Maximizing Modularity is hard*

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Abstract. Several algorithms have been proposed to compute partitions of networks into communities that score high on a graph clustering index called modularity. While publications on these algorithms typically contain experimental evaluations to emphasize the plausibility of results, none of these algorithms has been shown to actually compute optimal partitions. We here settle the unknown complexity status of modularity maximization by showing that the corresponding decision version is NP-complete in the strong sense. As a consequence, any efficient, i.e. polynomial-time, algorithm is only heuristic and yields suboptimal partitions on many instances.

1 Introduction

Partioning networks into communities is a fashionable statement of the graph clustering problem, which has been studied for decades and whose applications abound.

Recently, a new graph clustering index called *modularity* has been proposed [10]. It immediately prompted a number of follow-up studies concerning different applications and possible adjustments of the measure (see, e.g., [3, 4, 7, 13]). Also, a wide range of algorithmic approaches approaches has been considered, for example based on a greedy agglomeration [1, 8], spectral division [9, 12], simulated annealing [6, 11] and extremal optimization [2].

None of these algorithms, however, has been shown to be produce optimal partitions. While the complexity status of modularity maximization is open, it has been speculated [9] that it might be NP-hard due to similarity with the MAX-CUT problem.

In this paper, we provide the first complexity-theoretic argument as to why the problem of maximizing modularity is intractable by proving that it is NP-complete in the strong sense. This means that there is no correct polynomial-time algorithm to solve this problem for every instance unless P = NP. Therefore, all of the above algorithms eventually deliver suboptimal solutions, and there is no hope for an efficient algorithm that computes maximum modularity partitions on all problem instances. In a sense, our result thus justifies the use of heuristics for modularity optimization.

2 Modularity

Modularity is a quality index for clusterings defined as follows. We are given a simple graph G = (V, E), where V is the set of vertices and E the set of (undirected) edges. If not

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stated otherwise, n = |V| and m = |E| throughout. The degree $\deg(v)$ of a vertex $v \in V$ is the number of edges incident to v. A cluster or community $C \subseteq V$ is a subset of the vertices. A clustering $\mathcal{C} = \{C_1, \ldots, C_t\}$ of G is a partition of V into clusters such that each vertex appears in exactly one cluster. With a slight disambiguation, the modularity [10] $Q(\mathcal{C})$ of a clustering \mathcal{C} is defined as

$$Q(\mathcal{C}) = \sum_{C \in \mathcal{C}} \left[\frac{|E(C)|}{m} - \left(\frac{|E(C)| + \sum_{C' \in \mathcal{C}} |E(C, C')|}{2m} \right)^2 \right] , \tag{1}$$

where E(C, C') denotes the set of edges between vertices in clusters C and C', and E(C) = E(C, C). Note that C' ranges over all clusters, so that edges in E(C) are counted twice in the squared expression. This is to adjust proportions, since edges in E(C, C'), $C \neq C'$, are counted twice as well, once for each order of the arguments. Note that we can rewrite Eq. (1) into the more convenient form

$$Q(C) = \sum_{C \in C} \left[\frac{|E(C)|}{m} - \left(\frac{\sum_{v \in C} \deg(v)}{2m} \right)^2 \right] . \tag{2}$$

It reveals an inherent trade-off: to maximize the first term, many edges should be contained in clusters, whereas minimization of the second term is achieved by splitting the graph into many clusters of small total degrees. In the remainder of this paper, we will make use of this formulation.

3 NP-Completeness

To formulate our complexity-theoretic result, we need to consider the following decision problem underlying modularity maximization.

Problem 1 (MODULARITY) Given a graph G and a number K, is there a clustering C of G, for which $Q(C) \geq K$?

Note that we may ignore the fact that, in principle, K could be a real number in the range [0,1], because $4m^2 \cdot Q(\mathcal{C})$ is integer for every partition \mathcal{C} of G and polynomially bounded in the size of G.

Note also that modularity maximization cannot be easier than the decision problem, because determining the maximum possible modularity index of a graph immediately yields an answer to the decision question.

Our hardness result for MODULARITY is based on a transformation from the following decision problem.

