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# ON WEAKLY OPTIMAL PARTITIONS IN MODULAR NETWORKS

JORGE R. BUSCH, MARIANO G. BEIRÓ, AND J. IGNACIO ALVAREZ-HAMELIN

**ABSTRACT.** Modularity was introduced as a measure of goodness for the community structure induced by a partition of the set of vertices in a graph. Then, it also became an objective function used to find good partitions, with high success. Nevertheless, some works have shown a scaling limit and certain instabilities when finding communities with this criterion.

Modularity has been studied proposing several formalisms, as hamiltonians in a Potts model or laplacians in spectral partitioning. In this paper we present a new probabilistic formalism to analyze modularity, and from it we derive an algorithm based on weakly optimal partitions. This algorithm obtains good quality partitions and also scales to large graphs.

**Keywords:** *modularity, community structure, algorithms, complex systems*

## 1. INTRODUCTION

Finding communities is an important issue in complex systems, it is useful to classify and even to predict properties in biology or groups in sociology. A very successful method to find communities was based on *betweenness* [Freeman, 1977]. This divisive clustering method led to the problem of choosing a stopping criteria. So Newman introduced the modularity in [Newman and Girvan, 2004] and [Newman, 2004] as a measure of goodness of such partitions. This notion has shown to be rich from the theoretical viewpoint, and in practice it provided a unifying tool to compare partitions obtained by a diversity of methods. On the other hand, several methods have been devised to obtain partitions directly by modularity optimization. This problem has been shown to be NP-hard, and many of the algorithms developed to approach the optimum are diverse adaptations of some known algorithms for these problems, with the notable exception of Blondel *et al.* [Blondel et al., 2008]. From a theoretical viewpoint, and despite the complexity problem, modularity optimization has been shown to have some strong limitations, driving to partitions that do not conform to other intuitive or formal notions of community structure. These limitations are related to the scaling behavior of modularity, that causes long correlations in community structure, and unnatural seizures of communities.

In this paper we introduce, as in [Reichardt and Bornholdt, 2006], a generalization of the modularity function for weighted graphs, with a resolution parameter  $t$ . We give first some properties of this generalization analogous to known properties of the usual version. Then we introduce a notion of weak optimality of a partition

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and we study some properties of this notion, using our tools to put new light on some of the general limitations of modularity. We address the scaling limit problem for weakly optimal partitions, and we show some of its effects for some examples on binary trees. Finally, we describe a fast algorithm that gives weakly optimal partitions, explore its similarities with [Blondel et al., 2008], and compare the results with those obtained by other means. The result of this comparison is rather surprising: the values of modularity that we obtained for standard graphs are comparable, and in several cases better, than those obtained by other means. Of course this suggests that there is a stronger relation between weak optimality and optimality, explaining the performance of our algorithm and of [Blondel et al., 2008] (they also obtain weakly optimal partitions). This point deserves further investigation.

This paper is organized as follows. We introduce some probabilistic definitions in Section 2 and we analyze the consequences in Section 3. The next section presents our algorithm. We provide proofs for the lemmas in Section 5. Real complex networks are analyzed in Section 6, concluding our work in Section 7.

## 2. DEFINITIONS

**2.1. Some measures.** Let  $V$  be a finite set, and  $m : V \times V \rightarrow \mathbb{Z}_+$  be a non-negative integer function such that  $Z = \sum_{l,r} m(l,r) > 0$ . We assume throughout this work that  $m$  is, in addition, symmetric, that is  $m(l,r) = m(r,l)$  for  $(r,l) \in V \times V$ , and that  $\sum_r m(l,r) > 0$  for each  $l \in V$ . Then, we consider the oriented graph  $G = G(V, E)$  whose vertices are the elements of  $V$ , and whose edges are the pairs  $(l,r) \in V \times V$  such that  $m(l,r) > 0$ . That is,  $G$  provided with  $m$  is a weighted oriented graph, with the property that if  $(l,r) \in E$  then  $(r,l) \in E$ . There can be isolated points in  $G$ , but if  $v$  is isolated then  $m(v,v) > 0$  and there is a loop in  $v$ .

We define a probability measure  $m_E$  in  $V \times V$  by

$$m_E(l,r) = \frac{m(l,r)}{Z}$$

and additivity. We consider the marginal probabilities defined in  $V$  by

$$\begin{aligned} m_L(l) &= \sum_r m_E(l,r) \\ m_R(r) &= \sum_l m_E(l,r) \end{aligned}$$

and the product probability  $m_{LR}$  defined in  $V \times V$  by

$$m_{LR}(l,r) = m_L(l)m_R(r)$$

and additivity. Finally, for  $t > 0$  we shall consider the signed measure  $\mu_t$  in  $V \times V$  given by

$$\mu_t(S) = m_E(S) - tm_{LR}(S)$$

for  $S \subset V \times V$ . By the assumed symmetry of  $m$ , we have that  $m_L = m_R$ , and we denote this marginal probability measure by  $m_V$ , and  $m_{LR} = m_{VV}$ . Thus

$$\mu_t(S) = m_E(S) - tm_{VV}(S)$$

**2.2. Partitions.** We shall consider partitions  $\mathcal{C}$  of  $V$ , meaning a family of pairwise disjoint not empty sets  $C \subset V$  such that  $\cup_{C \in \mathcal{C}} C = V$ . We shall consider the usual (lattice) partial order between partitions of  $V$ ,  $\mathcal{C} \preceq \mathcal{C}'$  if  $\mathcal{C}'$  is a refinement of  $\mathcal{C}$ , or, which is the same, for any  $C \in \mathcal{C}$  it holds

$$C = \cup \mathcal{C}'_C$$

where  $\mathcal{C}'_C \doteq \{C' \in \mathcal{C}' : C' \subset C\}$ . Notice that with this partial order, there is always a minimal partition  $\mathcal{C}_0 \doteq \{V\}$  and a maximal partition  $\mathcal{C}_1 \doteq \{\{v\} : v \in V\}$ .

Given a partition  $\mathcal{C}$  of  $V$ , we associate to it a set of *diagonal* pairs  $(l, r) \in V \times V$ , by

$$D(\mathcal{C}) = \cup_{C \in \mathcal{C}} C \times C$$

and the set of *off diagonal* pairs

$$\bar{D}(\mathcal{C}) = V \times V \setminus D(\mathcal{C}) = \cup_{C, C' \in \mathcal{C}, C \neq C'} C \times C'$$

Consider a partition  $\mathcal{C}$  of  $V$ , and define  $c : V \rightarrow \mathcal{C}$  by  $c(v) = C$  if  $v \in C$ . Consider then the quotient graph  $G/\mathcal{C}$ , whose vertices are the elements of the partition, with weights defined by  $m' = m/\mathcal{C} : \mathcal{C} \times \mathcal{C} \rightarrow \mathbb{Z}_+$  by

$$m'(C, C') = \sum_{v \in C, v' \in C'} m(v, v')$$

Then, we obtain a signed measure  $\mu'_t$  in  $\mathcal{C} \times \mathcal{C}$ . Of course, if  $S' \subset \mathcal{C} \times \mathcal{C}$  and  $S = \{(v, v') \in V \times V : (c(v), c(v')) \in S'\}$ , then

$$\mu'_t(S') = \mu_t(S)$$

**Remarks 1.** Typically  $m$  will be the adjacency matrix of  $G$ . If we admit more general weights in our description it is to include in our framework this quotient graphs and the corresponding measures. This will show to be useful in the analysis of our algorithm, where we construct partitions starting from the maximal partition  $\mathcal{C}_1$  and advancing through smaller and smaller partitions by iteratively joining two of their elements (see Remarks 3).

