Walk modularity and community structure in networks

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Modularity maximization has been one of the most widely used approaches in the last decade for discovering community structure in networks of practical interest in biology, computing, social science, statistical mechanics, and more. Modularity is a quality function that measures the difference between the number of edges found within clusters minus the number of edges one would statistically expect to find based on random chance. We present a natural generalization of modularity based on the difference between the actual and expected number of walks within clusters, which we call *walk-modularity*. Walk-modularity can be expressed in matrix form, and community detection can be performed by finding leading eigenvectors of the walk-modularity matrix. We demonstrate community detection on both synthetic and real-world networks and find that walk-modularity maximization returns significantly improved results compared to traditional modularity maximization.

1 Introduction

The problem of detecting community structure within networks has received considerable attention over the last decade, largely due to the rapidly increasing accessibility of large, real-world network data sets in many fields, including biology, social sciences, statistical mechanics, citation networks, and many more [10, 11, 13, 18, 19]. A community, or cluster, may intuitively be thought of as a collection of nodes more densely connected to each other than with nodes outside the cluster. In real-world networks derived from biological, social, and internet data for example, one often does not know in advance how many separate communities are within the network, if any at all, nor how many nodes comprise each of the communities.

Several popular and effective algorithms for community detection in networks rely on the concept of modularity [1, 4, 6, 14, 15, 17]. The modularity function was initially designed as a quantitative measure of the quality of a given partition of a network [10]. The sensible observation motivating the modularity measure is that separate communities should have significantly fewer edges running between them than one would expect to find based on random chance. Equivalently, the number of edges connecting nodes within a community should be far greater than statistically expected. The modularity function is therefore defined as the difference between the edge density within groups of nodes minus the expected edge density of an equivalent network with the edges placed at random. Large, positive values of modularity indicate the presence of a good partition of a network into communities, and many community detection algorithms are based on searching for partitions which maximize the modularity function. In this work, we propose a natural generalization of modularity, that we call walkmodularity. A walk on a network begins at a starting vertex and continues going along edges, which may be repeated, until it reaches a specified last vertex. The number of edges traversed is called the length of the walk. The modularity generalization we propose is that the number of walks of a specified length connecting nodes within a community should be far greater than expected by random chance. Large, positive values of the walk-modularity function will indicate groups of nodes that are very tightly knit together. For walk length equal to one, the walk-modularity function reduces to the standard modularity measure, which just considers edges, and we refer to it as edge-modularity.

In the seminal paper of Newman [14], the modularity function was cast into a matrix formulation, yielding the so-called modularity matrix of a network. The modularity function can be maximized by computing leading eigenvectors of the modularity matrix, and high quality network partitions are obtained. For any specified walk length, we can define the walk-modularity matrix and can use it to find a good partition of a network into communities. The method of optimal modularity has several desirable features which have led to its widespread popularity. In particular, neither the number or sizes of the communities has to be specified in advance. These desirable features of the method of optimal modularity are retained when using the walk-modularity generalization.

2 Walk-Modularity

Two nodes in a network are connected by a length ℓ walk if you can start at one node and traverse ℓ consecutive edges to reach the other node. The generalized notion of modularity we propose is based on the idea that a community will have a statistically unexpected number of walks between nodes. We therefore express the walk-modularity as

> $Q_{\ell} =$ (number of walks of length ℓ within communities) - (expected number of such walks).

Partitions of a network with large positive values of Q_{ℓ} will indicate groups of nodes that are very tightly knit together. Suppose a network contains n nodes and has an adjacency matrix denoted by A. It is a well known fact that powers of the adjacency matrix can be used to count the numbers of walks between pairs of nodes in a graph. The i, j entry of the matrix A^{ℓ} is the number of walks of length ℓ between vertices iand j.

In order to calculate the expected number of walks, we need to consider an equivalent randomized network with which to compare the real network. The expected number of walks between vertices will depend on the choice of the so-called null model to which we compare our network. We will use the same null model described in the seminal paper of Newman [14]. In that work, an equivalent null model was considered where edges are placed entirely at random, subject to the constraint that the expected degree of each vertex in the null model is the same as the actual degree of the corresponding vertex in the real network. Let k_i be the degree of vertex i and let m be the total number of edges in the network. The expected number of edges between vertices i and j is then given by

$$P_{ij} = \frac{k_i \, k_j}{2m}$$

Powers of the expected adjacency matrix, P, will count the expected number of walks in the null model. The i, j entry of the matrix P^{ℓ} is the expected number of walks of length ℓ between vertices i and j.

