

Modularity optimization in community detection of complex networks

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Abstract – Detecting community structure in complex networks is a fundamental but challenging topic in network science. Modularity measures, such as widely used modularity function Q and recently suggested modularity density D , play critical roles as quality indices in partitioning a network into communities. In this letter, we reveal the complex behaviors of modularity optimization under different community definitions by an analytic study. Surprisingly, we find that in addition to the resolution limit of Q revealed in a recent study, both Q and D suffer from a more serious limitation, *i.e.* some derived communities do not satisfy the weak community definition or even the most weak community definition. Especially, the latter case, called as *misidentification*, implies that these communities may have sparser connection within them than between them, which violates the basic intuitive sense for a subgraph to be a community. Using a discrete convex optimization framework, we investigate the underlying causes for these limitations and provide insights on choices of the modularity measures in applications. Numerical experiments on artificial and real-life networks confirm the theoretical analysis.

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Introduction. – Many systems in real world can be represented as networks, in which nodes denote the objects of interest and edges that connect nodes describe the relationships between them. Examples range from social networks, technological networks to biological networks. These different types of complex networks have been revealed to have common topological features such as scale-free and small-world properties [1]. Importantly, many complex networks have community or modular structure, *i.e.*, networks consist of specific, relatively separate dense subgraphs [2]. Uncovering such community structure not only helps us understand the topological structure of large-scale networks, but also reveals the functionality of each component.

A large number of methods have been developed for detecting communities, which can be generally categorized into local and global methods. Local methods for community detection identify a subset of nodes as a community according to certain local connection conditions, independently from the structure of the rest of the network. Such methods include clique overlap-based hierarchical

clustering [3], clique percolation method [4], and subgraph fitness method [5]. Global methods for community detection optimize certain global quantitative functions encoding the quality of the overall partition of the network, such as information theoretical method [6], Potts model [7], and optimization of modularity measures [8,9]. One popular modularity measure is the modularity function Q developed by Newman [10] for evaluating how good a community partition is. Maximizing Q has been a widely accepted method for detecting community structure of complex networks [8,11,12]. However, Q has been exposed to resolution limit, *i.e.*, communities smaller than certain scale may not be revealed by optimization of Q even in the extreme case that they are cliques connected by single bridges [13]. Recently Li *et al.* proposed a quantitative measure called modularity density D to evaluate the community structure of networks [9]. Optimization of D does not show the resolution limit that Q suffers from on some examples.

In this letter, we analytically study the complex behaviors of modularity optimization under different community definitions. Surprisingly, we find that in addition to the resolution limit of Q revealed in [13], there is another serious limitation in Q and D , *i.e.* some derived

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communities do not satisfy the weak community definition [14] or even the most weak community definition [15]. Especially, the latter case, called as *misidentification*, violates the well-accepted basic intuitive sense for a subgraph to be a community. Using a discrete convex optimization framework, we investigate the underlying causes for these phenomena, and give insights on the choices of modularity measures in applications. Numerical experiments conducted on artificial and real-life networks confirm our theoretical analysis.

Community definition and modularity measures.

– Qualitatively, a community is a subgraph in a network whose nodes are more densely connected with each other than with nodes outside the subgraph [2,6,8]. Based on the quantitative setting of “densely” and “outside”, there are different community definitions. Radicchi *et al.* gave a quantitative community definition in a weak sense [14]. Given a network $G = (V, E)$ with node set V and edge set E , we denote $A = [a_{ij}]$ as its adjacency matrix. Let $P_K = \{V_1, V_2, \dots, V_K\}$ be a partition of the network, $V_s \in P_K$, and $\bar{V}_s = V \setminus V_s$, then V_s is a community in a weak sense [14] if

$$L(V_s, V_s) > L(V_s, \bar{V}_s), \quad (1)$$

where $L(V', V'') = \sum_{i \in V'} \sum_{j \in V''} a_{ij}$. In this weak community definition, the sum of degrees in V_s should exceed the sum of degrees towards the rest of the network. A much more loose definition is the most weak community definition proposed in [15]:

$$L(V_s, V_s) > \max_{t: t \neq s} \{L(V_s, V_t)\}, \quad (2)$$

which means that the sum of degrees in V_s should exceed the sum of degrees toward any one of other communities. We refer to V_s as an *extra weak community* if it does not meet (1) but meet (2). If a community identified by a method does not meet (2), we say that the method *misidentifies* the community.