**2.3. Modularity.** Now we define the modularity  $Q_t(\mathcal{C})$  at resolution  $t > 0$  of a partition  $\mathcal{C}$  by

$$Q_t(\mathcal{C}) = \mu_t(D(\mathcal{C}))$$

and its complement

$$\bar{Q}_t(\mathcal{C}) = \mu_t(\bar{D}(\mathcal{C}))$$

(see Figure 1)

**References 1.** If  $m(v, w)$  is the adjacency matrix of  $G$  and  $t = 1$ , then  $Q_t(\mathcal{C})$  is the usual Newman-Girvan modularity (see for example [Newman, 2006]). For weighted graphs and  $t = 1$ , it was defined in [Newman, 2004] (in this paper it is assumed that  $m(v, v) = 0$  for  $v \in V$ ). If we put  $\gamma = t$ , we obtain the generalization of the modularity introduced in [Reichardt and Bornholdt, 2006] (where  $m$  is the adjacency matrix). There is a subtle difference between our formalism and the one in this last paper: we represent the graph  $G$  and the weights  $m$  by the probability measure  $m_E$  (in this general setting this idea is, of course, not new: it is at the very origin of random graph theory), obtain the difference with the null model probability  $m_{VV}$  at the probability level, which gives  $\mu_t$ , and then apply it to  $D(\mathcal{C})$  to obtain the modularity. Instead, in [Reichardt and Bornholdt, 2006] the authors take means in the null model to bring it to the graph level, and they make the differences at this

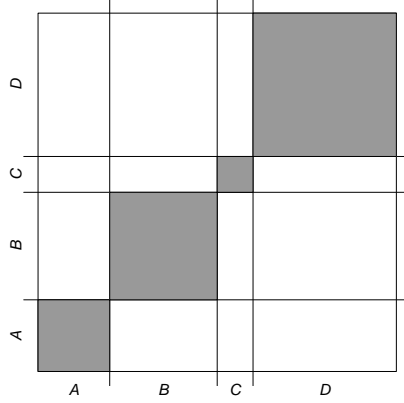


FIGURE 1. Here we illustrate the set  $D(\mathcal{C})$  associated to a partition  $\mathcal{C} = \{A, B, C, D\}$ .  $V$  is plotted in the interval  $[0, 1]$ , and we associate with each element  $X$  in the partition an interval of length  $m_V(X)$ . With this settings, you may think of  $m_{VV}$  as the area, and of  $m_E$  as another symmetric probability measure in the same square.

level to obtain the Hamiltonian. We hope that our approach will help intuition and analysis, because it puts emphasis in the additive nature of  $\mu_t$ .

Notice that the Newman-Girvan modularity is intimately related to Jacob Cohen's measure of agreement (1960) (see [Bishop et al., 2007], Chap 11). The statistical usage of this measure justifies the widely used terminology "null model" for the measure  $m_{VV}$ .

**2.4. Optimality.** We call a partition  $\mathcal{C}^*$  optimal for  $Q_t$  when  $Q_t(\mathcal{C}) \leq Q_t(\mathcal{C}^*)$  for any other partition  $\mathcal{C}$ .

We call a partition  $\mathcal{C}^*$  weakly optimal for  $Q_t$  when  $Q_t(\mathcal{C}) \leq Q_t(\mathcal{C}^*)$  for any partition  $\mathcal{C}$  such that  $\mathcal{C} \preceq \mathcal{C}^*$ .

We call a partition  $\mathcal{C}^*$  positive for  $\mu_t$  when  $\mu_t(C \times C) \geq 0$  whenever  $C$  is in  $\mathcal{C}$ .

We call a partition  $\mathcal{C}^*$  submodular for  $\mu_t$  when  $\mu_t(C \times C') \leq 0$  whenever  $C$  and  $C'$  are different sets in  $\mathcal{C}$ . When  $\mathcal{C}$  is submodular, we shall call its elements communities.

We call a partition  $\mathcal{C}$  internally connected when  $G(C)$  (i.e. the subgraph of  $G$  induced by  $C$ ) is connected for all  $C \in \mathcal{C}$ .

**References 2.** The problem of  $Q_1$  optimization has been shown to be NP-complete (see [Brandes et al., 2008]).

In [Reichardt and Bornholdt, 2006], the terms  $Z\mu_t(C \times C)$  and  $Z\mu_t(C \times C')$ ,  $C \neq C'$  are called cohesion and adhesion respectively. We shall not make further usage of this terminology.

### 3. SOME CONSEQUENCES

#### 3.1. Some useful relations.

**Lemma 1.** Let  $\mathcal{C}$  be a partition of  $V$ . Then

(i) For any  $C \in \mathcal{C}$ ,

$$\mu_t(C \times C) + \mu_t(C \times (V \setminus C)) = (1 - t)m_V(C)$$

(ii)  $Q_t(\mathcal{C}) + \bar{Q}_t(\mathcal{C}) = 1 - t$

**References 3.** See Equation 14 and its context in [Reichardt and Bornholdt, 2006] for a discussion of these relations.

### 3.2. Relations between optimality notions.

**Lemma 2.** Let  $\mathcal{C}$  be a partition of  $V$ , and let  $C, C' \in \mathcal{C}$  be different. Let  $\mathcal{D}$  be the partition obtained from  $\mathcal{C}$  by replacing  $C$  and  $C'$  by  $C \cup C'$ , that is

$$\mathcal{D} = (\mathcal{C} \setminus \{C, C'\}) \cup \{C \cup C'\}$$

Then

$$Q_t(\mathcal{D}) = Q_t(\mathcal{C}) + 2\mu_t(C \times C')$$

(see Figure 2)

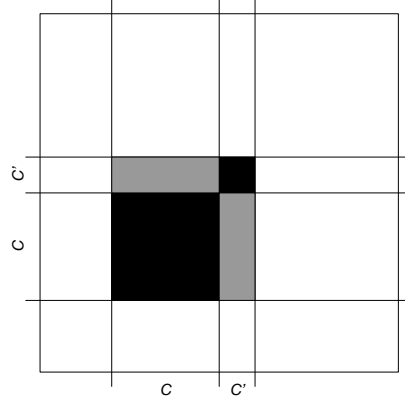


FIGURE 2. Here we illustrate Lemma 2. The terms associated in  $Q_t(\mathcal{C})$  to  $C$  and  $C'$  correspond to the black squares. When you join these sets to obtain  $\mathcal{D}$ , you replace these two terms by one, associated to the square formed by the black squares and the grey rectangles. The additivity and the symmetry of  $\mu_t$  make the rest.

**Lemma 3.**

- (i) If  $\mathcal{C}^*$  is optimal, it is weakly optimal.
- (ii)  $\mathcal{C}^*$  is submodular for  $\mu_t$  if and only if it is weakly optimal for  $Q_t$ .
- (iii) If  $\mathcal{C}^*$  is submodular for  $\mu_t$  and  $t \leq 1$ , then  $\mathcal{C}^*$  is positive for  $Q_t$ .

