

Limits of modularity maximization in community detection

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Modularity maximization is the most popular technique for the detection of community structure in graphs. The resolution limit of the method is supposedly solvable with the introduction of modified versions of the measure, with tunable resolution parameters. We show that multiresolution modularity is not suitable to detect communities in networks. This is due to two opposite coexisting effects: the tendency to merge small subgraphs, which dominates when the resolution is low; the tendency to split large subgraphs, which dominates when the resolution is high. In benchmark networks with heterogeneous distributions of cluster sizes, the simultaneous elimination of both biases is not possible and multiresolution modularity is not capable to recover the planted community structure, not even when it is pronounced and easily detectable by other methods, for any value of the resolution parameter.

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I. INTRODUCTION

The detection and analysis of communities in graphs [1, 2] is one of the most popular topics within the modern science of networks [3–10]. In the latest years an increasing number of large networked datasets including millions or even billions of vertices and edges have become available, and a traditional analysis based on local network properties and their global statistics (e.g., degree distributions and the like) provides but a partial description of the system and its function. Communities (also called *clusters* or *modules*) are subgraphs including vertices with similar features or function, and their identification may disclose not only such similarities among vertices, which are often hidden, but also how the system is internally organized and works.

Vertices belonging to the same community have a considerably higher probability of being linked to each other than vertices belonging to different clusters. Therefore a community appears as a region of the network with a high density of internal links, much higher than the average link density of the graph. The most popular method to detect communities in graphs consists in the optimization of a quality function, the modularity introduced by Newman and Girvan [11, 12]. Modularity quantifies the deviation of the internal link density of the clusters from the density one expects to find within the same groups of vertices in random graphs with the same expected degree sequence of the network at study. The idea is that vertices linked to each other in a random way should not form communities, as high values of the link density cannot be attained. Consequently, high values of modularity are supposed to indicate “suspiciously” high values of internal link densities for the subgraphs, which are then distinct from groups of randomly linked vertices and can be deemed as true communities. While this is actually not true [13, 14], the optimization of the measure has been widely used in the past years.

Recently it has been pointed out that modularity opti-

mization is plagued by serious biases. In particular, it has a resolution limit [15], that leads to the systematic merger of small clusters in larger modules, even when the clusters are well defined and loosely connected to each other. A more recent analysis of the resolution limit has led to the conclusion that the modularity landscape is “glassy”, and includes an exponentially growing (with system size) number of local maxima whose values are very close to the absolute maximum of the measure, even if the corresponding partitions may be topologically quite different from each other [16]. This implies on the one hand that it is not too difficult to find a good approximation of the modularity maximum for many techniques, on the other hand that the maximum is essentially unreachable. A recent comparative analysis of community finding algorithms has indeed revealed that modularity fails to properly identify clusters on benchmark graphs with built-in community structure, and that other methods are much more effective [17].

Nevertheless, modularity optimization is still being used. The main reason is the claim that the resolution limit can be removed by adopting suitable multiresolution versions of modularity, like those introduced by Reichardt and Bornholdt [18] and by Arenas, Fernández and Gómez [19]. In these variations, a tunable resolution parameter enables one to set the size of the clusters to arbitrary values, from very large to very small. However, real networks are characterized by the coexistence of clusters of very different sizes, whose distributions are quite well described by power laws [20–22]. Therefore there is no characteristic cluster size and tuning a resolution parameter may not help. Indeed, in this paper we show that multiresolution modularity is not capable to identify the right partition of the network in realistic settings and that therefore it does not solve the problems of modularity maximization in practical applications. The problem is that modularity maximization is not only inclined to merge small clusters, but also to break large clusters, and it seems basically impossible to avoid both

biases simultaneously.

The paper is structured as follows. In Section II we present a general analysis of some relevant mathematical properties of multiresolution modularity, with respect to the merger or split of subgraphs, leading to the identification of a range of values of the resolution parameter where modularity should be safe from the above-mentioned problems. In Section III we test the result on realistic benchmark graphs with community structure, showing that it is often impossible to find a value of the resolution parameter that delivers the planted partition. Conclusions are reported in Section IV.

