Bipartite Sparse Exchangeable Graphs for Machine Learning

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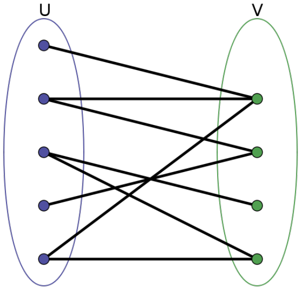
ML Group Meeting

Bipartite graphs

Definition

A bipartite graph is an ordered triple (V_U, V_I, E) where V_U, V_I are sets of vertices and $E \subseteq V_U \times V_I$ is a set of edges.



- $u \in V_U$ means that there is a vertex with label u in the graph.
- $t \in V_I$ means that there is a vertex with label t in the graph.
- $(u, t) \in E$ means that there is an edge between vertices u and t.
- Note that there are edges only between vertices of different part.
- I'll use the vocab of *users* and *items* to distinguish between parts of a graph.

Overview

- Many models in machine learning, e.g. models for topic modeling, probabilistic matrix factorization, feature allocation, define probability distribution over bipartite graphs

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- Many models in machine learning, e.g. models for topic modeling, probabilistic matrix factorization, feature allocation, define probability distribution over bipartite graphs
- Interested in inferring the parameters of distribution over bipartite graph from direct or indirect observation of the graph
- Recent work in statistical network modeling has introduced the sparse exchangeable (graphex) models as a new family of probability distributions over graphs (in particular, over bipartite graphs)

Big Picture

- What practical insights can be gained in light of the new sparse graph theory?
  - How to check for sparsity for a fixed size graph?
  - Can we scale inference for models belonging to this new model class?

Background

Example: Non-Negative Matrix Factorization

- Observed Data: Binary Adjacency matrix indicating if user i consumed item j
- Model: Probability of an edge depends only on the inner product of some latent user preference and item property
- Task: Make customized recommendations of items to users based on the observed graph

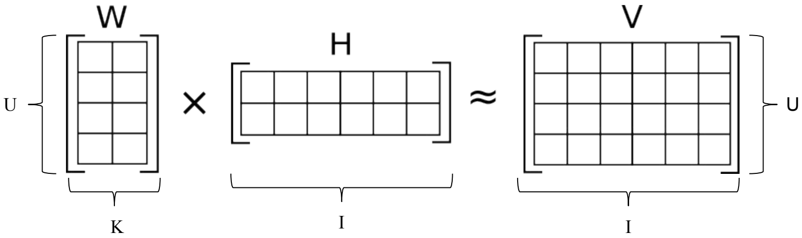

Figure: Non-Negative Matrix Factorization

Example: Non-Negative Matrix Factorization

Generative Model

For an observed adjacency matrix with n users and m items,

- Each user $i \in \{1, \ldots, n\} = V_U$
  User preference: $X_i \in \mathbb{R}_+^K$, is assigned iid with distribution $\Pr(X_i \in \cdot | \theta_U)$
- Each item $j \in \{1, \ldots, m\} = V_I$
  Item property: $Y_j \in \mathbb{R}_+^K$, is assigned iid with distribution $\Pr(Y_j \in \cdot | \theta_I)$
- Given the user preference and item property, include the edge (i, j) in E with probability $W(X_i^T Y_j)$, for e.g. $W(X_i^T Y_j) = 1 - e^{-X_i^T Y_j}$

Task: Learn likely values of $\{X_i\}, \{Y_j\}, \theta_U$, and θ_I

Dense Exchangeable Bipartite Graph Framework

Generative Model

Sample of a random graph $G_{n,m}$, where $n, m \in \mathbb{N}$, as follows:

- For each user vertex $i \in \{1, \ldots, n\}$, assign a latent feature $x_i \in \mathcal{X}$ iid with some distribution
- For each item vertex $j \in \{1, \ldots, m\}$, assign a latent feature $y_j \in \mathcal{Y}$ iid with some distribution
- Given the user feature and item feature, include the edge (i, j) independently with probability $W(x_i, y_j)$, where $W : \mathcal{X} \times \mathcal{Y} \to [0, 1]$ is called a graphon

Notes:

- Examples include, probabilistic matrix factorization, topic modeling, feature allocation
- Gives rise to graphs that are almost surely dense graphs, i.e., as the number of vertices increase, the ratio $\rho = \frac{|E|}{|V_U||V_I|}$ remains constant.

