NETWORK CLUSTERING BY EMBEDDING OF ATTRIBUTE-AUGMENTED GRAPHS

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Abstract. In this paper we propose a new approach to detect clusters in undirected graphs with attributed vertices. The aim is to group vertices which are similar not only in terms of structural connectivity but also in terms of attribute values. We incorporate structural and attribute similarities between the vertices in an augmented graph by creating additional vertices and edges as proposed in [5, 27]. The augmented graph is embedded in a Euclidean space associated to its Laplacian and apply a modified K-means algorithm to identify clusters. The modified K-means uses a vector distance measure where to each original vertex is assigned a vector-valued set of coordinates depending on both structural connectivity and attribute similarities. To define the coordinate vectors we employ an adaptive AMG (Algebraic MultiGrid) method to identify the coordinate directions in the embedding Euclidean space extending our previous result for graphs without attributes. We demonstrate the effectiveness of our proposed clustering method on both synthetic and real-world attributed graphs.

1. Introduction

Graph clustering is a main task in network analysis [21, 12, 17]; it aims to identify groups (clusters) of vertices with many edges among vertices inside the group and only few connections among vertices in different groups. In many real-world networks, such as social and biomedical networks, in addition to the vertex connectivity structure additional information related to some vertex features are often available; therefore, it is pertinent exploiting such additional information, often referred to as metadata, to improve the accuracy of clustering algorithms and/or to analyse the impact of the features on the clustering detectability. Many clustering methods have been extended to incorporate features information in the vertex similarities detection so that the clusters are not only densely connected but also very homogeneous in their attributes [1]. In this paper we present an extension of a recently proposed generalized spectral method [7] in order to deal with networks with categorical vertex attributes.

Next we introduce the problem setting and briefly summarize our approach.

Given a set of vertices $V$ and a set of $m$ categorical labels $L = \{l_1, \ldots, l_m\}$, a vertex-attributed graph is the 4-tuple $G = (V, E, W, L)$, where $E \subset V \times V$ is the edge set and $W : V \rightarrow \{1, \ldots, m\}$ is the attribute function.
and $W = (w_{ij})_{(i,j) \in E}$ is the (positive) edge weights matrix. Each vertex $v_i \in V$ is associated with an attribute vector $(l_1(v_i), \ldots, l_m(v_i))$, where $l_j(v_i)$ is the attribute value of vertex $v_i$ on attribute $l_j$. The cardinality or size of $G$ is the dimension $|V| = n$ of $V$.

In [7] we have formulated the clustering of an undirected graph, as a partition $V_1, \ldots, V_K$, in $K$ nonempty sets, so that $V_k \subset V$, $V_k \cap V_h = \emptyset$, $\forall k \neq h$ and $V_1 \cup \ldots \cup V_K = V$, which minimizes the following functional:

\begin{equation}
\text{RatioCut}(V_1, \ldots, V_K) = \frac{1}{2} \sum_{k=1}^{K} \frac{W(V_k, \overline{V_k})}{|V_k|},
\end{equation}

where $W(V_k, \overline{V_k}) = \sum_{i \in V_k, j \in \overline{V_k}} w_{ij}$, and $\overline{V_k}$ is the complement of $V_k$ in $V$. We observe that a graph partition which minimizes (1.1) corresponds to a partition which minimizes the weight of the edges between two different sets and maximizes the number of the vertices within a set. The solution of (a relaxed version of) this problem involves the eigenvectors of the (weighted) graph Laplacian that are used to define embedding of the graph into a Euclidean space of low dimension and use geometric means to construct clusters [13]. In [7], we have generalized this concept by looking at the spectrum of a generalized eigenvalue problem involving the (weighted) graph Laplacian and an adaptive AMG operator (solver) which provided a natural way to select the dimension of the embedding Euclidean space.

In this paper, our aim is to obtain a partition where the vertices within one set have similar attribute values. In order to achieve the purpose, we follow an approach based on the augmentation of the graph $G$ with new vertices representing the attribute values and new edges connecting original vertices to new vertices representing their attribute values. After this augmentation, we solve the minimization problem associated with the relaxed form of the functional (1.1) (as in [7]) now for the augmented graph by embedding into a low-dimensional space associated to the augmented graph Laplacian. A modified K-means algorithm is then applied in the embedding space, where a new distance measure between the original vertices is defined. Experimental results are obtained by using a large set of synthetic graphs generated by a Stochastic Block Model (SBM); we show that embedding the augmented graphs emphasizes both structural and attribute similarities among the graph vertices and the new vector distance allows the K-means algorithm to identify dense and homogeneous clusters also for graphs whose modular structure is weak. We also discuss comparison results with already available clustering methods and show the better behaviour of our method. Some tests on small and medium size real world attributed graphs confirm the validity of the approach.

The paper is organized as follows. In section 2 we summarize main features of a clustering algorithm already proposed by some of us to partition undirected graphs and whose extension to attributed graphs is the objective of this work. In section 3 we provide a description of a strategy which augments the original graph with new vertices and new edges depending on the attribute values associated to the original graph vertices. It was previously proposed in [27, 5], and can also be viewed as a coarse version of a graph disaggregation (cf., [15]). The authors in [27, 5] defined
a distance measure based on random walks on the augmented graph which allowed
them to then apply a geometric (spatial) clustering, i.e., K-means thus extending the
concept of closeness to vertices sharing the same label value. In section 3.1 starting
from a representation of original graph vertices in terms of a set of coordinates which
is obtained by embedding the augmented graph in a vector space associated to its
Laplacian, and then includes information on attributes, we define an extension of the
usual Euclidean distance, so that a version of K-means can be applied to identify
partitions of the attributed graph having homogeneous labels. In section 4 we discuss
results on synthetic graphs and on some real-world data sets. Section 5 contains
concluding remarks and possible future works.

2. Embedding in the space of algebraically smooth vectors for
graph Laplacian

In [7] we proposed a new method for efficient embedding of undirected graphs
in a low-dimensional Euclidean space spanned by an accurate approximation of the
smallest part of the spectrum of a linear operator associated to the graph Laplacian.
The method can be viewed as an extension of the classical spectral clustering which
employs a standard eigenvalue problem for graph Laplacian.

