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# Reformulation of a locally optimal heuristic for modularity maximization

Alberto Costa<sup>1</sup>, Sonia Cafieri<sup>2</sup>, Pierre Hansen<sup>1,3</sup>

<sup>1</sup> LIX, École Polytechnique, F-91128 Palaiseau, France  
costa@lix.polytechnique.fr

<sup>2</sup> École Nationale de l'Aviation Civile, F-31055 Toulouse, France  
sonia.cafieri@enac.fr

<sup>3</sup> GERAD, HEC, 3000 chemin de la Côte-S.te-Catherine, H3T 2A7 Montréal, Canada  
pierre.hansen@gerad.ca

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## 1 Introduction

A network, or graph,  $G = (V, E)$  consists of a set of vertices  $V = \{1, \dots, n\}$  and a set of edges  $E = \{1, \dots, m\}$  connecting vertices. One of the most studied problems in the field of complex systems is to find communities, or clusters, in networks. A community consists of a subset  $S$  of the vertices of  $V$  where inner edges connecting pairs of vertices of  $S$  are more dense than cut edges connecting vertices of  $S$  to vertices of  $V \setminus S$ . Many criteria have been proposed to evaluate partitions of  $V$  into communities. The best known of them appears to be the modularity, defined as follows by Newman and Girvan [9]:

$$Q = \sum_c Q_c = \sum_c \left( \frac{m_c}{m} - \frac{D_c^2}{4m^2} \right), \quad (1)$$

where  $Q_c$  is the modularity of the cluster  $c$ ,  $m_c$  is the number of edges with both end vertices within the cluster  $c$ ,  $D_c$  is the sum of the degrees of the vertices in the cluster  $c$ , and  $m$  is the number of edges of the whole network. The modularity is the difference between the fraction of edges within communities and the expected fraction of such edges in a random graph having the same distribution of degrees than the graph under study. In order to find a good partition into communities for a given network, according to Newman and Girvan one should maximize its modularity. This is a strongly NP-hard problem [3].

A few exact algorithms [1, 6, 10] and many heuristics have been proposed for network modularity maximization. They consist in divisive and agglomerative hierarchical clustering approaches [5, 8], as well as exact or approximate partitioning ones. In this paper, we focus on a recent locally optimal heuristic based on a hierarchical divisive approach [4]. We propose several ways to reformulate the model of [4] in order to accelerate the resolution by reducing efficiently the number of variables and constraints. Computation results are reported for a series of real-world problems from the literature in which the different reformulations are compared. It appears that computing times are very substantially reduced.

## 2 Initial model

The model used in the framework of the hierarchical divisive heuristic proposed in [4] to split a cluster  $(V_c, E_c)$  into two clusters maximizing the modularity, and based on the one proposed in [10], is the following:

$$\max \frac{1}{m} \left( m_1 + m_2 - \frac{1}{2m} \left( D_1^2 + \frac{D_c^2}{2} - D_1 D_c \right) \right) \quad (2)$$

$$\text{s.t. } X_{i,j,1} \leq Y_i \quad \forall (v_i, v_j) \in E_c \quad (3)$$

$$X_{i,j,1} \leq Y_j \quad \forall (v_i, v_j) \in E_c \quad (4)$$

$$X_{i,j,2} \leq 1 - Y_i \quad \forall (v_i, v_j) \in E_c \quad (5)$$

$$X_{i,j,2} \leq 1 - Y_j \quad \forall (v_i, v_j) \in E_c \quad (6)$$

$$m_s = \sum_{(v_i, v_j) \in E_c} X_{i,j,s} \quad \forall s \in \{1, 2\} \quad (7)$$

$$D_1 = \sum_{v_i \in V_c} k_i Y_{i,1} \quad (8)$$

$$Y_i \in \{0, 1\} \quad \forall v_i \in V_c \quad (9)$$

$$X_{i,j,s} \geq 0 \quad \forall (v_i, v_j) \in E_c, \forall s \in \{1, 2\}, \quad (10)$$

where the variable  $X_{i,j,s}$  is equal to 1 if the edge  $(v_i, v_j)$  is inside the community  $s$  (i.e., both vertices  $v_i$  and  $v_j$  are inside the community  $s$ ) and 0 otherwise,  $Y_i$  is equal to 1 if the vertex  $v_i$  is inside the community 1, and 0 otherwise, and  $k_i$  is the degree of the vertex  $v_i$ ; note that  $D_c$  is a parameter, and it is known before solving the problem.