Given a partition $P_K = \{V_1, V_2, \dots, V_K\}$, the modularity function Q [10] is defined as

$$Q = \sum_{s=1}^K \left[\frac{L(V_s, V_s)}{2L} - \left(\frac{L(V_s, V_s) + L(V_s, \bar{V}_s)}{2L} \right)^2 \right] \equiv \sum_{s=1}^K Q_s, \quad (3)$$

where $L = L(V, V)/2$ is the total number of edges in the network. This measure provides a way to determine if or not a partition is good enough to decipher the community structure of a network. Generally, a larger Q corresponds to a better community structure.

In contrast, for a given partition P_K , the modularity density D [9] is defined as

$$D = \sum_{s=1}^K \frac{L(V_s, V_s) - L(V_s, \bar{V}_s)}{|V_s|} \equiv \sum_{s=1}^K D_s, \quad (4)$$

where $|V_s|$ is the number of nodes in community s . Note that, compared with Q , the denominator of D incorporates the number of nodes in a community.

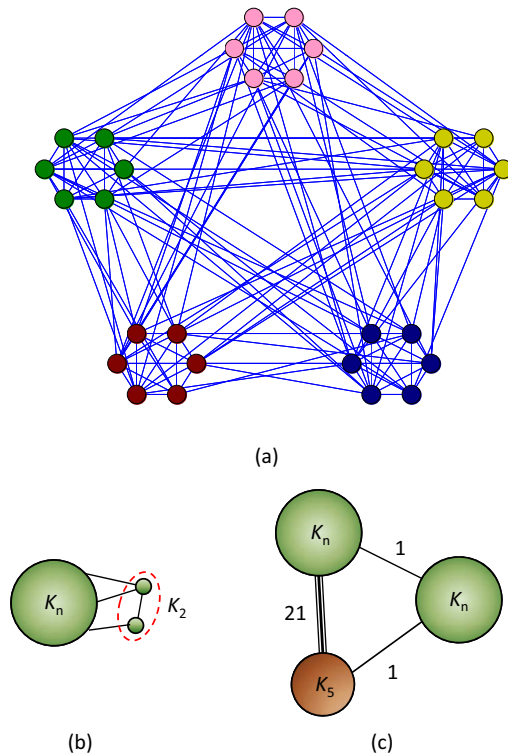


Fig. 1: (Colour on-line) Examples on which optimization of Q or D violates the weak or most weak community definition.

Despite the good performance of Q and D in many practical networks, they may lead to apparently unreasonable partitions in some cases. We observe that optimization of Q and D leads to some communities failing to satisfy the weak community definition (1) or even the most weak community definition (2) in some networks. An example is given in fig. 1(a), where there are five 6-cliques, any two of which are connected by 8 edges. Let P_5 denote the partition where each 6-clique is a community, and P_1 denote the whole network as a community. It is easy to see that $Q(P_5) = 44/155 > 0 = Q(P_1)$, which implies that maximizing Q partitions the network into five extra weak communities. Figure 1(b) shows another example in which extra weak communities are not qualified communities in the basic qualitative sense. Q partitions the network into 2 communities (K_n and K_2) when $n \geq 3$, while D partitions it into 2 communities (K_n and K_2) when $n \geq 10$. An example for the misidentification of Q or D is shown in fig. 1(c), where Q (respectively, D) partitions the network into three communities (two K_n and one K_5) when $n \geq 16$ (respectively, $n \geq 21$), in which K_5 is a subgraph violating the most weak community definition. Next, we give a theoretical analysis to show that these phenomena in optimizing Q and D exist in a wide range of network structure.

