Fast and reliable inference algorithm for hierarchical stochastic block models

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I. INTRODUCTION

Network clustering reveals the organization of a network or corresponding complex system with elements represented as vertices and interactions as edges in a (directed, weighted) graph. Although the notion of clustering can be somewhat loose, network clusters or groups are generally considered as nodes with enriched interactions [18, 20] and edges sharing common patterns [1]. Statistical inference often treats groups as latent variables, with observed networks generated from latent group structure, termed a stochastic block model [22]. Regardless of the definitions, statistical inference can be either translated to modularity maximization, which is provably an NP-complete problem [4].

Here we present scalable and reliable algorithms that recover hierarchical stochastic block models fast and accurately. Our algorithm scales almost linearly in number of edges, and inferred models were more accurate that other scalable methods.

II. MODELS

a. Stochastic block model We represent a network data as an adjacency matrix A, where each element A_{ij} captures the relationship between vertices $i, j \in V$. Let n be a number of vertices, n = |V|, and m be a number of (un)directed edges, or non-zero entries of (upper triangular) A. For a binary and undirected network, A_{ij} takes on a value 1 if i and j interact, 0 otherwise. We assume that the set V decomposes into an arbitrary K disjoint subsets. We give a unique index $1, \ldots, K$ to these subsets. For simplicity let g_i denotes membership mapping of vertex i to a certain group, with $g_i \in [K]$. Assume each group (or block) is identifiable by a $K \times K$ block matrix θ and $\theta_{ab} \in [0, 1]$ for all $a, b \in [K] \times [K]$. We can define the data likelihood as

$$p(A|g,\theta) = \prod_{i < j} \theta_{g_i g_j}^{A_{ij}} (1 - \theta_{g_i,g_j})^{1 - A_{ij}}.$$

b. Degree-corrected stochastic block model In some situations, a degree-corrected stochastic block model (DSBM) provides more appealing group structures in a real-world network [14]. Again, we represent a network as an adjacency matrix A; a vertex set V decomposes into K disjoint subsets; the membership function is $g, g : V \to [K]$. However, A_{ij} may takes on values of non-negative real number, and block-block relationships are captured by a $K \times K$ matrix λ and $\lambda_{ab} \in \mathbb{R}^+$ for all $a, b \in [K] \times [K]$.

Our DSBM generalizes a regular SBM, weighting edges based on degrees of endpoints by ρ_{ij} for each A_{ij} . Here we define $\rho_{ij} \equiv d_i d_j / \sum_{j'} d_{j'}$. Note the denominator determines the scaling of edge weight, but does not strongly influence inference results. We define the data likelihood to have each block-block relationship follow the Poisson distribution:

$$p(A|g,\lambda) = \prod_{i < j} \frac{(\lambda_{g_i,g_j}\rho_{ij})^{A_{ij}}}{A_{ij}!} e^{-\lambda_{g_i,g_j}\rho_{ij}}.$$

c. Hierarchical group-group structure Extensive empirical studies such as [18] suggest that the size of a group is limited to a certain number, meaning that $n/K < \infty$ and $K \to \infty$ as $n \to \infty$. Therefore a full modeling of the block matrices λ and θ is inherently formidable [5] since K^2 can easily exceed n and m. However, most state-of-the-art algorithms require $O(K^2)$ operations per pair and iteration (e.g., [2]), which essentially scales in $O(n^2K^2) \approx O(n^4)$. A model can be reduced that may include only within-group relationships, e.g., diagonalization of the matrix θ [12], so that we achieve O(mK) runtime where m is number of edges. This strategy is useful if groups are identifiable by just "within-group" edges, and edges between groups are sampled with some background probability.

Hierarchical assumption provides balance between the full and the diagonal block-block relationships. We adopt the idea of [6] and model the hierarchical group-group relations by a binary dendrogram (see Fig.1). For instance, the relationship between group a and b is captured by lowest common ancestor LCA(a, b) in the binary dendrogram and



FIG. 1: Hierarhical stochastic block model. (a) We assume that group-group relationships are shared hierarchically. (b) A full block matrix. (c) A shrunken block matrix by the hierarchical model.

associated parameters. The model complexity of hierarchical structure scales in O(K) while modeling group-group interactions.