Let $D = diag(d_i)_{i=1}^{n}$, with $d_i = \sum_{j=0}^{n} w_{ij}$, be the diagonal matrix of weighted
vertex degrees of $G$, the graph Laplacian of $G$ is the matrix $L = D - W \in \mathbb{R}^{n \times n}$. We
observe that $L$ is a symmetric, positive semi-definite M-matrix, and its spectrum is a
main tool for studying the graph [23]. In particular, in spectral clustering, a graph is
embedded in the Euclidean space spanned by the first $K$ eigenvectors corresponding
to the first $K$ smallest eigenvalues of $L$; this embedding allows to apply standard
spatial clustering algorithms, e.g., the K-means optimization algorithm, giving good
approximations of optimal partitioning for well-clustered graphs [20].

As low-dimensional space for graph embedding, we use the space spanned by some
vectors, referred to as algebraically smooth vectors generated by an iteration process.
We use the bootstrap process coming from an Algebraic MultiGrid (AMG) operator
associated to the graph Laplacian. Note that we always consider the graph Laplacian
of a connected graph; in the case of graphs with more than one connected component,
we apply our method to each of its connected components. Furthermore, we also
eliminate singularity of the graph Laplacian by a rank-1 update which gives symmetric
positive definite (s.p.d.) graph Laplacian matrix $L_S = L + \lambda e \cdot e^T$, where $e$ is a vector
of dimension $n$ having unit (nonzero) components only for a single pair of indices $i$
and $j$ corresponding to an arbitrarily chosen edge $(i, j) \in E$. In the following, we
briefly summarize the theoretical basis of our method and its formulation.

In the theory of AMG [22], an $\epsilon-$smooth vector of the matrix $L_S$ is defined as follows:

**Definition 2.1.** Let $M$ be a s.p.d. smoothing operator, i.e., the iteration matrix of a
relaxation method convergent in the $L_S$-norm\(^1\) and given $\epsilon \in (0, 1)$, we say that the
vector $u$ is algebraically $\epsilon$-smooth with respect to $L_S$ if

\[
\|(I - M^{-1}L_S)u\|_{L_S}^2 \geq (1 - \epsilon)\|u\|_{L_S}^2.
\]

\(^1\)The $A-$norm of the vector $u$, where $A$ is a s.p.d. matrix is defined as $\|u\|_A = \sqrt{u^T A u}$. 
We note that \(\|(I - M^{-1}L_S)u\|_{L_S} \leq \|u\|_{L_S}\) (since \(M\) is a convergent smoother). That is, \(u\) is in the near-nullspace of \(M^{-1}L_S\) in the sense that \(M^{-1}L_Su\) has a much smaller norm than \(u\).

Such a vector can be obtained by performing a few iterations of the smoother \(M\), i.e.

\[
(2.1) \quad u = u^t = (I - M^{-1}L_S)u^{t-1},
\]

starting from a random vector \(u^0\) for a sufficiently large \(t\).

The above concept was generalized in [7] in the sense that we used an operator \(B\) (in fact a sequence of operators that gradually approximate \(L_S\)) corresponding to the iteration matrix \(M\) and considered the respective algebraically smooth vectors.

Given the matrix \(L_S\), we first define a two-level method for solving the linear system \(L_Sx = b\), where \(x \in \mathbb{R}^n\) is the unknown vector and \(b \in \mathbb{R}^n\) is a given right-hand side term. Let \(V_c \subset \mathbb{R}^n\) be the space spanned by a set of smooth vectors \(\{u_r\}_r\) of \(L_S\) with respect to the operator \(M\). Let \(\{\phi_i\}_{i=1}^n\) provide a basis of \(V_c\), and let \(P = [\phi_1, \ldots, \phi_n]\) be the interpolation matrix mapping vectors from \(V_c\) to \(V \subset \mathbb{R}^n\) and \((L_S)c = P^T L_S P\) the corresponding coarse matrix. We define a two-level operator \(B\) corresponding to the iteration matrix

\[
I - B^{-1}L_S = (I - M^{-T}L_S)(I - P(L_S)^{-1}P^T L_S)(I - M^{-1}L_S),
\]

which leads to the formula

\[
B^{-1} = \overline{M}^{-1} + (I - M^{-T}L_S)P(L_S)^{-1}P^T (I - L_S M^{-1}),
\]

where \(\overline{M} = M(M + M^T - L_S)^{-1}M^T\) is the so-called symmetrized smoother, such that \(I - \overline{M}^{-1}L_S = (I - M^{-T}L_S)(I - M^{-1}L_S)\).

The following spectral equivalence result holds [22]:

\[
v^T L_S v \leq v^T B v \leq C v^T L_S v, \quad \forall v \in V
\]

where the optimal constant \(C\) is given by the formula:

\[
(2.2) \quad C = \max_{v \in V} \frac{\|v - \pi v\|_{L_S}^2}{\|v\|_{L_S}^2}.
\]

Here \(\pi : V \mapsto V_c \subset V\) is a projection in the \(M\)-inner product, i.e., \(\pi = P(P^T M P)^{-1}P^T M\).

The following theorem [7] holds:

**Theorem 2.1.** Consider the operator \(B\) defined by the two-level algorithm with smoother \(M\), symmetrized smoother \(\overline{M}\), and coarse space \(V_c\). Let \(\rho\) be the convergence rate of the iterative process having \(B\) as iteration matrix. Consider the generalized eigenvalue problem:

\[
(2.3) \quad L_S q_k = \lambda_k M q_k,
\]

where \(0 \leq \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_s < \lambda_{s+1} \leq \cdots \leq \lambda_{\max}\), and assume that the coarse space \(V_c\) contains the first \(s \geq 1\) eigenvectors \(q_k\). Then, the following estimate holds for the spectral equivalence constant \(C\):

\[
C \leq \frac{1}{1 - \rho} \approx \frac{1}{\lambda_{s+1}}.
\]
The above result assures that if $B$ is a method with a sufficiently small convergence rate, then eigenvectors in $(2.3)$ can effectively be replaced (as argued in [7]) by the algebraically smooth vectors generated by the iteration process based on $B$. More specifically, in [7] we proposed an iterative procedure which justified the use, in place of the eigenvectors $q_k$, of a sequence of smooth vectors with respect to $L_S$. These vectors are obtained during a bootstrap procedure whose final aim was to construct a composite AMG operator $B$ leading to a sufficiently small spectrally equivalence constant $C$. For sake of completeness, we summarize here main features of the bootstrap procedure and the resulting graph embedding algorithm.