Problem 2 (3-Partition) Given 3k positive integer numbers a_1, \ldots, a_{3k} such that the sum $\sum_{i=1}^{3k} a_i = kb$ and $b/4 < a_i < b/2$ for an integer b and for all $i = 1, \ldots, 3k$, is there a partition of these numbers into k sets, such that the numbers in each set sum up to b?

We will show that an instance $A = \{a_1, \ldots, a_{3k}\}$ of 3-Partition can be transformed into an instance (G(A), K(A)) of MODULARITY, such that G(A) has a clustering with

modularity at least K(A), if and only if a_1, \ldots, a_{3k} can be partitioned into k sets of sum $b = \frac{1}{k} \sum_{i=1}^{k} a_i$ each.

It is crucial that 3-Partition is strongly NP-complete [5], i.e. the problem remains NP-complete even if the input is represented in unary coding. This implies that no algorithm can decide the problem in time polynomial even in the sum of the input values, unless P = NP. More importantly, it implies that our transformation need only be pseudo-polynomial.

The reduction is defined as follows. From an instance A of 3-Partition, construct a graph G(A) with k cliques (completly connected subgraphs) H_1, \ldots, H_k of size $a = \sum_{i=1}^{3k} a_i$ each. For each element $a_i \in A$ we introduce a single element vertex, and connect it to a_i vertices in each of the k cliques in such a way that each clique member is connected to exactly one element vertex. It is easy to see that each clique vertex then has degree a and the element vertex corresponding to element $a_i \in A$ has degree ka_i . The number of edges in G(A) is $m = \frac{k}{2}a(a+1)$. See Fig. 1 for an example. Note that the size of G(A) is polynomial

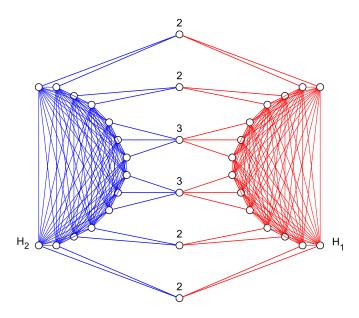


Fig. 1. An example graph G(A) for the instance $A = \{2, 2, 2, 2, 3, 3\}$ of 3-Partition. Edge colors indicate edges to and within the k = 2 cliques H_1 (red) and H_2 (blue). Vertex labels indicate the corresponding numbers $a_i \in A$.

in the unary coding size of A, so that our transformation is indeed pseudo-polynomial.

Before specifying bound K(A) for the instance of Modularity, we will show three properties of maximum modularity clusterings of G(A). Together these properties establish the desired characterization of solutions for 3-Partition by solutions for Modularity.

Lemma 1. In a maximum modularity clustering of G(A), none of the cliques H_1, \ldots, H_k is split.

Proof. We consider a clustering C that splits a clique $H \in \{H_1, \ldots, H_k\}$ into different clusters and then show how to obtain a clustering with strictly higher modularity. Suppose

that $C_1, \ldots, C_r \in \mathcal{C}$, r > 1, are the clusters that contain vertices of H. For $i = 1, \ldots, r$ we denote by

- n_i the number of vertices of H contained in cluster C_i ,
- $-m_i = |E(C_i)|$ the number edges between vertices in C_i ,
- f_i the number of edges between vertices of H in C_i and element vertices in C_i ,
- d_i be the sum of degrees of all vertices in C_i .

The contribution of C_1, \ldots, C_r to $Q(\mathcal{C})$ is

$$\frac{1}{m}\sum_{i=1}^{r}m_{i}-\frac{1}{4m^{2}}\sum_{i=1}^{r}d_{i}^{2}.$$

Now suppose we create a clustering \mathcal{C}' by rearranging the vertices in C_1, \ldots, C_r into clusters C', C'_1, \ldots, C'_r , such that C' contains exactly the vertices of clique H, and each C'_i , $1 \leq i \leq r$, the remaining elements of C_i (if any). In this new clustering the number of covered edges reduces by $\sum_{i=1}^r f_i$, because all vertices from H are removed from the clusters C'_i . This labels the edges connecting the clique vertices to other non-clique vertices of C_i as intercluster edges. For H itself there are $\sum_{i=1}^r \sum_{j=i+1}^r n_i n_j$ edges that are now additionally covered due to the creation of cluster C'. In terms of degrees the new cluster C' contains a vertices of degree a. The sums for the remaining clusters C'_i are reduced by the degrees of the clique vertices, as these vertices are now in C'. So the contribution of these clusters to Q(C') is given by