For the hierarchical SBM (hSB), the likelihood function is defined

$$p(A|g,\boldsymbol{\theta}) = \prod_{i < j} \theta_{\text{LCA}(g_i,g_j)}^{A_{ij}} (1 - \theta_{\text{LCA}(g_i,g_j)})^{1 - A_{ij}}$$
(1)

where the θ parameters follow the conjugate Beta distribution,

$$p(\theta|a_0, b_0) = \mathsf{Beta}(\theta|a_0, b_0) = \frac{\Gamma(a_0 + b_0)}{\Gamma(a_0)\Gamma(b_0)} \theta^{a_0 - 1} (1 - \theta)^{b_0 - 1}.$$

For the hierarchical DSBM (hDSB), the likelihood function is defined

$$p(A|g,\lambda) = \prod_{i < j} \frac{(\lambda_{\text{LCA}(g_i,g_j)}\rho_{ij})^{A_{ij}}}{A_{ij}!} e^{-\lambda_{\text{LCA}(g_i,g_j)}\rho_{ij}},$$
(2)

where the rate parameters follow the Gamma distribution,

$$p(\lambda|a_0, b_0) = \mathsf{Gam}(\lambda|a_0, b_0) = \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0 - 1} e^{-\lambda b_0}.$$

III. MODEL INFERENCE

A. Variational Bayes inference

It is intractable to search over all binary dendrogram models. Instead, we restrict the model space to a class of complete binary trees with a fixed yet sufficiently deep depth. We then apply variational inference algorithms: mean-field approximation [24] and locally collapsed variational inference [23].

We rewrite the likelihood of a tree model T (Eq.2) by introducing latent variables, z_{ia} indicating membership of a vertex *i* in a group *a* if $z_{ia} = 1$, otherwise $z_{ia} = 0$.

$$p(A|z,\lambda) = \prod_{i < j} \prod_{r \in \mathcal{T}} \left[\frac{\lambda_r \rho_{ij}}{A_{ij}!} e^{-\lambda_r \rho_{ij}} \right]^{z_{ia} z_{jb} \mathbb{I}_{\{\text{LCA}(a,b)=r\}}}$$

We approximate the posterior distribution of *z* and λ by the following surrogate distribution:

$$q(z,\lambda|\mu,\alpha,\beta) = \prod_{i=1}^{n} q(\mathbf{z}_{i}|\mu_{i}) \prod_{r \in \mathcal{T}} q(\lambda_{r}|\alpha_{r},\beta_{r})$$
(3)

where $q(\mathbf{z}_i|\mu_i) = \prod_{k=1}^{K} \mu_{ia}^{z_{ia}}$ and $q(\lambda_r|\alpha_r, \beta_r) = \mathsf{Gam}(\lambda_r|\alpha_r, \beta_r)$. As in [23], we distinguish random variables $\{\mathbf{z}_i\}$ as local variables and $\{\lambda_r\}$ as global variables.

a. Global update Given $\langle z_{ia} \rangle \equiv \mu_{ia}$, by the generalized mean-field theory [24], we have variational distributions $q(\lambda_r | \alpha_r, \beta_r)$, for all *r*, characterized by

$$\alpha_r = a_0 + \sum_{a,b} \sum_{i < j} \mathbb{1}_{\{r = \text{LCA}(a,b)\}} \mu_{ia} \mu_{jb} A_{ij}, \quad \beta_r = b_0 + \sum_{a,b} \sum_{i < j} \mathbb{1}_{\{r = \text{LCA}(a,b)\}} \mu_{ia} \mu_{jb} \rho_{ij}.$$
(4)

We can take expectation with respect to the variational Gamma distributions, $\langle \lambda_r \rangle = \alpha_r / \beta_r$ and $\langle \ln \lambda_r \rangle = \psi(\alpha_r) - \ln \beta_r$, where $\psi(\cdot)$ denotes the digamma function. We let

$$\eta_r \equiv (\ln \lambda_r, -\lambda_r)^{\top} \tag{5}$$

for convenience.

b. Local update by mean-field theory Let us consider that we update the probability μ_i of assignment of a vertex *i* to a certain group *a*, given all other latent assignments $\{\mu_j : j \neq i\}$ and the global variables fixed. Note that this probability depends on the global variables η_r located along the path from the leaf *a* to the root of the tree model, which we denote by $\Pi(a)$.

