Stochastic Blockmodel with Cluster Overlap, Relevance Selection, and Similarity-Based Smoothing

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Introduction

• Stochastic Blockmodel

- **A** Generative model
- Expresses objects as a low dimensional representation $\mathit{U}_{i},\mathit{U}_{j}$
- Models the link probability of a pair of objects $P(A_{ij}) = f(U_i, U_j, \boldsymbol{\theta})$
- e.g., latent class model, mixed membership stochastic blockmodel

• Applications

- Revealing structures in networks
- (Overlapping) Clustering, Link prediction

Introduction

- Overlapping stochastic blockmodels
	- Objects have hard memberships in multiple clusters.

- Contributions of this paper
	- Extend the overlapping stochastic blockmodel to bipartite graphs
	- **Relevance selection mechanism**
	- Make use of additionally available object features
	- Nonparametric Bayesian approach

Background

- Indian Buffet Process (IBP) (Griffiths et al. 2011)
	- N objects, K clusters, overlapping clustering $\mathbf{U} \in \{0,1\}^{N \times K}$.
	- Object: customer, cluster: dish
	- The first customer selects $Poisson(\alpha)$ dishes to begin with
	- \bullet Each subsequent customer n :
		- Selects an already selected dish k with probability $\frac{m_k}{n}$
		- Selects $Poisson(\alpha/n)$ new dishes

The Proposed Model

Basic Model

• Bipartite graph ($N \times M$ binary adjacency matrix, $|\mathcal{A}| = N$, $|\mathcal{B}| = M$)

$$
\begin{array}{rcl}\n\mathbf{U} & \sim & \mathcal{IBP}(\alpha_u) \\
\mathbf{V} & \sim & \mathcal{IBP}(\alpha_v) \\
\mathbf{W} & \sim & \mathcal{N} \text{or} (0, \sigma_w^2) \\
\mathbf{A} & \sim & \mathcal{B} \text{er}(\sigma(\mathbf{U} \mathbf{W} \mathbf{V}^\top))\n\end{array}
$$

- $\mathcal{IBP}(\alpha)$: IBP prior distribution, \mathcal{N} or $(0,\sigma^2)$: Gaussian distribution,
- $\sigma(x) = \frac{1}{1+\exp(-x)}$, $Ber(p)$: Bernoulli distribution,
- $-$ U $\in \{0,1\}^{N \times K}$, V $\in \{0,1\}^{M \times L}$: cluster assignment matrices

$$
P(A_{nm} = 1) = \sigma(\mathbf{u}_n \mathbf{W} \mathbf{v}_m^{\top})
$$

= $\sigma(\sum_{k,l} u_{nk} W_{kl} v_{ml})$

- W_{kl} : the interaction strength between two nodes due to their memberships in cluster k and cluster l

 $P(A_{nm} = 1) = \sigma(W_{12} + W_{13} + W_{32} + W_{33})$

Basic Model

Unipartite graph $(\mathbf{A} \in \{0,1\}^{N \times N})$

U ~
$$
\mathcal{IBP}(\alpha_u)
$$

\n**W** ~ $\mathcal{N}or(0, \sigma_w^2)$
\n**A** ~ $\mathcal{Ber}(\sigma(\mathbf{U}\mathbf{W}\mathbf{U}^{\top}))$

$$
P(A_{nm} = 1) = \sigma(\mathbf{u}_n \mathbf{W} \mathbf{u}_m^{\top})
$$

= $\sigma(\sum_{k,l} u_{nk} W_{kl} u_{ml})$

- $IBP(\alpha)$: IBP prior distribution, \mathcal{N} or $(0,\sigma^2)$: Gaussian distribution,
- $\sigma(x) = \frac{1}{1+\exp(-x)}$, $Ber(p)$: Bernoulli distribution,
- $\mathsf{L} \ \ \mathsf{U} \in \{0,1\}^{N \times K}$: cluster assignment matrix $\mathsf{P} (\mathsf{A}_{nm} = 1) = \sigma (\, W_{12} \! + \! W_{13} \! + \! W_{32} \! + \! W_{33})$

Relevance Selection Mechanism

- **•** Motivation
	- In real-world networks, there may be some noisy objects (e.g., spammer)
	- May lead to bad parameter estimates
- Maintain two random binary vectors $\mathbf{R}^{\mathcal{A}} \in \{0,1\}^{N \times 1}$, $\mathbf{R}^{\mathcal{B}} \in \{0,1\}^{M \times 1}$

Relevance Selection Mechanism

- **•** Background noise link probability $\phi \sim \text{Beta}(a, b)$
- If one or both objects $n \in A$ and $m \in B$ are irrelevant
	- A_{nm} is drawn from $\mathcal{B}er(\phi)$
- \bullet If both *n* and *m* are relevant,
	- A_{nm} is drawn from $\mathcal{B}er(p) = \mathcal{B}er(\sigma(\mathbf{u}_n\mathbf{W}\mathbf{v}_m^{\top}))$

$$
\begin{array}{rcl}\n\phi & \sim & \mathcal{B}\text{et}(a, b) \\
R_n^A & \sim & \mathcal{B}\text{er}(\rho_n^A), \quad R_m^B \sim \mathcal{B}\text{er}(\rho_m^B) \\
\mathbf{u}_n & \sim & \mathcal{IBP}(\alpha_u) \quad \text{if } R_n^A = 1 \text{; zeros otherwise} \\
\mathbf{v}_m & \sim & \mathcal{IBP}(\alpha_v) \quad \text{if } R_m^B = 1 \text{, zeros otherwise} \\
\rho & = & \sigma(\mathbf{u}_n \mathbf{W} \mathbf{v}_m^\top) \\
A_{nm} & \sim & \mathcal{B}\text{er}(\rho^{R_n^A R_m^B} \phi^{1 - R_n^A R_m^B})\n\end{array}
$$