### 3 Reformulations

#### 3.1 Power of two reformulation

The heuristic proposed in [4] works by recursively splitting a cluster into two clusters in an optimal way (in the sense that the computed bipartition corresponds to the best possible modularity). The model is a quadratic integer programming one, with a convex relaxation. The only non-linear term is  $D_1^2$ . The usual Branch-and-Bound approach implemented in CPLEX [7] is to relax the integrality constraints, solve the continuous quadratic program obtained and then branch. Alternately, one may linearize  $D_1^2$  by replacing it with its expansion in power of two, as proposed for mixed-integer quadratic programming in [2]:

$$D_1 = \sum_{i=0}^t 2^i a_i, \quad a_i \in \{0, 1\}. \quad (11)$$

Therefore, the term  $D_1^2$  in (2) can be written as:

$$D_1^2 = \sum_{l=0}^t 2^l a_l \cdot \sum_{h=0}^t 2^h a_h = \sum_{l=0}^t \sum_{h=0}^t 2^{l+h} a_l a_h = \sum_{l=0}^t \sum_{h=0}^t 2^{l+h} R_{lh} = \sum_{l=0}^t 2^{2l} a_l + \sum_{l=0}^t \sum_{h<l} 2^{l+h+1} R_{lh}, \quad (12)$$

where  $R_{lh}$  is the linearization variable for  $a_l a_h$ ; hence, we have to adjoin the following constraints to our model:

$$\begin{aligned} R_{lh} &\geq a_l + a_h - 1, \quad \forall l \in \{0, \dots, t\}, \forall h \in \{0, \dots, l-1\} \\ R_{lh} &\geq 0, \quad \forall l \in \{0, \dots, t\}, \forall h \in \{0, \dots, l-1\}. \end{aligned}$$

To estimate  $t$ , recall that the maximum value which can be assumed by  $D_1$  is the sum of the degrees of all the vertices in the current cluster, that is  $D_c$ . Moreover, from (11) the maximum possible value for  $D_1$  is  $2^{t+1} - 1$ . Hence,  $t$  can be computed as:

$$2^{t+1} - 1 \geq D_c \quad \Rightarrow \quad t = \lceil \log_2(D_c + 1) - 1 \rceil. \quad (13)$$

### 3.2 Change of variables

The model of [4] uses variables assigning edges or vertices to a specific community. When bipartitioning, as there are only two communities to be determined at each iteration, one can use other variables  $S_{i,j}$ , associated with the fact that the two end vertices  $v_i$  and  $v_j$  of an edge belong to the same cluster or not (i.e.,  $S_{i,j} = 1$  if  $Y_i = Y_j$ , and 0 otherwise). This leads to the following reformulation:

$$\max \frac{1}{m} \left( \sum_{(v_i, v_j) \in E_c} (2S_{i,j} - Y_i - Y_j) + |E_c| - \frac{1}{2m} \left( D_1^2 + \frac{D_c^2}{2} - D_1 D_c \right) \right) \quad (14)$$

$$\text{s.t. } S_{i,j} \leq Y_i \quad \forall (v_i, v_j) \in E_c \quad (15)$$

$$S_{i,j} \leq Y_j \quad \forall (v_i, v_j) \in E_c \quad (16)$$

$$D_1 = \sum_{v_i \in V_c} k_i Y_i \quad (17)$$

$$Y_i \in \{0, 1\} \quad \forall v_i \in V_c. \quad (18)$$

### 3.3 Symmetry breaking

To avoid considering twice equivalent solutions, one fixes a vertex to belong to the first (or second) community. It appears that the vertex with largest degree is a good choice.

