Restricted Boltzmann Stochastic Block Model: A Generative Model for Networks with Attributes

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Abstract
In most practical contexts network indexed data consists not only of a description about the presence/absence of links, but also attributes and information about the nodes and/or links. Building on success of Stochastic Block Models (SBM) we propose a simple yet powerful generalization of SBM for networks with node attributes. In a standard SBM the rows of latent community membership matrix are sampled from a multinomial. In RB-SBM, our proposed model, these rows are sampled from a Restricted Boltzmann Machine (RBM) that models a joint distribution over observed attributes and latent community membership. This model has the advantage of being simple while combining connectivity and attribute information, and it has very few tuning parameters. Furthermore, we show that inference can be done efficiently in linear time and it can be naturally extended to accommodate, for instance, overlapping communities. We demonstrate the performance of our model on multiple synthetic and real world networks with node attributes where we obtain state-of-the-art results on the task of community detection.

1 Introduction
In this paper we propose a communities based statistical model for networks that have observable attributes associated with each node (also known as node covariates). We use the phrase networks with attributes to refer to such networks. Many real world networks can be modeled in this way. For example, consider a social network: the nodes represent people and the edges represent friendship. Additionally, each person has observable attributes like age, current affiliation, gender, hometown, and so on.

The notion of community relies (at least partially) on the similarity between nodes of a network. If one makes a reasonable assumption that similar nodes have a higher tendency to connect to each other, then the observed connections offer a surrogate to this similarity measure. Traditionally, community detection algorithms like spectral clustering (von Luxburg 2007) exploit the observed connectivity pattern in a network to discover communities. However, networks are usually sparse, and thus looking only at the adjacency matrix of a network provides a very noisy signal about node similarities. For example, for Cora dataset that we use in our experiments, a spectral clustering method will always yield poor performance irrespective of how the number of communities is chosen (performance has been reported in Table 2). This is mainly due to the presence of many nodes that only have degree one (i.e., many isolated links).

On the other hand, node attributes often provide additional information about similarity between nodes (Yang, McAuley, and Leskovec 2013). A community detection method that takes these observed attributes into account is thus likely to find more meaningful communities as opposed to a method that only considers the underlying connectivity pattern. Hence, development of models and algorithms tailored towards networks with attributes is important. There are at least two approaches for incorporating node attributes while detecting communities: (i) modifying the cost function (like modularity score (Newman 2003)) of an existing community detection algorithm to include information about node attributes, and (ii) posing the problem of community detection as the problem of performing inference in an appropriate statistical model that can incorporate domain knowledge (see Section 2 for more details).

In this paper, we consider the second approach, but rather than making domain specific assumptions, we propose a simple and flexible generative model that can be used to model networks of different types. Our approach combines the well known Stochastic Block Model (SBM) (Holland, Laskey, and Leinhardt 1983) for modeling network connections with a variant of Restricted Boltzmann Machines (RBM) (Fischer and Igel 2012) for modeling the relationship between community membership of a node and its observable attributes. We call this model Restricted Boltzmann Stochastic Block Model (RB-SBM).

While other generative models that extend SBMs to networks with attributes have been proposed (Binkiewicz, Vogelstein, and Rohe 2017), these approaches usually employ a very simple model of attributes that limits model flexibility. Owing to the use of RBMs, our approach is more flexible.
in terms of modeling the joint distribution between node attributes and community membership. Another class of models assumes that node attributes are fixed and known and hence these models are not truly generative in nature (Newman and Clauset 2016; Zhang et al. 2018). Finally, there are multiple application specific generative models like the models for document networks (Liu, Niculescu-Mizil, and Gryc 2009; Chang and Blei 2009) as we discuss in Section 2.

Our model applies to both directed and undirected networks. We assume that the edges are unweighted, the node attributes are binary and there are no self loops or multiple edges. The proposed model can be very naturally extended beyond this (albeit at a higher computational cost), but for sake of concreteness and clarity we do not consider these extensions here and only briefly mention them in Appendix D. Furthermore, many real world problems can be modeled using networks that satisfy these constraints.

Our model can be used to generate networks with attributes along with ground truth communities that can help in testing the performance of new and existing community detection algorithms that take node attributes into account. Furthermore, we derive an inference procedure for our model using the Variational Expectation Maximization strategy (Section 4). This procedure runs in linear time in the number of nodes and edges, and is therefore suitable for application in large networks. We demonstrate the utility of our model on several synthetic and real world networks with attributes in Section 5.

Our contributions: (i) We propose a simple and flexible generative model for networks with attributes (Section 3) that may provide a stepping stone for development of more sophisticated models (Section 6, Appendix D), (ii) We derive an efficient approximate inference method for the proposed model (Section 4), (iii) We empirically validate the proposed model on the task of community detection and demonstrate through a qualitative case study that it can provide interpretable insights about the data (Section 5). Our approach outperforms existing approaches on Cora and Citeseer networks in terms of NMI score with respect to known ground truth community memberships.

2 Related Work

Approaches for community detection in networks with attributes can be divided into two main categories - those that are more algorithmic in nature and those based on probabilistic models. This paper belongs to the second category.

Algorithmic approaches usually modify existing algorithms for community detection in networks without attributes to make them suitable for networks with attributes. As an example, (Zhou, Cheng, and Yu 2010; Ruan, Fuhr, and Parthasarathy 2013) use node attributes to augment the set of edges in the network. Existing community detection algorithms are then used on this augmented network. Covariate Assisted Spectral Clustering (CASC) (Binkiewicz, Vogelstein, and Rohe 2017) uses spectral clustering algorithm (von Luxburg 2007) on a similarity matrix that combines both node attributes and connectivity information. Spectral clustering has been adapted to networks with attributes in many different ways, see references within (Binkiewicz, Vogelstein, and Rohe 2017) for more details.

Some other approaches modify the objective function of an existing algorithm to include node attributes. For example, (Zhang, Levina, and Zhu 2016) propose joint community detection criteria, which can be seen as a modification of modularity score for networks with attributes. See references within (Li, Yeung, and Zhang 2011; Akoglu et al. 2012; Zhang, Levina, and Zhu 2016) for other similar approaches. Along similar lines, (Li et al. 2018) proposed Community Detection in attributed graphs: an Embedding approach (CDE) that relies on simultaneous non-negative matrix factorization of node-attribute and adjacency matrices.

In general, approaches based on probabilistic models offer more insights as compared to algorithmic approaches. For example, using our approach one can naturally find the role played by different node attributes in characterizing various communities. Both discriminative (Yang et al. 2009) as well as generative probabilistic models (Cohn and Hofmann 2001; Erosheva, Fienberg, and Lafferty 2004; Chang and Blei 2009; Liu, Niculescu-Mizil, and Gryc 2009; Balasubramanyan and Cohen 2011; Xu et al. 2012; Yang, McAuley, and Leskovec 2013) have been proposed.

However, statistical models are usually more domain specific. For instance, most of the probabilistic models for this task have been tailored towards document networks. In this context, each node represents a document and these documents are connected to each other via hyperlinks or citations. These methods usually employ variants of Latent Dirichlet Allocation (LDA) (Blei, Ng, and Jordan 2003) to model textual node attributes. For example, (Erosheva, Fienberg, and Lafferty 2004) proposed a model that we will call LDA-Link-Word (LLW) following (Yang et al. 2009). The model uses LDA for modeling documents and uses the notion of communities for modeling links. (Yang et al. 2009) use a node popularity based conditional link model (PCL) and combine it with PLSA (Probabilistic Latent Semantic Analysis, which is similar to LDA) to model documents. They call this model PCL-PLSA. They also have a discriminative variant of the model which replaces PLSA with a discriminative content model to obtain PCL-DC.