For simplicity, let

$$d_{ia} \equiv \sum_{j} A_{ij} \mu_{ja}, \quad \mathbf{s}_{ia} \equiv (d_{ia}, \sum_{j} \mu_{ja} \rho_{ij})^{\top}.$$
(6)

At some $r \in \Pi(a)$, we may use the aggregated statistics:

$$\mathbf{s}_{ir} \equiv \sum_{b} \mathbb{1}_{\{r = \text{LCA}(a,b)\}} \mathbf{s}_{ib},\tag{7}$$

which allows us to write the update equation sufficiently as

$$\mu_{ia} \propto \exp\{\sum_{r \in \Pi(a)} \langle \eta_r \rangle^\top \mathbf{s}_{ir}\}$$
(8)

subject to $\sum_{a=1}^{K} \mu_{ia} = 1$ and $\mu_{ia} \ge 0$.

c. Local update by collapsed variational inference Alternatively, we may update μ_{ia} by collapsing the global variables with respect to the global variational distributions. Again, we consider assigning a vertex *i* to group *a* and use s_{ir} (Eq.7) collected along the path Π from the root of the tree to the group *a*. However, instead of using the expected natural parameters (Eq.5), we integrate them out.

$$\mu_{ia} \propto \prod_{r \in \Pi(a)} \langle p(\mathbf{s}_{ir} | \lambda_r) \rangle_{q(\lambda | \alpha_r, \beta_r)}$$
(9)

where

$$\langle p(\mathbf{s}_{ir}|\lambda_r)\rangle_{q(\lambda|\alpha_r,\beta_r)} \propto \int \exp\{\eta_r^{\top}\mathbf{s}_{ir}\}q(\eta_r|\alpha_r,\beta_r)\,d\lambda_r.$$

Since our model space has fixed size, we need not sample as proposed in [23], but just normalize μ_i to satisfy the constraints: $\sum_k \mu_{ia} = 1$ and $\mu_{ia} \ge 0$.

B. Dynamic programming

The overall algorithm alternates between global and local updates. We approximate $q(\lambda_r | \alpha_r, \beta_r)$ by Eq. 4, then locally update $q(\mathbf{z}_i | \mu_i)$ by Eq. 8 for meanfield, or 9 for locally collapsed variational inference.

a. Lazy evaluation of the sufficient statistics To have it efficiently evaluate required statistics in the global update (Eq.4), we calculate the following statistics at the leaf-level,

$$d_{ia} = \sum_{j} A_{ij} \mu_{ja}, \quad n_{ia} = \mu_{ia}, \quad \operatorname{vol}_a = \sum_{i} \mu_{ia} d_i,$$

then, for internal r, we can easily accumulate them using lower-level results,

$$d_{ir} = d_{ileft(r)} + d_{iright(r)}, \quad n_{ir} = n_{ileft(r)} + n_{iright(r)}, \quad vol_r = vol_{left(r)} + vol_{right(r)}.$$

We can rewrite the update equations (Eq.4) with respect to d, n, vol as follows. At the leaf group a, d

$$\alpha_a = a_0 + \sum_i d_{ia}\mu_{ia}, \quad \beta_a = b_0 + \frac{1}{4m}\sum_i d_i\mu_{ia}(\operatorname{vol}_a - d_i\mu_{ia})$$

and for internal group *r*,

$$\alpha_r = a_0 + \sum_i n_{i\text{left}(r)} d_{i\text{right}(r)}, \quad \beta_r = b_0 + \frac{1}{2m} \sum_i d_i n_{i\text{left}(r)} (\text{vol}_{\text{right}(r)} - d_i n_{i\text{right}(r)}).$$

b. Deterministic local update In practice, a majority of vertices can play a single role, i.e., $\langle \mathbf{z}_i \rangle$ has only one non-zero element filled with the value 1. We evaluate μ_i by (Eq.8) or (Eq.9). Then we set $\mu_{ia^*} = 1$ for $a^* = \arg \max_a \sum_{r \in \Pi(a)} \langle \eta_r \rangle \mathbf{s}_{ir}$; $mu_{ia} = 0$ for $a \neq a^*$.