**References 4.** Lemma 2, which in our framework is an immediate consequence of the additivity of  $\mu_t$ , is a key tool in [Fortunato and Barthélemy, 2007] (see Equation 15 in this paper), in [Reichardt and Bornholdt, 2006] (see Equation 5 in this paper) and in [Kumpula et al., 2007] (see Equation 7 in this paper).

The relation between optimality and submodularity is addressed in [Reichardt and Bornholdt, 2006] (see Equation 19 and its context in this paper).

**References 5.** *This is to justify the use of the term submodular. A real set function  $\mu$  defined in a family  $\mathcal{D}$  of sets, closed under unions and intersections, is called submodular when*

$$\mu(X \cup Y) + \mu(X \cap Y) \leq \mu(X) + \mu(Y)$$

for  $X, Y \in \mathcal{D}$  (see [Fujishige, 2005]). If  $\mathcal{C}$  is a partition of  $V$ , and  $\mathcal{D}$  is the family formed by the unions of elements of  $\mathcal{C}$ , then the set function defined by

$$X \mapsto \mu_t(X \times X)$$

is submodular in  $\mathcal{D}$  when  $\mathcal{C}$  is submodular for  $\mu_t$  according to our definition.

**Lemma 4.** *Let  $t > 0$  and let  $\mathcal{C}$  be any partition of  $V$ . Let, for each  $C \in \mathcal{C}$ ,  $\mathcal{D}_C$  be the partition of  $C$  associated to the connected components of  $G(C)$ . This defines a partition  $\mathcal{D}$  of  $V$ . Then  $\mathcal{D}$  is internally connected and  $Q_t(\mathcal{D}) \geq Q_t(\mathcal{C})$ .*

**References 6.** *This useful result means that when we look for optimal partitions, we can restrict our search to internally connected partitions. It generalizes Lemma 3.4 in [Brandes et al., 2008].*

**3.3. Basic inequalities for  $Q_t$ .** Denote

$$\rho(C) = m_E(C \times (V \setminus C))$$

Then we have

**Lemma 5.** *If  $0 < t$  and  $C \subset V$ , then*

- (1)  $m_V(C) = m_E(C \times C) + \rho(C) \leq m_E(C \times C) + 2\rho(C) \leq 1$
- (2)  $\mu_t(C \times C) = m_E(C \times C)(1 - t(m_E(C \times C) + 2\rho(C))) - t\rho^2(C)$
- (3)  $\mu_t(C \times C) \leq m_E(C \times C)(1 - tm_V(C))$
- (4)  $\mu_t(C \times C) \leq m_E(C \times C)(1 - 2t\rho(C))$

and, if in addition  $t \leq 1$ , then

- (5)  $\mu_t(C \times C) \geq -t\rho^2(C)$

(see Figure 3)

**Lemma 6.** *Let  $\mathcal{C}$  be a partition of  $V$ , and  $0 < t$ , then*

- (6)  $Q_t(\mathcal{C}) \leq 1 - t \sum_{C \in \mathcal{C}} m_V^2(C) \leq 1 - t/|\mathcal{C}|$
- (7)  $Q_t(\mathcal{C}) \leq m_E(D(\mathcal{C}))(1 - 2t \min_{C \in \mathcal{C}} \rho(C))$

and, if in addition  $t \leq 1$ , then

- (8)  $Q_t(\mathcal{C}) \geq (-t/2)(1 - m_E(D(\mathcal{C})))$

**References 7.** *Suppose that  $m(v, w)$  is the adjacency matrix of  $G$  and  $t = 1$ . Then  $Q_t(\mathcal{C})$  is the usual modularity of the partition  $\mathcal{C}$ . The inequality in 6 gives then  $Q_t(\mathcal{C}) \leq 1 - 1/|\mathcal{C}| < 1$  (see [Brandes et al., 2008], Lemma 3.1 and Corollary 6.4, and [Fortunato and Barthélemy, 2007], Fla. 11). In this case the additional hypothesis for Equation 8 is true, and the inequality gives  $Q_t(\mathcal{C}) \geq -(1 - m_E(D(\mathcal{C}))) / 2$  which (as  $1 - m_E(D(\mathcal{C})) \leq 1$ ) gives the lower bound in Lemma 3.1 of [Brandes et al., 2008].*

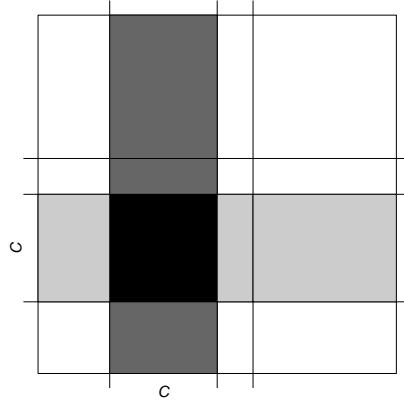


FIGURE 3. Here we illustrate Equation 1. The dark gray region, when you apply to it  $m_E$ , gives  $\rho(C)$ . If you add  $m_E$  applied to the black region, you obtain  $m_V(C)$  (recall that  $m_V$  is the marginal probability of  $m_E$ ). If you add now  $m_E$  applied to the light gray region (which is also  $\rho$ ), of course this, being a probability, is less than 1.

**Lemma 7.** *Let  $\mathcal{C}$  be a partition of  $V$ , submodular for  $\mu_t$ . Then*

$$Q_t(\mathcal{C}) \geq (1 - t)$$

*thus, if  $t \leq 1$ ,  $Q_t(\mathcal{C}) \geq 0$ .*

### 3.4. Bounds for the size of the communities in submodular partitions: scaling limit.

**Lemma 8.** *Let  $\mathcal{C}$  be a partition of  $V$ , submodular for  $\mu_t$ , with  $|\mathcal{C}| \geq 2$ . Then*

(i) *If  $C, C' \in \mathcal{C}$  are different, then*

$$(9) \quad m_V^2(C \cup C') \geq \frac{4m_E(C \times C')}{t}$$

(ii) *Assume that  $G$  is connected, let  $c^*$  denote the value of the minimum cut, with weights  $m$ , in  $G$ . Then, for all  $C \in \mathcal{C}$  it holds*

$$(10) \quad \left(m_V(C) - \frac{1}{2}\right)^2 \leq \frac{1}{4} - \frac{c^*}{tZ}$$

$$(11) \quad \left(\frac{1}{|\mathcal{C}|} - \frac{1}{2}\right)^2 \leq \frac{1}{4} - \frac{c^*}{tZ}$$

$$(12) \quad \frac{c^*}{tZ} < m_V(C) < 1 - \frac{c^*}{tZ}$$

$$(13) \quad |\mathcal{C}| < \frac{tZ}{c^*}$$

**References 8.** *In Eq. 9, we showed that if two communities  $C, C'$  are connected (i.e if  $m_E(C \times C') > 0$ ) then*

$$m_V(C \cup C') \geq 2\sqrt{\frac{m_E(C \times C')}{t}}$$



*This is our version of the fundamental scaling limit found, for  $t = 1$ , in [Fortunato and Barthélemy, 2007] (see the discussion in pp. 38-39). For a general  $t$  (called  $\gamma$  in this paper) this scaling limit was considered in [Kumpula et al., 2007]. Notice that this bound is for the union of two connected communities. Later on we show by a toy example that a similar bound for one community does not hold. This example also shows that it is not easy to obtain, from this scaling limit, bounds on the number of communities.*

