{t=1}^{N_I} T(D_t).
\]

The difficulty of this method centres on the use of the edgeUpdate function in equation (10). This algorithm proceeds as follows. At each step \( t \), we ask what the impact of the addition of a new edge to an existing graph is in terms of shortest path relationships. Our algorithm answers this question by two successive breadth-first searches (BFS) around the vertices incident to the edge added at each \( t \). Firstly, we conduct a BFS around \( v_2 \) and check whether the shortest path between \( v_1 \) and each of the \( m \)th degree neighbors of \( v_2 \) are shortened by the addition of a new edge between \( v_1 \) and \( v_2 \). Secondly, we conduct a BFS centred at \( v_1 \), where we check if the shortest paths between all the neighbors of \( v_2 \), which were modified in the first stage and the \( m \)th degree neighbors of \( v_1 \) are shortened by the introduction of the new edge. The full edge updating algorithm of \( D_t \) is described in pseudocode in Figure 1. For simplicity, we represent the algorithm when each \( D_t \) is coded as a full matrix. However, a list representation can also be adopted to minimise storage space. Moreover, we have also provided a graphical description of our edge updating algorithm for density-integration in Figure 2. A C++ version of this algorithm is freely available as part of the NetworkAnalysis package on the R platform (http://cran.r-project.org/package=NetworkAnalysis).
Algorithmic Analysis

When storing the graph of interest as an adjacency matrix, Dijkstra’s algorithm has efficiency in $O(|V|^2)$. Since density-integration would require invoking that algorithm $N_I = N_V(N_V - 1)/2$ times, the efficiency would, in that case, be in $O(|V|^4)$. If coding the graph as a matrix, our proposed algorithm does not perform better than a combination of Dijkstra’s algorithm. As the efficiency of a BFS is $O(|V|^2)$ and we perform $N_I$ such searches, it follows that in the worst-case scenario, the efficiency of our proposed method would also be $O(|V|^4)$. However, if the graph of interest is coded as a list, each BFS is in $O(|E| + |V|)$, and therefore the entire recursive shortest-path algorithm has an efficiency of $O(|V|^2|E| + |V|^3)$. By contrast, a combination of Dijkstra’s algorithms based on an adjacency list only reduces to $O(|V|^2|E| \log |V|)$ or $O(|V|^2|E| + |V|^3 \log |V|)$ using the Fibonacci heap. Thus, our algorithm outperforms a combination of $N_I$ Dijkstra’s algorithms when the graph of interest is coded as a list.

Conclusion

In this paper, we have described a recursive shortest path algorithm for weighted graphs, which can be used for the integrating topological metrics with respect to density. This proposed method can readily be generalized to directed networks. In such a case, one simply needs to define a graph $G = (V, E, W)$, where the elements of $E(G)$ are ordered pairs of vertices. The edgeUpdate function in equation (10) can then be modified in order to check for directed shortest paths instead of undirected ones. Given the growing interest of natural scientists in graph topological properties and the large availability of weighted networks, the utilization of algorithms of the type described in this paper is likely to become ubiquitous.

Acknowledgments

This work was supported by a fellowship from the UK National Institute for Health Research (NIHR) Biomedical Research Centre for Mental Health (BRC-MH) at the South London and Maudsley NHS Foundation Trust and King’s College London. This work has also been funded by the Guy’s and St Thomas’ Charitable Foundation as well as the South London and Maudsley Trustees. the authors also would like to thank two reviewers for their valuable input.

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### Inputs:
$D$, {$v_1, v_2$}.

### Output:
$D$.

#### Initialization:
1. Set $N = \text{D.ncol}()$;
2. $d_{v_1v_2} = d_{v_2v_1} = 1$;

#### BFS around $v_2$:
3. Set $S_G = v_1 \cup v_2$, $S^{(0)} = v_2$;
4. FOR $(m = 1, \ldots, N - 2)$ DO
   5. $\Delta = \bigcup_{v \in S^{(m-1)}} \delta(v)/S_G$;
   6. FOR $(v \in \Delta)$ DO
      7. IF $(d_{v_1v} \geq m + 1)$
         8. $d_{v_1v} = d_{vv_1} = m + 1$; Add $v$ to $S^{(m)}$; Add $v$ to $S_G$;
   END IF;
9. END FOR;
10. IF $S^{(m)} = \emptyset$ BREAK;
11. END FOR;

#### BFS around $v_1$:
12. Set $S_G = S_G/v_1$, $S^{(0)} = v_1$;
13. FOR $(m = 1, \ldots, N - 2)$ DO
   14. $\Delta = \bigcup_{v \in S^{(m-1)}} \delta(v)/S_G$;
   15. FOR $(v \in \Delta)$ DO
       16. FOR $(u \in S_G)$ DO
          17. IF $(d_{uv} \geq d_{u_1v} + m)$
             18. $d_{uv} = d_{u_1v} + m$; $d_{vu} = d_{v_1u} + m$; Add $v$ to $S^{(m)}$;
       END IF;
19. END FOR;
20. END FOR;
21. IF $S^{(m)} = \emptyset$ BREAK;
22. END FOR;

#### Return $D$;

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Figure 1. Updating of $D$ inserting one edge at a time, here denoted $v_1v_2$. The set $S_G$ is the set of visited vertices, whereas $S^{(m)}$s are the sets of unvisited edge corresponding to the $m$th degree neighborhoods of the previously modified vertices, and $\Delta$ is the set of relevant vertices at every level of the BFS. Both $\Delta$, $S_G$ and the $S^{(m)}$s should be regarded as containers, where adding implies inserting a new element in a set.
Figure 2. Graphical representation of the edge updating algorithm to modify the shortest path matrix, \( D \), one edge at a time. In panel (a), a new edge, \( v_4v_5 \), is added to an existing graph, which is otherwise composed of two disconnected components. In panel (b), we conduct a BFS around \( v_5 \) with respect to \( v_4 \), updating \( D \) accordingly with the new shortest paths between \( v_4 \) and \( v_5 \) and its first and second degree neighbors represented in red, yellow and purple, respectively. In panel (c), we conduct a BFS around \( v_4 \) with respect to the vertices, which were modified in phase I of edgeUpdate, denoted in blue. The first and second degree neighbors of \( v_4 \) are here denoted in orange and purple, respectively. In each panel, the corresponding modifications in the matrix of shortest paths are reported on the right-hand side. The presence of a dashed line between two vertices indicates that we test whether the inclusion of \( v_4v_5 \) shortens the shortest path between these two vertices.