Non-linear Attributed Graph Clustering by Symmetric NMF with PU Learning

Seiji Maekawa1, Koh Takeuchi2, Makoto Onizuka1

1Graduate School of Information Science and Technology, Osaka University, 1–5 Yamadaoka, Suita, Osaka, Japan
2NTT Communication Science Laboratories, 2–4 Hikaridai, Seika, Soraku, Kyoto, Japan

{maekawa.seiji, onizuka}@ist.osaka-u.ac.jp, koh.t@acm.org

Abstract

We consider the clustering problem of attributed graphs. Our challenge is how we can design an effective and efficient clustering method that precisely captures the hidden relationship between the topology and the attributes in real-world graphs. We propose Non-linear Attributed Graph Clustering by Symmetric Non-negative Matrix Factorization with Positive Unlabeled Learning. The features of our method are three holds. 1) it learns a non-linear projection function between the different cluster assignments of the topology and the attributes of graphs so as to capture the complicated relationship between the topology and the attributes in real-world graphs. 2) it leverages the positive unlabeled learning [Liu et al. 2003] to take the effect of partially observed positive edges into the cluster assignment, and 3) it achieves efficient computational complexity, $O((n^2 + mn)kt)$, where $n$ is the vertex size, $m$ is the attribute size, $k$ is the number of clusters, and $t$ is the number of iterations for learning the cluster assignment. We conducted experiments extensively for various clustering methods with various real datasets to validate that our method outperforms the former clustering methods regarding the clustering quality.

Introduction

Graph is a fundamental data structure for representing vertices and their relationships. Graph data appear everywhere in many application domains, such as web graph [Flake et al. 2002], social network [Fortunato 2010], protein complexes [Brohee and Van Helden 2006], traffic planning [George, Kim, and Shekhar 2007], computer vision [Jain et al. 2016], and gene expressions [Ben-Dor and Yakhini 1999; Kulis et al. 2009]. The authors of [Sahu et al. 2017] conducted an online survey and showed that graph database is becoming increasingly prevalent across many application domains and, in particular, the graph clustering is the most widely used technique in machine learning and data mining fields.

Graphs in the real world usually have attributes on vertices. Actually, the graph databases support attributed graphs [Francis et al. 2018; Sevenich et al. 2016]. However, most of the graph clustering techniques [Newman 2006; Xu et al. 2007; Karypis and Kumar 1998b] do not leverage the attributes of vertices since their design is limited to simple graphs without having attributes. Therefore, these techniques can not extract precise clusters without leveraging the attributes.

There are emerging researches that tackle the clustering problem for attributed graphs [Huang et al. 2017; Xu et al. 2012; Akoglu et al. 2012; Parimala and Lopez 2015; Zhou, Cheng, and Yu 2009; Zhou, Cheng, and Yu 2010]. Despite the considerable improvements made by the existing methods, they have not fully leveraged the virtue of attributed real-world graphs. That is, there are two missing aspects of the attributed graphs we should consider for designing effective clustering methods. First, the topology and the attributes of real-world graphs have a complicated relationship with each other, that is, they would have different cluster structures in general, because the topology and attributes are obtained from different viewpoints of the similarity of vertices. Second, typical graphs usually have a subset of positive edges, since real-world graphs follow the open world assumption, that is “absence of information is interpreted as unknown information, not as negative” (Keet 2013). For example, a social graph may not reflect precisely the social connections in the real world: we can only observe positive connections between people such as “likes” and “friendships”, but cannot observe negative ones [Hsieh, Natarajan, and Dhillon 2015]. In addition, there is a possibility of missing positive edges among pairs of vertices where no edges were observed in the graph.