Hierarchical group structure allows us to efficiently search for the maximum assignments of vertices. While we perform a depth-first search over the binary tree model, the algorithm keeps track of maximum score *M*, corresponding group assignment *k*, and sufficient statistics **s** (See Alg.1 for details).

Alg 1 Deterministic latent variable inference

```
repeat
        for all i \in V do
                 d_{ik} \leftarrow \sum_i A_{ii} \mu_{ik} for all k
                 (M, k_{\max}, \mathbf{s}) \leftarrow MAXGRADPATH(root of \mathcal{T})
                 \forall k \neq k_{\max}, \mu_{ik} \leftarrow 0 \text{ but } \mu_{ik_{\max}} \leftarrow 1
       end for
until convergence of \{n_k\}
function MAXGRADPATH(r)
       if r is leaf-level, cluster k then
                 \begin{split} \mathbf{s} &\leftarrow (d_{ik}, d_i \mathrm{vol}[k]/2m) \\ M &\leftarrow \langle \eta_k \rangle^\top \, \mathbf{s} \, (\mathrm{Eq.8}), \, \mathrm{or} \, \ln \langle p(\mathbf{s}|\lambda) \rangle_{q(\lambda|\alpha_k, \beta_k)} \, (\mathrm{Eq.9}) \end{split} 
                 return (M, k, s)
       else
                (M_{\text{left}}, k_{\text{left}}, \mathbf{s}_{\text{left}}) \leftarrow \text{MAXGRADPATH}(\text{left}(r))
                 (M_{\text{right}}, k_{\text{right}}, \mathbf{s}_{\text{right}}) \leftarrow \text{MAXGRADPATH}(\text{right}(r))
                M_{\text{left}} \leftarrow M_{\text{left}} + \langle \eta_r \rangle^\top \mathbf{s}_{\text{right}} \text{ (Eq.8), or } \ln \left\langle p(\mathbf{s}_{\text{right}} | \lambda) \right\rangle_{q(\lambda | \alpha_r, \beta_r)} \text{ (Eq.9)}
                 M_{\text{right}} \leftarrow M_{\text{right}} + \langle \eta_r \rangle^{\top} \mathbf{s}_{\text{left}} (Eq.8), or \ln \langle p(\mathbf{s}_{\text{left}} | \lambda) \rangle_{q(\lambda | \alpha_r, \beta_r)} (Eq.9)
                 M_{\text{max}} \leftarrow \max{\{M_{\text{left}}, M_{\text{right}}\}}, \text{ and } k_{\text{max}} \leftarrow \arg\max_{k' \in \{\text{left, right}\}} M_{k'}
                return (M_{\text{max}}, k_{\text{max}}, \mathbf{s}_{\text{left}} + \mathbf{s}_{\text{right}})
       end if
end function
```

c. Probabilistic local update The similar lazy-evaluation approach can be applied to the probabilistic latent variable update for μ_{ia} . With memoization of partial log-scores (Eq.9 or Eq.8), we can exactly evaluate μ within two passes of tree traversal (see Alg.2 for details).

Both global and local update steps scale in O(mK). The deterministic update converges faster (in 5 to 10 iterations), while the probabilistic one converges in tens of iterations.

d. Pruning unnecessarily branching subtrees Allowing sufficient depth of the tree model, we may generate an over-complicated model fitted to noisy observation. To reduce model complexity, we apply final pruning steps. At each subtree of the full model, we compared this subtree with the collapsed model under the single group. We determine whether to collapse or not via the Bayse factor, or log-ratio of the marginal likelihood [13]. This automatically determines the number of groups from the data.