## 4 Compact model

Applying all the reformulations presented in the previous sections leads to the following compact model:

$$\max \frac{1}{m} \left( \sum_{(v_i, v_j) \in E_c} (2S_{i,j} - Y_i - Y_j) + |E_c| - \frac{1}{2m} \left( \sum_{l=0}^t 2^{2l} a_l + \sum_{l=0}^t \sum_{h < l} 2^{l+h+1} R_{l,h} + \frac{D_c^2}{2} - D_1 D_c \right) \right) \quad (19)$$

$$\text{s.t. } S_{i,j} \leq Y_i \quad \forall (v_i, v_j) \in E_c \quad (20)$$

$$S_{i,j} \leq Y_j \quad \forall (v_i, v_j) \in E_c \quad (21)$$

$$R_{l,h} \geq a_l + a_h - 1 \quad \forall l \leq t, \forall h < l \quad (22)$$

$$R_{l,h} \geq 0 \quad \forall l \leq t, \forall h < l \quad (23)$$

$$D_1 = \sum_{l=0}^t 2^l a_l \quad (24)$$

$$D_1 = \sum_{v_i \in V_c} k_i Y_v \quad (25)$$

$$Y_g = 0, \quad g = \arg \max \{k_i, \forall v_i \in V_c\} \quad (26)$$

$$Y_i \in \{0, 1\} \quad \forall v_i \in V_c \quad (27)$$

$$a_l \in \{0, 1\} \quad \forall l \leq t. \quad (28)$$

This model has  $|V_c| + t + 1$  binary variables,  $|E_c| + \frac{t^2 + t}{2} + 1$  continuous variables and  $2|E_c| + t^2 + t + 3$  constraints, while the initial model has  $|V_c|$  binary variables,  $2|E_c| + 3$  continuous variables and  $6|E_c| + 3$  constraints.

## 5 Results

Table 1 presents the comparison of computing times for the initial model and the final one. Results have been obtained on a 2.4GHz Intel Xeon CPU of a computer with 24 GB RAM

running Linux and CPLEX 12.2 [7].  $M$  denotes the number of clusters, and  $Q$  the modularity; computing times are in seconds. Note that slight discrepancies may arise in the values of  $M$  and  $Q$ ; they are due to the fact that optimal bipartitions are not necessarily unique. It appears that the computing time is reduced by a factor of 2 to over 265.

Network	Network		Initial model			Compact model		
	n	m	$M$	$Q$	time	$M$	$Q$	time
Karate	34	78	4	0.4188	0.32	4	0.4188	<b>0.16</b>
Dolphins	62	159	4	0.5265	1.45	4	0.5265	<b>0.65</b>
Les misérables	77	254	8	0.5468	4.47	8	0.5468	<b>0.67</b>
A00 main	83	135	7	0.5281	0.71	7	0.5281	<b>0.37</b>
P53 protein	104	226	7	0.5284	16.82	7	0.5284	<b>1.55</b>
Political books	105	441	4	0.5263	16.74	5	0.5244	<b>2.66</b>
Football	115	613	10	0.6009	238.47	10	0.6009	<b>82.21</b>
A01 main	249	635	15	0.6288	563.41	15	0.6288	<b>38.12</b>
USAir97	332	2126	8	0.3596	113545.00	8	0.3596	<b>428.40</b>
Netscience main	379	914	20	0.8470	11.83	20	0.8470	<b>5.24</b>
S838	512	819	15	0.8166	24.48	15	0.8166	<b>6.40</b>
Power	4941	6594	40	0.9394	3952.72	41	0.9396	<b>567.07</b>

TAB. 1: Results obtained with the hierarchical divisive heuristic using respectively the original formulation and the compact reformulation.

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