II. THE PROBLEM OF MERGING AND SPLITTING CLUSTERS

A. Multiresolution modularity

We do not expect that our results are significantly affected by the specific modularity formula one chooses. Here we adopt the generalized modularity Q_λ proposed by Reichardt and Bornholdt [18], which reads

$$Q_\lambda = \sum_S \left[\frac{k_{in}^S}{2M} - \lambda \left(\frac{k_{tot}^S}{2M} \right)^2 \right], \quad (1)$$

where the sum runs over all the clusters, $2M$ is the total degree of the network, k_{tot}^S is the sum of the degrees of vertices in module S and k_{in}^S is twice the number of internal edges in module S . So, we have $k_{tot}^S = k_{in}^S$ only if the module is disconnected from the rest of the graph. Here λ works like a resolution parameter: high values of λ lead to smaller modules because the term $(k_{tot}^S/2M)^2$ in the sum of Eq. (1) becomes more important and its minimization, induced by the maximization of Q_λ , favors smaller clusters.

We ask when it is proficuous for modularity to keep two subgraphs together or separate. For this, we need to compute the difference $\Delta Q_\lambda = Q_\lambda(\text{partition with merged subgraphs}) - Q_\lambda(\text{partition with separated subgraphs})$: if $\Delta Q_\lambda > 0$ modularity would be higher for the partition where the subgraphs are merged, otherwise the split would be more convenient.

We indicate with A and B the two subgraphs (see Fig. 1). Let Q_λ^{A-B} and Q_λ^{AUB} denote the value of modularity when A and B are kept separated and merged, respectively.

$$Q_\lambda^{A-B} = \left[\sum_{S \neq A, B} \dots \right] + \frac{k_{in}^A}{2M} + \frac{k_{in}^B}{2M} - \lambda \left(\frac{k_{in}^A + l + v}{2M} \right)^2 - \lambda \left(\frac{k_{in}^B + r + v}{2M} \right)^2, \quad (2)$$

where v denotes the number of links joining A with B , l the number of links joining A with the rest of the network

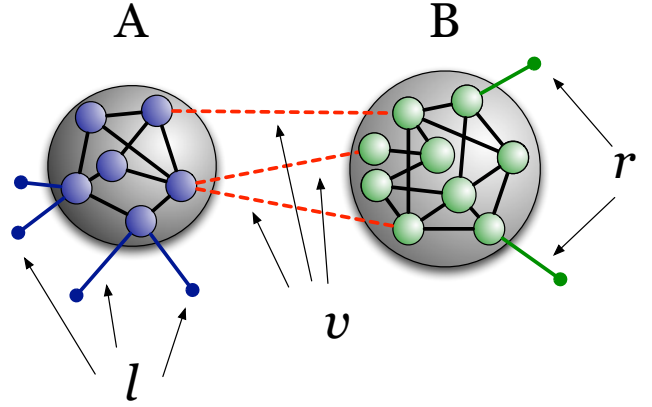


Figure 1: (Color online) Schematic representation of the problem of merging versus splitting subgraphs. Here A and B are two subgraphs, the problem is whether one yields a higher value for modularity by merging them in a single subgraph or by keeping them separated. The parameters involved in the decision are the number of internal links in A and B (multiplied by 2), k_{in}^A and k_{in}^B , the number of links v between A and B (here $v = 3$), the number of links l between A and vertices belonging neither to A nor to B (here $l = 4$), and its equivalent r for B (here $r = 2$).

(excluding B) and r is the equivalent of l for B . For Q_λ^{AUB} we have:

$$Q_\lambda^{AUB} = \left[\sum_{S \neq A, B} \dots \right] + \frac{k_{in}^A}{2M} + \frac{k_{in}^B}{2M} + \frac{2v}{2M} - \lambda \left(\frac{k_{in}^A + l + v + k_{in}^B + r + v}{2M} \right)^2. \quad (3)$$

The difference $\Delta Q_\lambda = Q_\lambda^{AUB} - Q_\lambda^{A-B}$ reads

$$\Delta Q_\lambda = \frac{2v}{2M} - \lambda \frac{k_{in}^A k_{in}^B + l k_{in}^B + r k_{in}^A + l r}{2M^2} - \lambda \frac{v(k_{in}^A + k_{in}^B + l + r) + v^2}{2M^2}. \quad (4)$$

To simplify a little Eq. (4) we can define $\Delta = 2M \Delta Q_\lambda$

$$\Delta = 2v - \lambda \frac{k_{in}^A k_{in}^B + l k_{in}^B + r k_{in}^A + l r}{M} - \lambda \frac{v(k_{in}^A + k_{in}^B + l + r) + v^2}{M}. \quad (5)$$

Modularity is higher for A and B merged if and only if $\Delta > 0$.