Not all probabilistic models are specific to document networks. As an example, (Yang, McAuley, and Leskovec 2013) proposed Community Detection in Networks with Node Attributes (CESNA) for networks where node attributes are binary and communities can overlap.

All of these models either assume that community memberships determine attributes or the other way round. In contrast, we model the joint distribution between node attributes and community memberships directly thereby avoiding this assumption. Also, we believe that the use of RBM makes our approach applicable across multiple domains as opposed to being restricted to for example, document networks.

3 Proposed Model

The RB-SBM model is generative and describes a network with \( N \) nodes represented by a simple graph, where each
node/vertex is endowed with $M$ binary attributes. Furthermore, there is a latent structure that specifies the community membership of each of the nodes, namely, each node belongs to exactly one of the $K$ communities.

Let $A \in \{0, 1\}^{N \times N}$ be the binary adjacency matrix of the network (no self loops are allowed), $Y \in \{0, 1\}^{N \times M}$ be the binary attribute matrix and $Z \in \{0, 1\}^{N \times K}$ be the community membership matrix that satisfies $\sum_n z_{nk} = 1$ for all $n$. Each node belongs to exactly one community. We will use $\theta$ to denote the parameters of our statistical model (these will be specified later).

Our model combines a Restricted Boltzmann Machine (RBM) (Fischer and Igel 2012) to model the joint distribution over $Y$ and $Z$ and a Stochastic Block Model (SBM) (Holland, Laskey, and Leinhardt 1983) to model the connections in $A$ given $Z$ and $Y$. A high level graphical description of the model is provided in Figure 1.

### 3.1 Modeling Interaction between $Y$ and $Z$

We assume that the joint probability mass function $P_\theta(Y, Z)$ factorizes into $\prod_{n=1}^{N} P_\theta(Y_n, Z_n)$ where $Y_n$ and $Z_n$ represent the $n^{\text{th}}$ row of $Y$ and $Z$ respectively. We model the joint distribution over $Y_n$ and $Z_n$ using a RBM. However, due to the restriction that each node belongs to exactly one community, $Z_n$ will be a one-hot encoded vector and hence the usual formulation of RBM which uses binary values for both visible and hidden units cannot be used directly. A trivial change in the computation of partition function solves this issue. With $W \in \mathbb{R}^{M \times K}$, $u \in \mathbb{R}^M$, and $v \in \mathbb{R}^K$ as the parameters of RBM, the joint distribution of $Y_n$ and $Z_n$ is given by:

$$P_\theta(Y_n = y, Z_n = z) = \frac{\exp \left( y W z^T + y u^T + z v^T \right)}{\Psi(W, u, v)} .$$  

(1)

Here $\Psi(W, u, v)$ is the normalization constant (also known as partition function). Unlike the commonly used RBM, in our case $\Psi(W, u, v)$ does not involve a sum over all possible binary values of $Z_n$, therefore

$$\Psi(W, u, v) = \sum_{y \in \{0, 1\}^M} \sum_{v_y \in \{0, 1\}^K} \exp \left( (y W)_k + y u^T + v_k \right) ,$$  

(2)

where, $y$ is treated as a row vector and $(y W)_k$ and $v_k$ are the $k^{\text{th}}$ terms of the vectors $y W$ and $v$ respectively. Further, unlike in a usual RBM, we can efficiently compute $\Psi(W, u, v)$ in $O(K M)$ time (see Appendix A.2). It is also easy to see that (see Appendix A.1):

$$P_\theta(Y_{nm} = 1 | Z_{nk} = 1) = \frac{1}{1 + e^{-w_{nk} - u_m}} \quad \text{and} \quad P_\theta(Z_{nk} = 1 | Y_n = y) = \frac{e^{\sum_{m=1}^{K} w_{mk} y_m + v_k}}{\sum_{k'=1}^{K} e^{\sum_{m=1}^{K} w_{mk'} y_m + v_{k'}}} .$$  

(3)

(4)

One can use (3) and (4) for Gibbs sampling to draw a sample from the joint distribution over attributes and community membership that is modeled by the RBM.

### 3.2 Modeling Connections in the Network

We use the Stochastic Block Model to model the presence/absence of edges in the network. Usually, in a SBM it is assumed that the community membership of nodes $Z_n$ are sampled independently and identically distributed (i.i.d.) from a multinomial distribution $\pi$ over $K$ communities. Then, conditioned on the community membership of the two end points $i$ and $j$, an edge is sampled with probability $Z_i Z_j^T$ independently for all values of $i$ and $j$. Here, $B$ is the block matrix that is used in the SBM. In our case, rather than obtaining the community membership of nodes from $\pi$, we sample them from the RBM using (3) and (4).

The block matrix $B$ plays a crucial role in determining the properties of the network that is being modeled. For instance, if one is looking for the traditional assortative communities, then entries on the leading diagonal of $B$ should be higher than other entries. One can similarly impose different structures on $B$ to capture different types of properties like hierarchical communities, disassortative communities and so on. Although different formulations are possible, we take a Bayesian point of view and impose a Beta prior on all entries of the $B$ matrix. The user can specify the $\alpha \in \mathbb{R}_{+}^{K \times K}$ and $\beta \in \mathbb{R}_{+}^{K \times K}$ hyperparameters of the prior on $B$ by using domain specific knowledge about the problem.

### 3.3 Full description of RB-SBM

The generative process of our model can be summarized as follows:

(i) Sample $B_{k\ell} \sim \text{Beta}(\alpha_{k\ell}, \beta_{k\ell})$ for $k, \ell = 1, \ldots, K$

(ii) Sample $Y_n, Z_n$ for all $n$ from the RBM in (1)

(iii) Sample $A_{ij} \sim \text{Bernoulli}(Z_i B Z_j^T)$ for all $i \neq j$.

Using the independence assumptions implied by the graphical model given in Fig. 1, one can write the probability density function\(^1\) of $A$, $Y$, $Z$, $B$ as:

$$P_\theta(A, Y, Z, B) = P_\theta(B) P_\theta(Y, Z) P_\theta(A | B, Z) .$$  

(5)

The parameters are $\theta = \{W, u, v\}$. These parameters are used by the RBM. Additionally, the model uses three hyperparameters - $\alpha$, $\beta$ and $K$. The first two describe the prior on $B$ whereas $K$ is the number of communities. Although, (5) depends on the hyperparameters as well, we have suppressed this in the notation to avoid clutter. While performing inference in the model, we consider $\alpha$, $\beta$ and $K$ to be fixed constants that are provided by the user. Note that both RBM and SBM are known to have good representation power and hence our model can be used to generate a large class of networks with various properties. In addition, as we will see in Section 4, this way of combining a RBM and a SBM allows for an efficient inference procedure. Next we highlight some noteworthy features of this model.

**Directly modeling $P_\theta(Y, Z)$:** While in certain settings it is reasonable to assume a direction on the edge that connects $Y$ and $Z$ in the graphical model, such an assumption need

\(^1\)Formally this is the Radon-Nikodym derivative with respect to a dominating measure consisting of the product of counting measures (for the first three arguments) and Lebesgue measure (for the last argument).
not always hold in practice. For example, in a friendship network, while people form communities based on shared attributes, they also acquire attributes because of the membership to different communities due to the influence of peers. Modeling the joint distribution directly captures both type of interactions between \(Y\) and \(Z\).

**Reduction to SBM:** RB-SBM reduces to SBM if one sets \(W = 0\) and \(v_k = \ln \pi_k \forall k\), where \(\pi\) is the multinomial distribution from which community memberships are sampled i.i.d. in a SBM. It can be verified that in such a setting the marginal distribution for the RBM is \(P_\theta(Z_{nk} = 1) = \pi_k\) and hence if one ignores the observed attributes, the generated network \((A, \tilde{Z})\) will come from an SBM with parameters \((\pi, B)\) (see Appendix A.3).