We take the above two aspects into account and propose NAGC, Non-linear Attribute Graph Clustering by Symmetric Non-negative Matrix Factorization with Positive Unlabeled Learning. To achieve high clustering quality, 1) our method flexibly captures the complex relationship among the topology and the attributes by learning a non-linear projection function among their different cluster assignments, and 2) our method leverages PU learning [Elkan and Noto 2008; Liu et al. 2003; Hsieh, Natarajan, and Dhillon 2015] to take the effect of partial positive edges and no edge observations into the cluster assignment. To the best of our knowledge, our method is the first method that applies the idea of PU learning to the graph clustering. Our method can precisely capture clustering results by revealing the relationship
between the topology and the attributes in real-world graphs. As for the efficiency, we carefully design the learning model of our method so that its cost does not contain the quadratic effect of the number of attributes. Thus, our method is scalable to the number of attributes, which is usually large in real-world graphs (See the statistics of the graphs in Table 2 in the experiment section).

We extensively made experiments for various clustering methods over various real datasets with ground truth. We compared our method with the former clustering methods in terms of the clustering quality by leveraging the different but related cluster structures among the topology and the attributes. We also confirm that our method is stable against the hyperparameter selection.

The rest of this paper is organized as follows. We introduce fundamental techniques for our method, Non-negative Matrix Factorization, Symmetric Non-negative Matrix Factorization, and Biased Matrix Completion in the preliminary section. We propose our method in the section of non-linear factorization, and Biased Matrix Completion in the preliminary section. We can put an orthogonal constraint on factor matrices to get precise clusters. This method is limited to consider linear relationships among clusters of vertices and attributes.

Symmetric Non-negative Matrix Factorization

The goal of graph clustering is to find a partition of vertices in a graph where the similarity between vertices is high within the same cluster and low across different clusters. To capture such a cluster structure embedded in a graph, Kuang et al proposed Symmetric Non-negative Matrix Factorization (SNMF) (Kuang, Yun, and Park 2015; Kuang, Ding, and Park 2012), and showed an interesting relationship among SNMF and graph clustering methods including the spectral clustering (Ng, Jordan, and Weiss 2002).

SNMF estimates a cluster assignment matrix \( U \) by minimizing a non-convex loss function that uses \( S \) as input:

\[
\min_{U \geq 0} \left\| S - UV^T \right\|_F^2
\]

In the same manner as NMF, we can obtain a clustering result by assigning \( i \)-th vertex to the \( k_i \)-th cluster that has the largest value in \( u_i \), that means \( k_i = \arg\max \{ u_{i,l} \mid l = 1, \ldots, k \} \).

Biased Matrix Completion

Hsieh et al. (Hsieh, Natarajan, and Dhillon 2015) considered a matrix completion problem when only a subset of positive relationships is observed, such as recommender systems and social networks where only “likes” or “friendships” are observed. The problem is an instance of PU (positive-unlabeled) learning (Elkan and Noto 2008; Liu et al. 2003), i.e. learning from only positive and unlabeled examples that has been studied in the classification problems. They introduced the \( \rho \)-weighted loss for a bipartite graph \( G' = (V', E') \) comprising a set of vertices \( V' = \{ 1, 2, \ldots, n \} \) and edges \( E' = \{ (i, j) \mid (i, j) \subseteq [n] \times [m] \} \):

\[
\ell_{\rho}(z_{i,j}) = \rho 1_{(i,j) \in E'}(z_{i,j} - 1)^2 + (1 - \rho) 1_{(i,j) \notin E'} z_{i,j}^2
\]

where \( \rho = [0, 1] \), \( 1_{(i,j) \in E'}(\cdot) \), and \( 1_{(i,j) \notin E'}(\cdot) \) are a bias weight, an indicator function for positive edges, and an indicator function for unlabeled edges, respectively. This loss can change a weight for reconstruction errors among positive and unlabeled edges. When we set \( \rho = 0.5 \), it treats the positive and unlabeled entities equally. With this loss, they proposed a biased matrix completion as:

\[
\min_{Z \ni Z^\prime} \sum_{(i,j) \in E'} \rho (z_{i,j} - 1)^2 + \sum_{(i,j) \notin E'} (1 - \rho) z_{i,j}^2
\]

where \( \lambda \geq 0 \) is a hyperparameter. To the best of our knowledge, no method based on SNMF has employed the biased formulation of matrix completion problems.
Table 1: Definition of main symbols.

