Improved community structure detection using a modified fine tuning strategy

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Abstract. - The community structure of a complex network can be determined by finding the partitioning of its nodes that maximizes modularity. Many of the proposed algorithms for doing this work by recursively bisecting the network. We show that this unduely constrains their results, leading to a bias in the size of the communities they find and limiting their effectivness. To solve this problem, we propose adding a step to the existing algorithms that does not increase the order of their computational complexity. We show that, if this step is combined with a commonly used method, the identified constraint and resulting bias are removed, and its ability to find the optimal partitioning is improved. The effectiveness of this combined algorithm is also demonstrated by using it on real-world example networks. For a number of these examples, it achieves the best results of any known algorithm.

The problem of detecting and characterizing the community structure of complex networks has recently attracted a great deal of interest [1–10]. The structure of a network is important for how it functions [2]. Often networks have a modular structure in which the nodes can be partitioned into highly connected groups that have common properties or work together to achieve specific behavior. This is true for many different types of networks including social, biological, and telecommunication networks. For example, recent work suggests the importance of modularity for the functioning of metabolic and transcriptional regulatory networks [11–14]. However, identifying the various communities or modules in a network, i.e. its community structure, can be difficult. This is especially true for large networks which can frequently be partitioned in multiple, almost equally good ways. In these cases it becomes very important to eliminate or reduce all biases and undue constraints from the method used to detect communities.

Various algorithms have been proposed for the partitioning of complex networks into communities [3,4,10,15-41]. Many of these algorithms are based on the idea of maximizing a measure called modularity Q [3]. Finding the partitioning with the absolute maximum modularity has been proven to be an NP-hard problem [42],

and is thus intractable for large networks. It is therefore of interest to find a fast algorithm for obtaining a network partitioning that nearly maximizes modularity. One of the best methods currently in use is the leading eigenvalue method introduced by Newman [27, 28]. This is a bisectioning method, like most other proposed methods. It begins by dividing the nodes into two communities and then recursively divides each of those communities in two until no further increase modularity can be achieved. Each bisection is done by first making a "guess" at the best way to divide the community into two, followed by a "fine-tuning" that systematically considers moving each of the nodes to the other community until no further improvement in modularity can be achieved. Note that once a community is generated and fine-tuned the partition between it and all other communities is fixed. It can only be divided further into smaller communities; none of its nodes are ever placed in other existing communities. As we will see, this constraint generates a bias in the results that limits the modularity of the resulting partitioning.

To address this problem, we introduce an additional tuning step in the algorithm. This additional tuning, which is done each time after all communities have been bisectioned and fine-tuned, systematically considers moving

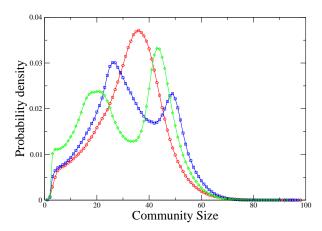


Fig. 1: (Color online) Community size distribution for Erdős-Rényi random networks with 400 nodes and average degree 4. The results were obtained using the q=2 leading eigenvector method with fine-tuning, which is a bisectioning algorithm, (blue squares), the q=3 trisectioning variant of that algorithm (green diamonds), and our improved algorithm that combines the q=2 variant with "final-tuning" (red circles).

each node of the network to all other existing communities or into a new community of its own. Using this additional "final-tuning", the value of modularity is consistently improved. The computational cost of final-tuning is very modest and the algorithm can be used to study large networks. To demonstrate its usefulness we will use it to determine the community structure of some known example networks. As we will see, the results indicate that our algorithm is competitive with the best existing community detection methods, and for some networks gives partitionings with modularity larger than that obtained with any other known method.