Define g_i to be the community to which vertex *i* belongs. The walk-modularity, Q_ℓ , for walks of length ℓ can be written

$$Q_{\ell} = \frac{1}{2m_{\ell}} \sum_{i,j} \left[(A^{\ell})_{ij} - (P^{\ell})_{ij} \right] \delta(g_i, g_j) ,$$

where $\delta(r, s) = 1$ if r = s or zero otherwise. Walk-modularity only compares the actual number of walks versus the expected number of walks for vertices within the same community. We choose to normalize walk-modularity by

$$m_\ell = \frac{1}{2} \sum_{i,j} (A^\ell)_{ij} \; .$$

Note that for $\ell = 1$, the walk-modularity Q_1 reduces to the standard definition of modularity given in [10], which we refer to as edge-modularity. The walk length, ℓ , will turn out to be a natural parameter in the clustering algorithm that provides the ability to control how tightly knit a community of nodes should be.

3 Spectral Optimization of Walk-Modularity

To find community structure in a network, we wish to maximize the walk-modularity over all possible partitions of the network. A large number of community detection techniques have been based on maximizing edge-modularity, such as in [1, 6, 7, 17], although [7] proved that the decision problem of finding a clustering with modularity exceeding a given value is **NP**-complete. Clustering algorithms attempting to maximize modularity focus on heuristics and approximations to approach the optimum value. There are many heuristic algorithms for maximizing edge-modularity, using techniques such as linear programming, vector programming, greedy agglomeration approaches, extremal optimization, and spectral optimization [1, 3, 6, 7, 14, 15]. In what follows, we employ the spectral optimization procedure from [14] adapted to work for walk-modularity, which proved to be the simplest optimization technique to implement while giving very high quality results.

Closely following the discussion in [14, 15], we first consider the problem of partitioning the network into just two groups of nodes. Define a length n index vector **s**

such that

$$s_i = \begin{cases} +1 & \text{if vertex } i \text{ belongs to group } 1, \\ -1 & \text{if vertex } i \text{ belongs to group } 2. \end{cases}$$

Noting that the quantity $\delta(g_i, g_j) = \frac{1}{2}(s_i s_j + 1)$ is 1 if nodes *i* and *j* are in the same group, and 0 otherwise, we can write the walk-modularity as

$$Q_{\ell} = \frac{1}{4m_{\ell}} \sum_{i,j} \left[(A^{\ell})_{ij} - (P^{\ell})_{ij} \right] (s_i s_j + 1)$$

= $\frac{1}{4m_{\ell}} \sum_{i,j} \left[(A^{\ell})_{ij} - (P^{\ell})_{ij} \right] s_i s_j + \frac{1}{4m_{\ell}} \sum_{i,j} \left[(A^{\ell})_{ij} - (P^{\ell})_{ij} \right]$

If we define the walk-modularity matrix as

$$B = A^{\ell} - P^{\ell}$$

then

$$Q_{\ell} = \frac{1}{4m_{\ell}} \mathbf{s}^T B \mathbf{s} + \frac{1}{4m_{\ell}} \sum_{i,j} B_{ij} \tag{1}$$

Since large, positive values of walk-modularity indicate the presence of a good division of the network, the goal is to obtain the index vector \mathbf{s} which maximizes the value of Q_{ℓ} . This amounts to optimizing $\mathbf{s}^T B \mathbf{s}$ since the second term in (1) does not depend on the choice of \mathbf{s} . Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ be the eigenvalues of B, with associated orthonormal eigenvectors $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n$. Expressing \mathbf{s} as a linear combination of the eigenvectors $\mathbf{s} = \sum_{i=1}^n a_i \mathbf{u}_i$ with $a_i = \mathbf{u}_i^T \mathbf{s}$, we obtain

$$\mathbf{s}^T B \mathbf{s} = \left(\sum_{i=1}^n a_i \mathbf{u}_i^T\right) B\left(\sum_{i=1}^n a_i \mathbf{u}_i\right) = \sum_{i=1}^n a_i^2 \lambda_i.$$

Hence, the task of choosing **s** to maximize Q_{ℓ} is equivalent to choosing positive values a_i^2 to place as much weight as possible on the term in the sum with the largest positive eigenvalue, namely λ_1 . Since $a_1 = \mathbf{u}_1^T \mathbf{s}$, we choose **s** to be as close to parallel with \mathbf{u}_1 as possible. Thus, as in [14], the choice of **s** is

$$s_i = \begin{cases} +1 & u_i^{(1)} \ge 0\\ -1 & u_i^{(1)} < 0 \end{cases}$$

where $u_i^{(1)}$ is the *i*-th entry of \mathbf{u}_1 . Therefore, nodes are placed into either group 1 or group 2 depending on the sign of their corresponding entry in the leading eigenvector of the walk-modularity matrix. If the overall value of walk-modularity is $Q_{\ell} \leq 0$ then the network should not be partitioned in two.