| Variable | Explanation |
|----------|-------------|
| $S \in \mathbb{R}^{n \times n}$ | adjacency matrix |
| $X \in \mathbb{R}^{m \times n}$ | attribute matrix |
| $U \in \mathbb{R}^{n \times k_1}$ | cluster assignment matrix |
| $V \in \mathbb{R}^{m \times k_2}$ | attribute factor matrix |
| $H \in \mathbb{R}^{k_1 \times k_2}$ | cluster assignment transfer matrix |
| $W \in \mathbb{R}^{n \times m}$ | mask matrix of $S$ |
| $k_1 \in \mathbb{N}$ | number of clusters |
| $k_2 \in \mathbb{N}$ | number of clusters for attributes |
| $\lambda \geq 0$ | balancing parameter between the topology and the attributes |
| $\rho \in [0, 1]$ | bias weight for $S$ |
| $t \in \mathbb{N}$ | number of iterations |

Non-linear Attribute Graph Clustering

In this section, we propose a variant of NMF that can find a reasonable cluster assignment by considering the complex relationship between the topology and the attributes. We also attempt to mitigate the serious problem of the partial positive edges that prevents us from capturing a precise assignment by leveraging the idea of the biased matrix completion. Table 1 lists the main symbols and their definitions.

Our method jointly decomposes the adjacency matrix $S$ and the attribute matrix $X$ into factor matrices with learning a non-linear projection function. This function can transfer a cluster assignment extracted from the adjacency matrix to that from the attribute matrix. Here, we define our method as a minimization problem of a non-convex loss.

$$\min_{U, V, H \geq 0} \mathcal{L}_\rho(S - UU^\top) + \frac{\lambda}{2} \| X - f(UH)V^\top \|^2_F$$ (6)

where $f$ denotes an element-wise non-linear activate function. We use $\mathcal{L}_\rho(Z)$ to denote an approximation error of the adjacency matrix $S$ with the $\rho$-weighted loss.

$$\mathcal{L}_\rho(Z) = \sum_{(i,j) \in E} \rho(z_{i,j} - 1)^2 + (1 - \rho) \sum_{(i,j) \notin E} z_{i,j}^2$$ (7)

We employ the sigmoid function as a non-linear activation function in this paper: $f(x) = \frac{1}{1 + e^{-x}}$. This choice can be generalized to any non-linear functions. Note that, in the second term of Eq. (6), $f(UH)$ plays the role of the cluster assignment matrix for the attribute matrix. By transforming $U$ with $f$ and $H$, our method enables to capture the complex relationship among the topology and the attributes. Our method works as SNMF when $\lambda = 0$ and $\rho = 0.5$. We illustrate our proposed method in Figure 1.

Since our loss is non-convex for $U$, $V$, and $H$, we derive a parameter estimation procedure that alternatively updates each parameter by utilizing the method of Lagrange multipliers (Ding et al. 2006). Following the standard theory of constrained optimization, we introduce Lagrangian multipliers $\alpha \in \mathbb{R}^{n \times k_1}$, $\beta \in \mathbb{R}^{m \times k_2}$, and $\gamma \in \mathbb{R}^{k_1 \times k_2}$ for the non-negative constraints $U, V, H \geq 0$. We define the Lagrangian function of our proposed method as:

$$\mathcal{L}(U, V, H; \alpha, \beta, \gamma) = \mathcal{L}_\rho(S - UU^\top) + \frac{\lambda}{2} \| X - f(UH)V^\top \|^2_F + \text{Tr}(\alpha^\top U) + \text{Tr}(\beta^\top V) + \text{Tr}(\gamma^\top H)$$ (8)

For each parameter $U$, $V$, and $H$, we derive partial differentials of the Lagrangian function.