Modularity Q is defined as [3]

$$Q = \frac{1}{2m} \sum_{i,j} B_{ij} \delta_{C(i),C(j)} \tag{1}$$

where $B_{ij} = A_{ij} - k_i k_j / (2m)$ are the elements of the "modularity matrix" and C(i) is the community to which node i belongs. Here m is the total number of links in the network, k_i is the degree of node i, A_{ij} are the elements of the adjacency matrix, and δ is the Kronecker delta function. This definition of modularity is based on the idea that links between nodes in the same community are dense and that there are only sparse links between nodes in different communities. It is equal to the fraction of links that connect nodes in the same community minus what that fraction would be on average if the communities remained fixed but the links were randomly distributed.

The leading eigenvalue method [27,28] produces a guess for the initial bisectioning of a network by rewriting the modularity Q in terms of a vector S whose elements S_i take the values ± 1 depending on which of the two communities node i belongs to. Using the fact that $\delta_{C(i),C(j)} =$

 $(S_iS_i+1)/2$, Eq. 1 becomes

$$Q = \frac{1}{4m} S^T B S. (2)$$

The problem now becomes to choose the vector S that maximizes Q. If the elements of S were unconstrained, then the best choice would be to make S equal to the eigenvector corresponding to the largest eigenvalue of B. However, since they are constrained to be ± 1 , the method assigns the sign of S_i to correspond to the sign of the ith component of the eigenvector with the largest eigenvalue. The particular form of the modularity matrix B makes the power method a fast and efficient way to calculate the leading eigenvector [27, 28].

To refine the initial guess, a "fine-tuning" based on the Kernighan-Lin algorithm [43] is used. Once a community has been split in two, fine-tuning proceeds by computing for each node l the difference in modularity δQ associated with moving it from its sub-community to the other,

$$\delta Q = -\frac{S_l}{m} \sum_{i \neq l} B_{li} S_i. \tag{3}$$

The move resulting in the highest δQ (even if negative) is performed and recorded. If multiple moves result in the highest δQ one of them is picked at random. The procedure is then repeated, each time considering only the nodes that have not yet been moved and recording the new partitioning, until each node has been moved once. At this stage, the intermediate partitioning with the highest modularity is retained. The entire "fine-tuning" procedure is repeated at least once, until no further increase in modularity can be achieved. The move resulting in the largest modularity is then made, but, if the modularity after fine-tuning is less than the modularity before, the partitioning given by the initial guess is restored. Subsequent bisectionings of existing communities are done with an analogous procedure, except that instead of maximizing Q they attempt to maximize

$$\Delta Q = \frac{1}{4m} S^T B^{(C)} S,\tag{4}$$

where

$$B_{ij}^{(C)} = B_{ij} - \delta_{ij} \sum_{k \in C} B_{ik} \tag{5}$$

is the modularity matrix for community C and $i, j \in C$.

As far as maximizing modularity is concerned, the leading eigenvalue method arguably offers the best balance between speed and accuracy of all methods currently in use. It is inferior only to simulated annealing but much faster [6], and, for some networks, to greedy algorithms [6, 38] as discussed below.

However, there is a bias in the method that limits its effectiveness. This bias can be demonstrated by considering the distribution of community sizes that it finds in an ensemble of random networks. The blue squares in Fig. 1

show the community size distribution obtained using the leading eigenvalue method with fine-tuning for an ensemble of 10^6 random (Erdős-Rényi) networks. The size of these networks is N=400 and their average degree is k=4. To avoid complications with the community detection process, only fully connected networks have been considered. The distribution has two peaks, one around N/8, and another one around N/16. Thus, the method is biased in favor of finding communities of those sizes. Since, 8 and 16 are both powers of 2, this suggests that the bias is due to the bisectioning nature of the algorithm.