$$\frac{1}{m} \sum_{i=1}^{r} \left(m_i + \sum_{j=i+1}^{r} n_i n_j - f_i \right) - \frac{1}{4m^2} \left(a^4 + \sum_{i=1}^{r} (d_i - n_i a)^2 \right) ,$$

so that

$$Q(C') - Q(C) = \frac{1}{m} \left(\sum_{i=1}^{r} \sum_{j=i+1}^{r} n_i n_j - f_i \right) + \frac{1}{4m^2} \left(\left(\sum_{i=1}^{r} 2d_i n_i a - n_i^2 a^2 \right) - a^4 \right)$$
$$= \frac{1}{4m^2} \left(4m \sum_{i=1}^{r} \sum_{j=i+1}^{r} n_i n_j - 4m \sum_{i=1}^{r} f_i + \left(\sum_{i=1}^{r} n_i \left(2d_i a - n_i a^2 \right) \right) - a^4 \right)$$

Using the fact that $2\sum_{i=1}^r \sum_{j=i+1}^r n_i n_j = \sum_{i=1}^r \sum_{j\neq i} n_i n_j$, substituting $m = \frac{k}{2}a(a+1)$ and rearranging terms we get

$$Q(C') - Q(C) = \frac{a}{4m^2} \left(-a^3 - 2k(a+1) \sum_{i=1}^r f_i + \sum_{i=1}^r n_i \left(2d_i - n_i a + k(a+1) \sum_{j \neq i} n_j \right) \right)$$

$$\geq \frac{a}{4m^2} \left(-a^3 - 2k(a+1) \sum_{i=1}^r f_i + \sum_{i=1}^r n_i \left(n_i a + 2kf_i + k(a+1) \sum_{j \neq i}^r n_j \right) \right).$$

For the last inequality we use the fact that $d_i \ge n_i a + k f_i$. This inequality holds because C_i contains at least the n_i vertices of degree a from the clique H. In addition it contains

both the clique and element vertices for each edge counted in f_i . For each such edge there are k-1 other edges connecting the element vertex to the k-1 other cliques. Hence, we get a contribution of kf_i in the degrees of the element vertices. Combining the terms n_i and one of the terms $\sum_{j\neq i} n_j$ we get

$$Q(C') - Q(C) \ge \frac{a}{4m^2} \left(-a^3 - 2k(a+1) \sum_{i=1}^r f_i + \sum_{i=1}^r n_i \left(a \sum_{j=1}^r n_j + 2k f_i + ((k-1)a + k) \sum_{j \ne i}^r n_j \right) \right)$$

$$= \frac{a}{4m^2} \left(-2k(a+1) \sum_{i=1}^r f_i + \sum_{i=1}^r n_i \left(2k f_i + ((k-1)a + k) \sum_{j \ne i}^r n_j \right) \right)$$

$$= \frac{a}{4m^2} \left(\sum_{i=1}^r 2k f_i (n_i - a - 1) + ((k-1)a + k) \sum_{i=1}^r \sum_{j \ne i}^r n_i n_j \right)$$

$$\ge \frac{a}{4m^2} \left(\sum_{i=1}^r 2k n_i (n_i - a - 1) + ((k-1)a + k) \sum_{i=1}^r \sum_{j \ne i}^r n_i n_j \right),$$

For the last step we note that $n_i \leq a-1$ and $n_i-a-1 < 0$ for all $i=1,\ldots,r$. So increasing f_i decreases the modularity difference. For each vertex of H there is at most one edge to a vertex not in H, and thus $f_i \leq n_i$.