**Constraints on \(Y_n\) and \(Z_n\):** We assume that attributes are binary since a large class of attributes can be encoded using binary vectors. Even the continuous valued attributes can be discretized and represented as binary attributes. Although, continuous relaxations of RBMs do exist, we opted for the binary variant in favor of simplicity and ease of inference (also see Appendix D).

**Utility of the model:** Note that in our model, while the attributes and community membership come from a joint distribution, the observed edges in the network are only a function of community membership. This is a reasonable assumption to make considering the traditional definition of a community. If the observed network \(A\) is dense enough (or equivalently, the entries of \(B\) are sufficiently large) one can ignore the attributes and use a traditional community detection algorithm like Spectral Clustering (von Luxburg 2007) to recover the communities. However, most real world networks are very sparse. In such cases, information from the node attributes can also be exploited to recover the communities, and in these cases the model becomes especially useful. Note that there are other approaches that explicitly augment the observed networks based on \(Y\) to alleviate the sparsity problem (Ruan, Fuhr, and Parthasarathy 2013). However, in our approach we do not use any explicit augmentation (refer to Table 2 for a comparison against (Ruan, Fuhr, and Parthasarathy 2013) on community detection task). Our approach naturally combines the node attributes and network connectivity to recover the underlying communities as we will show in the next section.

### 4 Inference

In practice, one observes only the connectivity structure and node attributes (i.e. \(A\) and \(Y\)), while the community membership \(Z\) and block structure \(B\) is hidden from us. The main objective of inference is to discover the underlying community structure (i.e. \(Z\) and \(B\)) that summarizes the network. Inference is concerned with the computation of \(P_\theta(Z, B | A, Y)\), which can then be used for tasks like assigning each node to the **most probable** community. For RB-SBM, exact computation of \(P_\theta(Z, B | A, Y)\) is intractable since while calculating \(P_\theta(A, Y)\) one needs to perform a summation over \(K^N\) choices. Thus, we resort to approximate inference techniques and use Variational Inference (Blei, Kucukelbir, and McAuliffe 2017).

Given \(A\) and \(Y\) we would like to find a distribution over the unobserved variables \(Z\) and \(B\) along with a point estimate of the parameters \(W, u\) and \(v\). We use a variational EM algorithm (Bishop 2006) that alternates between the following two steps:

**(i) E-step:** Find an approximation to the posterior distribution over \(Z\) and \(B\) keeping \(W, u\) and \(v\) fixed.

**(ii) M-step:** Find point estimates of \(W, u\) and \(v\) while assuming the distribution over \(Z\) and \(B\) found in step (i) fixed.

To understand this in more detail, let \(\mathcal{L}(\theta) = \ln P_\theta(A, Y)\) be the log probability of the observed data for fixed \(A\) and \(Y\). It is intractable to compute \(\mathcal{L}(\theta)\) and hence rather than maximizing \(\mathcal{L}(\theta)\) directly, we will maximize a lower bound on \(\mathcal{L}(\theta)\) that can be computed easily. We use \(Q(Z, B)\) to refer to the distribution that will approximate the true posterior \(P_\theta(Z, B | A, Y)\). One can write

\[
\mathcal{L}(\theta) = E_Q[\ln P_\theta(A, Y)] \\
= E_Q[\ln P_\theta(A, Y, Z, B) - \ln P_\theta(Z, B | A, Y)] \\
= E_Q[\ln \frac{P_\theta(A, Y, Z, B)}{Q(Z, B)} - \ln \frac{P_\theta(Z, B | A, Y)}{Q(Z, B)}] \\
= \mathcal{L}_Q(\theta) + KL(Q(Z, B) || P_\theta(Z, B | A, Y)) \\
\geq \mathcal{L}_Q(\theta),
\]

where, \(\mathcal{L}_Q(\theta) = E_Q[\ln P_\theta(A, Y, Z, B) - \ln Q(Z, B)]\). The term \(\mathcal{L}_Q(\theta)\) is also known as ELBO (Blei, Kucukelbir, and McAuliffe 2017). In the E-step, \(\theta\) is held constant and ELBO is maximized over \(Q\), while in the M-step, \(Q\) is held constant and ELBO is maximized over \(\theta\). Next we describe these two steps.

#### 4.1 E-step

We assume that the distribution \(Q\) belongs to the mean field family of distributions (Blei, Kucukelbir, and McAuliffe 2017), i.e.,

\[
Q(Z, B) = \prod_{n=1}^{N} q_n(Z_n) \prod_{k, \ell} q_{k\ell}(B_{k\ell}).
\]

Under this assumption, one can show that a coordinate ascent technique can be used to get the distributions \(q_n^*\) and...
\(q_{k\ell}^*\), for \(n = 1, \ldots, N\) and \(k, \ell = 1, \ldots, K\), that approximately maximize \(\mathcal{L}_Q(\theta)\) for a fixed \(\theta\) by setting (Blei, Kucukelbir, and McAuliffe 2017):

\[
q_n^*(Z_n) \propto \exp[\mathbb{E}_{Q_{-n}}[\ln P_\theta(A, Y, Z, B)]]
\]

\[
q_{k\ell}^*(B_{k\ell}) \propto \exp[\mathbb{E}_{Q_{-k\ell}}[\ln P_\theta(A, Y, Z, B)]],
\]

where \(\mathbb{E}_{Q_{-n}}[\cdot]\) represents expectation with respect to all distributions on the right hand side of (7) except \(q_n\) for the given value of \(n\). Similarly \(\mathbb{E}_{Q_{-k\ell}}[\cdot]\) represents the expectation with respect to all distributions except \(q_{k\ell}\). One can iterate over \(n, k\) and \(\ell\) in some specific order and update the corresponding distributions using (8).

The expectations given in (8) can be solved in closed form. These expressions have been derived in Appendix B. This relies on conjugacy arguments for exponential families and shows that \(q_{k\ell}\) is a Beta distribution for all \(k\) and \(\ell\).

In a single E-step, we update \(q_n\) only for a randomly chosen subset of \(n\) nodes. One would want \(\omega\) to be small enough so that E-step can be completed in a reasonable amount of time while at the same time being large enough to make sufficient amount of progress before the next M-step. We experimentally found that the value of \(\omega = \min\{N, 256\}\) works well in all our experiments even in the case when \(N\) is as large as 100000 (Section 5.1). Since \(\omega\) is a fixed constant which is dependent on the number of nodes in the network, the overall complexity of the E-step is \(O(N + |E|)\), where \(|E|\) is the number of edges in the network. Details about complexity analysis have been given in Appendix B.

### 4.2 M-step

In the M-step, the distribution \(Q\) is held constant and \(\mathcal{L}_Q(\theta)\) is maximized over \(W, u\) and \(v\). We do this by computing the gradient of \(\mathcal{L}_Q(\theta)\) with respect to these parameters and performing gradient ascent. In a single M-step, we perform \(\xi\) gradient ascent updates to approximately maximize \(\mathcal{L}_Q(\theta)\). We empirically observed that \(\xi = 1\) suffices for all our experiments and hence we use that value. Larger values of \(\xi\) can be used, but without any significant gains.

The gradients can be expressed as (see Appendix C):

\[
\nabla_{u_n} \mathcal{L}_Q(\theta) = \sum_{n=1}^N (y_{nm} - E_{P_{RBM}}[Y_{nm}]),
\]

\[
\nabla_{v_k} \mathcal{L}_Q(\theta) = \sum_{n=1}^N (q_{nk} - E_{P_{RBM}}[Z_{nk}]),
\]

\[
\nabla_{w_{nk}} \mathcal{L}_Q(\theta) = \sum_{n=1}^N (y_{nm}q_{nk} - E_{P_{RBM}}[Y_{nm}Z_{nk}]).
\]

Above \(P_{RBM}\) denotes the joint probability distribution over attributes and community memberships that is encoded by the RBM learned so far, and \(q_{nk}\) has been used as a shorthand notation for \(q_{nk}(Z_n)\) evaluated at a one hot vector \(z\) for which \(z_k = 1\).