Eq. (5) is rather general but we are just interested in testing modularity for some special cases, for which calculations are easy. Here in particular, we will consider the case $l = r = \eta$ and $k_{in}^A = k_{in}^B = \xi$. Eq. (5) becomes

$$\Delta = 2v - \lambda \frac{(\xi + v + \eta)^2}{M}. \quad (6)$$

B. Splitting clusters

Despite the different approaches to the problem of detecting clusters in networks, there are some general ideas which are shared by most scholars. One of them is that a random graph has no communities, so it should not be split by an algorithm in smaller pieces. Another shared belief is that a complete graph (or clique), i.e. a graph whose vertices are all connected to each other, is a perfect community (due to the fact that the internal link density reaches the highest possible value of 1). So, if cliques are just loosely connected to each other, one would expect that a good method should detect them as separate clusters. We would like to find the mathematical conditions, in particular the choice of the resolution parameter λ , that satisfy both requisites. In this subsection we search for the condition to avoid the splitting of random subgraphs, while the condition to avoid the merger of cliques will be given in the next subsection.

Let us consider a random subgraph \mathcal{S} with total degree $2M_S$, which is part of a larger network with total degree $2M$. The goal is to check under which condition \mathcal{S} is split by optimizing modularity. Here for simplicity we consider only bi-partitions. The expected optimal modularity Q_2 for the bipartition of a random graph has been computed by Reichardt and Bornholdt [23]

$$Q_{RB} = 0.78 \frac{\langle \sqrt{k} \rangle_{\mathcal{S}}}{\langle k \rangle_{\mathcal{S}}}, \quad (7)$$

where the brackets indicate expectation values over the ensemble of random graphs with the same expected degree sequence of the subgraph at study.

We now express Q_2 in terms of the number of edges v between the clusters of the bipartition with optimal modularity. We obtain

$$2M_S Q_2 = 2M_S - 2v - \frac{k_A^2 + k_B^2}{2M_S} = \frac{2k_A k_B}{2M_S} - 2v, \quad (8)$$

where k_A (k_B) is the total degree of module A (B). Since modularity is optimal when the two modules are of about equal size, i.e. when $k_A \approx k_B \approx M_S$, we have:

$$2M_S Q_2 = M_S - 2v, \quad (9)$$

from which we can derive v ,

$$v = M_S \left(\frac{1}{2} - Q_2 \right). \quad (10)$$

For $Q_2 = 0$ we would have $v = M_S/2$, which is the expected average number of links joining two modules of equal size, arbitrarily chosen. Eq. (10) implies that optimizing modularity decreases the number of expected links between the modules, with respect to arbitrary bi-partitions, while it increases the internal density of links of the modules. One also sees that, for v to be positive, $Q_2 \leq 0.5$. Actually, in the calculation of Reichardt and Bornholdt, this holds only if $\langle k \rangle$ is big enough. To give

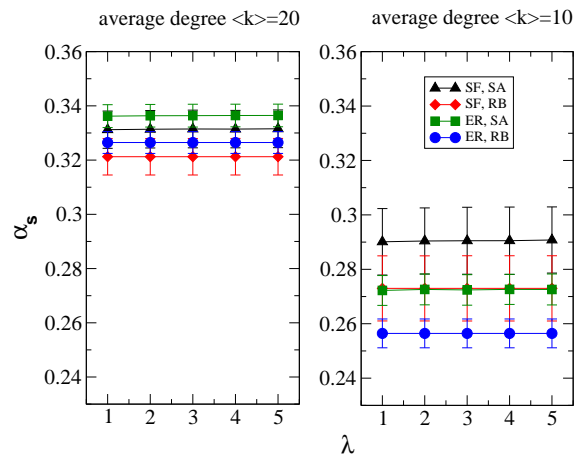


Figure 2: (Color online) The plot shows α_S measured on Erdős-Rényi and scale free graphs. For each type of graph we plot the analytical estimate of Reichardt and Bornholdt (RB) and a numerical estimate obtained by optimizing modularity with simulated annealing (SA) [13]. The minimum cut $v = \alpha_S \times M_S$ was measured by optimizing modularity for different values of λ . To optimize modularity, we are looking for small values of v and equal values of k^A and k^B , so tuning λ just controls the importance of either requirement. However, simulations show that the dependence on λ is quite weak, validating our approximation $k^A \approx k^B$.