Optimization analysis of Q and D . – To analyze the complex behaviors of Q and D , we formulate the optimization of Q and D as two two-stage nonlinear

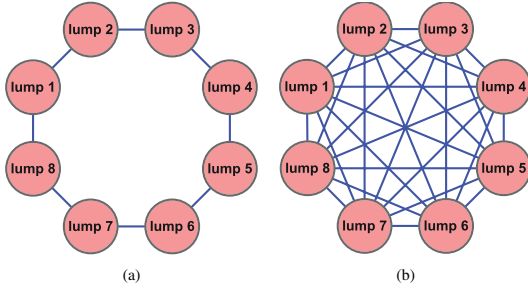


Fig. 2: (Colour on-line) Two exemplar networks: (a) ring of lumps and (b) *ad hoc* network.

programming problems, respectively,

$$Q_{II}: \max_K Q_I(K) = \max_K \max_{P_K} \sum_{s=1}^K Q_s, \quad (5)$$

$$D_{II}: \max_K D_I(K) = \max_K \max_{P_K} \sum_{s=1}^K D_s, \quad (6)$$

where $P_K = \{V_1, V_2, \dots, V_K\}$ is a partition of the network.

Obviously, analytically solving these two optimization models on a general complex network is impossible. As in [9,13], we make the following analysis on two widely used exemplar networks: a ring of dense lumps [13] and an *ad hoc* network [10,16], which are shown in fig. 2. The network *ring of lumps* consists of $N(N \geq 8$ and $N = 2^k, k \in \{3, 4, 5, \dots\})$ dense lumps, each with m nodes and l_{in} edges. Between two adjacent lumps there are l_{bw} edges. When $l_{bw} = 1$ and the lumps are cliques, the ring of lumps becomes a ring of cliques which has been discussed in [9,13]. The *ad hoc* network consists of N dense subgraphs, and there are l_{bw} edges between each pair of dense subgraphs. Hence, the total number of edges in this network is $L = Nl_{in} + N(N-1)l_{bw}/2$. In addition, we assume that the edges in the lumps or between the lumps are evenly distributed.

Suppose that we partition the whole network into K communities with each community containing N_i lumps, where $N_1 + \dots + N_K = N$. By substituting the variables N_i and the number of edges and nodes in each candidate community into (5) and (6), we found that optimization models (5) and (6) become two two-stage discrete convex/concave programming problems. Specifically, for the ring of lumps, the first-stage optimization model in (5) is a discrete convex programming in the feasible region $F = \{1, 2, 4, \dots, N/2^{s+1}, N/2^s, N/2^{s-1}, \dots, N\}$, whose solution can be obtained by solving its K-K-T equations [17]. $Q_I(K)$ is a discrete concave function, so the solution of the second-stage optimization model in (5) can be given by the derivative of $Q_I(K)$ at zero. In a similar way, the first-stage optimization in (6) is a convex programming problem which can be solved from its K-K-T equations. $D_I(K)$ is a discrete concave function, thus D_{II} is a discrete convex programming and can be easily solved. For the *ad hoc* network, similar analysis can be done. The only difference is that the

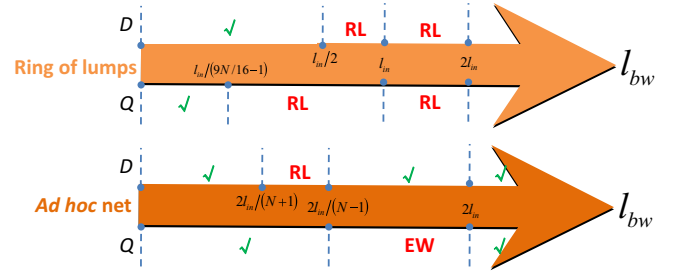


Fig. 3: (Colour on-line) Modularity optimization of Q and D on two exemplar networks. RL and EW respectively mean the resolution limit region and the extra weak community region. Green “√” means the partition is correct in terms of the weak definition.

convexity/concavity of the first-stage optimization and the second-stage optimization in (5) and (6) depends on the relations between l_{in} and l_{bw} . Here we omit the details.