In order to check if this is true, we introduce a generalized version of the leading eigenvector method inspired by the Potts model [44] that recursively divides a network into q subsets. For q=2 it is equivalent to the method described above. In the generalized method each of the elements of S are from a set $\{P_1,...,P_q\}$ of (q-1)-dimensional unit vectors such that $[(q-1)P_i\cdot P_j+1]/q=\delta_{i,j}$. These are the vertices of a regular q-simplex centered at the origin. Modularity is now written as

$$Q = \frac{q-1}{2mq} S^T B S, \tag{6}$$

with the multiplication between elements of S understood as a dot product. Equations 3 and 4 are generalized similarly. The initial guess for S is made assuming that an eigenvector of B (or $B^{(C)}$) is equally likely to point in any direction in \mathbb{R}^N . Hence, normalized eigenvectors are uniformly distributed on the (N-1)-hypersphere of radius one, and the probability density for any component of an eigenvector is given by

$$p_N(x) = \frac{1}{I_{N-2}} (1 - x^2)^{\frac{N-3}{2}},$$
 (7)

where $I_N = \sqrt{\pi} \Gamma(N/2+1/2)/\Gamma(N/2+1)$. The variance of this density is 1/N. In the limit of large N, this approaches a Gaussian distribution whose cumulative probability function will be denoted by $F_N(x)$. Now, divide the real axis into q intervals defined by $\mathcal{I}_j = \{x|(j-1)/q \leq F_N(x) < j/q\}$ and arrange the set of vectors $\{P_j\}$ in increasing order of their number of positive components. Then, if U is the eigenvector corresponding to the largest eigenvalue, the initial guess for the q-partitioning is made by choosing $S_i = P_j$ if $U_i \in \mathcal{I}_j$. Fine-tuning is easily generalized as well. This is done, once a community has been split into q sub-communities, simply by considering moving each node from its guessed sub-community to each of the other q-1 possibilities.

Here we consider results of only the q=3 variant of the generalized method. This is a trisectioning algorithm. In the q=3 case, the elements of S are from the set $\{(1,0),(-1/2,\sqrt{3}/2),(-1/2,-\sqrt{3}/2)\}$ and $\delta_{C(i),C(j)}=(2S_i\cdot S_j+1)/3$. If U is the eigenvector corresponding to the largest eigenvalue, we choose $S_i=(1,0)$ if $F_N(U_i)\geq 2/3$, $S_i=(-1/2,\sqrt{3}/2)$ if $1/3\leq F_N(U_i)<2/3$, and $S_i=(-1/2,-\sqrt{3}/2)$ if $F_N(U_i)<1/3$. The green diamonds in Fig. 1 shows the community size distribution

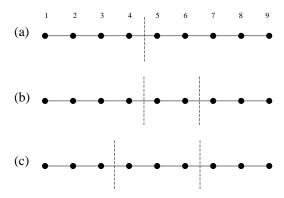


Fig. 2: Partitions of a simple network (a) after one bisection using any simple bisectioning algorithm, (b) final result with simple bisectioning, and (c) the optimal partitioning that maximizes modularity. The optimal partitioning results if bisectioning is combined with final-tuning.

obtained using this trisectioning method for the ensemble of random networks described above. Two peaks are now seen near N/9 and N/27, indicating a bias for finding communities of these sizes. Since, 9 and 27 are powers of 3, this bias is due to the trisectioning nature of the algorithm. This result indicates that the peaks found using bisectioning and trisectioning are artifacts of the methods, which are constrained to only allow division of existing communities and never move nodes to other existing communities. The same flaw is undoubtedly present in other community detection methods that involve simple bisectioning.

To better understand the problem, consider the simple example in Fig. 2 of a linear network with nine nodes connected by eight links. Fig. 2a shows the partitioning after one bisection. Further bisectioning divides the community with five nodes into two sub-communities as shown in Fig. 2b. The modularity of this configuration is Q = 51/128. However, this is not the partitioning that maximizes modularity. The partitioning shown in Fig. 2c exhibits the largest modularity $Q_{max} = 53/128$. This partitioning will never be found with a simple bisectioning algorithm. This is because nodes 4 and 5 are assigned to different communities at the first bisectioning, and can never be moved into the same community after that. However, they are in the same community in the optimal partitioning. In more general terms, if the partitions set during a division are not optimal, there is no chance to correct them. These partitions unduly constrain the community detection algorithm.