The bootstrap procedure builds a composite linear solver $\overline{B}$ obtained from a multiplicative composition of a number of AMG operators $B_r$. The operator $\overline{B}$ is defined from the error propagation matrix

\begin{equation}
I - \overline{B}^{-1}L_S = (I - B_r^{-1}L_S)\ldots (I - B_1^{-1}L_S)(I - B_0^{-1}L_S),
\end{equation}

where each $B_r$ is an AMG operator, i.e., a standard V-cycle involving a simple smoother such as the weighted Jacobi or the Gauss-Seidel method, and a hierarchy of coarse matrices exploiting coarsening based on compatible weighted matching in the form studied in [9, 8]. To construct the operator $B_r$, we first generate an algebraically smooth vector $u_r$. The first smooth vector is constructed based on the smoother $M$ for $L_S$ as described in (2.1). At step $r > 0$, we apply few iterations based on the currently available composite solver $\overline{B}$ consisting of the already built $r-1$ components; i.e., $u = u^t = (I - \overline{B}^{-1}L_S)u^{t-1}$, starting from a random vector $u^0$. Once the vector $u_r$ is available, the operator $B_r$ is defined as a V-cycle AMG where the construction of its hierarchy of coarse spaces is driven by the vector $u_r$ using coarsening based on compatible weighted matching [9, 8].

The process is iterated several times until $M$ vectors $\{u_r\}_{r=1}^M$ are computed; the number $M$ of computed vectors depends on the desired convergence factor $\varrho$ that we impose on the composite solver $B_{BAMG} = \overline{B}$ in (2.4) to exhibit after $M$ composite steps. As a result, for a given $\varrho \in (0, 1)$, the number $M$ of components (equivalently the number of smooth vectors associated with the components $B_r$) are such that by construction, we have:

\[ \|I - B_{BAMG}^{-1}L_S\|_{L_S} \leq \varrho. \]

In order to generate a set of orthogonal vectors spanning the graph embedding space, we finally apply a Singular Value Decomposition (SVD) to the computed set of vectors $\{u_r\}_{r=1}^M$ and use the corresponding left-singular vectors $\{u_r\}_{r=1}^{p_r}$ as basis for the embedding space. In addition to this set we add the vector of all ones, which is the null vector of $L$, and we also use this vector as the starting one in the bootstrap process. After embedding, we apply any standard spatial clustering procedure to identify possible vertex clusters of the original graph. Our method of choice is the widely used K-means algorithm, as detailed in [7] (see Algorithm 2).

Note that our procedure exploits increasingly accurate coarse spaces which provide improved approximations to the generalized eigenvalue problem (2.3). This is the case since the operator $B$ changes at each bootstrap step until we reach a final operator which has a sufficiently small spectral equivalence constant (2.2). The achieved convergence tolerance determines how many bootstrap steps to perform, and as a result...
gives a criterion how to choose the dimension of the embedding space. For the more standard spectral clustering it is not as clear how many eigenvectors to compute in advance in order to get satisfactory clustering results. Therefore, our method exhibits a desired property in practice and we view it as an advantage over the more standard spectral clustering approaches. We additionally observe that our method has a linear computational complexity with a proportionality constant that grows with the number of built smooth vectors which makes our approach more competitive for large networks.

In the following, we describe the extension of the method based on the bootstrap AMG to undirected graphs with vertex attributes.

### 3. Attribute-augmented Graphs

Let $G = (V, E, W, L)$ be a vertex-attributed graph, where $L$ is the set of attribute values, i.e., the set of vectors $(l_1(v_i), \ldots, l_m(v_i))$ with $m$ values associated to each vertex $v_i \in V$, and let $\text{Dom}(l_j) = \{l_{j,1}, \ldots, l_{j,n_j}\}$ be the $n_j$ distinct values of the attribute $l_j$. Algorithm 1 builds an augmented graph with additional vertices $V_a$, edges $E_a$ and edge weights $W_a$. It implements the method from [27, 5], and can be viewed also as a coarsened version of an attribute-based graph disaggregation algorithm [15]. In summary, Algorithm 1 builds the augmented graph defined as follows:

**Definition 3.1.** Let $G = (V, E, W, L)$ be a vertex-attributed graph, where $L$ is the set of attribute values, i.e., the set of vectors $(l_1(v_i), \ldots, l_m(v_i))$ with $m$ values associated to each vertex $v_i \in V$, and let $\text{Dom}(l_j) = \{l_{j,1}, \ldots, l_{j,n_j}\}$ be the $n_j$ distinct values of the attribute $l_j$. The augmented graph $G^H_A = (V \cup V_a, E \cup E_a, W_a)$, constructed in Algorithm 1 has its components defined as:

1. $V_a = \{(v_{j,k}) \mid j, k = 1, \ldots, n_j\}$ is the set of vertices representing the distinct attribute values $(l_{j,k})_{j=1}^{m,n_j}$ of the vertices in $G$;
2. $E_a$ is the set including the edges $(v_i, v_{j,k}) \forall j = 1, \ldots, m \iff l_j(v_i) = v_{j,k}$, which connect the vertex $v_i$ with his attribute value $v_{j,k}$;
3. $W_a$ is a real matrix including possible weights for the edges in $E \cup E_a$.

We note that the cardinality of the augmented graph $G^H_A$ is equal to $n_{new} = n + \sum_{j=1}^{m} n_j$, where $n_j \leq n$ is the number of different values of the attribute $l_j$, and the number of edges is $n_{e_{new}} = ne + nm$, where $ne$ is the number of edges in $G$. We also observe that in our implementation of the method and in the experiments discussed in section 3 we consider unweighted graphs, where matrix $W$ and $W_a$ corresponds to the adjacency matrix of the original graph and of the augmented graph, respectively. On the other hand, the extension of the code to the weighted graphs is straightforward while the impact of possible weights on the edges could have large impact on the final clusterings for any employed method.

In Fig. 1 we show a small undirected graph with 3 different labels and the corresponding augmented graph. The original graph has the vertex set $V = \{v_1 = 1, v_2 = 2, v_3 = 3, v_4 = 4\}$ and the edge set $E = \{(1, 2), (1, 3), (1, 4), (2, 4), (2, 3)\}$, then $|V| = n = 4$ and $|E| = ne = 5$; the vertices are characterized by the labels defined in Table 1. In this case, we have $m = 3$, $\text{Dom}(l_1) = \{M, F\}$, $\text{Dom}(l_2) = \{R, D, I\}$,
Algorithm 1: Graph augmentation based on vertex attributes.