an idea of the numbers that one could have, $Q_2 \approx 0.17$ when all vertices have degree $k = 20$, so $v \approx 0.33 \times M_S$ which is actually a not too bad approximation also for other degree distributions (for all vertices having degree $k = 10$, $v \approx 0.25 \times M_S$). Let us call α_S this proportionality factor between v and M_S ,

$$v = \alpha_S M_S \quad \text{and} \quad k_{in}^A = k_{in}^B = (1 - \alpha_S) M_S. \quad (11)$$

From Eqs. (7), (10) and (11) we get

$$\alpha_S = \frac{1}{2} - 0.78 \frac{\langle \sqrt{k} \rangle_{\mathcal{S}}}{\langle k \rangle_{\mathcal{S}}}. \quad (12)$$

In Fig. 2 we compare the values of α_S from Eq. (12) with numerical estimates derived by putting in Eq. (10) the maximum modularity Q_2 , derived with simulated annealing. The calculation of Q_2 is carried out for different values of λ , but the results seem to be essentially independent of λ . We consider both Erdős-Rényi (ER) and scale-free (SF) graphs, with 1000 vertices and average degree $\langle k \rangle = 20$ (left panel) and 10 (right panel). The SF graphs have degree exponent 2. As we can see from Fig. 2, the analytical estimate of Eq. (12) yields a good approximation of α_S .

Let us now consider our splitting-merging problem, considering A and B as candidates. We set $\eta = 1$, which means that only two links come out of \mathcal{S} (ideally one from A , the other from B). In this case, we would like to

have $\Delta > 0$, to avoid the split of the random subgraph \mathcal{S} . From Eq. (6) and Eqs. (11) we get (remember that $\xi = k_{in}^A = k_{in}^B$):

$$2\alpha_S M_S > \frac{\lambda(M_S + 1)^2}{M}. \quad (13)$$

If $M_S \gg 1$, this becomes

$$\lambda < \frac{2\alpha_S M}{M_S}. \quad (14)$$

Alternatively, we can incorporate the correction factor $[M_S/(M_S + 1)]^2 \approx 1$ in α_S , so that we call α_S what is actually $\alpha_S[M_S/(M_S + 1)]^2$. If the subgraph is a clique, $\alpha_S \approx 0.5$, and modularity can even split a clique when

$$\lambda \gtrsim \frac{M}{M_S}. \quad (15)$$

C. Merging clusters

Let us now consider two equal sized subgraphs connected with one edge ($v = 1$ and $\eta = 1$) and let $k_{in}^A = k_{in}^B = \xi_C$. Eq. (6) becomes:

$$\Delta = 2 - \lambda \frac{(\xi_C + 2)^2}{M}. \quad (16)$$

In this case we want $\Delta < 0$ (we wish to keep the two subgraphs separated), which implies

$$\lambda > \lambda_C = \frac{2M}{(\xi_C + 2)^2}. \quad (17)$$

If ξ_C is very small, λ has to be very big (for $\lambda_C > 1$ the subgraphs cannot be resolved by standard modularity, which corresponds to $\lambda = 1$, and we recover the resolution limit of Ref. [15]). On the other hand if ξ_C is large, the subgraphs will be resolved for a large range of λ -values.

If the subgraphs are two cliques of n_C nodes each, for instance, $\xi_C = n_C(n_C - 1)$.

D. Condition on the ineliminability of the bias

We now put together conditions (14) and (17). We have that

$$\lambda_2 < \lambda < \lambda_1, \quad (18)$$

where

$$\lambda_1 = \frac{2\alpha_S M}{M_S} \quad \text{and} \quad \lambda_2 = \frac{2M}{(\xi_C + 2)^2}. \quad (19)$$

Above λ_1 , modularity splits random subgraphs, below λ_2 it puts together subgraphs even if they are connected by just one link (even in the case in which they are cliques).