**Remarks 2.** *For one community, the best bounds that we could obtain are in Eq. 12. Given these lower bounds, of course we obtain also an upper bound for  $|C|$  in Eq. 13. These bounds are not tight, but they are suggestive of a qualitative behavior:*

- *As we shall show in our Daisy example below, there may exist very big and very small communities. The scaling limit shows that small communities will be joined to the big ones, and not between them.*
- *When  $m$  is the adjacency matrix of  $G$ ,  $c^*$  is the connectivity, and our bounds suggest that for higher connectivities the sizes of the communities are less disperse.*
- *The behavior of the bounds with respect to  $t$  are also suggestive: for big  $t$ , we find more communities, smaller, and with more dispersed sizes, as we shall later see in the examples.*

3.4.1. *Daisy example.* (see Figure 4) Consider a star with a center  $c$  of degree

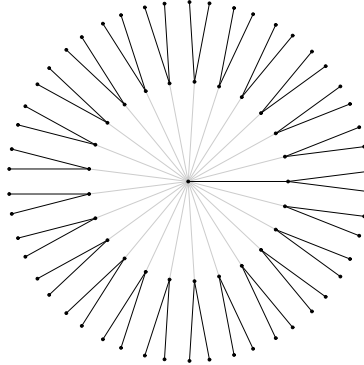


FIGURE 4. Daisy example with  $r = 1$ . Here black lines represent edges internal to a community, and gray lines represent edges between communities. In this case there is only one big community, formed up by the central vertex and one petal, and 24 small communities associated to the remaining petals.

$m = 25r$ , and  $m$  homologous  $T_i$  formed by one vertex joined to the center and two leaves. Let  $\mathcal{C}$  be an internally connected partition of  $V$ , and assume that no element of  $\mathcal{C}$  reduces to a leaf (see [Brandes et al., 2008], Lemma 3.3: notice that this lemma does *not* generalize to arbitrary  $t > 1$ ). Call  $C_0$  the community where  $c$  lies. Then  $C_0$  is formed up by the center and  $n < m$  of the  $T_i$ , and the remaining

elements of the partition are the remaining  $C_j = V(T_j)$ . Thus,

$$\mu_t(C_0 \times T_j) = \frac{1}{6m} \left( 1 - t \frac{5(m+5n)}{6m} \right)$$

Then the pair  $C_0, T_j$  is submodular when  $n \geq r(6/t - 5)$ . Let us first consider the case  $t = 1$ . It is easy to show that you obtain a  $Q_1 = \frac{4}{25}(4 - \frac{1}{6r})$  optimal partition taking  $n = r$  and the remaining  $24r$   $T_i$  as components. If you increase  $r$ , you obtain as many modules  $T_i$  with total degree 5 as you wish. Of course, the number of communities in this example,  $24r + 1$ , is of the same order that  $Z = 150r$ .

On the other hand, we would like to add this example to the section on counter-intuitive behavior of modularity optimization in [Brandes et al., 2008]. The strong asymmetry in the community structure, despite the strong symmetry in the graph, and the arbitrary selection of  $r$  homologous  $T_i$  for the central community, are technical artifacts. This is essentially due to the presence of a center joined to a myriad of small isolated communities, conditions that we can not rule out from the real world.

Let  $t_n = \frac{6}{5+n/r}, 0 \leq n \leq r$  (notice that  $1 = t_r < \dots < t_0 = 6/5$ ). Then the partition  $\mathcal{C}_n^*$  optimal for  $Q_{t_n}$  has  $n$   $T_i$ 's in the central community, and  $m - n$  small communities  $T_j$ . This shows the influence of  $t$  in the scaling limit.

**3.4.2. On complete binary trees.** Let  $G$  be a tree and let  $m$  be its adjacency matrix. Then for any internally connected partition  $\mathcal{C}$  of  $V$   $G/\mathcal{C}$  is also a tree, and we have

$$Q_1(\mathcal{C}) = 1 - \frac{2(|\mathcal{C}| - 1)}{Z} - \frac{1}{|\mathcal{C}|} - \sum_{C \in \mathcal{C}} (m_V(C) - \frac{1}{|\mathcal{C}|})^2$$

This follows from our definition of  $Q_1$ , noticing that

$$m_E(D(\mathcal{C})) = 1 - m_E(\bar{D}(\mathcal{C})) = 1 - \frac{2(|\mathcal{C}| - 1)}{Z}$$

because the number of edges between communities is, in this case,  $|\mathcal{C}| - 1$ , and that

$$m_{VV}(D(\mathcal{C})) = \sum_{C \in \mathcal{C}} m_V^2(C) = \frac{1}{|\mathcal{C}|} + \sum_{C \in \mathcal{C}} \left( m_V(C) - \frac{1}{|\mathcal{C}|} \right)^2$$

by the well known relation between central and noncentral second order moments.

Let  $s = |\mathcal{C}|$ , and consider the function

$$\varphi(s) = \frac{2(s-1)}{Z} + \frac{1}{s}$$

This function has its minimum at

$$s^* = \left\lfloor \frac{1 + \sqrt{1 + 2Z}}{2} \right\rfloor$$

(here  $\lfloor \cdot \rfloor$  denotes the *floor* function). Of course from this we obtain the general bound for the optimal  $Q_1$  of a tree

$$Q_1^* \leq 1 - \varphi(s^*)$$

**References 9.** *This estimate is similar to the results obtained in [Fortunato and Barthélemy, 2007] in a very special case (see Equation 9 and its context in this paper).*

This bound is tight for complete binary trees, because these particular graphs are almost regular, and then the second order moment

$$\frac{1}{s} \sum_{C \in \mathcal{C}} \left( m_V(C) - \frac{1}{s} \right)^2$$

may be considered negligible. This is not the case for our Daisy example where we find, for  $r = 1$ ,  $Q_1^* = 0.613$  and  $1 - \varphi(s^*) = 0.782$ .

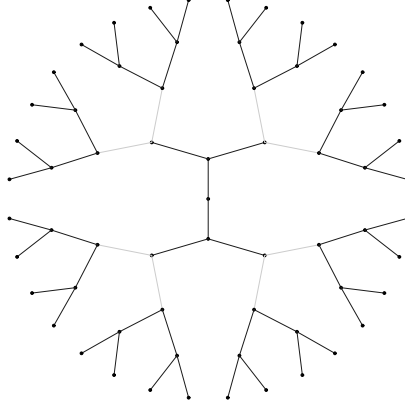


FIGURE 5. Here we show a complete binary tree of height 5 and its corresponding partition  $\mathcal{C}_h$  (in this case  $h = 2$ ). The black edges are internal to a community, the gray ones are between communities.