Data: vertex-attributed graph \( G = (V, E, W, L) \), \( n = |V| \), \( ne = |E| \), \( m \): number of label classes in \( L \), \( weight(\cdot) \): real function depending on vertices and attribute values

Result: augmented graph \( G_A^H = (V \cup V_a, E \cup E_a, W_a) \), \( n_{\text{new}} = |V \cup V_a| \), \( ne_{\text{new}} = |E \cup E_a| \)

for \( j = 1, \ldots, m \) do
  identify \( \text{Dom}(l_j) = \{l_{j,1}, \ldots, l_{j,n_j}\} \) as the set of distinct values of the label \( l_j \);
end

\( E_a = \emptyset \), \( V_a = \emptyset \), \( W_a = W \);

for \( j = 1, \ldots, m \) do
  for \( k = 1, \ldots, n_j \) do
    \( V_a = V_a \cup \{v_{j,k}\} \);
    for \( i = 1, \ldots, n \) do
      if \( l_j(v_i) = l_{j,k} \) then
        \( E_a = E_a \cup \{e_{\text{new}} = (v_i, v_{j,k})\} \);
        \( W_a(e_{\text{new}}) = weight(e_{\text{new}}) \);
      end
    end
  end

\( n_{\text{new}} = n + \sum_{j=1}^{m} n_j \);
\( ne_{\text{new}} = ne + mn \);

Figure 1. Original (left) and Augmented Graph (right).

\( \text{Dom}(l_3) = \{C, M, J\} \), \( n_1 = 2 \) and \( n_2 = n_3 = 3 \). Algorithm [1] builds the set of 8 new vertices, enumerated with consecutive integers from 5 to 12. We have \( V_a = \{v_{1,1} = M = 5, v_{1,2} = F = 6, v_{2,1} = R = 7, v_{2,2} = D = 8, v_{2,3} = I = 9, v_{3,1} = C = 10, v_{3,2} = M = 11, v_{3,3} = J = 12\} \). The set of new edges reads: \( E_a = \)
Finally, the augmented graph $G'_A$ has a total of $n_{new} = 12$ vertices and a total of $n e_{new} = 17$ edges. Both, the original graph and the augmented graphs have no edge weights.

In the augmented graph (see Definition 3.1) two original vertices $v_{i1}$ and $v_{i2}$, referred to as structure vertices, can be close either if they are connected through other structure vertices, or if they share attribute vertices as neighbors, or both. In [27, 5] the authors have defined a unified distance measure on the augmented graph using random walks, which estimates the pairwise vertex closeness in the graph through both structure and attribute edges. Using their distance measure, they apply a modified K-means algorithm constituting the so-called Structural/Attribute clustering algorithm (SA-cluster).

In this paper, we follow a different approach which can be seen as a generalization of a spectral clustering algorithm extending the method proposed in [7] to deal with vertex-attributed graphs. In details, after augmentations we compute the s.p.d modified graph Laplacian $L_s$ of the augmented graphs $G'_A$ and embed the graphs in the subspace spanned by the smooth vectors of $L_S$ associated to a composite AMG operator $B_{BAMG}$ as in (2). These smooth vectors, having $n_{new}$ entries are used to represent the original $n$ structure vertices in terms of a set of $1 + m$ scalar components, where the first component is related to the original graph structure information and the resulting $m$ are related to the vertex attributes. In this way, each original (structure) vertex is associated to $m$ additional (attribute) vertices, and can be viewed as a node of $m + 1$ disaggregated vertices (in analogy to [15]). Another analogy can be seen with the representation of a vector field in a physical (2D or 3D) space domain where the value of the field in a space point is represented by a node vector of (2 or 3) scalar components. The latter point of view was our motivation to define later the distance metric (3.1) which is another key ingredient of our method.

3.1. Vertex block-coordinates and new vector-valued Euclidean distance measure.

3.1.1. Vertex block-coordinates. Starting from the augmented graph $G'_A$ associated with the attributed graph $G$, let $\pi_r = (\pi'_1, \ldots, \pi'_n, \ldots, \pi'_{n_{new}}) \in \mathcal{R}^{n_{new}}$ be a smooth vector computed for the augmented graph Laplacian of $G'_A$. We recall that the vertices of the augmented graph come with double subscripts; namely, structure vertex $v_i$ is indexed as $v_{i,1}$ whereas all its attribute neighbors $v_{j,k}$ are indexed such that for attribute $j = 1, 2, \ldots, m$ we have $l_j(v_i) = v_{j,k}$ (the value from the domain of $l_j$).
According to this convention (applying it to the indices of the smooth vectors), we can partition the values of any smooth vector in blocks, where each block will correspond to a structure vertex and its \( m \) attribute neighbors. That is, we can form block coordinate vectors \( v^r_i = (\pi^r_{i,j})_{j=1}^{m+1} \) for each structure vertex \( v_i \) and each smooth vector \( \pi_r \) where, as already indicated, we let \( \pi^r_{i,1} = \pi^r_i \), and \( \pi^r_{i,j+1} = \pi^r_{j,k} \) if \( l_j(v_i) = v_{j,k} \), \( \forall j = 1, \ldots, m \). In this way, the original graph vertices will have the same coordinate \( \pi^r_{j,k} \) if they share the same attribute value \( v_{j,k} \) on a given attribute \( l_j \), so that vertices sharing an attribute value belong to the same hyperplane corresponding to that value.

In Fig. 2 we draw in a 3D space a picture of the coordinates representing the 4 original graph vertices obtained by using only 1 smooth vector generated by the bootstrap algorithm applied to the augmented graph Laplacian. We fix the coordinate related to the structure information on \( x \)-axis and use a combination of the other 3 coordinates associated to the attributes as \( y \)- and \( z \)-coordinates. We also draw the planes corresponding to the same attribute values, so that vertices sharing attribute coordinates belong to the same plane.

3.1.2. Distance metric. After assigning to each structure vertex \( v_i \) a block “augmented” smooth vector component \( v^r_i \in \mathbb{R}^{1+m} \), it is straightforward to define a distance between any two structure vertices \( v_{i_1} \) and \( v_{i_2} \) based on these \((1+m)\)-vector coordinates.