The solutions K_Q^* and K_D^* of the optimization models (5) and (6) on two networks are summarized in fig. 3 in terms of resolution limit and extra community phenomenon. In the case of the ring of lumps, the optimal solution of model (5) is

$$K_Q^* = \left\langle \sqrt{\frac{l_{in} + l_{bw}}{l_{bw}}} \sqrt{N} \right\rangle_F, \quad (7)$$

which is a point in F nearest to $\sqrt{\frac{l_{in} + l_{bw}}{l_{bw}}} \sqrt{N}$. Similarly, the optimal solution of model (6) is

$$K_D^* = \left\langle \frac{(l_{in} + l_{bw})N}{4l_{bw}} \right\rangle_F. \quad (8)$$

When $l_{bw} < l_{in}/(9N/16-1)$ (derived from $K_Q^* = N$), both modularity measures can identify known communities, with each lump as a community. When l_{bw} is larger than $l_{in}/(9N/16-1)$ and less than $l_{in}/2$ (derived from $K_D^* = N$), D is still able to identify the known communities but Q identifies a collection of lumps as a community. In terms of the weak community definition, D suffers from the resolution limit when $l_{bw} \in (l_{in}/2, l_{in})$ which depends on network structure, whereas Q has resolution limit when $l_{bw} \in (l_{in}/(9N/16-1), l_{in})$ which depends on both network structure and network scale. It implies that for a large scale network, Q is more likely to fail to find smaller qualified communities. When $l_{in} < l_{bw} < 2l_{in}$, the lumps do not satisfy the weak definition. Both Q and D has the resolution limit in terms of the most weak definition since either K_Q^* or K_D^* does not equal N . When $l_{bw} > 2l_{in}$, the lumps do not satisfy the most weak definition anymore. Optimal solutions are achieved neither at N nor at 1.

As we see, when $l_{bw} > l_{in}/(9N/16-1)$, Q identifies a collection of lumps as a community. The number of communities is proportional to \sqrt{N} . This result can be verified by the example in [13], where the authors only considered the case $l_{bw} = 1$. In fact, when $l_{bw} = 1$, we have $l_{in}/(N-1) < 1$ that leads to $l_{in} < (N-1)$ which implies

that the number of detected communities is larger than $\sqrt{Nl_{in} + N - 1}$, consistent with the result in [13].

Through the same analysis framework, for the *ad hoc* network, the optimal solution of model (5) is

$$K_Q^* = \begin{cases} N, & l_{bw} < 2l_{in}, \\ 1, & l_{bw} > 2l_{in}. \end{cases} \quad (9)$$

The optimal solution of model (6) is

$$K_D^* = \begin{cases} N, & l_{bw} < 2l_{in}/(N+1), \\ 1, & l_{bw} > 2l_{in}/(N+1). \end{cases} \quad (10)$$

Note that each lump in the *ad hoc* network does not satisfy the weak definition anymore when $l_{bw} \geq 2l_{in}/(N-1)$. We can see that both Q and D correctly identify known communities with each lump as a community when $l_{bw} < 2l_{in}/(N+1)$. However, when $l_{bw} \in (2l_{in}/(N+1), 2l_{in}/(N-1))$, Q still works but D has the resolution limit since it groups all lumps into a single community. Fortunately, this is a very narrow interval whose length decreases with the increase of the network scale. When $l_{bw} > 2l_{in}/(N-1)$ which means that lumps do not satisfy the weak community definition anymore, D works well under the weak definition (or equivalently, D has a resolution limit under the most weak definition until $l_{bw} = 2l_{in}$), but Q identifies the lumps as extra weak communities until $l_{bw} = 2l_{in}$. When $l_{bw} > 2l_{in}$, the lumps do not satisfy the most weak definition anymore. Both Q and D correctly identify the whole network as a community.