To show this, let  $G$  be a complete binary tree of height  $n$ , for which  $Z = 2^{n+2} - 4$ , let  $h = \lceil (n - 2)/2 \rceil$  (here  $\lceil \cdot \rceil$  stands for the *ceil* function) and let us consider the partition  $\mathcal{C}_h$  of  $V$  formed by  $R_h$ , the vertex set of the complete binary subtree of height  $h$ , and the connected components that remain when you remove  $R_h$  from  $G$  (see Figure 5). Then  $|\mathcal{C}_h| = 1 + 2^{h+1}$ . ( $\mathcal{C}_h$  is a weakly optimal partition, and very nearly optimal. We shall later show some cases for which it is not optimal, see Section 6.1). Rather than a detailed and cumbersome proof of the fact, we show in the following table that  $Q_1(\mathcal{C}_h) \approx 1 - \varphi(s^*)$ , and that this approximation is better when  $n$  increases.

$n$	$1 - \varphi(s^*)$	$Q_1(\mathcal{C}_h)$
3	0.5357143	0.505102
5	0.7620968	0.757024
6	0.8297258	0.824263
10	0.9562724	0.9539936
20	0.9986194	0.998536

TABLE 1. Upper bounds and results for partitions  $\mathcal{C}_h$

## 4. BUILDING UP SUBMODULAR PARTITIONS

4.1. **Basis for an algorithm.** Let  $\mathcal{C}$  be a partition of  $V$ . Let

$$t(\mathcal{C}) = \max \frac{m_E(C \times C')}{m_{VV}(C \times C')}$$

where  $\max$  is extended to all pairs  $(C, C') \in \mathcal{C} \times \mathcal{C}$  such that  $C \neq C'$ . (if  $|\mathcal{C}| = 1$ , we set  $t(\mathcal{C}) = 0$ ). We call  $t(\mathcal{C})$  the resolution of  $\mathcal{C}$ .

**Lemma 9.** *Let  $\mathcal{C}, \mathcal{D}$  be partitions of  $V$  and  $t > 0$ . Then*

- (i)  $\mathcal{C}$  is submodular for  $\mu_t$  if and only if  $t \geq t(\mathcal{C})$ .
- (ii) If  $\mathcal{C} \preceq \mathcal{D}$ , then  $t(\mathcal{C}) \leq t(\mathcal{D})$ .
- (iii)  $t(\mathcal{C}) \leq t(\mathcal{C}_1)$
- (iv)  $t(\mathcal{C}) = 0$  if and only if  $\mathcal{C} \preceq \mathcal{B}$ , where  $\mathcal{B}$  is the partition of  $V$  associated to the connected components of  $G$ .

Let  $\mathcal{C}$  be a partition of  $V$  and  $t \geq t(\mathcal{C})$ . We shall use

$$\begin{aligned} \alpha(\mathcal{C}) &\doteq m_{VV}(D(\mathcal{C})) = \sum_{C \in \mathcal{C}} m_V^2(C) \\ Z_0(\mathcal{C}) &\doteq \{(C, C') \in \mathcal{C} \times \mathcal{C}, C \neq C' : \mu_t(C, C') = 0\} \end{aligned}$$

Then we have

**Lemma 10.** *If  $t \geq t(\mathcal{C}) > 0$ , then  $t = t(\mathcal{C})$  if and only if  $Z_0(\mathcal{C}) \neq \emptyset$ .*

**Lemma 11.** *Let  $\mathcal{C}$  be a partition of  $V$  with  $t = t(\mathcal{C}) > 0$  and let  $(C, C') \in Z_0(\mathcal{C})$ . Define a new partition  $\mathcal{D}$  of  $V$  by*

$$\mathcal{D} \doteq (\mathcal{C} \setminus \{C, C'\}) \cup \{C \cup C'\}$$

*Then  $\mathcal{D} \prec \mathcal{C}$  is submodular for  $\mu_t$  and*

$$\begin{aligned} |\mathcal{D}| &= |\mathcal{C}| - 1 \\ |Z_0(\mathcal{D})| &< |Z_0(\mathcal{C})| \\ Q_t(\mathcal{D}) &= Q_t(\mathcal{C}) \\ \alpha(\mathcal{D}) &= \alpha(\mathcal{C}) + 2m_{VV}(C \times C') \end{aligned}$$

*For  $s < t$ , we obtain*

$$Q_s(\mathcal{D}) = Q_t(\mathcal{D}) + (t - s)\alpha(\mathcal{D}) > Q_s(\mathcal{C})$$

**Lemma 12.** *Let  $\mathcal{C}$  be a partition of  $V$ , and let  $t = t(\mathcal{C}) > 0$ . Apply iteratively the scheme described in the previous lemma, until you obtain a new partition  $\mathcal{D} \prec \mathcal{C}$  of  $V$  such that  $Z_0(\mathcal{D}) = \emptyset$ .*

*Then,*

$$\begin{aligned} \alpha(\mathcal{D}) &> \alpha(\mathcal{C}) \\ t(\mathcal{D}) &< t \\ Q_t(\mathcal{D}) &= Q_t(\mathcal{C}) \\ Q_{t(\mathcal{D})}(\mathcal{D}) &= Q_t(\mathcal{C}) + \alpha(\mathcal{D})(t - t(\mathcal{D})) \end{aligned}$$

*For  $s < t$ , we obtain once more*

$$Q_s(\mathcal{D}) > Q_s(\mathcal{C})$$

Our algorithm is based in the last two lemmas. Starting at  $\mathcal{C} = \mathcal{C}_1$ , and  $t = t(\mathcal{C}_1)$ , we apply iteratively the scheme described in Lemma 11 until we obtain a partition  $\mathcal{D}$  such that  $t(\mathcal{D}) < t(\mathcal{C})$ . Now, we update  $t$  to  $t(\mathcal{D})$ ,  $\mathcal{C}$  to  $\mathcal{D}$ , and iterate. The algorithm goes on while  $t(\mathcal{D}) \geq 1$  and the final result is the last  $\mathcal{D}$ , a submodular partition for  $\mu_1$ .

**Remarks 3.** *After the first steps of the algorithm, we usually obtain only one partition for each resolution. Let us denote  $\mathcal{C}_t$  to the first partition with resolution  $t$ . Then,  $Q_t \doteq Q_t(\mathcal{C}_t)$  and  $Q_{1t} \doteq Q_1(\mathcal{C}_t)$ . The function  $t \rightarrow Q_t$  is strictly decreasing and convex, hence  $1/t \rightarrow Q_t$  is increasing and concave (see Figure 9). The function  $1/t \rightarrow Q_{1t}$  is strictly increasing (see Lemma 11, Lemma 12 and Figure 8).*

*At the end of each step, giving a partition  $\mathcal{D}$ , all the partitions  $\mathcal{D}'$  considered satisfy  $\mathcal{D}' \preceq \mathcal{D}$ . This means that you can update the graph to be  $G/\mathcal{D}$  (doing the corresponding update in the weights), with a relevant gain in speed and memory.*

**References 10.** *Later on we shall compare the performance and results of our algorithm with others.*

*Here we want to describe briefly its relation with the algorithm described in [Blondel et al., 2008], that is similar in various aspects.*

*Let  $\mathcal{C}, \mathcal{D}$  be two partitions of  $V$ , with  $\mathcal{C} \preceq \mathcal{D}$ . Call  $\mathcal{C}$  submodular for  $\mu_t$  with respect to  $\mathcal{D}$  when if  $C, C' \in \mathcal{C}$  and  $D \subset C$  then:*

$$\mu_t(D \times (C \setminus D)) \geq \mu_t(D \times C')$$

*Notice that when  $\mathcal{D} = \mathcal{C}$  this is the ordinary submodularity for  $\mu_t$  (see Figure 6).*