In the range between λ_1 and λ_2 it should be possible to avoid both biases. However, if

$$\lambda_1 < \lambda_2, \quad (20)$$

the biases cannot be both simultaneously lifted. Eq. (20) holds when, by setting $M_S/\alpha_S = \beta_S$,

$$(\xi_C + 2)^2 < \beta_S. \quad (21)$$

Note that Eq. (21) does not depend on the size of the whole network, either in terms of vertices or edges.

To be more concrete we consider a simple example. We examine a network made out of two identical cliques of n_C vertices each and an internally random subgraph of n_S vertices and average degree $\langle k \rangle_S$. The three clusters are all connected to each other by one edge only (see Fig. 3).

In Fig. 4 we plot the relation between n_C and n_S coming

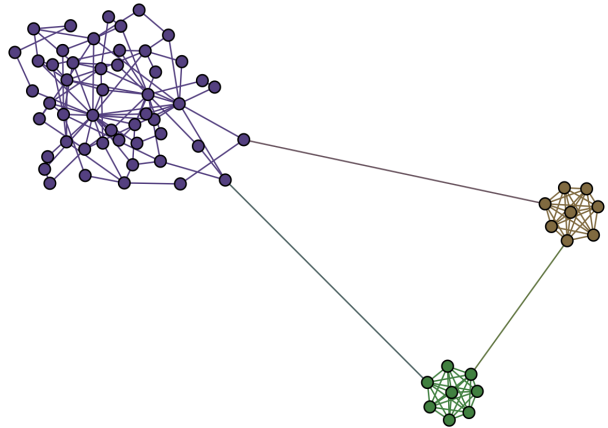


Figure 3: (Color online) Schematic network with two cliques and a random subgraph, which are the natural communities of the network.

from the equality $\lambda_1 = \lambda_2$ (obtained turning the inequality of Eq. (21) to an equality) for some values of $\langle k \rangle_S$. We used Eq. (12) to evaluate α_S , with the approximation $\langle \sqrt{k} \rangle_S = \sqrt{\langle k \rangle_S}$ and the relations $\xi_C = n_C(n_C - 1)$ and $M_S = n_S \langle k \rangle_S / 2$. For any given value of $\langle k \rangle_S$, the inequality of Eq. (21) holds above the corresponding curve.

In Fig. 5 we plot λ_1 and λ_2 as a function of n_S , for $n_C = 13$ and $\langle k \rangle_S = 100$. For λ_1 we show two curves, one corresponding to the exact function, determined numerically, while for the other we have used the theoretical approximation of α_S described above. The lines divide the $\lambda - n_S$ plane in four areas, characterized by the presence or absence of the two biases. As we can see, the portion of the plane in which both biases are simultaneously absent (gray area) is quite small.

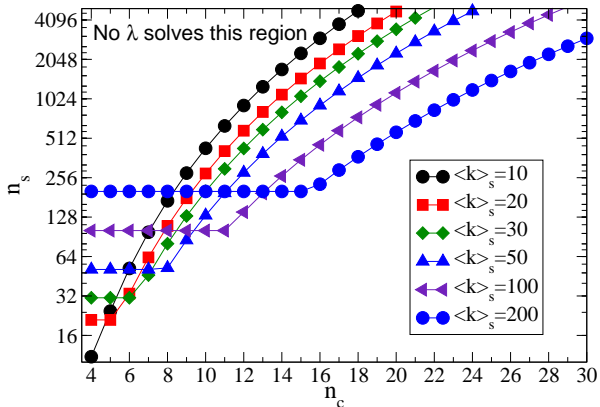


Figure 4: (Color online) This plot shows Eq. (21) as a function of n_S and n_C for the simple network with three clusters of Fig. 3. Above the curves modularity cannot find the right partition for any value of λ .

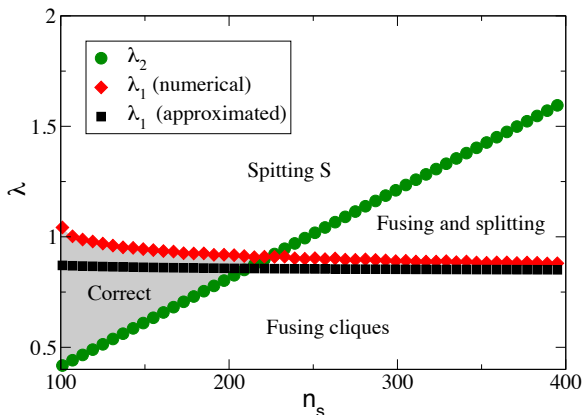


Figure 5: (Color online) Threshold parameters λ_1 and λ_2 as a function of n_S ($n_C = 13$, $\langle k \rangle_S = 100$). The theoretical line for λ_1 is obtained by approximating α_S as described in the text. We see that $\lambda_1 > \lambda_2$, up to $n_S \approx 230$, so that no λ can eliminate the biases for bigger values of n_S . When $n_S \lesssim 230$, the biases can be both eliminated only in the shadowed area between the curves.