$$\frac{\partial \mathcal{L}}{\partial U} = -2\rho S - \lambda \{(XV) \odot f'(UH)\}H^\top + 2\rho (UU^\top \odot W)U + 2(1 - \rho)(UU^\top \odot W')U + \lambda \{(f(UH)V^\top V) \odot f'(UH)\}H^\top + \alpha$$ (9)

$$\frac{\partial \mathcal{L}}{\partial V} = -\lambda X^\top f(UH) + \lambda V f(UH)^\top f(UH) + \beta$$ (10)

$$\frac{\partial \mathcal{L}}{\partial H} = -\lambda U^\top \{f'(UH) \odot (XV)\} + \lambda U^\top \{f'(UH) \odot f(UH)\}V^\top V + \gamma$$ (11)

where $W \in \mathbb{R}^{n \times n}$ is a mask matrix whose elements are set as $w_{i,j} = 1$ if $s_{i,j} \neq 0$ or $w_{i,j} = 0$ otherwise and $W' = 1 - W$. The KKT complementarity conditions for the non-negative constraints of parameters are:

$$\alpha \odot U = 0, \beta \odot V = 0, \gamma \odot H = 0$$ (12)

$$\frac{\partial \mathcal{L}}{\partial U} = 0, \frac{\partial \mathcal{L}}{\partial V} = 0, \frac{\partial \mathcal{L}}{\partial H} = 0$$ (13)

By satisfying these conditions, we can derive multiplicative


Algorithm 1 NAGC algorithm

**Input:** $S, X, k_3, k_2, \lambda, t$

**Output:** clustering result $C$

1. Preprocess: $S, X$
2. Initialize: $U, V, H$
3. while $t' < t$ do
   4. # alternatively update parameters
      5. $U(t'+1) \leftarrow$ update $(U(t'))$ by Eq. (14)
      6. $V(t'+1) \leftarrow$ update $(V(t'))$ by Eq. (15)
      7. $H(t'+1) \leftarrow$ update $(H(t'))$ by Eq. (16)
8. end while
9. while $n' < n$ do
   10. # assign each vertex to the clusters
    11. $c_{n'} \leftarrow \arg\max_l\{u_{n'l} | l = (1, \ldots, k)\}$
12. end while

update rules for each parameter.

$$
U \leftarrow U \odot \left[2\rho SU + \lambda\{(XV) \odot f'(UH)U^\top\}\odot
\left[2\rho(UU^\top \odot W)U + 2(1-\rho)(UU^\top \odot W')U + \lambda\{(f(UH)V^\top V) \odot f'(UH)\}U^\top\right]\right]
\hspace{1cm} (14)
$$

$$
V \leftarrow V \odot \{X^\top f(UH)\} \odot \{Vf(UH)^\top f(UH)\}\odot
\left[U^\top \{f'(UH) \odot (XV)\}\odot
\left[U^\top \{f'(UH) \odot f(UH)\}V^\top V\right]\odot
\right]$$
\hspace{1cm} (15)

$$
H \leftarrow H \odot \left[U^\top \{f'(UH) \odot (XV)\}\odot
\left[U^\top \{f'(UH) \odot f(UH)\}V^\top V\right]\odot
\right]$$
\hspace{1cm} (16)

Our loss is convex with respect to $V$ and $H$, however, as mentioned in (Kuang, Ding, and Park 2012), the loss is a fourth-order non-convex function with respect to $U$. That means, it is difficult to guarantee the monotonic convergence of our parameter estimation method; thus we expect a good convergence property that every limit point is a stationary point. We show the parameter estimation and clustering algorithm for our proposed method in Algorithm 1.

Since non-convex minimization problems have multiple local minima, we employ two popular methodologies for initializing the parameters $U, V$ and $H$. One is to use random values that is a typical way for matrix factorization. The other is to put the result of k-means as initial values of $U$ and $V$. $H$ is initialized by random values in both cases because there is no corresponding information to $H$.