One can either explicitly compute the expectation with respect to \(P_{RBM}\) in the second term of (9) for all parameters or approximate it using Monte-Carlo estimation. We present the computation of gradients using both strategies in Appendix C. While the exact gradient computation is slightly faster, the gradient approximation via Gibbs sampling is numerically more stable.

When Monte-Carlo estimation is used, as is the standard practice with RBMs (Fischer and Igel 2012), we use \(\eta\) persistent Gibbs chains which sample from \(P_{RBM}\) using (3) and (4) to obtain \(\eta\) samples at each M-step. These samples are then used to approximate the gradients in (9). Once the gradients have been computed, the standard gradient ascent updates can be made with learning rate \(\epsilon\) which is a user specified hyperparameter. The choice of learning rate is important, but there is a wide range of values for which the optimization procedure is stable and converges at a reasonable pace. Namely we used \(\epsilon = 1/N\) in all experiments (as the ELBO scales linearly with \(N\)).

### 5 Experiments

#### 5.1 Synthetic Networks

We generated synthetic networks with attributes using our model following the sampling procedure outlined in Section 3 for different values of \(N\). We used \(\alpha_{k\ell} = 1\) for all \(k, \ell\) and \(\beta_{k\ell} = \sqrt{N}\) if \(k = \ell\) and \(10\sqrt{N}\) otherwise. This choice roughly implies that the sparsity of sampled networks will be \(O(1/\sqrt{N})\). The factor of 10 ensures that as \(N\) becomes large, within community edges are roughly 10
times more likely as compared to across community edges. To choose the parameters of the RBM we suppose each of the \( M \) attributes might have an assortative role (two nodes with the same attribute are more likely in the same community), a disassortative role, or a neutral role. For each community \( k \), each attribute \( m \) was assigned the corresponding role with probabilities respectively \( p_+ \), \( p_- \) and \( p_0 \) (where \( p_+ + p_- + p_0 = 1 \)). The value of \( w_{mk} \) was set to +5, 0 or -5 respectively. We used the value of \( p_+ = 0.1, p_- = 0.1 \) and \( p_0 = 0.8 \) for these experiments. The vector \( u \) was set to -2 for all elements and \( v \) was set to 0.

We used \( M = 100, K = \log_2 N, \omega = \min\{256, N\} \) and \( \epsilon = 1/N \) for these experiments. Gradients were computed by using exact calculations for expectation in (9) as given in Appendix C.2. We also used gradient clipping where all the gradients were clipped in the range \([-5, 5]\) to increase the numerical stability of inference procedure. We have also experimented with the Gibbs sampling approach here and the results were qualitatively the same. All the experiments were executed on an Intel Core i7-6700 machine with 4 GB of usable main memory.

Figure 2 shows the average total time taken by the inference procedure to execute one iteration of E and M steps as a function of the number of edges on the \( x \)-axis. The running time is linear in the number of edges.

Figure 3 shows the Normalized Mutual Information (NMI) scores of the detected communities against the number of iterations for the first 1000 iterations. Different curves correspond to different values of \( N \).

Table 1: Details about real world network datasets used in our experiments. Citations: \(^a\) (Lu and Getoor 2003), \(^b\) (Yang, McAuley, and Leskovec 2013)

| Dataset | \#N | \#E | \#M | \#K |
|---------|-----|-----|-----|-----|
| Cora\(^a\) | 2708 | 5429 | 1433 | 7 |
| Citeseer\(^b\) | 3312 | 4732 | 3703 | 6 |
| Philosophers\(^a\) | 1497 | 44996 | 6357 | Unknown |

Table 2: Performance of RB-SBM on community detection. We have reported the mean NMI scores with standard deviation. For all other approaches the figures have been taken from the respective papers and it is not clear if the reported scores are mean-scores or max-scores. Cosine similarity kernel is used for spectral clustering when only node attributes are considered. Generative models have been prefixed with (\(*\)). It can be seen that our approach outperforms all other approaches that we have compared against. Citations: \(^a,b\) Spectral Clustering (von Luxburg 2007), \(^c\) (Binkiewicz, Vogelstein, and Rohe 2017), \(^d\) (Ruan, Fuhr, and Parthasarathy 2013), \(^e\) (Yang, McAuley, and Leskovec 2013), \(^f\) (Erosheva, Fienberg, and Lafferty 2004), \(^g\) (Yang et al. 2009), \(^h\) (Li et al. 2018)

| Method | Cora | Citeseer |
|--------|------|----------|
| SC\(^c\) (only network) | 0.030 | 0.191 |
| SC\(^c\) (only attributes) | 0.169 | 0.202 |
| CASC\(^c\) | 0.110 | 0.182 |
| CODICIL\(^d\) | 0.368 | 0.286 |
| (\(*\)CESNA\(^e\) | 0.269 | 0.022 |
| (\(*\)LLW\(^f\) | 0.359 | 0.192 |
| (\(*\)PCL-PLSA\(^g\) | 0.390 | 0.220 |
| PCL-DC\(^h\) | 0.512 | 0.292 |
| CDE\(^i\) | 0.504 | 0.299 |
| (\(*\)RB-SBM (Gibbs) \(\pm\)) | 0.521 \(\pm\) 0.008 | 0.412 \(\pm\) 0.007 |
| (\(*\)RB-SBM (Exact) \(\pm\)) | 0.511 \(\pm\) 0.001 | 0.401 \(\pm\) 0.008 |

5.2 Real World Networks

We performed community detection on datasets given in Table 1 (more details are given in Appendix E) to partition the set of nodes into non-overlapping communities using RB-SBM. For all datasets, we initialized \( \alpha = 1 \) and \( \beta_{kl} = 1 \)
if $k = \ell$ and 10 otherwise. While in Section 5.1, $\alpha$ and $\beta$ were set to generate sparse networks, here we use the values given above as a generic prior that indicates that we are looking for assortative communities. The initial value of $q_n(Z_n = z)$ was set to $1/K$ for all $n = 1, \ldots, N$ and all one hot vectors $z$. For Cora and Citeseer, the number of ground truth communities is known and hence we fixed $K$ to that value for these datasets. For Philosophers network we selected $K = 20$. For all datasets, the inference procedure was run for $\tau = 1000$ iterations. The final values of $q_n$ were used to infer community memberships of all nodes by setting $z_n = z$ where $z = \arg\max_z q_n(Z_n = z)$.

For these experiments, gradients in (9) were approximated by using Gibbs sampling with $\eta = 100$ persistent chains by accepting every $\gamma = 10^6$ sample. These values of $\eta$ and $\gamma$ were chosen because beyond these chosen values, the running time of the inference procedure increases without affecting the final performance significantly. The performance of our method is not very sensitive to these choices.

The order in which the factors of $Q$ in (7) are updated while performing coordinate ascent decides whether one should initialize $q_n$ or $q_{k \ell}$ at the beginning of the inference procedure. A bad initialization of $q_{k \ell}$ can lead to numerical overflow problems while computing the exponential in (8) for updating $q_n$ (see Appendix B). Thus, in all our experiments we update $q_{k \ell}$ for all $k, \ell = 1, \ldots, K$ before updating any of the $q_n$’s. The initialization of $q_n$’s that has been discussed above is generic and has been empirically observed to work on multiple datasets.