Exploiting Pairwise Similarities

- We may have access to side information
	- e.g., a similarity matrix between objects
- The IBP does not consider the pairwise similarity information.
	- Customer *n* chooses an existing dish regardless of the similarity of this customer with other customers.
- \bullet Two objects *n* and *m* have a high pairwise similarity \Rightarrow **u**_n and **u**_m should also be similar.
	- Encourages a customer to select a dish if the customer has a high similarity with all other customers who chose that dish.
	- Let the customer select many new dishes if the customer has low similarity with previous customers.

Exploiting Pairwise Similarities

- Modify the sampling scheme in the IBP based generative model
	- The probability that object *n* gets membership in cluster k will be proportional to $\frac{\sum_{n' \neq n} S_{nn'}^A u_{n'k}}{\sum_{n'=1}^n S_{nn'}^A}$.

 $\sum_{n'=1}^{n} S_{nn'}^{A}$: effective total number of objects,
 $\sum_{n'\neq n} S_{nn'}^{A} u_{n'k}$: effective number of objects (other than *n*) that belong to cluster k

- IBP:
$$
\frac{\sum_{n' \neq n} u_{n'k}}{n} = \frac{m_k}{n}
$$

 \bullet The number of new clusters for object *n* is given by Poisson $(\alpha/\sum_{n'=1}^n S_{nn'}^A)$.

If the object n has low similarities with the previous objects, encourage it more to get memberships in its own new clusters

- IBP: $Poisson(\alpha/n)$

The Final Model

• ROCS (Relevance-based Overlapping Clustering with Similarity-based-smoothing)

- $\; Sim \mathcal{IBP}(\alpha_u, \mathsf{S}^A) \!\!: \;$ similarity information augmented variant of the IBP
- For inference, we use MCMC (Gibbs sampling)

o Tasks

- **The correct number of clusters**
- Identify relevant objects
- Use pairwise similarity information
- Overlapping clustering
- Link prediction

o Baselines

- Overlapping Clustering using Nonnegative Matrix Factorization (OCNMF) (Psorakis et al. 2011)
- Kernelized Probabilistic Matrix Factorization (KPMF) (Zhou et al. 2012)
- Bayesian Community Detection (BCD) (Mørup et al. 2012)
- Latent Feature Relational Model (LFRM) (Miller et al. 2009)

- **•** Synthetic Data
	- 30 relevant objects, 20 irrelevant objects
	- Three overlapping clusters

• Overlapping clustering

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Table 1: Link Prediction on Synthetic Data

Results Summary

- ROCS perfectly identifies relevant/irrelevant objects
- ROCS identifies the correct number of clusters
- For link prediction task, ROCS is better than other methods in terms of both 0-1 test error and AUC score.

Facebook Data

- An ego-network in Facebook (228 nodes)
- User profile (e.g., age, gender, etc.) select 92 features.
- **Known number of clusters: 14**

Table 2: Link Prediction on Facebook Data

- BCD overestimated the number of clusters (20-22 across multiple runs). \bullet
- LFRM and ROCS almost correctly inferred the ground truth number of clusters (13-15 across multiple runs).

- Drug-Protein Interaction Data
	- Bipartite graph (200 drug molecules, 150 target proteins)
	- Drug-drug similarity matrix, Protein-protein similarity matrix

Method \vert 0-1 Test Error $\left(\frac{0}{0}\right)$ \vert AUC KPMF | 16.65 (\pm 0.36) | 0.8734 (\pm 0.0133) LFRM \vert 2.75 (\pm 0.04) \vert 0.9032 (\pm 0.0156) ROCS | 2.31 (\pm 0.06) | 0.9276 (\pm 0.0142)

Table 3: Link Prediction on Drug-Protein Interaction Data

- OCNMF and BCD are not applicable for bipartite graphs.
- LFRM here denotes ROCS without similarity information.
- KPMF takes into account the similarity information but does not assume overlapping clustering.

- Lazega Lawyers Data
	- Directed graph, social networks (71 partners)
	- Each entry has features (gender, office-location, age, etc.)

Method	0-1 Test Error $(\%)$	AUC.
OCNMF	35.36 (± 20.71)	0.6388 (± 0.1527)
KPMF	34.69 (± 1.13)	$\overline{0.7203 \ (\pm 0.0229)}$
BCD	16.58 (± 0.56)	$0.7876 \ (\pm 0.0168)$
LFRM	14.05 (\pm 2.04)	$\overline{0.8025 \ (\pm 0.0205)}$
ROCS	$\overline{12.98}$ (\pm 0.32)	$\overline{0.8248}$ (\pm 0.01642)

Table 4: Link Prediction on Lazega-Lawyers Data

Even weak similarity information can yield reasonable improvements in the prediction accuracy

Conclusions

Conclusions

• ROCS: a flexible model for modelling unipartite/bipartite graphs.

- Each object can belong to multiple clusters (hard membership).
- Nonparametric Bayesian approach.
- Irrelevant objects can be dealt with in a principled manner.
- Pairwise similarity between objects can be exploited to regularize the cluster memberships of objects.
- **Future work: make the model scalable.**

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