Computational complexity

Here, the computational complexity is discussed. We stop our algorithm at $t$ iterations, then the overall cost for SNMF is $O(n^2kt)$ (Kuang, Yun, and Park 2015, Kuang, Ding, and Park 2012). JWNMF that is the state-of-the-art method for the attributed graph clustering needs $O((n^2 + m^2 + mn)kt)$ (Huang et al. 2017) because it computes extra parameters for the joint factorization and parameter selections. Our proposed method does not need to calculate $A$ in Eq. (17) thus the overall cost for updating rules is equal to $O((n^2 + mn)kt)$ where $k = \max(k_1, k_2)$ and $k \ll n$. Therefore, our proposed method is much faster than JWNMF and almost the same as the original SNMF when $m \ll n$.

Experiments

The first goal of the experiments is to show our method outperforms JWNMF (Huang et al. 2017), the state-of-the-art method for attributed graph clustering. Let us start from the visualized clustering result for WebKB dataset (see the following subsection for the details of the dataset), which is shown in Fig. 2. We observe that both two methods successfully assign the clusters to the vertices located near the center. However, JWNMF fails to assign the precise clusters to many surrounding vertices ("x" indicates the assignment error in the figure). We investigated the reason and found that JWNMF ignores the effect of most attributes and this prevents JWNMF to learn the precise cluster assignment. This is caused by the limitation of JWNMF: it only learns a simple relationship between the topology and the attributes to have the same clustering structure. In contrast, our method successfully assigns the precise clusters. It learns a nonlinear projection function among the different cluster assignments of the topology and the attributes.

The WebKB dataset is not a special case our method works well. Our second goal of the experiments is to evaluate the clustering quality and efficiency of our method for various datasets. We evaluate our method with the former methods, JWNMF and BAGC (Xu et al. 2012), those are designed for attributed graphs. We also evaluate simple graph clustering methods without using attributes, METIS (Karypis and Kumar 1998a) and SNMF, and attribute-based clustering methods, NMF and k-means, so that how much only the topology or attributes of the graphs contribute to the clustering quality. We used publicly available codes for the existing methods in our experiments. To investigate the details of the quality improvement achieved by our method, we also evaluate the effectiveness...
of PU learning and the effect of the hyperparameters. We perform five restarts for each method and calculate the average and standard deviation of the results.

Datasets
Four real-world datasets with the ground truth are employed in our experiments. WebKB$^1$ is the web graph of four universities: the label for a vertex indicates the owner university of the page. The attributes of a vertex represent the words appeared in the page. Citeseer and Cora (see also footnote$^3$ for detail) are citation networks. The label for a vertex corresponds to a research field of the paper. The attributes of a vertex consist of the words appeared in the paper. Polblog$^4$ is a network of hyperlinks between blogs on US politics: the label of a vertex indicates whether the blog is liberal or conservative. The attributes of a vertex represent the sources of the blogs. Table 2 summarizes the characteristics of the four datasets. The density column in the table indicates (# of observed edges)/(# of possible edges), that is $|E|/n^2$.

Table 2: Summary of the datasets.

| Dataset   | Vertex $n$ | Edge $|E|$ | Attribute $m$ | Label $k_1$ | Density $|E|/n^2$ |
|-----------|------------|---------|---------------|-------------|-----------------|
| WebKB     | 877        | 1480    | 1703          | 4           | 0.18%           |
| Citeseer  | 3312       | 4600    | 3703          | 6           | 0.04%           |
| Cora      | 2708       | 5278    | 1433          | 7           | 0.07%           |
| polblog   | 1490       | 16630   | 7             | 2           | 0.75%           |

Measurements
We utilize the Adjusted Rand Index (ARI) (Yeung and Ruzzo 2001), which is a typical measurement used for assessing the clustering quality with ground truth labels. Generally, higher ARI indicates better clustering results. In addition to ARI, we also employ the modularity (Newman 2006) and average entropy for cluster validation with respect to the topological aspect and attribute aspect of clusters, respectively. Intuitively, higher modularity indicates there are dense connections in the same cluster but sparse connections between different clusters. Lower average entropy indicates there are similar attribute values in the same cluster but dissimilar attribute values between different clusters.