III. TESTS ON BENCHMARK GRAPHS

We want now to check the practical consequences of the limits of multiresolution modularity. For that we take the LFR benchmark, a model of graphs with built-in community structure that we have recently introduced [24]. It is an extension of the *planted ℓ -partition model* introduced by Condon and Karp [25]. Each graph has power law

distributions of degree and community size, which are common features of real graphs with community structure. The degree of mixture between clusters is measured by the *mixing parameter* μ , expressing the ratio between the number of neighbors of a vertex outside its community and the total number of neighbors. So $\mu = 0$ indicates that clusters are topologically disconnected from each other, as each vertex has neighbors within its community only, while $\mu = 1$ indicates that vertices are connected only to vertices outside their group, so the groups are not communities. Vertices are linked to each other at random, compatibly with the constraints on the distributions of degree and community size and to the fact that μ has to be (approximately) the same for all vertices. So the clusters are essentially random subgraphs.

We want to specialize Eq. (5) to the LFR benchmark graphs. Let us consider a cluster \mathcal{S} with n_b nodes, total degree $2m_b$ and internal degree $2M_{Sb}$. We split it into two equal-sized subgraphs such that the internal degree of either part is the same: $k_{in}^A = k_{in}^B$. Moreover, for simplicity we assume that the split is done such to keep an equal number of edges between each of the subgraphs and the rest of the network: $l = r$. We have $M_{Sb} = (1 - \mu)m_b$, $l = r = \mu m_b$, $v = \alpha_{Sb} M_{Sb} = \alpha_{Sb}(1 - \mu)m_b$. The condition of non-splitting is:

$$2v > \lambda \frac{(M_{Sb} + l)^2}{M}, \quad (22)$$

which is:

$$2\alpha_{Sb}(1 - \mu)m_b > \lambda \frac{m_b^2}{M}. \quad (23)$$

So,

$$\lambda < \lambda_1 \quad \text{where} \quad \lambda_1 = 2\alpha_{Sb}(1 - \mu) \frac{M}{m_b}. \quad (24)$$

We now search for the condition that leads to the merger of two clusters of an LFR benchmark graph. For that we should know how many edges they share, which depends on the graph size and the number of clusters. We call v_{xy} the number of edges between modules x and y and $2m_x$ and $2m_y$ their total degrees. Eq. (5) becomes

$$\Delta = 2v_{xy} - \lambda \frac{4m_x m_y}{M}. \quad (25)$$

The condition to keep the clusters separated is $\lambda > \lambda_2$, where

$$\lambda_2 = \frac{M v_{xy}}{2m_x m_y}. \quad (26)$$

So, the two biases can be simultaneously removed iff $\lambda_1 > \lambda_2$, which amounts to

$$2\alpha_{Sb}(1 - \mu) \frac{M}{m_b} > \frac{M v_{xy}}{2m_x m_y}. \quad (27)$$

The inequality of Eq. (27) has to hold for all triples of clusters x , y and b , and this is usually unlikely to happen. In order to show that, we check whether multiresolution modularity is able to deliver the planted partition of the LFR benchmark graphs for any value of the resolution parameter λ . The results are shown in Figs. 6 and 7. We plot the fraction of vertices which are incorrectly classified by modularity as a function of λ . We just consider misclassifications caused by merging (circles) or splitting (squares) the clusters of the planted partition of the graphs. We see that, for small values of λ , modularity merges many clusters and essentially splits none, whereas for large λ there is a dominance of splitting over merging. The plots clearly show that, for every value of λ , there will be some misclassification due to cluster merging, splitting or both. The fraction of affected vertices does not go below 10% but it can be considerably larger. Fig. 6 refers to graphs with 10000 vertices, but the situation does not improve if we go to larger graph sizes (50000 vertices for the benchmark graphs used for Fig. 7). We point out that we have chosen low values of the mixing parameter μ (0.1 and 0.3), corresponding to clusters which are well separated from each other. Modern algorithms for community detection (like Infomap [26] and OSLOM [27]) would easily find the correct partitions in the graphs we have used for the tests of Figs. 6 and 7 (see Ref. [17]). One may object that our estimate of the modularity maximum for each graph is just an approximation of the actual result, whose search is an NP-complete problem [28]. However, we have checked in each case that the partitions found have a higher modularity than the planted partition of the benchmark graphs.