By rearranging and using the fact that $a \geq 3k$ we get

$$Q(C') - Q(C) \ge \frac{a}{4m^2} \sum_{i=1}^r n_i \left(2k(n_i - a - 1) + ((k - 1)a + k) \sum_{j \ne i}^r n_j \right),$$

$$= \frac{a}{4m^2} \sum_{i=1}^r n_i \left(-2k + ((k - 1)a - k) \sum_{j \ne i}^r n_j \right),$$

$$\ge \frac{a}{4m^2} ((k - 1)a - 3k) \sum_{i=1}^r \sum_{j \ne i}^r n_i n_j,$$

$$\ge \frac{3k^2}{4m^2} (3k - 6) \sum_{i=1}^r \sum_{j \ne i}^r n_i n_j,$$

$$> 0,$$

as we can assume k > 2 for all relevant instances of 3-Partition. This shows that any clustering can be improved by merging each clique completely into a cluster. This proves the lemma.

Next, we observe that the optimum clustering places at most one clique completely into a single cluster.

Lemma 2. In a maximum modularity clustering of G(A), every cluster contains at most one of the cliques H_1, \ldots, H_k .

Proof. Consider a maximum modularity clustering. The previous lemma shows that each of the k cliques H_1, \ldots, H_k is entirely contained in one cluster. Assume that there is a cluster C which contains at least two of the cliques. If C does not contain any element vertices, then the cliques form disconnected components in the cluster. In this case it is easy to see that the clustering can be improved by splitting C into distinct clusters, one for each clique. In this way we keep the number of edges within clusters the same, however, we reduce the squared degree sums of clusters.

Otherwise, we assume C contains l > 1 cliques completely and in addition some element vertices of elements a_j with $j \in J \subseteq \{1, \ldots, k\}$. Note that inside the l cliques $\frac{l}{2}a(a-1)$ edges are covered. In addition, for every element vertex corresponding to an element a_j there are la_j edges included. The degree sum of the cluster is given by the la clique vertices of degree a and some number of element vertices of degree ka_j . The contribution of C to Q(C) is thus given by

$$\frac{1}{m} \left(\frac{l}{2} a(a-1) + l \sum_{j \in J} a_j \right) - \frac{1}{4m^2} \left(la^2 + k \sum_{j \in J} a_j \right)^2.$$

Now suppose we create C' by splitting C into C'_1 and C'_2 such that C'_1 completely contains a single clique H. This leaves the number of edges covered within the cliques the same, however, all edges from H to the included element vertices eventually drop out. The degree sum of C'_1 is exactly a^2 , and so the contribution of C'_1 and C'_2 to Q(C') is given by

$$\frac{1}{m} \left(\frac{l}{2} a(a-1) + (l-1) \sum_{j \in J} a_j \right) - \frac{1}{4m^2} \left(\left((l-1)a^2 + k \sum_{j \in J} a_j \right)^2 + a^4 \right).$$

Considering the difference we note that

$$Q(C') - Q(C) = -\frac{1}{m} \sum_{j \in J} a_j + \frac{1}{4m^2} \left((2l - 1)a^4 + 2ka^2 \sum_{j \in J} a_j - a^4 \right)$$

$$= \frac{2(l - 1)a^4 + 2ka^2 \sum_{j \in J} a_j - 4m \sum_{j \in J} a_j}{4m^2}$$

$$= \frac{2(l - 1)a^4 - 2ka \sum_{j \in J} a_j}{4m^2}$$

$$\geq \frac{9k^3}{2m^2} (9k - 1)$$

$$> 0,$$

as k > 0 for all instances of 3-Partition.

Since the clustering is improved in each case, it is not optimal. This is a contradiction.

The previous two lemmas show that any clustering can be strictly improved to a clustering that contains k clique clusters, such that each one completely contains one of the cliques H_1, \ldots, H_k (possibly plus some additional element vertices). In particular, this

must hold for the optimum clustering as well. Now that we know how the cliques are clustered we turn to the element vertices.

As they are not directly connected, it is never optimal to create a cluster consisting only of element vertices. Splitting such a cluster into singleton clusters, one for each element vertex, reduces the squared degree sums but keeps the edge coverage at the same value. Hence, such a split yields a clustering with strictly higher modularity. The next lemma shows that we can further strictly improve the modularity of a clustering with a singleton cluster of an element vertex by joining it with one of the clique clusters.

Lemma 3. In a maximum modularity clustering of G(A), there is no cluster composed of element vertices only.