Parameter Settings
In our experiments, we made a grid search for each dataset to select parameters, $\lambda$, $k_2$, and $\rho$, those give the best performance. $\lambda$ is chosen from the set \{10$^{-10}$, 10$^{-8}$, 10$^{-7}$, 10$^{-6}$, 10$^{-5}$, 10$^{-4}$, 10$^{-3}$, 10$^{-2}$, 0.1, 1, 10, 100\} by following the settings used in [Huang et al. 2017]. The model does not work well when $\lambda > 100$. We set $k_1$ at the number of ground truth labels for each dataset. $k_2$ is chosen from the set \{5, 7, 10, 15, 20\} so that we can learn the model more precisely than the number of clusters. $\rho$ is chosen from the set \{0.5, 0.55, 0.75, 0.95, 0.995\}.

To mitigate the different scales between $S$ and $X$, we normalize $S$ by multiplying each element of $S$ with $\frac{|X|}{|S|}$. The number of the iterations $t$ is fixed at 100 in all the experiments.

Clustering quality
Table 3 shows the results of evaluating the clustering quality by using the average and standard deviation of ARI. We confirmed that our method initialized by k-means results (Prop.) outperforms all the competing methods for all datasets. This result validates the effectiveness of the non-linear projection and PU learning to the clustering quality. The results of our method without PU learning (Prop. (w/o PU)) clarify the advantage of the non-linear projection: it performs better than the competing methods except for Cora dataset. In addition, the initialization by k-means result always improves the performance, see the gain from Prop.∗ (initialized by random values) to Prop. (initialized by k-means result).

JWNMF took the second place for WebKB dataset but resulted in poor performance on other datasets. METIS, that is a graph clustering method, achieved the second or third places for WebKB, Cora, and Polblog datasets. In contrast, for Citeseer dataset, NMF and k-means, those are attribute-based clustering methods, took the second and third places, respectively. These results indicate that either the topology or attributes of the graphs contribute largely to the clustering quality, but it is more effective to combine both of them.

To investigate more on the difficulty of the attributed graph clustering, we show that the topology and the attributes of real-world graphs have different cluster structures. Table 4 gives the modularity and the average entropy for the clustering result of WebKB dataset. We also include the ARI in the table for comparison, which is the same result as in Table 3. Our method achieves the highest ARI but does not achieve either the best modularity or the best average entropy. This result implies that, when we design an effective clustering method for attributed graphs, we should not optimize the model only to either the topology or the attributes. Instead, we need to take both effects of the topology and attributes.

As for BAGC, the ARI is the lowest among all the methods in all the datasets. It achieves better entropy than other attributed graph clustering methods do (our method and JWNMF), however, it fails to learn the model fully from the graph topology. We also note on the evaluation of PAICAN (Bojchevski and Günnemann 2018), one of the latest methods designed for outlier detection and clustering of attributed graphs. Despite an extensive search we made on the hyperparameters, PAICAN resulted in poor performance in our experiments, so we exclude its results from Table 3.

Hyperparameter Discussion
We discuss the effect of the hyperparameters of our method. We show the results of the variation of our method initialized by k-means result. Fig. 5 shows the effect of $\lambda$ to the

$^1$http://linqs.cs.umd.edu/projects//projects/lbc/index.html
$^3$http://www-personal.umich.edu/~mejn/netdata/
Table 3: The average and standard deviation (in parenthesis) of ARI. The methods annotated with * indicate the parameters are initialized by random values. The boldface font represents the best performance for each dataset.