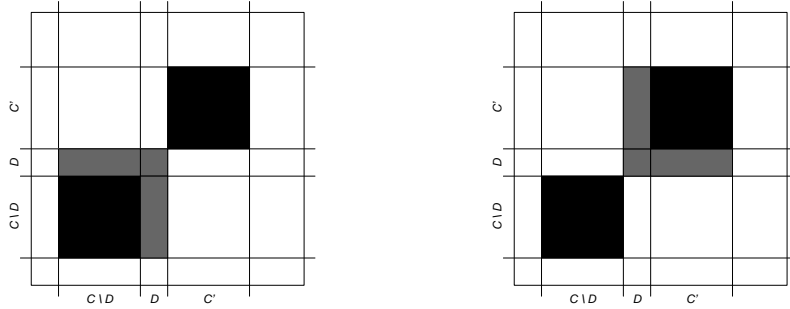


FIGURE 6. Here we illustrate the effect in  $Q_t$  of the replacement in  $\mathcal{C}$  of  $C$  by  $C \setminus D$  and  $C'$  by  $C' \cup D$ : we loose  $2\mu_t(D \times (C \setminus D))$ , we gain  $2\mu_t(D \times C')$ .

*Fixed  $D \subset C$ , select  $C'$  as to maximize*

$$\mu_t(D \times C') - \mu_t(D \times (C \setminus D))$$

*and define*

$$M_D(\mathcal{C})$$

*as the partition obtained from  $\mathcal{C}$  by replacing, when the maximum is strictly positive ( $M_D(\mathcal{C}) = \mathcal{C}$  in the other case),  $C$  by  $C \setminus D$  (eliminating it if it happens to be empty) and  $C'$  by  $C' \cup D$ . Of course,*

$$Q_t(M_D(\mathcal{C})) \geq Q_t(\mathcal{C})$$

(with equality holding only if  $M_D(\mathcal{C}) = \mathcal{C}$ ) and  $M_D(\mathcal{C}) \preceq \mathcal{D}$ . Notice that there is no reason for  $M_D(\mathcal{C})$  to be internally connected, even if  $\mathcal{C}$  is. Consider the elements of  $\mathcal{D}$  numerated,  $D_1, \dots, D_n$ , and let

$$M_{\mathcal{D}} = M_{D_n} \dots M_{D_1}$$

If we start with  $\mathcal{C} = \mathcal{D}$  and define

$$\mathcal{C}^{(k)} = M_{\mathcal{D}}^k(\mathcal{C})$$

from some  $k_0$  on all the  $\mathcal{C}^{(k)}$  are the same (because we are in a finite setting and  $Q_t$  increases in each iteration), and  $M_{\mathcal{D}}^\infty(\mathcal{D}) = \mathcal{C}^{(k_0)}$  is submodular for  $\mu_t$  with respect to  $\mathcal{D}$ . This is what the authors of [Blondel et al., 2008] called one “pass”. They start (as us) from  $\mathcal{D}^{(0)} = \mathcal{C}_1$ , the maximal partition, and by one pass they obtain  $\mathcal{D}^{(1)} = M_{\mathcal{D}}^\infty(\mathcal{D})$ . Then, they update  $\mathcal{D}$  to  $\mathcal{D}^{(1)}$  and proceed again the same, getting  $\mathcal{D}^{(2)} = M_{\mathcal{D}^{(1)}}(\mathcal{D}^{(1)})$ . Proceeding recursively in this way, at some time they obtain  $\mathcal{D}$  such that  $\mathcal{D} = M_{\mathcal{D}}(\mathcal{D})$ , which means that  $\mathcal{D}$  is submodular for  $\mu_t$ . Notice, as the authors of [Blondel et al., 2008] did, that after a  $\mathcal{D}$  update, all the partitions  $\mathcal{D}'$  considered satisfy  $\mathcal{D}' \preceq \mathcal{D}$ . This means that you can update the graph to be  $G/\mathcal{D}$  (doing the corresponding update in the weights), with a relevant gain in speed and memory. This happens also in our algorithm (see Remarks 3).

In [Blondel et al., 2008] the authors only consider the case  $t = 1$ , thus they obtain a partition that is submodular for  $\mu_1$ . Their algorithm is very fast, and able to deal with huge networks. They assert, and show by some example, that the intermediate community structures given by the algorithm overcome the scaling-limit problem. Perhaps the advantage, if any, of our algorithm, lies in that we obtain our intermediate community structures with strict control on the resolution. Notice that all our intermediate partitions are, by construction, internally connected. This is not necessarily the case for those obtained in [Blondel et al., 2008].

## 5. ON THE PROOFS

### 5.1. Section 3.

5.1.1. *Lemma 1.* For the first statement, notice that both  $m_E$  and  $m_{VV}$  have marginal probability  $m_V$ . The second statement follows from the first, adding for all  $C \in \mathcal{C}$ .

5.1.2. *Lemma 2.* We have already shown in Figure 2 how this Lemma follows, by graphical evidence, from the additivity of  $\mu_t$ .

5.1.3. *Lemma 3.*

- (i) This follows immediately from the definitions.
- (ii) If  $\mathcal{C}^*$  is weakly optimal, then from Lemma 2 it follows that  $\mu_t(C \times C') \leq 0$  for  $C, C' \in \mathcal{C}^*, C \neq C'$ , whence  $\mathcal{C}^*$  is submodular.

Then, if  $\mathcal{C}^*$  is submodular and  $\mathcal{D} \preceq \mathcal{C}^*$ , for any  $D \in \mathcal{D}$

$$\mu_t(D \times D) \leq \sum_{C \in \mathcal{C}_D^*} \mu_t(C \times C)$$

and it follows that

$$\begin{aligned} Q_t(\mathcal{D}) &\leq \sum_{D \in \mathcal{D}} \sum_{C \in \mathcal{C}_D^*} \mu_t(C \times C) \\ &= Q_t(\mathcal{C}^*) \end{aligned}$$

Hence,  $\mathcal{C}^*$  is weakly optimal.

(iii) This is immediate from the first statement in our Lemma 1.

5.1.4. *Lemma 4.* Let  $C \in \mathcal{C}$  and  $D, D' \in \mathcal{D}_C$ . By our definition of  $\mathcal{D}_C$ , there are no edges in  $D \times D'$ , whence  $m_E(D \times D') = 0$  and it follows that  $\mu_t(D \times D') \leq 0$ . Then

$$\mu_t(C \times C) \leq \sum_{D \in \mathcal{D}_C} \mu_t(D \times D)$$

for all  $C \in \mathcal{C}$ , whence  $Q_t(\mathcal{C}) \leq Q_t(\mathcal{D})$ .

5.1.5. *Lemma 5.* In Figure 3 we have already shown by graphical evidence that the first statement holds. The second statement follows by replacing  $m_V(C)$  in  $\mu_t(C \times C) = m_E(C \times C) - tm_V^2(C)$  by  $m_E(C \times C) + \rho(C)$ . The remaining statements in the Lemma are easy consequences of these two.