In order to divide a network into more than just two communities, we will employ a recursive approach where we keep dividing groups in two until we find indivisible communities. In order to decide whether a particular group should be further divided, we must examine the change in walk-modularity that would result. Proceeding again as in [14], we consider a group g with n_g nodes, and calculate the change in walkmodularity that would result from further division of the group into two pieces,

$$\begin{split} \Delta Q_{\ell} &= \frac{1}{2m_l} \left[\frac{1}{2} \sum_{i,j \in g} B_{ij} (s_i s_j + 1) - \sum_{i,j \in g} B_{ij} \right] \\ &= \frac{1}{4m_l} \left[\sum_{i,j \in g} B_{ij} s_i s_j - \sum_{i,j \in g} B_{ij} \right] \\ &= \frac{1}{4m_l} \sum_{i,j \in g} \left[B_{ij} - \delta_{ij} \sum_{k \in g} B_{ik} \right] s_i s_j \\ &= \frac{1}{4m_l} \mathbf{s}^T B^{(g)} \mathbf{s} \end{split}$$

In a recursive approach for dividing a network into multiple communities, maximizing the contribution to walk-modularity from subdivision of communities can be approached using the same leading eigenvector method as before, but using the matrix $B^{(g)}$ at each step. Furthermore, a recursive community detection algorithm should refuse to make any subdivisions for which the change in walk-modularity is negative, which can be determined by explicitly calculating the value of ΔQ_{ℓ} at each step. Communities for which $\Delta Q_{\ell} \leq 0$ are called indivisible. In this manner, the spectral approach can be applied to divide a network into multiple indivisible communities without the need to specify in advance the number or sizes of the communities.

4 Examples

To demonstrate that walk-modularity is a very effective generalization of edge-modularity for finding communities, we applied the spectral optimization algorithm described in the previous section to both computer generated test cases and real-world networks. It is very important to emphasize that, because our focus is conducting a consistent comparison between edge-modularity and walk-modularity, only the leading eigenvector algorithm is used for the tests in sections 4.1 and 4.2. No other enhancements for modularity maximization were included in this work. The only parameter which varies from test to test is the walk length ℓ . The real-world test networks examined in section 4.2 are culled from the data in [13, 21]. These two networks are commonly used as examples of real-world networks in community-detection literature [1, 2, 3, 6, 7, 10, 14, 15, 17]. The synthetic test networks in section 4.1 are randomly generated using either a variation on the standard Erdős-Rényi model of random networks or generated following the benchmark test described in [12], which has previously been used to benchmark community-detection algorithms in [1, 5, 9, 16], among others.

4.1 Synthetic Networks

Walk-modularity significantly outperforms edge-modularity on the synthetic networks we examine in this section. The first synthetic test shown is a modified Erdős-Rényi random network with n = 500 nodes with a K_{20} complete subgraph connected to it (Fig. 1). The probability of an edge between two nodes in the random network seen in figure 1 is 0.10. The probability of an edge connecting a node in the K_{20} subgraph to a node in the random network is 0.5. The average degree of nodes in the complete subgraph are roughly the same as the average degree of nodes in the random network. To consider a node as either misplaced or placed correctly, the two communities were defined to be the embedded K_{20} and the Erdős-Rényi random network. If the community detection algorithm placed a node from the complete subgraph in the same community as the rest of the network, or vice versa, the node is counted as misplaced.



Figure 1: Random network (n = 500) with an embedded K_{20} . The two communities found by edge-modularity, $\ell = 1$, have 50 misplaced nodes (top left). The two communities found by walk-modularity with $\ell = 2$ have 11 misplaced nodes (top right). When $\ell = 3$ there is only 1 misplaced node (bottom left), and when $\ell = 4$ every single node is placed correctly (bottom right).



Figure 2: Communities as defined by the benchmark test with parameters $n = 500, \mu = 0.15, \bar{k} = 25$.

In other words, we are trying to compare how well the algorithms can find an embedded complete subgraph. In this test, we find that walk-modularity significantly outperforms edge-modularity in that simply increasing the length of walks considered from $\ell = 1$ to $\ell = 3$ results in a decrease from 50 misplaced nodes to merely 1 misplaced node. When $\ell = 4$, walk-modularity correctly places every single node into the two communities.

We next demonstrate the benchmark tests from [12]. This synthetic test simulates a real-world network by placing each node in a well-defined community following a userspecified average degree, \bar{k} , and then randomly rewires nodes between communities according to a mixing parameter μ . The result is a network with several communities with an approximate proportion of $1 - \mu$ edges among each community and μ edges between any one community and the others. One such network is pictured in figure 2, for parameters $n = 500, \mu = 0.15$, and $\bar{k} = 25$. Again, walk-modularity significantly outperforms edge-modularity in this test case, although the number of nodes misplaced is somewhat difficult to quantify due to the variable number of communities that may be found. Figure 2 shows the communities as they were originally defined by the benchmark test. Figure 3 shows the communities found by edge-modularity, and figure 4 shows the result of the walk-modularity maximization with $\ell = 8$.