Proof. Consider a clustering C of maximum modularity and suppose that there is an element vertex v_i corresponding to the element a_i , which is not part of any clique cluster. As argued above we can improve such a clustering by creating a singleton cluster $C = \{v_i\}$. Suppose C_{min} is the clique cluster, for which the sum of degrees is minimal. We know that C_{min} contains all vertices from a clique H and eventually some other element vertices for elements a_j with $j \in J$ for some index set J. The cluster C_{min} covers all $\frac{a(a-1)}{2}$ edges within H and $\sum_{j\in J} a_j$ edges to element vertices. The degree sum is a^2 for clique vertices and $k\sum_{j\in J} a_j$ for element vertices. As C is a singleton cluster, it covers no edges and the degree sum is ka_i . This yields a contribution of C and C_{min} to Q(C) of

$$\frac{1}{m} \left(\frac{a(a-1)}{2} + \sum_{j \in J} a_j \right) - \frac{1}{4m^2} \left(\left(a^2 + k \sum_{j \in J} a_j \right)^2 + k^2 a_i^2 \right).$$

Again, we create a different clustering C' by joining C and C_{min} to a new cluster C'. This increases the edge coverage by a_i . The new cluster C' has the sum of degrees of both previous clusters. The contribution of C' to Q(C') is given by

$$\frac{1}{m} \left(\frac{a(a-1)}{2} + a_i + \sum_{j \in J} a_j \right) - \frac{1}{4m^2} \left(a^2 + ka_i + k \sum_{j \in J} a_j \right)^2,$$

so that

$$Q(C') - Q(C) = \frac{a_i}{m} - \frac{1}{4m^2} \left(2ka^2 a_i + 2k^2 a_i \sum_{j \in J} a_j \right)$$

$$= \frac{1}{4m^2} \left(2ka(a+1)a_i - 2ka^2 a_i - 2k^2 a_i \sum_{j \in J} a_j \right)$$

$$= \frac{a_i}{4m^2} \left(2ka - 2k^2 \sum_{j \in J} a_j \right).$$

At this point recall that C_{min} is the clique cluster with the minimum degree sum. For this cluster the elements corresponding to included element vertices can never sum to more

than $\frac{1}{k}a$. In particular, as v_i is not part of any clique cluster, the elements of vertices in C_{min} can never sum to more than $\frac{1}{k}(a-a_i)$. Thus,

$$\sum_{j \in J} a_j \le \frac{1}{k} (a - a_i) < \frac{1}{k} a,$$

and so Q(C') - Q(C) > 0. This contradicts the assumption that C is optimal.

We have shown that for the graphs G(A) the clustering of maximum modularity consists of exactly k clique clusters, and each element vertex belongs to exactly one of the clique clusters. Finally, we are now ready to state our main result.

Theorem 3. Modularity is strongly NP-complete.

Proof. For a given clustering \mathcal{C} of G(A) we can check in polynomial time whether $Q(\mathcal{C}) \geq K(A)$, so clearly MODULARITY \in NP.

For NP-completeness we transform an instance $A = \{a_1, \ldots, a_{3k}\}$ of 3-Partition into an instance (G(A), K(A)) of Modularity. We have already outlined the construction of the graph G(A) above. For the correct parameter K(A) we consider a clustering in G(A) with the properties derived in the previous lemmas, i.e. a clustering with exactly k clique clusters. Any such clustering yields exactly (k-1)a inter-cluster edges, so the edge coverage is given by

$$\sum_{C \in \mathcal{C}^*} \frac{|E(C)|}{m} = \frac{m - (k-1)a}{m} = 1 - \frac{2(k-1)a}{ka(a+1)} = 1 - \frac{2k-2}{k(a+1)}.$$

Hence, the clustering $C = (C_1, \ldots, C_k)$ with maximum modularity must minimize

$$\deg(C_1)^2 + \deg(C_2)^2 + \ldots + \deg(C_k)^2$$
.