Let \( n_c \) be the number of smooth vectors obtained by the bootstrap AMG applied to the augmented graph Laplacian \( L_S \) and let \( v_{i_1} = (\pi^r_{i_1,j})_{j=1,r=1}^{m+1,n_c} \) and \( v_{i_2} = (\pi^r_{i_2,j})_{j=1,r=1}^{m+1,n_c} \) be the block-coordinates of the vertices, then we let

\[
dist(v_{i_1}, v_{i_2}) = \sqrt{\sum_{r=1}^{n_c} \| \pi^r_{i_1} - \pi^r_{i_2} \|^2},
\]

where \( \| \pi^r_{i_1} - \pi^r_{i_2} \|^2 \) is the square of the usual Euclidean distance between the block components \((\pi^r_{i_1,j})_{j=1}^{m+1} \) and \((\pi^r_{i_2,j})_{j=1}^{m+1} \). Once we have a distance measure defined, we are able to apply a standard \( K \)-means clustering algorithm for the set of structure vertices.

We implemented all the functionalities needed to apply our new clustering algorithm for attributed graph in the software framework described in [8]. The extended code to deal with graphs, including our clustering procedures also employing networks with attribute vertices, has been made available with the new name BCMatch4Graphs at [https://github.com/bootcmatch/BCMatch4Graphs](https://github.com/bootcmatch/BCMatch4Graphs).

4. Numerical Results

In the present section, we study the clustering quality of our method described in section 3 on both synthetic and some real-life attributed graphs available from public repositories.

Also, we compare our algorithm with several existing clustering methods, whose implementation is freely available, some of which also use information on vertices attributes. We consider both, methods that do not incorporate attribute information
and others that do employ such attribute information. More specifically, we consider the following attribute-free methods:

- Louvain method (Lou) is a greedy optimization method that attempts to maximize the modularity of a partition of the graph by a multilevel algorithm [3];
- Fast Greedy method (FG) is also a greedy method which tries to maximize modularity by a hierarchical agglomeration algorithm [6];
- BCMG is our original method, available in BCMatch4Graphs and based on the bootstrap AMG for the Laplacian graph [7]. We point out that default algorithmic parameters for setup of the method are applied, as discussed in [4] while a required accuracy of $10^{-6}$ is fixed for the final operator in [2,4].
Then we consider the following clustering methods that employ information on vertices attributes:

- **Newman** is the method described in [19]. It uses a techniques of Bayesian statistical inference to fit a suitable network model to the available data, trying to find a possible partition correlated to the attributes;
- **BAGC** is a model-based approach to attributed graph clustering. It also relies on a Bayesian probabilistic model which tries to fit both structural and attribute aspects of networks [25];
- **BCMAG** is the new clustering method based on the augmented graph described in this paper and implemented in BCMatch4Graphs. The bootstrap algorithm for augmented graph embedding is applied in the same conditions of the above BCMG method.

We note that Lou and FG are implemented in the R package igraph. BAGC is available on the git hub repository [26]. Software implementing Newman is available as supplementary material of [19]. Finally, let us point out that we were not able to compare our results with the SA-cluster method described in [27, 5] because, at the best of our knowledge, the related code is not available.

### 4.1. Simulation framework.

In order to assess the overall proposed methodology we started from a Stochastic Block Model SBM [14] to generate random graphs. Assume there are q sets of vertices in a graph, a SBM is specified by the expected fraction of vertices in each set \( n_a \), \( 1 \leq a \leq q \), and by the probability \( p_{ab} \) of an edge between set \( a \) and set \( b \) \( \forall a,b \in [1,\ldots,q] \). These probabilities form a matrix \( P \) that is commonly referred to as affinity matrix. We focus on a simple well-known (cf., [11]) SBM called **planted** graph. The planted model is a special SBM case in which the values of the probability in the affinity matrix \( P \) are equal to a constant \( p_{\text{in}} \) on the diagonal and equal to another constant \( p_{\text{out}} \) off the diagonal; thus, two vertices within the same set share an edge with probability \( p_{\text{in}} \), while two vertices in different sets share an edge with probability \( p_{\text{out}} \). In particular, if \( p_{\text{in}} > p_{\text{out}} \) the model is called assortative, while if \( p_{\text{in}} < p_{\text{out}} \) the model is called dis-assortative. In our simulations we assume an assortative structure, so that \( p_{\text{in}} > p_{\text{out}} \). We generate a SBM random graph \( G \) of \( n \) vertices partitioned into \( q \) sets, \( C_1,\ldots,C_q \), with adjacency matrix \( A_{ij} = 1 \) if there is an edge between vertices \( i \) and \( j \), and 0 otherwise; more specifically, we consider Bernoulli trials for each potential edge with the probabilities given by the affinity matrix, so that the corresponding adjacency matrix has entries defined as follows:

\[
A_{rs} | \ r \in C_a \ s \in C_b \sim \text{Bern}(p_{ab}), \ \forall r,s \in [1,\ldots,n]
\]  

(4.1)

where for \( a,b \in [1,\ldots,q] \):

\[
p_{ab} = \begin{cases} p_{\text{in}} & \text{if } a = b \\ p_{\text{out}} & \text{otherwise} \end{cases}
\]

(4.2)

Note that the probabilities are defined in such a way that the average vertex degree is a given \( c \). Each vertex has a label in \([1,\ldots,q]\), indicating which set it belongs to. A
study presented in [11] identifies conditions under which polynomial-time algorithms can find a partition that is correlated with the planted partition. More specifically, this is possible when

\[ p_{in} - p_{out} > \frac{\sqrt{qp_{in} + q(q - 1)p_{out}}}{\sqrt{n}}. \]

This implies that, depending on the generative parameter values, this condition might not be satisfied. It is often convenient to work with a scaled affinity matrix so that \( c_{ab} = np_{ab} \), and then we can write \( p_{in} = \frac{c_{in}}{n} \) and \( p_{out} = \frac{c_{out}}{n} \). In this case, the average degree of the graph can be expressed as:

\[ c = \sum_{a,b} c_{ab}p_{a}p_{b}, \]

that in our case can be simplified as:

\[ c = \frac{q - 1}{q} c_{out} + \frac{1}{q} c_{in}. \]

Rewriting (4.3) in terms of \( c_{in} \) and \( c_{out} \), we have:

\[ c_{in} - c_{out} > q\left[ c_{in} + (q - 1)c_{out}\right], \]

and from (4.4) we finally obtain:

\[ c_{in} - c_{out} > q\sqrt{c}. \]

We observe that when \( c_{in} \) is much greater than \( c_{out} \) the graph shows a strong cluster structure, while such structure becomes weaker when \( c_{in} \) is close to \( c_{out} \), then in the following we are implicitly measuring the strength of the set/cluster structure by the difference \( c_{in} - c_{out} \).