The problem can be solved by using an additional modified fine-tuning step similar to the one described above but involving all partitions. This modified fine-tuning, which we call "final-tuning," is performed at the end of every round of divisions in the course of which all communities that resulted from the previous round have been divided once. In the final-tuning procedure, the differences in modularity associated with moving every node of

the network from its sub-community to every other subcommunity are computed, and the move resulting in the highest modularity difference is performed and recorded. As in the case of fine-tuning, if multiple moves result in the highest modularity difference one of them is picked at random. The procedure is repeated on the nodes that have not yet been moved until each node has been moved once, at the end retaining the intermediate configuration with the highest modularity. Equation 3 can be used to calculate the difference in modularity δQ when switching one node to an arbitrary community, by defining community C as the union of the origin and destination communities. However, it is usually faster to calculate δQ directly from Eq. 1 [7]. That is, by subtracting the modularity calculated with node l in community Y from the modularity calculated with l in its original community X we find

$$\delta Q = \frac{1}{m} \left(\sum_{i \in Y} A_{li} - \sum_{i \in X} A_{li} - \frac{k_l (K_Y - K_X + k_l)}{2m} \right), (8)$$

where K_X and K_Y are the sums of the degrees of all nodes in communities X and Y respectively, and k_j is the degree of node j. The speed of final-tuning can be improved by only considering moving nodes to the communities of the nodes which they are connected to, or into a community of their own.

To incorporate final-tuning into the community detection, we suggest the following algorithm.

- 1. Apply any previous method, for example the leading eigenvalue method with fine-tuning, to attempt to divide each of the existing communities.
- 2. Use Eq. 8 to calculate δQ caused by all possible moves of any single node to all other existing communities, or into a community of its own.
- 3. Find the move that leads to the largest δQ (even if negative) and make the move. If multiple moves result in the largest δQ pick one of them randomly. Fix the community assignment for the node moved.
- 4. Repeat steps 2-3, but in step 2 only consider moving nodes whose community assignment has not yet been fixed. Continue repeating until every node is moved once and only once.
- 5. Choose the intermediate configuration with the largest Q.
- 6. Repeat 2-5 until no further improvement of Q is achieved.
- 7. Compare the modularity of the resulting partition to the modularity after step 1. If the latter is larger, then revert to the partitioning after step 1.
- 8. Repeat 1-7 until no further improvement of Q is achieved.

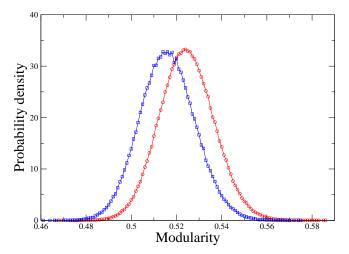


Fig. 3: (Color online) Modularity distribution for Erdős-Rényi random networks with 400 nodes and average degree 4. The results were obtained using the q=2 leading eigenvector method with fine-tuning (blue squares), and by combining it with "final-tuning" (red circles).

The computational complexity of the leading eigenvalue algorithm with fine-tuning is O[N(N+m)] for one bisection [27]. Since the expected number of bisections is $O(\log N)$, the overall complexity of the community detection procedure is $O[N(N+m)]\log N$ [27]. The additional workload due to investigating all possible moves between communities in a final-tuning step is generally $O[N^2]$. Thus, if the leading eigenvalue algorithm with fine-tuning is used in step 1, then combining it with final-tuning does not change the overall order of computational complexity.