5.1.6. *Lemma 6.* Here all is consequence of Lemma 5. In addition we used some general well known inequalities, that we state here for ever:

Let  $x_i, y_i$  be positive real numbers,  $i = 1, \dots, n$ . Then

- (i)  $\sum_i x_i^2 \geq \frac{(\sum_i x_i)^2}{n}$
- (ii)  $\sum_i x_i y_i \leq (\max_i x_i)(\sum_i y_i)$

5.1.7. *Lemma 7.* This follows from Lemma 1 if you notice that, when  $\mathcal{C}$  is submodular for  $\mu_t$ ,  $\bar{Q}_t(\mathcal{C}) \leq 0$ .

5.1.8. *Lemma 8.*

(i) By the submodularity, we have

$$m_E(C \times C') - tm_V(C)m_V(C') \leq 0$$

whence  $m_V(C)m_V(C') \geq \frac{m_E(C \times C')}{t}$ . Now

$$m_V^2(C \cup C') = (m_V(C) + m_V(C'))^2 \geq 4m_V(C)m_V(C')$$

and the result follows.

(ii) By the submodularity, for each  $C, C' \in \mathcal{C}$  we have

$$m_E(C \times C') \leq tm_V(C)m_V(C')$$

Sum for all  $C' \neq C$ , to obtain

$$m_E(C \times (V \setminus C)) \leq tm_V(C)(1 - m_V(C))$$

Now  $Zm_E(C \times (V \setminus C))$  is a cut in  $G$ , whence

$$\frac{c^*}{tZ} \leq m_V(C)(1 - m_V(C))$$

Complete squares in the right, and the first inequality follows.

As  $\sum_{C \in \mathcal{C}} m_V(C) = 1$ , we have

$$\min_{C \in \mathcal{C}} m_V(C) \leq \frac{1}{|\mathcal{C}|} \leq \max_{C \in \mathcal{C}} m_V(C)$$

so that the second inequality follows from the first.

From the first inequality, we obtain

$$|m_V(C) - \frac{1}{2}| \leq \sqrt{\frac{1}{4} - \frac{c^*}{tZ}} = \frac{1}{2} \sqrt{1 - \frac{4c^*}{tZ}}$$

whence, using the well known  $\sqrt{1-x} < 1 - x/2$  for  $x > 0$ , we obtain

$$|m_V(C) - \frac{1}{2}| \leq \frac{1}{2} - \frac{c^*}{tZ}$$

and the third inequality follows. The last inequality follows from this one immediately.

## 5.2. Section 4.

### 5.2.1. Lemma 9.

- (i) This is obvious from the definitions.
- (ii) If  $\mathcal{C} \preceq \mathcal{D}$  and  $\mathcal{D}$  is submodular for  $\mu_t$ , it follows immediately from the additivity of  $\mu_t$  that  $\mathcal{C}$  is also submodular for  $\mu_t$ .
- (iii) This follows from the previous point.
- (iv)  $t(\mathcal{C}) = 0$  means that  $m_E(C \times C') = 0$  when  $C, C' \in \mathcal{C}, C \neq C'$ . But then the connected components of  $G(C)$  are, for any  $C \in \mathcal{C}$ , connected components of  $G$ , whence the statement.

### 5.2.2. Lemma 10. This follows at once from the definitions.

5.2.3. *Lemma 11.* All our statements follow easily from the construction of  $\mathcal{D}$ , perhaps with the exception of  $Z_0(\mathcal{D}) < Z_0(\mathcal{C})$ . For this, notice that  $Z_0(\mathcal{D})$  is obtained from  $Z_0(\mathcal{C})$  by deleting all pairs where some coordinate is  $C$  or  $C'$ , and adding the pairs of the form  $(C \cup C', D')$  for which  $\mu_t((C \cup C') \times D') = 0$ , and  $D'$  is neither  $C$  nor  $C'$ . But  $\mu_t((C \cup C') \times D') = \mu_t(C \times D') + \mu_t(C' \times D') = 0$  implies that  $\mu_t(C \times D') = \mu_t(C' \times D') = 0$ , so that for each pair that we eventually add, we have deleted two (the same argument applies, of course, reversing the order in the coordinates). As we have deleted from  $Z_0(\mathcal{C})$  at least  $(C, C')$ , the statement follows.

### 5.2.4. Lemma 12. All the statements are easy consequences of the previous lemmas.

## 6. APPLICATION TO NETWORKS

We implemented our algorithm for building submodular partitions in C++; the source code is available on SourceForge [DeltaCom, 2010].

Here, we compare our results with those obtained by other methods: the algorithm of Newman based on the spectrum of the modularity matrix [Newman, 2006]; the algorithm by Duch and Arenas using extremal optimization [Duch and Arenas, 2005]; the fast, greedy algorithm of [Clauset et al., 2004]; and the hierarchical fast-unfolding method of [Blondel et al., 2008]. We omit previous algorithms, like the betweenness-based Girvan-Newman method, the spectrum-based ones and the simulated annealing method of Guimerà *et al.* [Guimerà and Nunes Amaral, 2005], which are rather slow and size limited. We analyze binary trees and some real networks.

**6.1. Binary trees revisited.** In section 3.4.2 we had found an upper bound for modularity on complete binary trees. Here, we apply our algorithm to them, and show the results in Table 2, with a comparison to Blondel's algorithm [Blondel et al., 2008]. Both provide similar results, and quite close to the bounds in Table 1.

We also provide a visualization of a submodular community partition for trees of height 5, in Figure 7. Notice the subtle differences with the  $\mathcal{C}_h$  partition in Figure 5.



$n$	Blondel	this paper
5	0.758195	0.758195
6	0.821712	0.821051
7	0.876850	0.877364
10	0.953032	0.953219

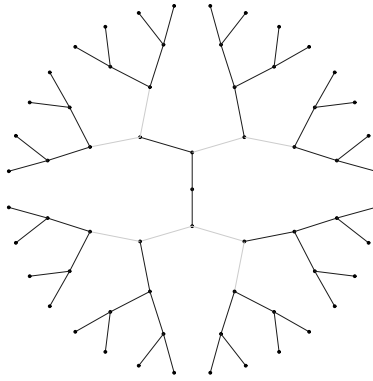
TABLE 2. Newman’s modularity for binary trees of height  $n$ .

FIGURE 7. Communities obtained by Blondel’s algorithm and by this paper. We remark that for a tree of height 5, both achieve the same result.

**6.2. Real networks.** Table 3 displays the results of  $Q_1$  for different common test networks: a karate club network studied by Zachary [Zachary, 1977], a network of email interchanges at university compiled by Guimerà *et al.* [Guimerà *et al.*, 2003], a metabolic network from the *C. elegans* [Duch and Arenas, 2005], a set of scientific co-citations in arXiv [CUP, 2003], a trust network of users of the PGP algorithm [Boguñá *et al.*, 2004], a coauthorship network on condensed matter physics [Newman, 2001], the nd.edu domain of the www [Albert *et al.*, 1999], a web graph from Google [Leskovec *et al.*, 2008] and an Internet map at the inter-router level obtained with DIMES [DIMES, 2005]. This comparison table is similar to those found in [Newman, 2006] and [Duch and Arenas, 2005].