From above analysis, we conclude that for a class of networks represented by the ring of lumps, optimization of both Q and D has resolution limit and cannot resolve small communities smaller than a scale. The range of network structure that D suffers from resolution limit is smaller than Q . Both Q and D may identify some extra weak communities in this type of large and dense networks. For a class of networks represented by the *ad hoc* network, Q identifies extra weak communities in a large range of network structure, while D performs well except a narrow resolution limit interval. Although in evenly distributed *ad hoc* networks, no communities are found to violate the most weak definition, in an unevenly distributed network (*e.g.* fig. 1(c)), it is very likely that some derived communities by optimization of Q and D do not satisfy the most weak definition. In the next section, we conduct numerical experiments to confirm the theoretical analysis and show that these phenomena in optimization of Q and D are common in artificial and real-life networks.

Experimental results. – Although the exemplary networks have special topology structures, the conclusion obtained on them provides insights into general complex networks. In this section, we conduct computational experiments by using a simulated annealing (SA)

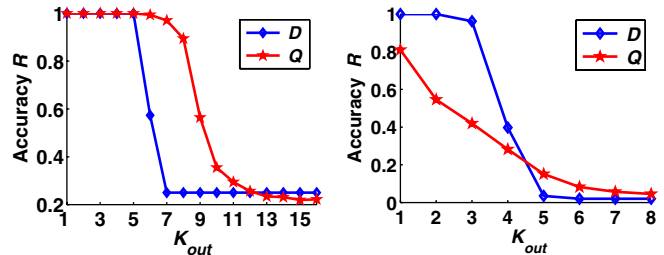


Fig. 4: (Colour on-line) Comparison of Q and D in terms of accuracy on 4-community (left) and 50-community (right) *ad hoc* networks, where accuracy R denotes the fraction of nodes correctly classified into the original communities.

procedure as in [11] to confirm that those limitations exist in optimization of Q and D on general complex networks and point out the types of networks that Q and D suit for.

Artificial networks. We first use a benchmark set of computer-generated networks as examples [2], in which each network has 128 nodes divided into 4 communities, each with 32 nodes. Edges are placed randomly with two fixed probabilities k_{in} and k_{out} such that the average degree of a node is 16. The average edge connection of each node to nodes in other communities is denoted by k_{out} . For each k_{out} , 10 random *ad hoc* networks are generated. The derived partitions are evaluated by the fraction of nodes correctly classified into the original communities (denoted as R).

The average accuracy over 10 *ad hoc* networks is summarized in fig. 4(a). We can see that when k_{out} is small, *i.e.* the networks have distinct communities, both modularity measures have good performance in identifying known communities. When k_{out} becomes large, especially when $k_{out} > 8$, the known communities in original networks become very ambiguous, and the detected partitions by both measures are quite different from the original ones. When $6 < k_{out} < 10$, Q seems to have better performance than D . This is natural, since we can see from their definitions that D puts more penalty on outward edges of communities than Q . Figure 5(a) and fig. 5(b) show the extra weak communities identified by Q and D , where the community numbers include both communities satisfying the weak definition (denoted as T) and the communities failing to satisfy the weak definition (denoted as F). We can see that D has no extra weak community phenomenon, whereas when $k_{out} > 8$, some communities detected by Q are extra weak communities. This computational result is consistent with the theoretical analysis.

The *ad hoc* networks described above only have four communities, so the resolution limit in Q does not appear. Now we generate another set of *ad hoc* networks with 50 communities of size 8. The average node degree in these communities is 8. The results are summarized in fig. 4(b). We can see that, due to the resolution limit of Q , *i.e.*, the tendency to group several known dense subgraphs into