The strength of division of a graph into clusters can be measured by the modularity [18]. It can be broadly defined as the fraction of the edges that fall within the given set minus the expected value of such fraction if edges were distributed at random, in details:

\[ Q = \frac{1}{2ne} \sum_{ij} [A_{ij} - \frac{c_{i}c_{j}}{2ne}]\delta(C_{i},C_{j}), \]

where \( ne \) is the number of edges in the whole graph, \( c_{i}, c_{j} \) are the degree of vertices \( i \) and \( j \) respectively, \( A = \langle A_{ij}\rangle_{ij} \) is the adjacency matrix of the graph, \( \delta(C_{i},C_{j}) \) is equal to 1 if vertices \( i \) and \( j \) belong to the same cluster and 0 otherwise. Graphs with high modularity have dense connections between vertices within clusters but sparse connections across clusters. We observe that \( Q \in [-1, 1] \) and it is often used to evaluate the quality of a partition obtained by a clustering method. Furthermore, many clustering methods are based on optimization algorithms which try to maximize modularity, e.g. Lou and FG.

In some cases it is expected that a graph has natural partition into clusters referred to as ground truth. Clustering methods aim to estimate such a true partition. In our simulation framework the ground truth is known and a high modularity corresponds
to \( c_{in} >> c_{out} \), while a low modularity corresponds to \( c_{in} \sim c_{out} \). We varied the difference \( c_{in} - c_{out} \) above and below the so-called detectability threshold \( q \sqrt{c} \), given a specific set of average degrees \( c \in [5, 10, 15, 20] \) and number of clusters \( q \in [2, 3, 4, 5] \). In the following discussion, we use the true labels, i.e., the index of the cluster that a vertex belongs to as vertex attribute, so vertices in the same cluster have the same attribute.

4.2. Evaluation Metrics. In order to analyze the obtained results, we employ standard metrics which allow us to compare two different clusterings and then quantify the performance of the clustering algorithms when the ground truth is given. Let \( \mathcal{C}' \) be the ground truth, and \( \mathcal{C} \) be the estimated partition obtained by a given clustering method, in the following we define Normalized Mutual Information (introduced in [10]), Entropy and Gain.

Given the graph \( G \) and two partitions \( \mathcal{C} = \mathcal{C}_1, \ldots, \mathcal{C}_K \) and \( \mathcal{C}' = \mathcal{C}'_1, \ldots, \mathcal{C}'_{K'} \), with \( K \) and \( K' \) non empty sets, respectively, we consider

- \( p(k) \) to be the probability of a vertex to belong to group \( \mathcal{C}_k \).
- \( p(k, k') \) to be the probability that a vertex belongs to set \( \mathcal{C}_k \) from \( \mathcal{C} \) and to the group \( \mathcal{C}'_{k'} \) from partition \( \mathcal{C}' \).

If we set \( n_k = |\mathcal{C}_k| \) and \( n_{k, k'} = |\mathcal{C}_k \cap \mathcal{C}'_{k'}| \), we can define \( p(k) = n_k/n \) and \( p(k, k') = n_{k, k'}/n \).

\( NMI \) is defined as:

\[
NMI(\mathcal{C}, \mathcal{C}') = \frac{I(\mathcal{C}, \mathcal{C}')}{H(\mathcal{C}) + H(\mathcal{C}')},
\]

where \( H(\mathcal{C}) \) is the entropy associated with partition \( \mathcal{C} \):

\[
H(\mathcal{C}) = -\sum_{k=1}^{K} p(k) \log(p(k)),
\]

and \( I(\mathcal{C}, \mathcal{C}') \) is the mutual information between \( \mathcal{C} \) and \( \mathcal{C}' \), i.e., the information that one partition has about the other:

\[
I(\mathcal{C}, \mathcal{C}') = \sum_{k=1}^{K} \sum_{k'=1}^{K'} p(k, k') \log \frac{p(k, k')}{p(k)p(k')}.
\]

Note that \( NMI \in [0, 1] \), and two partitions can be considered in good agreement when \( NMI \approx 1 \).

Given the entropy \( H(\mathcal{C}) \) and \( H(\mathcal{C}') \) of two clusterings, the cluster-specific entropy of \( \mathcal{C}' \), that is the conditional entropy of \( \mathcal{C}' \) with respect to cluster \( \mathcal{C}_k \), is defined as:

\[
H(\mathcal{C}'|\mathcal{C}_k) = -\sum_{k'=1}^{K'} \frac{n_{k, k'}}{n_k} \log \left( \frac{n_{k, k'}}{n_k} \right),
\]

The conditional entropy of \( \mathcal{C}' \) given clustering \( \mathcal{C} \) is then defined as the weighted sum:

\[
H(\mathcal{C}'|\mathcal{C}) = \sum_{k=1}^{K} \frac{n_k}{n} H(\mathcal{C}'|\mathcal{C}_k) = -\sum_{k=1}^{K} \frac{n_k}{n} \sum_{k'=1}^{K'} \frac{n_{k, k'}}{n_k} \log \left( \frac{n_{k, k'}}{n_k} \right).
\]
The (4.9) suggests that the more cluster’s members are split into different partitions, the higher the conditional entropy. If \( C' \) represents the ground truth, for a perfect clustering the conditional entropy value, which for the sake of brevity we refer to as entropy in the rest of the paper, should be zero.