If $q_n(Z_n = z)$ becomes very small for all $n$ and a particular $z$ for which $z_n = 1$ during the first few iterations, then community $k$ effectively dies. We observed that: (i) this was a common occurrence because of numerical issues and (ii) a dead community never comes back to life. Thus, we would like to avoid very small values in $q_n$ during the initial stages when $Q$ and the RBM parameters are essentially random. To do so we use the following simulated annealing heuristic. After E-step, we apply the following transformation:

$$h(x) = \begin{cases} x^\lambda & \text{if } 0 \leq x \leq \frac{1}{2} \\ \frac{1}{2} - (1 - x)^\lambda & \text{if } \frac{1}{2} < x \leq 1 \end{cases}$$

(10)

to $q_n(Z_n = z)$ for all one hot vectors $z$ and $n \in I$, where $I$ is the set indices of nodes that are being updated in the current E-step. After applying the transformation $h(.)$, $q_n$ is re-normalized so that its entries sum up to one. Note that at $\lambda = 1$, $h(x) = x$ and for $\lambda < 1$, $h(x) > x$ if $x \leq 1/2$ and $h(x) < x$ if $x > 1/2$. For $\lambda < 1$, this achieves the regularization effect that was desired above. In our experiments, we start with $\lambda = 0.3$ and increase it linearly to 1 as the number of iterations increases. Empirically, we observed that this gives us better results on all datasets.

Table 2 shows the NMI scores obtained by RB-SBM on Cora and Citeseer datasets where the ground truth communities are available. It can be seen that our approach outperforms all existing approaches that we have compared against with a much simpler model. A brief description for each of the competing approaches has been given in Section 2.

For the Philosophers network, the ground truth communities are not available and hence we present a qualitative analysis of the discovered communities. Due to space constraints, we only present two of these communities. Figure 4 shows the members and attributes of two communities that can be interpreted as “Islamic Philosophers” and “Legal Philosophers”. Most relevant attributes for each community were selected based on the weights $w_{mk}$ of the RBM for these two communities. It can be seen that the model was able to discover meaningful communities while at the same time highlighting the importance of various attributes for these communities.

### 6 Conclusion

In this paper, we presented a generative model for networks with attributes. Our model combines a RBM for modeling node attributes with a SBM for modeling node relationships. As both of these models are fairly expressive, the resultant model is simple yet flexible. One of the most attractive features of our approach is that the derived inference procedure runs in time that is linear in the number of nodes and edges in the network.

We believe that our proposed model serves as a stepping-stone for generalization of SBMs for networks with attributes and one can consider many extensions (Appendix D). For instance, it is possible to use other variants of SBM.
like Degree-Corrected SBM (Karrer and Newman 2011) or Mixed-Membership SBM (Airoldi et al. 2008) instead of the basic SBM currently used.

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A Supplementary Material for Section 3

In this section, we will present proofs for the claims made in Section 3.

A.1 Conditional Probabilities in RBM

Here, we will derive the expressions presented in (3) and (4). In RBMs, conditioned on the value of $Z_n$ (hidden units), the elements of $Y_n$ (visible units) are independent of each other. Hence, one can write:

$$P_{\theta}(Y_{nm} = 1 | Z_{nk} = 1) = \frac{P_{\theta}(Y_{nm} = 1, Z_{nk} = 1, Y_{nm} = \bar{y})}{\sum_{y_{nm} \in \{0, 1\}} P_{\theta}(Y_{nm} = y_{nm}, Z_{nk} = 1, Y_{nm} = \bar{y})}$$

$$= \frac{\exp\left(w_{mk} + u_m + \sum_{m' \neq m} (w_{m'k} + u_{m'}) \bar{y}_{m'} + v_k\right)}{\sum_{y_{nm} \in \{0, 1\}} \exp\left(w_{mk}y_{nm} + u_m y_{nm} + \sum_{m' \neq m} (w_{m'k} + u_{m'}) \bar{y}_{m'} + v_k\right)}$$

$$= \frac{\exp(w_{mk} + u_m)}{1 + \exp(w_{mk} + u_m)}$$

$$= \frac{1}{1 + \exp(-w_{mk} - u_m)}.$$

Here $\bar{Y}_{nm}$ is a random vector that has all entries from $Y_n$ except the $m^{th}$ entry. Similarly $\bar{y}$ is a vector of $M - 1$ binary values that represents an arbitrary value that can be taken by $Y_{nm}$.

In our case, we have a RBM that has $M$ binary units on one side (node attributes) and one categorical unit on the other side (community membership). We can derive the conditional probability of community membership given the node attributes as:

$$P_{\theta}(Z_{nk} = 1 | Y_n = y) = \frac{P_{\theta}(Z_{nk} = 1, Y_n = y)}{\sum_{k'} P_{\theta}(Z_{nk'} = 1, Y_n = y)}$$

$$= \frac{\exp\left(\sum_m (w_{mk} y_m + u_m y_m) + v_k\right)}{\sum_{k'} \exp\left(\sum_m (w_{mk'} y_m + u_m y_m) + v_{k'}\right)}$$

$$= \frac{\exp\left(\sum_m w_{mk} y_m + v_k\right)}{\sum_{k'} \exp\left(\sum_m w_{mk'} y_m + v_{k'}\right)}.$$

Note that given the value of $Z_n$, all the elements of $Y_n$ can be sampled independently in parallel. These conditional probabilities are used by the Gibbs sampling procedure for obtaining samples from the joint distribution that is modeled by the RBM.

A.2 Computation of Partition Function

Suppose that the RBM models a joint distribution over $Y_n \in \{0, 1\}^M$ and $Z_n \in \{0, 1\}^K$ such that $\sum_k Z_{nk} = 1$ as described in Section 3.1. First, we find the marginal distribution over $Z_n$:

$$P_{\theta}(Z_{nk} = 1) = \sum_{y \in \{0, 1\}^M} P_{\theta}(Y_n = y, Z_{nk} = 1)$$

$$= \frac{1}{\Psi(W, u, v)} \sum_{y \in \{0, 1\}^M} \exp\left(\sum_{m=1}^{M} (w_{mk} + u_m) y_m + v_k\right)$$

$$= \frac{\exp(v_k)}{\Psi(W, u, v)} \sum_{y \in \{0, 1\}^M} \prod_{m=1}^{M} \exp((w_{mk} + u_m) y_m)$$

$$= \frac{\exp(v_k)}{\Psi(W, u, v)} \prod_{m=1}^{M} (1 + \exp(w_{mk} + u_m)). \quad (11)$$

One can use the fact that $\sum_{k=1}^{K} P_{\theta}(Z_{nk} = 1) = 1$ to conclude that

$$\Psi(W, u, v) = \sum_{k=1}^{K} \exp(v_k) \prod_{m=1}^{M} (1 + \exp(w_{mk} + u_m)). \quad (12)$$
A.3 Reduction to SBM
Consider the case when \( \mathbf{W} = 0 \) and \( v_k = \ln \tau_k \) for \( k = 1, \ldots, K \). Using these values in (11) and cancelling out the common terms in numerator and denominator one gets \( P_\theta(Z_{nk} = 1) = \tau_k \). Thus, if one samples from this distribution, then the sampled community membership vectors will follow \( \pi \). Following the generative process outlined in Section 3 and ignoring the node attributes, the generated \( \mathbf{A} \) will be as if it has been sampled from a SBM with parameters \((\pi, \mathbf{B})\).