e. Initialization Variational inference algorithms not necessarily guarantee the convergence to global optima. To avoid bad local optima, we may restart the algorithm multiple times from random configuration. However, the model space grows super-exponentially and an algorithm may require exponentially many random restarts. Instead, we found that iterative bisections of network provide a good starting point. Since each bisection using the deterministic inference with 2 groups can be completed in O(m), we can finish the whole initialization in $O(m \log K)$.

```
repeat
      for all i \in [n] do
            d_{ik} \leftarrow \sum_j A_{ij} \mu_{jk} for all k
             CALCGRADPATH(root of \mathcal{T})
            SUMGRADPATH(root of \mathcal{T}, 0)
             \mu_{ik} \propto \exp\{\nabla[k]\}
      end for
until convergence
function CALCGRADPATH(r)
      if r is leaf-level, cluster k then
            \mathbf{s} \leftarrow (d_{ik}, d_i \text{vol}[k]/2m)
            return s
      else
            \mathbf{s}_{\text{left}} \leftarrow \text{CALCGRADPATH}(\text{left}(r))
            \mathbf{s}_{right} \leftarrow CALCGRADPATH(right(r))
            \delta_{\text{left}}[r] \leftarrow \langle \eta_r \rangle^\top \mathbf{s}_{\text{right}} \text{ (Eq.8), or } \ln \left\langle p(\mathbf{s}_{\text{right}} | \lambda) \right\rangle_{q(\lambda | \alpha_r, \beta_r)} \text{ (Eq.9)}
            \delta_{\text{right}}[r] \leftarrow \langle \eta_r \rangle^{\top} \mathbf{s}_{\text{left}} (Eq.8), or \ln \langle p(\mathbf{s}_{\text{left}} | \lambda) \rangle_{q(\lambda | \alpha_r, \beta_r)} (Eq.9)
            return (\mathbf{s}_{left} + \mathbf{s}_{right})
      end if
end function
function SUMGRADPATH(r, α)
      if r is bottom-level, cluster k then
            \mathbf{s} \leftarrow (d_{ik}, n_k)
            \nabla[k] \leftarrow \alpha + \langle \eta_k \rangle^\top \mathbf{s} (Eq.8), or \ln \langle p(\mathbf{s}|\lambda) \rangle_{a(\lambda|\alpha_k,\beta_k)} (Eq.9)
      else
            SUMGRADPATH(left(r), \alpha + \delta_{left}[r])
            SUMGRADPATH(right(r), \alpha + \delta_{right}[r])
      end if
end function
```

f. Approximation for speed up Although O(mK) runtime is practical for small K, a network of 10,000 nodes and 100,000 edges could have K as large as 1000. Therefore, full computation of each variational update could make the overall algorithm scales essentially in O(mn) (if O(n) = O(K)). We may reduce m as in the previous work [12] by stochastic variational inference. Here, we address different aspect, reducing K to some $k^* \ll K$.

Suppose we want to re-assign a vertex *i* by evaluating $\{\mu_{ik} : k \in [K]\}$. In assortative networks, vertices tend to form a group only with connected vertices. This allows us to locally carry out the computation of latent and global updates. Let *U* be a subset of leaf groups, to which the vertex *i* is connected, i.e., $U = \{k \in [K] : d_{ik} > 0\}$ (see Eq.6). Let $k_{\min} = \min U$ and $k_{\max} = \max U$. With a proper initial configuration (e.g., iterative bisections), we get $|U| \ll K$. Then, we can restrict MAXGRADPATH (Alg.1), and CALCGRADPATH and SUMGRADPATH (Alg.2) to a small subtree. We can call them from LCA(k_{\min}, k_{\max}). Moreover, this locality can be determined in constant time.

IV. RESULTS AND DISCUSSIONS

a. Simulation study The hDSB outperforms in various benchmark networks. We generated sparse network data with average degree 10 and maximum degree 100 using the LFR benchmark [17]. We also tested on benchmark networks with higher degrees (e.g., 30, 50, 100) and found that hDSB was still the best performing algorithm, and its performance can easily attain to the mutual information 1. However, this setting is far from real-world networks, so we omit the result. With the fixed degree distribution, we varied size of the networks (5000, 10000). We also varied the maximum size of groups (20, 50, 100, 150) while fixing the minimum size to 10. Although our method can provide mixed membership probability, we did not allow mixed membership to compare with other community detection methods.