Sparse Exchangeable Bipartite Graph Framework

Generative Model

Sample a random graph $G_{s,\alpha}$, where $s, \alpha \in \mathbb{R}_+$, as follows:

- Sample user features: a Poisson Process $\{(x_i, u_i)\}$ on $\mathcal{X} \times [0, s]$
- Sample item features: a Poisson Process $\{(y_j, t_j)\}$ on $\mathcal{Y} \times [0, \alpha]$
- Given the user feature and item feature, include the edge (u_i, t_j) independently with probability $W(x_i, y_j)$, where $W : \mathcal{X} \times \mathcal{Y} \to [0, 1]$ is a (generalized) graphon
- Throw away all vertices that failed to connect

Example

$W : \mathbb{R}_+ \times \mathbb{R}_+ \to [0, 1]$ is defined as: $W(x, y) = 1 - \exp(-xy)$
User Size: $s < s' \in \mathbb{R}_+$
Item Size: $\alpha < \alpha' \in \mathbb{R}_+$

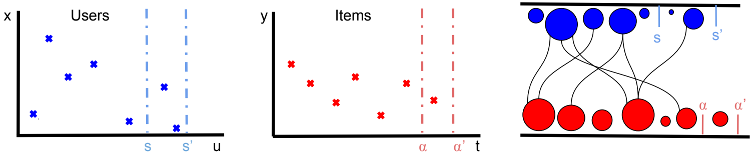

Figure: Sample from the generative model

Example

$$V_U^s = \{u_2, u_3, u_4\} \quad V_U^{s'} = \{u_2, u_3, u_4, u_5\}$$
$$V_I^\alpha = V_I^{\alpha'} = \{t_1, t_2, t_4, t_6\}$$
$$E^s = \{(u_2, t_1), (u_2, t_4), (u_2, t_6), (u_3, t_1), (u_4, t_2), (u_4, t_4)\}$$
$$E^{s'} = \{(u_2, t_1), (u_2, t_4), (u_2, t_6), (u_3, t_1), (u_4, t_2), (u_4, t_4), (u_5, t_4)\}$$

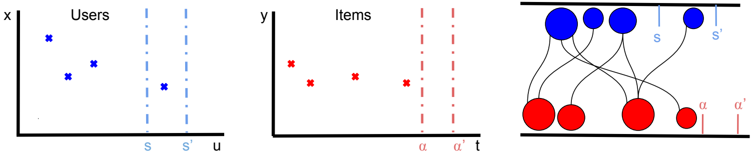

Figure: Sample from the generative model

Sampling Results

Questions

Sparsity is a property of sequences of graphs.

- How can we test if a given dataset is generated using a sparse model?
- How to sub-sample the dataset for test-train split?

p-Sampling a Graph

Definition

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Theorem (VR16)

Let $(G_{s,\alpha})_{s\in\mathbb{R}_+,\alpha\in\mathbb{R}_+}$ *be generated by* W*. If* $\mathrm{user\text{-}p\text{-}samp}(G_{s,\alpha}, r/s)$ *is an* r/s*-sampling of* G_s*, then*

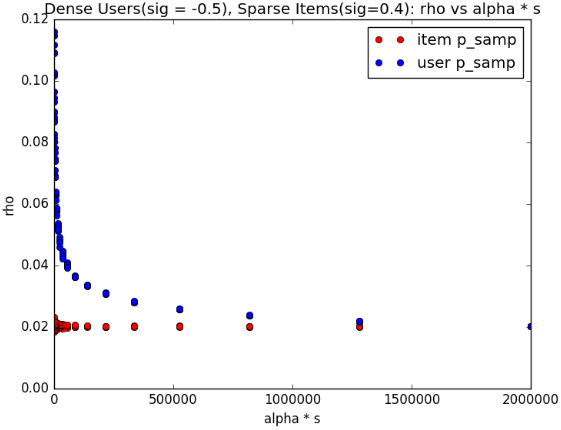
$$\mathrm{user\text{-}p\text{-}samp}(G_{s,\alpha}, r/s) \stackrel{d}{=} G_{r,\alpha}$$

Mutatis mutandis for $\mathrm{item\text{-}p\text{-}samp}$

Test for Sparsity

Recall: For densely generated graphs, $\rho = \frac{|E|}{|V_U| * |V_I|}$ remains constant.

For sparsely generated graphs, as user/item size decreases, ρ should increase.



