



**HAL**  
open science

## Reformulation of a locally optimal heuristic for modularity maximization

Alberto Costa, Sonia Cafieri, Pierre Hansen

► **To cite this version:**

Alberto Costa, Sonia Cafieri, Pierre Hansen. Reformulation of a locally optimal heuristic for modularity maximization. ROADEF 2012, 13ème congrès annuel de la Société Française de Recherche Opérationnelle et d'Aide à la Décision, Apr 2012, Angers, France. hal-00934798

**HAL Id: hal-00934798**

**<https://enac.hal.science/hal-00934798>**

Submitted on 8 Apr 2014

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# 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

**Keywords :** *binary decomposition, clustering, modularity maximization, reformulation.*

## 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.

## References

- [1] D. Aloise, S. Cafieri, G. Caporossi, P. Hansen, S. Perron and L. Liberti. Column generation algorithms for exact modularity maximization in networks. *Physical Review E*, 82(4), 046112, American Physical Society, 2010.
- [2] A. Billionnet, S. Elloumi and A. Lambert. Extending the QCR method to general mixed-integer programs. *Mathematical Programming A*, doi:10.1007/s10107-010-0381-7, Springer, 2010.
- [3] U. Brandes, D. Delling, M. Gaertler, R. Görke, M. Hoefer, Z. Nikoloski, and D. Wagner. On Modularity Clustering. *IEEE Transactions on Knowledge and Data Engineering*, 20(2):172-188, IEEE, 2008.
- [4] S. Cafieri, P. Hansen, L. Liberti. Locally optimal heuristic for modularity maximization of networks. *Physical Review E*, 83(5):056105, American Physical Society, 2011.
- [5] A. Clauset, M. E. J. Newman and C. Moore. Finding and evaluating community structure in very large networks. *Physical Review E*, 70(6), 066111, American Physical Society, 2004.
- [6] M. Grötschel and Y. Wakabayashi. A cutting plane algorithm for a clustering problem. *Mathematical Programming*, 45(1), 59-96, Springer, 1989.
- [7] IBM. ILOG CPLEX 12.2 *User's Manual*, IBM, 2010.
- [8] M. E. J. Newman. Modularity and community structure in networks. *Proceedings of the National Academy of Sciences of the U.S.A.*, 103(23), 8577-8582, 2006.
- [9] M. E. J. Newman and M. Girvan. Finding and evaluating community structure in networks. *Physical Review E*, 69(2):026113, American Physical Society, 2004.
- [10] G. Xu, S. Tsoka and L. G. Papageorgiou. Finding community structures in complex networks using mixed integer optimisation. *The European Physical Journal B - Condensed Matter and Complex Systems*, 60(2), 231-239, European Physical Society, 2007.