The effectiveness of including final-tuning in a community detection algorithm can be demonstrated first by noting that if it is used, then the optimal partitioning of the simple network in Fig. 2 (shown in Fig. 2c) is obtained. This is because final-tuning removes the undue constraints that exist in simple bisectioning methods. Second, combining final-tuning with the q=2 leading eigenvalue method and fine-tuning, the multiple peaks of the community size distribution for random networks disappear (Red circles in Fig. 1), leaving only a single peak as expected [7]. This indicates that the undue constraints have been removed. The resulting modularity is also significantly improved. Figure 3 compares the distribution of modularity of partitionings obtained with (red circles) and without (blue squares) final-tuning for the same ensemble of random networks. In both cases, the results approximately follow a Gaussian distribution, but the average maximum modularity increases from 0.515748 ± 0.000067 to 0.524293 ± 0.000057 with the use of the finial-tuning. The standard deviations of the two distributions are 0.012158 ± 0.000082 and 0.012022 ± 0.000068 , respectively. All errors are 2σ estimates. Note that using the leading eigenvalue method with q > 2 does not improve the q = 2results. (Data not shown.)

Table 1: Comparison of maximum modularity of some example networks found using our method of final-tuning combined with the q=2 leading eigenvalue method and fine-tuning, Q_{FT} , against the best previously known result obtained using any other algorithm, Q_{pub} . The source of the data for the network is cited next to its name, and the articles reporting the previous best results are cited under "Method."

| Network | Size | Q_{FT} | Q_{pub} | Method |
|------------------------|-------|----------|-----------|----------|
| Karate [45] | 34 | 0.420 | 0.420 | [40] |
| Jazz musicians [46] | 198 | 0.445 | 0.445 | [25, 40] |
| Metabolic [47] | 453 | 0.452 | 0.450 | [38, 40] |
| E-mail [48] | 1133 | 0.580 | 0.579 | [40] |
| Key signing $[49, 50]$ | 10680 | 0.867 | 0.878 | [38] |
| Physicists [51] | 27519 | 0.737 | 0.748 | [38] |

The networks are, respectively, the karate club of Zachary, a collaboration network of early Jazz musicians, a metabolic network of the nematode *Caenorhabditis elegans*, a network of e-mail contacts at a university, a trust network of mutual cryptography key signings, and a coauthourship network of condensed matter physicists. These same networks were studied in Ref. [27].

As a further test, we applied final-tuning, combined with the q=2 leading eigenvalue method and fine-tuning, to find the community structure of a number of real world example networks that have been studied in the literature [9, 25, 27, 38, 40, 45–51]. Note that, because the algorithm is partly stochastic, we have run hundreds of analyzes for each of the networks considered and chosen the partition with the largest modularity. Table 1 shows a comparison between our results (labeled "FT") and the best known published results (labeled "pub"). Although the increases in modularity may only seem modest, the estimated upper bounds for the maximum modularity for some of these networks [40] are very close to our results. For the two smallest networks, we find what is likely to be the optimal partitioning. For the two medium sized networks, our algorithm achieves results better than any other known algorithm. However, for the two largest networks a greedy algorithm performs better. Greedy algorithms work by combining communities, instead of dividing them. It is possible that combining a greedy algorithm with final-tuning would improve the results for the two largest networks as well. Note that for all examples studied our results using final-tuning combined with the leading eigenvalue method equaled or surpassed the best known results obtained using the leading eigenvalue method only.

In summary, we have shown that an undue constraint exists in many of the algorithms commonly used to detect the community structure of complex networks, and that this constraint limits the effectiveness of those algorithms for finding the network partitioning with the maximum modularity. To solve the problem, we proposed adding an

extra step into the community detection procedure that fine-tunes the partitioning by considering moving nodes to all other existing communities. This extra step requires only minor computational cost, and does not increase the order of the computational complexity of the overall algorithm. We demonstrated the effectiveness of our improved algorithm by showing that it eliminates the bias towards dividing random networks into communities of size $N/2^n$ that exists when a bisectioning algorithm is used. We also used it to determine the community structure of some known example networks and found that, except for the largest networks, it achieves the best results of any currently known algorithm. Finally, since finding the network partitioning with the largest modularity is an an NP-hard problem [42], we note that the approach we have used here to improve the approximate algorithms for solving the problem, namely of identifying and removing undue constraints that bias their results, may be helpful in improving approximate algorithms for solving other NPhard problems associated with complex networks such as finding the set of routes that maximizes the capacity of congested network transport [52–54].

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