Suppose we want to measure if a certain partition reduces the overall entropy and hence is more informative. The measure that we suggest to look at is called \textit{Information Gain}, or more simply, \textit{Gain}. Information Gain is the expected reduction in entropy caused by partitioning the vertices according to a given partition \( C \). It is defined as the difference between the absolute entropy of the clustering \( C' \) and the conditional entropy \( H(C'|C) \):

\[
IG(C', C) = H(C') - H(C'|C)
\]

\textbf{4.3. Clustering evaluation for SBM graphs.} In Figures 3-6, we show a summary of the results obtained for \( n = 400 \) vertices, \( q = 2, 4 \), and \( c = 5, 20 \). In our simulated data the ground truth labels are known and we plot the corresponding modularity in subfigure (A) of every plot. As you can see, our new method \textit{BCMAG} perfectly matches with the truth also under the detectability threshold, especially for \( q = 2 \). Furthermore, it improves results, in a more significant way when vertex degree and then graph density increases, with respect to the \textit{BCMG} method which does not employ attribute information. On the other hand, we expect that a method that does not use the attributes will fail below the detectability threshold. Indeed the two methods \textit{FG} and \textit{Lou}, that do not use the labels and tend to maximize the Modularity, show an overall overestimation of the Modularity in the case of sparse graphs (\( c = 5 \)).

The methods \textit{Newman} and \textit{BAGC}, although using vertices attributes, find partitions with a small Modularity. If we look at the \( NMI \), Entropy and Gain values, we can see that in all cases for \( q = 2 \), our new method \textit{BCMAG} has perfect values also below the detectability threshold, while for \( q = 4 \), some discrepancy is observed when \( c_{in} - c_{out} \) is very small. It is worth noticing that \textit{NMI} and Entropy values for \textit{Newman} and \textit{BAGC}, although using information on attributes, are not satisfactory especially for sparser graphs (\( c = 5 \)).

\textbf{Perturbation analysis.} In this section we investigate the effect of randomness in the ground truth (i.e., the given true partition), using a permutation strategy. We simulate the case in which the ground truth is affected by bias. Here we consider a single attribute representing the true partition. Ideally, a perfect attributed graph clustering method would be robust with respect to bias in the labels, in graphs where \( c_{in} - c_{out} \) is greater than the detectability threshold. We simulate such scenario via randomly permuting the ground truth labels by a percentage \( \alpha \in [0, 0.5] \) with incremental step 0.1, on the simulation case \( n = 400 \), number of groups \( q = 5 \) and average degree \( c = 10 \).

In Figure 7 we plot a \textit{NMI} curve for each level of perturbation of the labels, ranging from unperturbed (\( \alpha = 0\% \)) to the maximum level of perturbation (\( \alpha = 50\% \)). In particular, we show the results for \textit{BCMAG} in sub-figure (A), for \textit{Newman} in sub-figure (B) and for \textit{BAGC} in sub-figure (C).
Figure 3. Case $n = 400$, $q = 2$, $c = 5$. In each subplot we indicated the theoretical detectability threshold with a vertical dashed line, and Modularity (A), $NMI$ (B), Entropy (C) and Gain (D) corresponding to the different clustering approaches.

In sub-figure (A) we notice that the $NMI$ curves for $BCMAG$ at perturbation level $\alpha \geq 0.3$ have high variability before the detectability threshold. After the detectability threshold, we see that $NMI \in [0.7, 1]$ for perturbation level $\alpha < 0.5$. This result is very reassuring, because if there is no bias in the labels (i.e., $\alpha = 0$), our methodology obtains $NMI = 1$, even for graphs where $c_{in} - c_{out}$ falls below the detectability threshold, hence ensuring a perfect clustering regardless of the graph
structure. On the other hand, when the perturbation level increases the average NMI decreases, as expected, but it oscillates regardless of the $c_{in} - c_{out}$ when above the detectability threshold. In particular for $\alpha < 0.3$, NMI oscillates between the values 0.85 and 1. In subfigure (B) Newman methodology NMI shows an expected high variability when $c_{in} - c_{out}$ is below the detectability threshold, while above it Newman has a lower NMI when $c_{in} - c_{out}$ increases (the graph has a more modular structure)
and when the perturbation level decreases (there is lower bias in the labels). The drop in \( NMI \) is more evident at higher levels of perturbation. We can speculate that this is due to the fact that the biased labels are driving the clustering over the modular structure of the graph in this case. As you can see in sub-figure (C), \textit{BACG} has a greater \( NMI \) when \( c_{in} - c_{out} \) increases (the graph has a more modular structure) and when the perturbation level decreases (there is lower bias in the labels). As
a consequence of this, the best BCMAG clusterings ($NMI \approx 1$) corresponds to no perturbation and high $c_{in} - c_{out}$. Similarly the worst BCMAG clusterings ($NMI \approx 0$) corresponds to perturbation $\alpha = 0.5$ and high $c_{in} - c_{out}$.

4.4. Real networks. In this section we show the application of our new method on graphs originating by two real data networks that we indicate in the following as Lazega Lawyers and Yeast. A few indicators for these two networks are provided in
Case $n = 400$, $q = 5$ and $c = 10$. $NMI$ curves for each level of perturbation of the labels, ranging from unperturbed ($\alpha = 0\%$) to the maximum level of perturbation ($\alpha = 50\%$). We show the results for $BCMAG$ in sub-figure (A), for $Newman$ in sub-figure (B) and for $BAGC$ in sub-figure (C).

Table\[2\] In particular we indicate the network names, number of vertices $|V|$, number of edges $|E|$, sparsity (defined as $\frac{|E|}{(|V|(|V|-1)/2)}$), average vertex degree $c$, and number of attributes. Further details on experimental setting and discussion of results follow in the subsections.
Table 2. Features of real networks. For each network we show the name, number of vertices $|V|$, number of edges $|E|$, sparsity, average degree $c$ and number of available attributes $m$.

| Name     | $|V|$ | $|E|$ | sparsity | $c$ | $m$ |
|----------|------|------|----------|-----|-----|
| Yeast    | 2375 | 11693| 0.004    | 9.85| 1   |
| eladv    | 71   | 717  | 0.289    | 20.20| 7   |
| eladv36  | 36   | 289  | 0.459    | 16.06| 7   |
| friend36 | 36   | 187  | 0.297    | 10.39| 7   |

*Lazega Lawyers dataset.* The data *Lazega Lawyers* comes from a network study of corporate law partnership that was carried out in a Northeastern US corporate law firm between 1988-1991. It includes measurements of networks among the 71 attorneys (partners and associates) of the firm. In particular, we looked at the advice network (adv) and at the friendship network (friend). Various members’ attributes are also part of the dataset, including seniority, formal status, office in which they work, gender, law school attended, individual performance measurements (hours worked, fees brought in), attitudes concerning various management policy options, etc. The ethnography, organizational and network analyses of this case are available in [16]. The number 36 indicates that subset of data for 36 partners only were considered. In our analysis we considered 7 attributes, namely: status (1=partner; 2=associate), gender (1=man; 2=woman), office (1=Boston; 2=Hartford; 3=Providence), firm years, age, practice (1=litigation; 2=corporate), law school (1: Harvard, Yale; 2: Ucon; 3: other). The 7 attributes have a different number of distinct values, as summarized in Table 3.

| Attribute     | Distinct values |
|---------------|-----------------|
| Status        | 2               |
| Gender        | 2               |
| Office        | 3               |
| Firm years    | 27              |
| Age           | 33              |
| Practice      | 2               |
| Law school    | 3               |

Table 3. Attributes used in the analysis of the *Lazega Lawyers* networks and the corresponding number of distinct values.