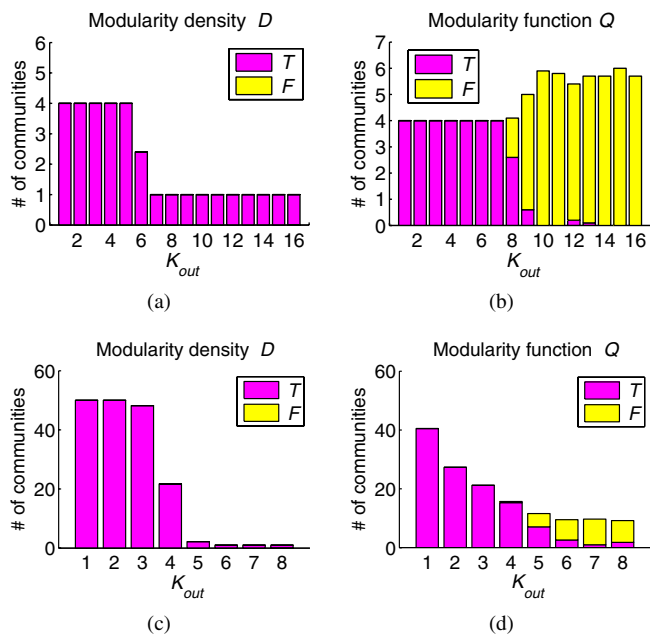


Fig. 5: (Colour on-line) Comparison of Q and D in terms of extra weak communities on 4-community ((a), (b)) and 50-community ((c), (d)) *ad hoc* networks, where T (F) denotes communities satisfying (failing to satisfy) the weak definition.

one community, Q has a bad performance even for the networks with small k_{out} . This result is consistent with the observation in [13]. In contrast, D has a good performance when k_{out} is small. With the increasing of k_{out} , D groups all communities into one since at this time the communities become very ambiguous. From fig. 5(c) and fig. 5(d), again we see that D does not suffer from extra weak community phenomenon, whereas optimization of Q can lead to extra weak communities. The comparison results also provide us some insights on the network characteristics that these two modularity measures suit for. For a dense network with obvious community structure, Q is a good choice, whereas for a large sparse network with small communities, it is better to use D . Consistent with our theoretical analysis, in evenly distributed *ad hoc* networks like the above 4-community network and 50-community network, optimization of Q may lead to extra weak communities, but has no misidentification phenomenon.

Real-life networks. We further examine the optimization of Q and D on several well studied real-life networks, such as the email network (EmailNet) [18], the jazz musician network (JazzNet) [19], and the scientific collaboration network (SciNet) [20]. In addition, we construct a transcriptional regulatory network in yeast from global ChIP-chip experiments [21,22], denoted as YeastTRN. A smaller network is extracted from YeastTRN by merely considering the regulatory relationships among transcription factors (represented by YeastTFR). The network partitions derived by optimization of Q and D are summarized in table 1, where the column n_Q (n_D) lists

Table 1: Results on the real-life networks by optimizing Q and D .

Network	Node	Edge	Q	n_Q	D	n_D
EmailNet	1133	5451	0.57	10(0)	63.16	31(1)
JazzNet	198	2742	0.44	4(1*)	52.84	4(1)
SciNet	118	200	0.75	7(0)	28.30	16(0)
YeastTRN	4441	12873	0.48	14(2)	15.78	15(1)
YeastTFR	162	663	0.35	6(3)	11.50	4(0)

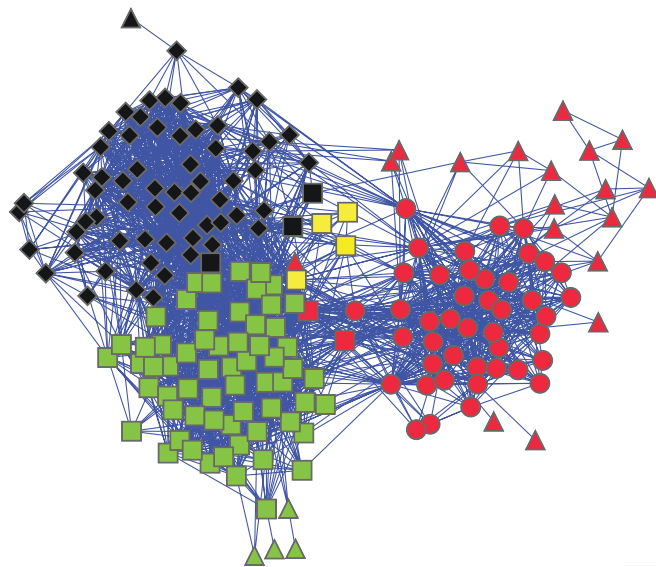


Fig. 6: (Colour on-line) Communities identified by optimization of Q and D on the jazz musician network.

the number of communities obtained by optimizing Q (D), and the figures in parentheses are the number of extra weak communities (those with stars denote the communities violating the most weak community definition).