IV. CONCLUSIONS

We have shown that the introduction of a resolution parameter does not solve the problems of Newman-Girvan modularity pointed out in the last years. This is due to the existence of two concurrent biases: the tendency to merge small clusters and to split large ones. We have seen that it is usually very difficult, and often impossible, to tune the resolution such to avoid both biases simultaneously. Tests on artificial benchmark graphs with community structure indeed show that a considerable fraction of vertices is misclassified, for any value of the resolution parameter, even when clusters are well separated and easily identified by other methods. Since, in practical applications, one knows very little about the community structure of the graphs at study, it is impossible a priori to quantify the systematic error induced by the use of modularity. Moreover, it is very hard to think of a possible way to “heal” the partition delivered by modularity, just because there are two sources of errors. If modularity simply combined smaller clusters in larger ones, as people have been thinking until now, one could hope to recover the real partition by looking inside the clusters delivered by modularity. Instead, since

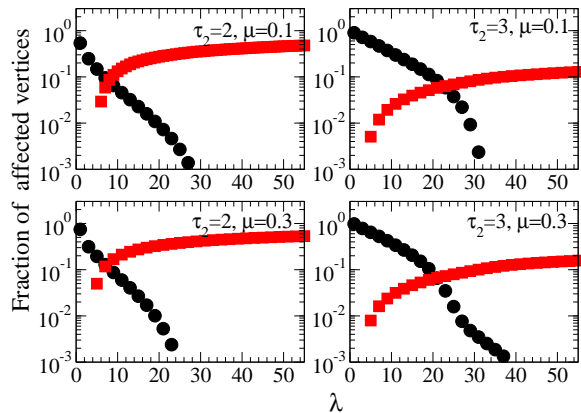


Figure 6: (Color online) Test of multiresolution modularity on LFR benchmark graphs. Each panel shows the fraction of misclassified vertices due to artificial mergers (circles) and splits (squares) of clusters, as a function of the resolution parameter λ . The panels correspond to different choices of the exponent τ_2 of the cluster size distribution of the graph and of the mixing parameter μ . Each point represents an average over 100 benchmark graphs. All graphs have 10000 vertices. The other parameters are: average degree $\langle k \rangle = 20$; maximum degree $k_{max} = 100$; minimum cluster size $c_{min} = 10$; maximum cluster size $c_{max} = 1000$; degree exponent $\tau_1 = 2$.

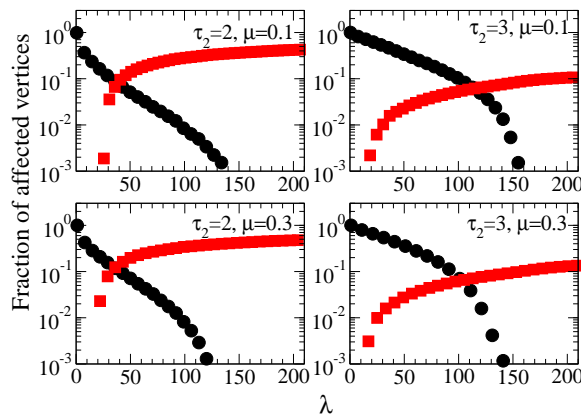


Figure 7: (Color online) Same as Fig. 6, but for LFR benchmark graphs of 50000 vertices. All other parameters are the same as for the graphs used in Fig. 6.

clusters can be both split and merged, the real partition must be recovered by splitting some clusters and merging others, and it is very difficult to understand which clusters contain smaller ones and which others are parts of larger clusters instead. These reasons suffice to be skip-

tical about the results obtained by using modularity in practice, with or without resolution parameters.

Acknowledgments

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