B Supplementary Material for E-step
In this section, we will derive the expressions for updating \( q_k^{} \) and \( q_{k\ell} \) that are used in Section 4. Using the independence assumptions implied by the graphical model given in Fig. 1, we can write the following expression for \( \ln P_\theta(\mathbf{A}, \mathbf{Y}, \mathbf{Z}, \mathbf{B}) \):

\[
\ln P_\theta(\mathbf{A}, \mathbf{Y}, \mathbf{Z}, \mathbf{B}) = \ln P_\theta(\mathbf{B}) + \ln P_\theta(\mathbf{Y}, \mathbf{Z}) + \ln P_\theta(\mathbf{A}|\mathbf{Z}, \mathbf{B})
\]

\[
= \sum_{k,\ell=1}^{K} -\ln B(\alpha_{k\ell}, \beta_{k\ell}) + (\alpha_{k\ell} - 1) \ln B_{k\ell} + (\beta_{k\ell} - 1) \ln(1 - B_{k\ell}) + \sum_{n=1}^{N} \left( \sum_{m=1}^{M} \sum_{k=1}^{K} Y_{nm} Z_{nk} w_{mk} + \sum_{m=1}^{M} u_m Y_{nm} + \sum_{k=1}^{K} v_k Z_{nk} \right) - N \ln \left( \sum_{y} \exp \left( \sum_{m=1}^{M} \sum_{k=1}^{K} y_m z_k w_{mk} + \sum_{m=1}^{M} u_m y_m + \sum_{k=1}^{K} v_k z_k \right) \right) + \sum_{i\neq j}^{K} \sum_{k,\ell=1}^{K} A_{ij} Z_{ik} Z_{j\ell} \ln B_{k\ell} + (1 - A_{ij}) Z_{ik} Z_{j\ell} \ln(1 - B_{k\ell}) \,
\]

(13)

Here, \( B(\cdot) \) is the Beta function.

B.1 Updating \( q_{k\ell}(B_{k\ell}) \)
The optimal value of \( q_{k\ell} \) is given by (8). In this section, we evaluate \( \mathbb{E}_{Q_{\rightarrow \cdot}}[\ln P_\theta(\mathbf{A}, \mathbf{Y}, \mathbf{Z}, \mathbf{B})] \). Using (13), the fact that \( Q \) belongs to mean field family of distributions and by linearity of expectation, one arrives at the following expression:

\[
\mathbb{E}_{Q_{\rightarrow \cdot}}[\ln P_\theta(\mathbf{A}, \mathbf{Y}, \mathbf{Z}, \mathbf{B})] = (\alpha_{k\ell} - 1) \ln B_{k\ell} + (\beta_{k\ell} - 1) \ln(1 - B_{k\ell}) + \sum_{i\neq j}^{K} \sum_{k,\ell=1}^{K} a_{ij} q_{ik} q_{j\ell} \ln B_{k\ell} + (1 - a_{ij}) q_{ik} q_{j\ell} \ln(1 - B_{k\ell}) + \text{const} \,.
\]

(14)

Note that \( \mathbf{A} \) and \( \mathbf{Y} \) are observed quantities and hence they are fixed. All the terms that do not depend on \( B_{k\ell} \) have been absorbed in the constant. We have used \( q_{nk} \) to denote \( q_n(Z_{nk} = 1) \). Using (14) in (8) and by omitting the constants, we get:

\[
q_{k\ell}(B_{k\ell} = b_{k\ell}) \propto \exp \left( \left( \sum_{i\neq j}^{K} a_{ij} q_{ik} q_{j\ell} + \alpha_{k\ell} - 1 \right) \ln b_{k\ell} + \left( \sum_{i\neq j}^{K} (1 - a_{ij}) q_{ik} q_{j\ell} + \beta_{k\ell} - 1 \right) \ln(1 - b_{k\ell}) \right) \,.
\]

(15)

This is the exponential family form of a Beta distribution. Thus, we can conclude that \( q_{k\ell} = \text{Beta}(\bar{\alpha}_{k\ell}, \bar{\beta}_{k\ell}) \), where

\[
\bar{\alpha}_{k\ell} = \sum_{i\neq j}^{K} a_{ij} q_{ik} q_{j\ell} + \alpha_{k\ell} \,.
\]

(16)

\[
\bar{\beta}_{k\ell} = \sum_{i\neq j}^{K} (1 - a_{ij}) q_{ik} q_{j\ell} + \beta_{k\ell} \,.
\]

(17)

Naively computing \( \bar{\alpha}_{k\ell} \) and \( \bar{\beta}_{k\ell} \) will incur \( O(N^2) \) cost which is prohibitively large for big networks, but there is an efficient way to compute these terms, namely

\[
\sum_{i\neq j}^{K} (1 - a_{ij}) q_{ik} q_{j\ell} = \sum_{i,j}^{K} q_{ik} q_{j\ell} - \sum_{i\neq j}^{K} a_{ij} q_{ik} q_{j\ell} - \sum_{n=1}^{N} q_{nk} q_{nt} - \sum_{(i,j) \in \mathcal{E}}^{K} q_{ik} q_{j\ell} - \sum_{n=1}^{N} q_{nk} q_{nt} \,.
\]

(18)

where \( \mathcal{E} \) is the set of edges in the network. Now both (16) and (17) can be computed in \( O(N + |\mathcal{E}|) \) time. One needs to compute (16) and (17) for all \( k; \ell = 1, \ldots, K \). Thus, the total cost of updating \( q_{k\ell} \) for all community pairs is \( O(K^2(N + |\mathcal{E}|)) \). However, the computation over all community pairs can be done in parallel and hence the effective time needed is \( O(|\mathcal{E}| + N) \). Note that all of these computations are exact and we have not used any approximation.
B.2 Updating $q_k(Z_n)$

Proceeding as in the case of $q_B$ updating, we get

$$E_{Q_{−\beta}}[\ln P_\theta(A,Y,Z,B)] = \sum_{m=1}^{M} \sum_{k=1}^{K} y_{sm} Z_{sk} w_{mk} + \sum_{k=1}^{K} v_k Z_{sk}$$

$$+ \sum_{i \neq s}^{K} \sum_{k,\ell=1}^{K} q_{ik} Z_{\ell k}(\Psi(\bar{\alpha}_{k\ell}) - \Psi(\bar{\alpha}_{k\ell} + \bar{\beta}_{k\ell}))$$

$$+ \sum_{i \neq s}^{K} \sum_{k,\ell=1}^{K} (1 - a_{i\alpha}) q_{ik} Z_{\ell k}(\Psi(\bar{\beta}_{k\ell}) - \Psi(\bar{\alpha}_{k\ell} + \bar{\beta}_{k\ell}))$$

$$+ \sum_{j \neq s}^{K} \sum_{k,\ell=1}^{K} a_{s\beta} Z_{sk} q_{j\ell}(\Psi(\bar{\alpha}_{k\ell}) - \Psi(\bar{\alpha}_{k\ell} + \bar{\beta}_{k\ell}))$$

$$+ \sum_{j \neq s}^{K} \sum_{k,\ell=1}^{K} (1 - a_{j\beta}) Z_{sk} q_{j\ell}(\Psi(\bar{\beta}_{k\ell}) - \Psi(\bar{\alpha}_{k\ell} + \bar{\beta}_{k\ell})) + \text{const}.$$ (19)

All the terms that do not depend on $Z_n$ have been absorbed in the constant. $\Psi(.)$ is the digamma function and we have used the fact that if a random variable $X \sim \text{Beta}(\alpha, \beta)$, then $E[\ln X] = \Psi(\alpha) - \Psi(\alpha + \beta)$. Also, note that if $X \sim \text{Beta}(\alpha, \beta)$, then $1 - X \sim \text{Beta}(\beta, \alpha)$.