| Method     | Input Type       | WebKB      | Citeseer    | Cora        | polblog     |
|------------|------------------|------------|-------------|-------------|-------------|
| Prop.      | Topology, Attribute | 0.995 (±0.002) | 0.280 (±0.027) | 0.348 (±0.022) | 0.626 (±0.037) |
| Prop. (w/o PU) | Topology, Attribute | 0.990 (±0.005) | 0.221 (±0.010) | 0.270 (±0.024) | 0.621 (±0.000) |
| Prop.*     | Topology, Attribute | 0.982 (±0.003) | 0.126 (±0.023) | 0.244 (±0.038) | 0.603 (±0.011) |
| JWNMF      | Topology, Attribute | 0.906 (±0.000) | 0.127 (±0.000) | 0.230 (±0.000) | 0.517 (±0.000) |
| JWNMF*     | Topology, Attribute | 0.909 (±0.002) | 0.082 (±0.009) | 0.227 (±0.011) | 0.504 (±0.011) |
| BAGC       | Topology, Attribute | 0.204 (±0.000) | 0.000 (±0.000) | 0.016 (±0.000) | 0.000 (±0.000) |
| METIS      | Topology         | 0.851 (±0.000) | 0.156 (±0.000) | 0.283 (±0.000) | 0.545 (±0.000) |
| SNNF       | Topology         | 0.840 (±0.100) | 0.067 (±0.020) | 0.211 (±0.028) | 0.498 (±0.059) |
| NMF        | Attribute        | 0.327 (±0.004) | 0.193 (±0.023) | 0.115 (±0.001) | 0.000 (±0.000) |
| k-means    | Attribute        | 0.260 (±0.131) | 0.190 (±0.044) | 0.093 (±0.034) | 0.000 (±0.000) |

Table 4: Modularity and average entropy results for WebKB dataset. The methods with * indicate the parameters are initialized by random values. The boldface font represents the best performance for each measure.

| Measure     | Modularity | Entropy | ARI  |
|-------------|------------|---------|------|
| Prop.       | 0.738      | 0.152   | 0.995|
| Prop. (w/o PU) | 0.737      | 0.152   | 0.990|
| Prop.*      | 0.737      | 0.152   | 0.982|
| JWNMF       | 0.739      | 0.153   | 0.906|
| JWNMF*      | 0.741      | 0.153   | 0.909|
| BAGC        | 0.224      | 0.150   | 0.204|
| METIS       | 0.732      | 0.153   | 0.851|
| SNNF        | 0.725      | 0.153   | 0.840|
| NMF         | 0.278      | 0.146   | 0.327|
| k-means     | 0.239      | 0.146   | 0.260|

clustering results. Other parameters are fixed at the values when ARI becomes highest for each λ. There is a peak in each dataset (λ = 10−4 on WebKB and λ = 10−5 on Cora) which indicates that the effect to the model is well balanced by λ between the topology and the attributes.

The effect of k2 to ARI is shown in Figs. 4. Fig. 4a shows that ARI slightly increases when k2 increases. ARI of the WebKB is enough high (almost 1) when k2 = 20. Fig. 4b shows that there is a peak of ARI on Cora when ρ = 0.95 and k2 = 10. ARI by our proposed method is always higher than ARI of other clustering methods for any k2. From Figs. and 4, we confirmed that ARI is stable against the selection of ρ (when ρ < 0.1) and k2 in a wide range. Thus, in practice, we suppose our method would perform well when λ and k2 may be simply chosen e.g., λ = 0.01 and k2 = k1.

As for the hyperparameter of PU learning, ρ has a large influence on the performance of our method as shown in Figs. 3 and 4. To evaluate the effectiveness of the Positive Unlabeled approach, we show the effect of ρ to ARI achieved by our method in Table 5. It shows that, when the density is high, the best ρ tends to be low in general.