4.2 Real-World Networks

The dolphins network from [13] is a social network of 62 dolphins from Doubtful Sound, New Zealand, with edges representing social relations between individuals, as estab-



Figure 3: Communities as detected by traditional edge-modularity, $\ell = 1$.



Figure 4: Communities as detected by walk-modularity with $\ell = 8$.

lished by observation over the course of a decade. During the decade of observation in this study, the network of dolphins split into two separate communities. In a partition of the dolphins network, a node is considered misplaced if the algorithm places it into



Figure 5: The dolphins network of [13]. Nodes are labeled with ± 1 according to the observed separation of the dolphin network by biologists. (Top) Nodes are colored according to the partitioning found by edge-modularity maximization. Misplaced nodes are colored red. (Bottom) Nodes are colored according to the partitioning found by walk-modularity maximization with $\ell = 10$. There is only a single misplaced node.

a different community than that observed by the biologists in [13]. Partitioning this network using edge-modularity finds 3 nodes misplaced, as in figure 5 (top). After increasing the length of walks considered to $\ell = 8$, the diameter of this network, the number of nodes misplaced drops to merely 2, and a value of $\ell = 10$ counts only a single misplaced node, figure 5 (bottom).

The karate club network from [21] is another social network, this time consisting of 34 members of a karate club, which once again split into two communities during the course of observation following a disagreement between the club's instructor and administrator. The nodes of this network represent individuals, and the edges friendships as determined by Zachary. As before, a node is considered misplaced if the algorithm places it in a community which differs from the observed partition. In this case, there is no effect found from increasing ℓ , although the results are no worse than with edge-modularity. The partition found from both walk-modularity with $\ell = 5$, the diameter of this network, and edge-modularity are the same, as shown in figure 6.



Figure 6: The karate club network of [21]. The nodes are colored relative to the partition found by the community detection algorithm, and the results are the same for both walk-modularity $\ell = 5$ and edge- modularity. The nodes are labelled ± 1 based on the observed partition, and colored red to indicate a node that was incorrectly placed relative to the observed.

For a given network, the user-controlled parameter ℓ can significantly impact the quality of the partition found by maximizing walk-modularity. In practice, we have found that choosing a value for ℓ somewhat near to the diameter of the network gives excellent results, as demonstrated in Table 1. Although it is typically computationally expensive to find the exact diameter of a network, there are several fast approximation algorithms [8, 20]. Moreover, we emphasize that even by using small values of $\ell > 1$, we obtained significant improvements in the observed quality of partitions. We summarize the test case results of this section in Table 1.

5 Conclusion

We introduced a new measure of the quality of a partition of a network into communities, which we call walk-modularity. Walk-modularity is a natural generalization of modularity because it considers the difference between the actual and expected number of walks of length ℓ within communities. Mathematically, it is a very simple and elegant generalization in that it only involves taking the ℓ -th powers of both the adjacency matrix and the expected adjacency matrix. As with traditional edge-modularity, walkmodularity can be maximized by finding the leading eigenvector of a matrix, called the walk-modularity matrix. Although we have only explored, in this paper, a single technique to maximize walk-modularity, it is a quantity that is compatible with maximization algorithms other than spectral maximization.

Even with small values of $\ell > 1$, we demonstrated with test cases that maximizing walk-modularity produces partitions with many fewer misplaced nodes than traditional edge-modularity. For a random network with an embedded complete graph, K_{20} , walkmodularity is capable of perfectly identifying the complete subgraph and separating it from the random network. Walk-modularity is also more successful in identifying

Network	Diameter	ℓ	Nodes Misplaced
Embedded K_{20}	3	1	50
		2	11
		3	1
		4	0
Benchmark Test [12]	4	1-3	> 100
n = 500		4	72
$\mu = 0.15$		5	92
$\bar{k} = 25$		6	40
		7	11
		8	9
Dolphins [13]	8	1-7	3
		8, 9	2
		10	1
Karate Club [21]	5	1-5	1

Table 1: Summary of the number of nodes placed in incorrect communities as the walk length parameter, ℓ , varies. In each case, as ℓ increases the community detection becomes more accurate.

the six communities in a randomly generated benchmark test where edge-modularity did not perform well. With two standard real-world community detection test cases, namely the dolphin network and the karate club network, walk-modularity performs in a manner comparable to the other most common community detection algorithms, and perhaps a bit better than edge-modularity in our comparison on the dolphin network.

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