From table 1 we can see that the extra weak community phenomenon of Q and D is common in real-life networks. By comparing the results of Q and D , we can see that Q more seriously suffers from this problem than D . This computational result is consistent with what we observed in the theoretical analysis. Furthermore, communities determined by optimizing Q in most of the networks are fewer than those detected by optimizing D , which may be due to the resolution limit of Q . A typical example is the jazz musician network describing the collaboration among jazz bands [19], in which nodes denote the bands and edges represent linked bands with at least one shared musician. Due to the black/white racial segregation and the cities that bands recorded in, the network can be divided into three communities in reality. We found that both Q and D partition this network into four communities (fig. 6). An extra weak community identified by D (triangle nodes) has 22 nodes consisting of several connected groups. An 4-node community identified by Q (yellow nodes) has 5 inner edges and 17, 30, 32 edges towards other

three communities, respectively and violates the most weak community definition. These results demonstrate that optimizing Q and D does lead to the extra weak communities and misidentification phenomenon in some real-life networks.

Table 1 shows that the extra weak community problem of Q and D is also common in biological networks. For YeastTFR, D gives a partition with four communities, whereas Q partitions the network into six communities, three of which are extra weak communities. We used the GO Term Finder to examine the significant function terms shared by TFs in a community. We counted the number of GO terms with p -value smaller than 1×10^{-9} in each community, and then calculated the average number of significant GO terms for a partition. The result shows that the partition given by D has 35 significant GO terms while the partition obtained by Q only has 25.6 significant GO terms, indicating that D is more effective in detecting biological functional modules than Q . In an extra weak community given by Q with 24 nodes, there are 29 significant GO terms with p -value less than 1×10^{-9} . In contrast, a correctly identified community of almost similar size is enriched with 37 significant GO terms. Furthermore, we randomly selected some sets of nodes with the similar size and the average number of significant GO terms in such random sets is 19.8, much lower than that of two types of communities mentioned above. It further indicates that the extra weak community problem may lead to unreasonable network partition and attention should be taken in applying modularity measures for community detection.

Conclusion and discussion. – We investigate modularity optimization for community identification through a discrete convex/concave programming framework in this letter. We show that the resolution limit of Q and D is closely related to the structure of the network. The modularity Q is much more sensitive to the resolution limit for a range of network structure than D . Importantly, we found that optimization of Q or D may violate the weak or even most weak community definition. Especially, they may misidentify the community structure of some networks. Our analysis provides insights into limitation and applicability of Q and D . Computational experiments on general complex networks confirm the theoretical analysis.

The violation of the weak or most weak community definition is partially caused by the fact that Q and D only globally evaluate a partition or community structure, without considering the local connections of individual subgraphs. Taking the weak definition as an example, given a partition $P = \{V_1, V_2, \dots, V_K\}$, if for any i , V_i satisfies the weak definition, then $D(P) > 0$ and $Q(P) > 0$. Note that the reverse of the statement is not correct, *i.e.*, if $D(P) > 0$ or $Q(P) > 0$, then it is not necessary for all V_i to satisfy the weak community definition. To make all the derived communities satisfy the weak or most weak community definition, it is natural to add the inequalities (1), (2) into optimization models (5), (6) as constrained

optimization problems. It should be noted that, when Q and D are used as independent indices to evaluate how good a given partition or community structure is, there is no way to simply combine a constraint into Q and D to overcome their limitations. Therefore, further research work is needed to develop better modularity functions.

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