The three networks are plotted in Figure 8 where the different colours refer to the cluster labels identified by the *Lou* methodology. In the Figures 10-12 we plot the Modularity and the Entropy associated to the methods *BCMAG, BCMG, BAGC* and *Lou*, respectively in subfigure (A) and (B) for different choice of the clusters’ number $q$. The 7 categories of attributes considered in the analysis of the 3 *Lazega Lawyers* networks show a different number of distinct values, and hence...
there is not an obvious choice of the number of clusters based on the attributes. As a consequence we show the number of clusters suggested by the Lou method and the associated Modularity and Entropy, computed as in \((4.8)\). We note that the available implementation of the Newman methodology can be used when only 1 attribute category is available. As we can see, the Modularity of BCMAG is on average the closest to Lou clustering in every case. On the other hand, the Entropy of BCMAG is the lowest, which indicates a better partition. In all cases the new method appears as a large improvement over our previous method BCMG which does not employ attributes information. It is worth noticing, that in all cases BCMAG shows the best entropy value when \(q = 7\), indicating a good agreement with the partition based on attribute categories. The corresponding clusterings are plotted in figure 9.

**Yeast dataset.** In this subsection, we apply the described methodologies to a comprehensive protein-protein interaction network, that we refer to as Yeast. This biological network aims to reveal many aspects of the complex regulatory network underlying the cellular function. This data set was compiled by [24], combining various sources. Only the interactions that have “high” and “medium” confidence are included in the analysis. The network is plotted in Figure 13, where the different colours refer to the 23 cluster labels identified by the Lou methodology. The data were downloaded from [2] and are also available in the R package igraphdata. We analysed the maximum connected component using as metadata the single label of the 13 protein classes described in [1]. Note that 39 out of the 2375 network proteins had not given class label. We considered each of them as belonging to an individual class. This resulted in a total of 2375 + 13 + 39 augmented graph nodes. In Figure 14 we plot the Modularity (sub-figure (A)) and the Entropy (sub-figure (B)) corresponding to the clustering provided by BCMAG, BCMG, BAGC, Newman, computed as in \((4.9)\) when \(C'\) is the ground truth represented by the attribute labels. We also provide values obtained by Lou and the attribute labels (as the ground truth), in this case the Entropy is computed as in \((4.8)\). In this example, as said, we have one single set of labels indicating the protein class. Intuitively, we could consider as number of clusters \(q = 13\) (vertical cyan line), corresponding to the distinct classes provided in the labels. In Figure 13, we plot the network where colours correspond to the different clusters identified with BCMAG when \(q = 13\). Alternatively, as in the previous example, we could use the number of clusters \(q = 23\) found by Lou (vertical brown line). As a consequence the most interesting area of the plots falls in the area \(13 \leq q \leq 23\). As we can see in sub-figure (A), the lowest Modularity corresponds to the protein labels clustering. This indicates that the attributes provide low separation between the proteins in this case. Note that the Modularity of all the methodologies is less oscillating when \(13 \leq q \leq 23\). Moreover, the Modularity values provided by Newman and BCMG are closer to the Modularity of Lou, while BCMAG and BAGC provide Modularity values that are closer to the labels Modularity. In particular, the BCMAG Modularity curve offers a trade off between using the labels or not. Indeed the BCMAG Modularity values are on average halfway between the horizontal cyan line (Lou Modularity) and the brown horizontal line (labels Modularity).
Lazega Lawyers Networks. The different colours refer to the Lou cluster labels. Subfigures (A), (B) and (C) show the adv, adv36 and friend36 networks respectively.

If we look at the Entropy in sub-figure (B), the general trend of the 4 methodologies BCMAG, BCMG, BAGC and Newman is to have a decreasing Entropy (conditioned on the true labels) for increasing number of clusters $q$. The lowest Entropy is reached by BCMAG for any $q \in [3, 31]$. The maximum absolute Entropy is associated with the labels partition (cyan horizontal line). As a consequence BCMAG has the maximum Gain and hence appears as the most informative clustering.
Conclusions

In this work we extend a clustering method for undirected graphs to employ possible additional information, such as vertex attributes, in order to improve clustering detection and quality. The new method relies on an already proposed augmentation of the graph which incorporates vertex attributes in the graph in terms of new vertices and
new edges. Starting from this augmentation we embed the graph in a low-dimensional vector space spanned by some near-null vectors computed by an adaptive AMG process approximating small eigenvalues of the augmented graph Laplacian. Each such vector is appropriately used to build $1 + m$ coordinates, where $m$ is the number of attributes, of the original graph vertices, so that vertices sharing an attribute value
Figure 12. Modularity (A) and Entropy (B) corresponding to the friendship network of the Lazega dataset, considering only 36 partners.

are in the same hyperplane defined by that value. We also defined a modified Euclidean distance so that the new method was able to detect clusters by applying a modified K-means optimization algorithm. Experimental results show that the new method largely outperforms the old approach which ignores the attributes and it is also better than some of the available methods employing attributes information. One limitation of our approach relies on the fact that it can only be computationally feasible for categorical attributed networks. Moreover our approach would require high computational cost when the number of distinct attributes values is high. Feature selection or attributes transformation could be explored to address these issues. Further development would be needed to handle missing data or sparse attributes.

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Figure 13. Yeast protein-protein interaction network. Colours correspond to the clusters labels: Lou (top) and BCMAG, with $q = 13$ (bottom).
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