**Efficiency**

Table 6 shows the runtimes of our method, JWNMF, and BAGC. The hyperparameter k2 is set to k1 in our method. First, we investigate the performance of our method without PU learning by setting ρ to 0.5 (Prop. (w/o PU) in the table). In this case, the first term (topology part) of the loss function Eq. (6) corresponds to 1/2∥S − UU†∥F, which is equivalent with the topology part of the JWNMF objective function Eq. (17). So, the runtime difference between Prop. (w/o PU) and JWNMF is caused by the different cost for the attribute part. The results in the table show that Prop. (w/o
Table 5: Effect of ρ on ARI achieved by our method with k-means initialization. The density indicates the (# of observed edges)/(# of possible edges), that is |E|/n^2. The boldface font represents the best performance for each dataset.

| Dataset | WebKB | Citeeseer | Cora | polblog |
|---------|-------|-----------|------|---------|
| Density |       |           |      |         |
| ρ = 0.5 | 0.990 | 0.221     | 0.270 | 0.621   |
| ρ = 0.75| 0.995 | 0.216     | 0.296 | 0.625   |
| ρ = 0.95| 0.512 | 0.254     | 0.348 | 0.626   |
| ρ = 0.995| 0.433 | 0.280     | 0.266 | 0.529   |

Table 6: Runtime [sec] of attributed graph clustering methods. Our method and JWNMF are implemented in Python3 and BAGC is implemented in Octave.

| Method   | WebKB | Citeeseer | Cora | polblog |
|----------|-------|-----------|------|---------|
| Prop.    | 2.62  | 54.32     | 29.13| 5.43    |
| Prop. (w/o PU) | 0.81  | 10.15     | 4.82 | 0.40    |
| JWNMF    | 8.80  | 60.71     | 13.33| 0.60    |
| BAGC     | 4.20  | 9.38      | 4.84 | 0.06    |

PU) is more efficient than JWNMF in all the datasets. This is because our method is more efficient for the learning cost for the attribute part.

Next, we investigate the cost of PU learning. Our method with PU learning (Prop.) requires more running time than without PU learning, Prop. (w/o PU). This is because the update rule for PU learning needs multiple times of the computation (O((n^2kt)) of the topology part.

Finally, we compared the performance of our method with others. Remember the discussion we made on the computational complexity. Our method is more efficient than JWNMF by O((n^2kt)). So, it is expected that our method is faster than JWNMF for the datasets if its number of attributes (m) is large. Indeed, the results show that our method is more efficient than JWNMF on WebKB and Citeeseer, which have many attributes and a relatively small number of vertices. As for BAGC, it is highly efficient but the clustering quality is very poor. Thus, our method achieves high efficiency and effectiveness at the same time.

Related Work

SNMF is recently extended to consider both a graph structure and attribute information for discovering clusters of data entities. JWNMF (Huang et al. 2017) factorizes both the topology and the attribute matrices at the same time. The objective is shown:

$$\min_{U, V, A \geq 0} \|S - UV^T\|_F^2 + \lambda \|XA - UV^T\|_F^2$$  \hspace{1cm} (17)

where λ and A = diag(a_1, a_2, \ldots, a_k) are a hyper parameter and an attribute selection matrix, respectively. There are two critical issues in JWNMF. The first issue is that the clustering quality is not high. JWNMF is limited to learn the single cluster assignment matrix U. Thus it does not fully capture the relationship between the topology and the attributes. The second issue is on the efficiency. JWNMF uses two model parameters λ and A for adjusting attributes weight to the learning model, but they are redundant and, moreover, the cost of learning A is expensive as O(m^2t) where m is the number of attributes.

We considered the clustering problem of attributed graphs. We designed an effective and efficient clustering method, NAGC, Non-linear Attribute Graph Clustering by Symmetric Non-negative Matrix Factorization with Positive Unlabeled Learning. The features of our method are three holds. 1) it learns a non-linear projection between the two latent embedding spaces of the topology and the attributes of graphs, 2) it leverages the positive unlabeled learning to take the effect of partially observed positive edges, and 3) it achieves efficient computational complexity, $O((n^2 + mn)kt)$ for learning the cluster assignment.

References

[Akoglu et al. 2012] Akoglu, L.; Tong, H.; Meeder, B.; and Faloutsos, C. 2012. PICS: Parameter-free identification of cohesive subgroups in large attributed graphs. In Proceedings of SIAM SDM.