Using (19) in (8) and by omitting the constants, one can write

$$q_{sk} \propto \exp \left( \sum_{m=1}^{M} y_{sm} w_{mk} + v_k ight)$$

$$+ \sum_{i \neq s}^{K} \sum_{\ell=1}^{K} q_{ik} \ell(\Psi(\bar{\alpha}_{k\ell}) - \Psi(\bar{\alpha}_{k\ell} + \bar{\beta}_{k\ell}))$$

$$+ \sum_{i \neq s}^{K} \sum_{\ell=1}^{K} (1 - a_{i\alpha}) q_{ik} \ell(\Psi(\bar{\beta}_{k\ell}) - \Psi(\bar{\alpha}_{k\ell} + \bar{\beta}_{k\ell}))$$

$$+ \sum_{j \neq s}^{K} \sum_{\ell=1}^{K} a_{s\beta} q_{j\ell}(\Psi(\bar{\alpha}_{k\ell}) - \Psi(\bar{\alpha}_{k\ell} + \bar{\beta}_{k\ell}))$$

$$+ \sum_{j \neq s}^{K} \sum_{\ell=1}^{K} (1 - a_{j\beta}) q_{j\ell}(\Psi(\bar{\beta}_{k\ell}) - \Psi(\bar{\alpha}_{k\ell} + \bar{\beta}_{k\ell})).$$ (20)

One can compute $\Psi(\bar{\alpha}_{k\ell}) - \Psi(\bar{\alpha}_{k\ell} + \bar{\beta}_{k\ell})$ and $\Psi(\bar{\beta}_{k\ell}) - \Psi(\bar{\alpha}_{k\ell} + \bar{\beta}_{k\ell})$ for all $k, \ell = 1, \ldots, K$ once at the beginning of the E-step. This can be done in $O(K^2)$ time. The inner summations over $\ell = 1, \ldots, K$ in (20) can also be computed once at the beginning of the E-step in $O(K^2)$ time. These values can be reused while computing the outer summations over $i$ and $j$ in (20). Thus, given these quantities, the unnormalized value of $q_{sk}$ can be computed in $O(M + N)$ time. Since we need to compute $q_{sk}$ for all values of $k$, the total time needed to update $q_k$ is $O(K^2 + K(M + N))$.

As before, the computations over all community pairs can be done in parallel. Also, the unnormalized value of $q_{sk}$ can be computed in parallel for all values of $k$. Thus the effective running time for these updates is $O(\omega N)$ where $\omega$ is the number of nodes in the random subset for which $q_k$ will be updated during the current E-step. Since, $\omega$ is a constant independent of $N$, we can omit it. Using all of this information, it can be seen that as claimed in Section 4.1, one iteration of E-step takes $O(N + |\mathcal{E}|)$ time.

C Supplementary Material for M-step

We will first derive the expression for gradients given in (9) and then present two ways of computing these gradients. Recall that

$$\mathcal{L}_Q(\theta) = E_Q[\ln P_\theta(A,Y,Z,B) - \ln Q(Z,B)]$$

$$= E_Q[\ln P_\theta(A,Y,Z,B)] + \text{const}.$$ (21)
The second term has been treated as a constant since it does not depend on \( W \), \( u \) or \( v \). As done in Appendix B, using the mean field assumption on \( Q \) and linearity of expectation one can compute

\[
\mathcal{L}_Q(\theta) = \sum_{n=1}^{N} \left( \sum_{m=1}^{M} \sum_{k=1}^{K} y_{nm} q_{nk} w_{mk} + \sum_{m=1}^{M} u_m y_{nm} + \sum_{k=1}^{K} u_k q_{nk} \right) - N \ln \left( \sum_{y,z} \exp \left( \sum_{m=1}^{M} \sum_{k=1}^{K} y_m z_k w_{mk} + \sum_{m=1}^{M} u_m y_m + \sum_{k=1}^{K} u_k z_k \right) \right) + \text{const}.
\]

All the terms that are independent of \( W \) have been absorbed in the constant. Differentiating (22) with respect to \( w_{mk} \) we get:

\[
\frac{\partial \mathcal{L}_Q(\theta)}{\partial w_{mk}} = \sum_{n=1}^{N} y_{nm} q_{nk} - N \sum_{y,z} \frac{1}{\Psi(W,u,v)} \exp \left( \sum_{m=1}^{M} \sum_{k=1}^{K} y_m z_k w_{mk} + \sum_{m=1}^{M} u_m y_m + \sum_{k=1}^{K} u_k z_k \right) y_m z_k
\]

\[
= \sum_{n=1}^{N} (y_{nm} q_{nk} - \mathbb{E}_{P_{\text{RBM}}}[Y_{nm} Z_{nk}]).
\]

It can be seen that (23) gives the expression for \( \nabla_{w_{mk}} \mathcal{L}_Q(\theta) \) that was given in (9). One can work out the expressions for \( \nabla_{u_{nk}} \mathcal{L}_Q(\theta) \) and \( \nabla_{v_{mk}} \mathcal{L}_Q(\theta) \) along the same lines.

In our case, we can efficiently compute \( P_{\theta}(Z_{nk} = 1) \) and \( \Psi(W,u,v) \) (Appendix A.2), we have two ways to compute the gradients presented in (9). Next we will describe these two strategies.

### C.1 Approximating the Gradients via Gibbs Sampling

We can compute the expectations in (9) by obtaining samples from the RBM using Gibbs sampling and then using these samples to get a Monte-Carlo estimate of the expected value. In our experiments, we run \( \eta \) Gibbs chains starting with values of \( y \) that have been randomly sampled from the observed \( Y_o \)’s. Our Gibbs chains are persistent in the sense that we do not reset the chains at the beginning of each M-step. For each M-step, we run all the \( \eta \) persistent Gibbs chains for \( \gamma \) steps and use the standard procedure (Fischer and Igel 2012) to approximate the expectations. We use \( \eta = 100 \) and \( \gamma = 10 \) in our experiments.

### C.2 Exact Computation of Gradients

We can also compute the gradients in the closed form. To see this, note that since the node attributes are binary and community memberships are categorical, we can write:

\[
\mathbb{E}_{P_{\text{RBM}}}[Y_{nm} Z_{nk}] = P_{\theta}(Y_{nm} = 1, Z_{nk} = 1),
\]

\[
\mathbb{E}_{P_{\text{RBM}}}[Z_{nk}] = P_{\theta}(Z_{nk} = 1),
\]

\[
\mathbb{E}_{P_{\text{RBM}}}[Y_{nm}] = P_{\theta}(Y_{nm} = 1).
\]

We have already computed \( P_{\theta}(Z_{nk} = 1) \) in Appendix A.2. Note that, although the expressions above include the index \( n \), the right hand side is not a function of \( n \) since all of them depend only on \( P_{\theta}(Z_{nk} = 1) \) as we will see next, and \( P_{\theta}(Z_{nk} = 1) \) is not a function of \( n \) as shown in (11).

To compute \( P_{\theta}(Y_{nm} = 1, Z_{nk} = 1) \), note that it can be written as:

\[
P_{\theta}(Y_{nm} = 1, Z_{nk} = 1) = P_{\theta}(Y_{nm} = 1|Z_{nk} = 1)P_{\theta}(Z_{nk} = 1),
\]

which can be computed using (3) and (11). Similarly, \( P_{\theta}(Y_{nm} = 1) \) can also be computed by using:

\[
P_{\theta}(Y_{nm} = 1) = \sum_{k=1}^{K} P_{\theta}(Y_{nm} = 1, Z_{nk} = 1).
\]

Due to the presence of a product over \( M \) terms in (11), this exact computation of gradient may encounter numerical stability issues for large values of \( M \). The approximate computation of gradients is numerically more stable.

We can compute (11) for all \( k = 1, \ldots, K \) in \( O(MK) \) time. Once this is available, both \( P_{\theta}(Y_{nm} = 1, Z_{nk} = 1) \) and \( P_{\theta}(Y_{nm} = 1) \) can be computed for all \( m = 1, \ldots, M \) and \( k = 1, \ldots, K \) in \( O(MK) \) time each. The approximate gradient computation also involves the overhead of running the Gibbs chain.