This requires to equilibrate the element vertices according to their degree as good as possible between the clusters. In the optimum case we can assign each cluster element vertices corresponding to elements that sum to $b = \frac{1}{k}a$. In this case the sum of degrees of element vertices in each clique cluster is equal to $k\frac{1}{k}a = a$. This yields $\deg(C_i) = a^2 + a$ for each clique cluster C_i , i = 1, ..., k, and gives

$$\deg(C_1)^2 + \ldots + \deg(C_k)^2 \ge k(a^2 + a)^2 = ka^2(a+1)^2.$$

Equality holds only in the case, in which an assignment of b to each cluster is possible. Hence, if there is a clustering C with Q(C) of at least

$$K(A) = 1 - \frac{2k - 2}{k(a+1)} - \frac{ka^2(a+1)^2}{k^2a^2(a+1)^2} = \frac{(k-1)(a-1)}{k(a+1)}$$

then we know that this clustering must split the element vertices perfectly to the k clique clusters. As each element vertex is contained in exactly one cluster, this yields a solution for the instance of 3-Partition. With this choice of K(A) the instance (G(A), K(A)) of Modularity is satisfiable only if the instance A of 3-Partition is satisfiable.

Otherwise, suppose the instance for 3-Partition is satisfiable. Then there is a partition into k sets such that the sum over each set is $\frac{1}{k}a$. If we cluster the corresponding graph by joining the element vertices of each set with a different clique, we get a clustering of modularity K(A). This shows that the instance (G(A), K(A)) of Modularity is satisfiable if the instance A of 3-Partition is satisfiable. This completes the reduction and proves the theorem.

4 Conclusion

We have shown that maximizing the popular modularity clustering index is strongly NP-complete. These results can be generalized to modularity in weighted graphs. We can consider the graph G to be completely connected and use weights of 0 and 1 on each edge to indicate its presence. Instead of the numbers of edges the definition of modularity then employs the sum of edge weights for edges within clusters, between clusters and in the total graph. This yields an equivalent definition of modularity for graphs, in which the existence of an edge is modeled with binary weights. An extension of modularity to arbitrarily weighted graphs is then straightforward. Our hardness result holds also for the problem of maximizing modularity in weighted graphs, as this more general problem class includes the problem considered in this paper as a special case.

Our hardness result shows that there is no polynomial-time algorithm optimizing modularity unless P = NP. Recently proposed algorithms [1,2,6,8,9,11,12] are therefore incorrect in the sense that they yield suboptimal solutions on many instances. Furthermore, it is a justification to use approximation algorithms and heuristics to cope with the problem. Future work includes a deeper formal analysis of the properties of modularity and the development of algorithms with performance guarantees.

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References

- A. Clauset, M. Newman, and C. Moore Finding community structure in very large networks. Phys. Rev. E 70, 066111, 2004.
- 2. J. Duch and A. Arenas. Community detection in complex networks using extremal optimization. Phys. Rev. E 72, 027104, 2005.
- 3. P. Fine, E. Di Paolo, and A. Philippides Spatially constrained networks and the evolution of modular control systems. 9th Intl. Conference on the Simulation of Adaptive Behavior (SAB'06).
- S. Fortunato and M. Barthélemy. Resolution limit in community detection. arXiv.org physics/0607100, 2006.
- 5. M. R. Garey and D. S. Johnson. Complexity results for multiprocessor scheduling under resource constraints. SIAM Journal on Computing 4:397-411, 1975.
- R. Guimerà, M. Sales-Pardo, and L. A. N. Amaral. Modularity from fluctuations in random graphs and complex networks. Phys. Rev. E 70, 025101, 2004.
- 7. S. Muff, F. Rao, and A. Caflisch. Local modularity measure for network clusterizations. Phys. Rev. E 72, 056107, 2005.
- M. Newman. Fast algorithm for detecting community structure in networks. Phys. Rev. E 69, 066133, 2004.

- 9. M. Newman. Modularity and community structure in networks. Proc. Nat. Akad. Sci. USA 103, 8577-8582, 2006.
- 10. M. Newman and M. Girvan. Finding and evaluating community structure in networks. Phys. Rev. E 69, 026113, 2004.
- 11. J. Reichardt and S. Bornholdt. Statistical mechanics of community detection. arXiv.org: cond-mat/0603718, 2006.
- 12. S. White and P. Smyth. A Spectral Clustering Approach To Finding Communities in Graph. Proc. 2005 SIAM Data Mining Conference, 2005.
- 13. E. Ziv, M. Middendorf, and C. Wiggins Information-theoretic approach to network modularity Phys. Rev. E 71, 046117, 2005.