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Reformulation of a locally optimal heuristic for modularity maximization

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

1 Introduction

A network, or graph, \( G = (V, E) \) consists of a set of vertices \( V = \{1, \ldots, n\} \) and a set of edges \( E = \{1, \ldots, m\} \) 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]:

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

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:

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max \( \frac{1}{m} \left( m_1 + m_2 - \frac{1}{2m} \left( D_1^2 + \frac{D_c^2}{2} - D_1D_c \right) \right) \) 

s.t. \( X_{i,j,1} \leq Y_i \) \( \forall (v_i, v_j) \in E_c \) 
\( X_{i,j,1} \leq Y_j \) \( \forall (v_i, v_j) \in E_c \) 
\( X_{i,j,2} \leq 1 - Y_i \) \( \forall (v_i, v_j) \in E_c \) 
\( X_{i,j,2} \leq 1 - Y_j \) \( \forall (v_i, v_j) \in E_c \) 
\( m_s = \sum_{(v_i, v_j) \in E_c} X_{i,j,s} \) \( \forall s \in \{1, 2\} \) 
\( D_1 = \sum_{v_i \in V_c} k_i Y_{i,1} \) 
\( Y_i \in \{0, 1\} \) \( \forall v_i \in V_c \) 
\( X_{i,j,s} \geq 0 \) \( \forall (v_i, v_j) \in E_c, \forall s \in \{1, 2\}, \) 

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]:

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

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

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

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

\[ R_{lh} \geq a_l + a_h - 1, \quad \forall l \in \{0, \ldots, t\}, \forall h \in \{0, \ldots, l - 1\} \]
\[ R_{lh} \geq 0, \quad \forall l \in \{0, \ldots, t\}, \forall h \in \{0, \ldots, l - 1\}. \]

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:

\[ 2^{t+1} - 1 \geq D_c \quad \Rightarrow \quad t = \lfloor \log_2(D_c + 1) \rfloor - 1. \]  (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:

$$\max \frac{1}{m} \left( \sum_{(v_i,v_j) \in E_c} (2S_{i,j} - Y_i - Y_j) + |E_c| - \frac{1}{2m} \left( D_1^2 + \frac{D_c^2}{2} - D_1D_c \right) \right)$$ (14)

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

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

$D_1 = \sum_{v_i \in V_c} k_iY_i$ (17)

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

$$\max \frac{1}{m} \left( \sum_{(v_i,v_j) \in E_c} (2S_{i,j} - Y_i - Y_j) + |E_c| - \frac{1}{2m} \left( \sum_{l=0}^{t} 2^{2l}a_l + \sum_{l=0}^{t} \sum_{h<l} 2^{l+h+1} R_{l,h} + \frac{D_c^2}{2} - D_1D_c \right) \right)$$ (19)

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

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

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

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

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

$D_1 = \sum_{v_i \in V_c} k_iY_i$ (25)

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

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

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

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

References