We observe that our algorithm gives better results in terms of modularity relative to the method of Clauset *et al.*. For big networks, we also improve results by Newman and Duch-Arenas (not so for the smallest networks).

For larger real networks many of these methods fail, as their algorithmic complexity is too high. In those cases, we provide a comparison with the Blondel fast algorithm [Blondel *et al.*, 2008], which is also scalable and publicly available. It gives the best results for very large networks, as far as we know.

To end this section, figures 8 to 11 display how the resolution  $t$  and the modularity  $Q$  evolve for different networks.

Network	Size	Newman	Duch-Arenas	Clauset <i>et al.</i>	Blondel	this paper
karate	34	0.419	0.419	0.381	0.419	0.405
dolphins	62	–	–	–	0.519	0.506
email	1133	0.572	0.574	0.494	0.457	0.524
metabolic	453	0.435	0.434	0.402	0.438	0.419
arxiv	9377	–	0.770	0.772	0.813	0.797
key signing	10680	0.855	0.846	0.733	0.884	0.864
condmat	27519	0.723	0.679	0.668	0.750	0.723
web-nd	325729	–	–	–	0.935	0.935
web-google	875712	–	–	–	0.978	0.968
ir_dimes	976025	–	–	–	0.845	0.839

TABLE 3. Comparison of Newman’s modularity for some real networks using different algorithms.

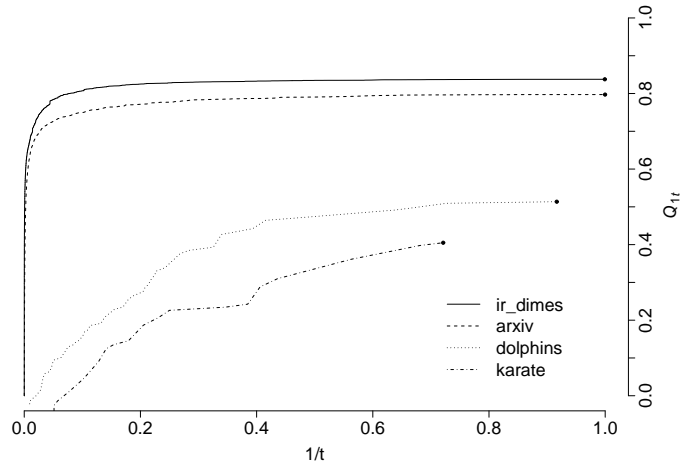


FIGURE 8. Evolution of  $Q_1(\mathcal{C}_t)$  for some networks. We see that the last resolution strongly depends on the size of the network. Even for big networks, the optimal values are reached near 1. Notice that the first few values of  $Q_{1t}$  are negative; we do not plot them.

## 7. CONCLUSIONS

In this paper we have shown several properties of the modularity with resolution parameter for weighted graphs, using systematically our version of the definition. Several of these properties were known in special cases, as we have mentioned in detail in our reference sections; some of them are new. We introduced a notion of weak optimality of a partition, and we described an algorithm to obtain weakly

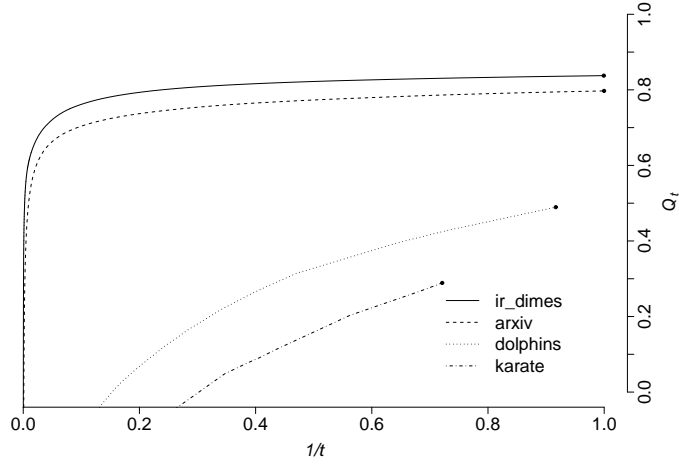


FIGURE 9. Evolution of  $Q_t(\mathcal{C}_t)$  for some networks. Notice that the first values of  $Q_t$  are negative. We do not plot them.

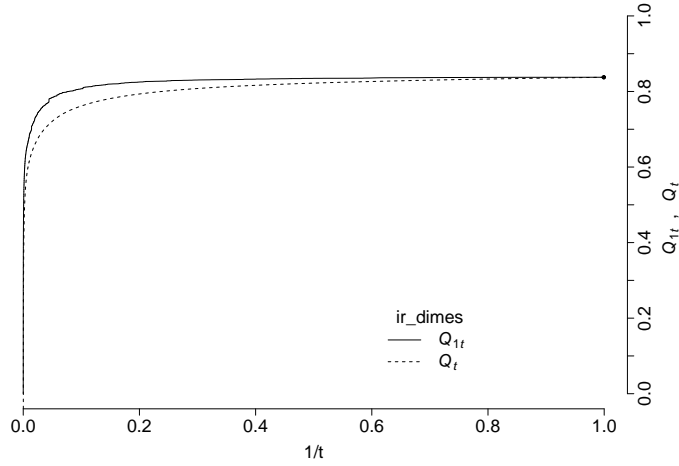


FIGURE 10. Comparison of  $Q_t(\mathcal{C}_t)$  and  $Q_1(\mathcal{C}_t)$  for the ir\_dimes network. The closeness of both curves for  $t = 1$  is attributable to a small second order moment of the sizes  $m_v(\mathcal{C})$ , and to the great number of communities.

optimal partitions. We have shown that this algorithm is able to deal with huge networks, and that the resulting values of modularity are comparable to those obtained by some of the known optimization algorithms.

We showed that the known limitation of modularity optimization, its scaling limit, is also a limitation for weak optimality. The introduction of the resolution parameter  $t$  partially solves this limitation: for  $t > 1$  there are weaker restrictions,

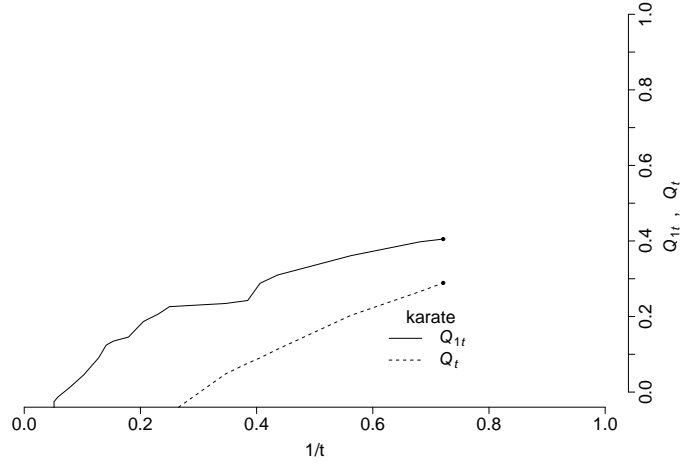


FIGURE 11. For karate, a small network, we see a greater contrast between  $Q_1(\mathcal{C}_t)$  and  $Q_t(\mathcal{C}_t)$ .

but we feel that it is necessary to make a deeper modification in the modularity to obtain, through its optimization, community structures that satisfy natural specifications.

#### ACKNOWLEDGMENTS

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