For the case of exact computations, since the first term in the gradient involves a sum over \( N \), the overall time complexity of a single M-step is \( O(NK + MK) \). One can again perform these computations in parallel over all values of \( k \).
D Extensions of RB-SBM

In this section we present a brief overview of how RB-SBM can be extended in various ways. We leave detailed experiments for future work.

D.1 Continuous Attributes

RB-SBM requires the node attributes to be binary. Although we argue in Section 3 that a large class of networks can be modeled this way, it is straightforward to extend RB-SBM to accommodate continuous attributes. In this section, we present this extension. We will assume that the node attributes are bounded and hence they can be rescaled to lie in the range $[0, 1]$.

The only reason RB-SBM assumes binary node attributes is to perform Gibbs sampling using (3) and (4) during the M-step. Apart from these two equations, the inference procedure does not rely on the attributes being binary anywhere else. Thus, all that is needed is to derive the Gibbs sampling equations for the case of continuous attributes.

Using notation from Appendix A.1, one can write:

$$P_{\theta}(Y_{nm} = y|Z_{nk} = 1) = P_{\theta}(Y_{nm} = y|Z_{nk} = 1, \bar{Y}_{nm} = \bar{y})$$

$$= \frac{\int_{0}^{1} P_{\theta}(Y_{nm} = y', Z_{nk} = 1, \bar{Y}_{nm} = \bar{y})dy'}{\int_{0}^{1} P_{\theta}(Y_{nm} = y', Z_{nk} = 1)dy'}$$

$$= \frac{\int_{0}^{1} \exp \left( (w_{mk} + u_m)y + \sum_{m' \neq m} (w_{m'k} + u_{m'})\bar{y}_{m'} + v_k \right)dy'}{\int_{0}^{1} \exp \left( (w_{mk} + u_m)y + \sum_{m' \neq m} (w_{m'k} + u_{m'})\bar{y}_{m'} + v_k \right)dy'}$$

$$= \frac{w_{mk} + u_m}{\exp(w_{mk} + u_m) - 1} \exp\left( (w_{mk} + u_m)y \right).$$

The value of node attributes can now be easily sampled using inverse sampling. It is easy to see that (4) remains unchanged. Note that this does not affect the running time of the inference procedure and hence inference can still be performed in linear time.

D.2 Mixed-Membership

In this setup we combine RBM with mixed-membership SBM (MMSBM) (Airoldi et al. 2008). As opposed to SBMs where each node belongs to a single community, in MMSBM each node has an associated probability vector $\phi_n \in \Delta^K$ that captures the degree to which node $n$ belongs to each of the $K$ communities. Here $\Delta^K$ is a $K - 1$ dimensional simplex. To decide whether to connect nodes $i$ and $j$ or not, a community membership is sampled for each of the corresponding endpoints from $\phi_i$ and $\phi_j$ respectively. Then, based on the sampled community memberships, the corresponding entry of block matrix $B$ is chosen as before.

We now wish to model the joint distribution between observed attributes $Y_n$ and mixed-membership vector $\phi_n$ for each node $n$. We again use a variant of RBM to do this. In this variant of RBM the hidden units together form a vector that belongs to $\Delta^K$ rather than forming a one-hot vector as in Section 3. We will first derive the Gibbs sampling equation for this variant of RBM. Note that since $\phi_n \in \Delta^K$ there are only $K - 1$ free variables in $\phi_n$. Thus, sampling a single variable is meaningless, hence, we sample two variables at a time. Without loss of generality we will always sample a combination of $\phi_{nk}, \phi_{nK}$ for $k \in \{1, 2, \ldots, K - 1\}$.

Let $\phi_{nk}$ denote all entries of vector $\phi_n$ except the $k^{th}$ and $K^{th}$ entries and $S_{nk}$ be the sum of all entries in $\bar{\phi}_{nk}$. When $\phi_{nk} = a$ for $a \in [0, 1 - S_{nk}]$, $\phi_{nK} = 1 - a - S_{nk}$. Thus, by sampling $a$, we can update both $\phi_{nk}$ and $\phi_{nK}$. To sample $a$, we use:

$$P_{\theta}(\phi_{nk} = a, \phi_{nK} = 1 - a - S_{nk} | Y_n) = P_{\theta}(\phi_{nk} = a, \phi_{nK} = 1 - a - S_{nk} | Y_n, \bar{\phi}_{nk})$$

$$= \frac{\int_{0}^{1 - S_{nk}} P_{\theta}(\phi_{nk} = a', \phi_{nK} = 1 - a' - S_{nk}, Y_n, \bar{\phi}_{nk})da'}{\int_{0}^{1 - S_{nk}} \exp \left( a(v_k - v_K + \sum_{m=1}^{M} (W_{mk} - W_{mK})y_{nm}) \right)da'}$$

This value can be easily computed and a sample can be drawn using inverse sampling. One can iterate over the indices $1, 2, \ldots, K - 1$ in some order to sample the vector $\phi_n$. Note that the sampling procedure for attributes given $\phi_n$ remains unchanged. With this new Gibbs sampling procedure, the M-step can be performed as before.
To perform E-step, one can follow the derivation given in (Airoldi et al. 2008). However, this time, the vectors $\phi_n$ are sampled from the RBM rather than being sampled from a Dirichlet prior. Thus, the conjugacy arguments no longer hold and unless one makes additional assumptions, a closed form solution cannot be obtained. One can still compute ELBO as before and optimize it using gradient ascent.

The time complexity of this inference procedure is quadratic in the number of nodes. Finding a more efficient inference procedure is an interesting avenue for future research.

### D.3 Overlapping-Communities

In mixed-membership SBM a node cannot exhibit high membership for more than one community simultaneously. In some practical scenarios this is not a good modeling assumption. Consider for instance a person who is part of two reading groups. Being in one reading group may not necessarily reduce the affinity of that person towards the other reading group. The overlapping SBM (OSBM) (Latouche, Birmele, and Ambroise 2011) models such scenarios where a node can simultaneously be part of multiple communities.

To extend RB-SBM for overlapping communities, we use the standard variant of RBM where the community membership vector is no longer restricted to being a one-hot encoded vector and it can be any arbitrary binary vector. These overlapping communities then serve as an input to OSBM. One can use the standard RBM equations for performing M-step. The E-step can be performed by closely mimicking the procedure followed in (Latouche, Birmele, and Ambroise 2011).

However, this inference procedure again runs in time that is quadratic in the number of nodes and finding a more efficient inference procedure is an interesting problem that we defer to future work.

### E Dataset Description

**Cora:** Cora (Lu and Getoor 2003) is a citation network containing 2708 nodes and 5429 edges. The nodes correspond to scientific publications and a directed edge from node $i$ to node $j$ indicates that $j$ was cited by $i$. Each node is also equipped with a vector of 1433 observed binary attributes where each attribute corresponds to the presence/absence of a word from the vocabulary in the content of the documents. The nodes have been classified into 7 ground truth communities corresponding to different domains in computer science.

**Citeseer:** Citeseer (Lu and Getoor 2003) is another citation network that has the same semantics as the Cora network described above. It has 3312 nodes, 3703 attributes per node, 4732 edges and 6 ground truth communities.

**Philosophers:** This network was created in the same way as in (Yang, McAuley, and Leskovec 2013). Entries for all philosophers listed on Wikipedia were crawled based on alphabetical index. Nodes correspond to Philosophers and there is a directed edge from philosopher $i$ to philosopher $j$ if $i$'s Wikipedia page contains a link to $j$’s Wikipedia page. All the non-philosopher entries on Wikipedia to which at least 10 and at most 50% of the philosopher’s web pages point to, define the node attributes. These attributes indicate the presence of links to non-philosopher entries and hence are binary. This network has 1497 nodes and each node has 6357 attributes.