Fig.2 compares hDSB with locally collapsed variational inference (hDSB-lcvi), hDSB with mean-field (hDSB-mf), *k*-metis provided with true *K* [15] (Metis), hSB with mean-field (hSB), and modularity maximization [7] (CNM). We measured the normalized mutual information (NMI) [16] between the inferred and the ground truth groups. The



FIG. 2: The benchmark result. **x-axis**: noise parameter (the μ parameter of LFR [17]); **y-axis**: normalized mutual information [16]; **Top titles**: the maximum size of a group; **Right titles**: total number of vertices. See the text for details.

NMI scales in between 0 and 1, and higher value means higher similarity.

In overall, the performance of hDSB dominates the other methods. The effect of different latent variable inference was not so significant. For networks with balanced group structure, with the maximum group size ≤ 50 , Metis algorithm performs nearly as well as hDSB. However, it requires the number of groups as a parameter, and real-world networks may contain heterogeneous group structures. The degree-correction provides more realistic group structure than regular SBM; in fact, we found that it prevents from over-segmentation. Not surprisingly, since CNM algorithm relies on local greedy steps, it was most sensitive to noise and resolution limit problem [10] (under-segmentation).

b. Cross-validation: link prediction tests We used 6 real-world datasets (2 biological and 4 social networks): NCAA: NCAA college football network [11]; NetSci: coauthorship network on the network science [21]; Hep-Th: co-authorship network on the High-Energy Theory Archive [20]; Cond: co-authorship network on the Condensed Matter Archive [20]; Reactome: co-reaction network [8]; CoExp: Genemania co-expression network [19].

With true group structure unknown, performance may be assessed by link prediction. We removed links chosen uniformly from the observed network. For large networks, such as Hep-TH, Cond, CoExp, we chose the same number of non-links. For smaller networks, NCAA, NetSci, Reactome, we chose non-links while preserving the original ratio of links to non-links. We preprocessed the networks by iteratively removing vertices with degree ≤ 2 , since these vertices do not form a group.

In addition to the methods used in the benchmark study, we considered the sampling method of hierarchical random graph [6] (HRG) and the link community optimization by the maximum likelihood [3] (LC). These methods do not provide a fixed group structure, rather scores s_{ij} for a pair ij, and a high scoring pair means a possible link. For the algorithms that provide a group structure, we estimated the score s_{ij} by group-wise frequency,

$$\hat{\theta}_{ab} = \frac{\# \text{ links observed between one end in group } a \text{ and the other in group } b}{\# \text{ possible links between groups } a \text{ and } b}$$

For instance, a pair *ij* takes $\hat{\theta}_{ab}$ as a score if *i* and *j* belong to groups *a* and *b* respectively. We allowed 10 random restarts for LC method. Metis and LC require pre-specified number of blocks or colors. We performed discrete grid search over the parametric space and reported the best results. As a summary statistic, we estimated the area under the precision-recall curve (AUPRC) [9]. AUPRC scales in [0, 1] on the small datasets (NCAA, NetSci, and Reactome); [0.5, 1] on the large networks (Hep-Th, Cond2005, CoExp).

Fig.3 shows the results on these networks. Either hDSB or hSB was consistently top-ranked on all datasets over all range of missing links. Notably hSB performed best in some networks. We may conclude that groups of hSB are as robust as hDSB, and groups of the benchmark networks can be reasonably further decomposed into smaller groups. In the NCAA network, our algorithms even outperformed the exhaustive sampling method (HRG). Link community optimization (LC) works poorly in both scalability and accuracy if a network consists of many groups. It



FIG. 3: The missing link prediction results. *x*-axis: a fraction of missing links; *y*-axis: area under the precision recall curve; (n,m): n = number of vertices and m = number of edges.

appears that the proposed algorithm of Ball & Newman [3] can easily overfit the training data. A similar argument was also made previously [12].



FIG. 4: Runtime of the algorithms.

c. Runtime Fig.4 shows runtime [25] as a function of number of edges. We ran Alg. 2 with full or restricted calculation. While the full version increases almost quadratically (red dots), runtime of the restricted grows linearly (blue triangles) on simulation and real-world networks. In terms of accuracy, the restricted version worked equally well.

Acknowledgments

Source codes available at https://code.google.com/p/hsblock/ or from the authors by e-mail.

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