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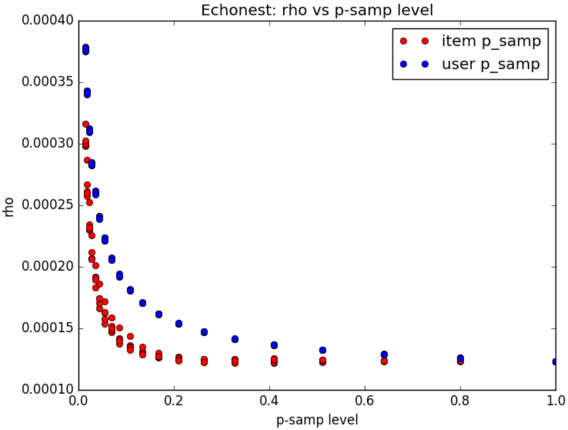
Yes! : Echonest: Music data set with 1 million users and 385,000 songs, with 48 million observations. Each observation is the number of times a user played a song.



Test for Sparsity

Netflix: Movie data set with 480,000 users and 17,770 movies, with 100 million observations.

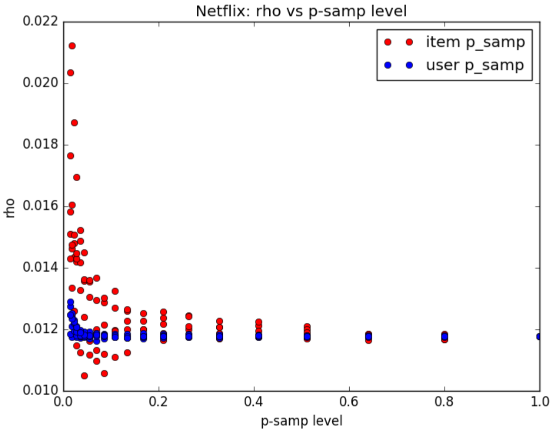


Figure: Netflix

Insights related to Train-Test Split

How do we split graph datasets like Echonest, Netflix?

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- Existing Approach: Randomly holdout some fraction of the edges
  - Makes the recommendation task easier: more likely to select edges from high degree users and high degree items.
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- Existing Approach: Randomly holdout some fraction of the edges
  - Makes the recommendation task easier: more likely to select edges from high degree users and high degree items.
  - Unfairly penalizes generative models: Posterior distribution would be incorrect because of biased sampling
- Proposed Approach: Based on $p-$sampling
  - Split the edge set into Train and Test set by p-sampling users
  - Run the training procedure to infer item properties. Fix the item properties once training finishes.
  - Split Test set into lookup and heldout set by p-sampling items
  - Run the training procedure to infer users preferences in the lookup set (keeping item properties fixed)
  - Perform the prediction task on heldout set.

Extended Example: Sparse Non-Negative Matrix Factorization

Application: Sparse Non-Negative Matrix Factorization

Recall:

- Observed Data: Adjacency matrix g where g_{ij} indicates user i consumed item j

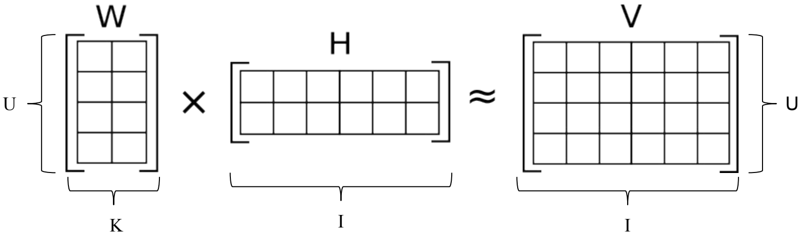


Figure: Non-Negative Matrix Factorization

Application: Non-Negative Matrix Factorization

Main Idea

Users and items have a $K-$dimensional latent feature

- Each user i has total popularity P_i and feature affinity $(\phi_{ik})_{k=1}^K$
- Each item j has total popularity P'_j and feature affinity $(\varphi_{jk})_{k=1}^K$
- Probability of edge (i, j) is given as $1 - exp(-P_i P'_j \sum_k \phi_{ik}\varphi_{jk})$

Note: Inclusion probability of edge (i, j) is the probability of a non-zero draw from a Poisson distribution with mean $P_i P'_j \sum_k \phi_{ik}\varphi_{jk}$

Digression: Generalized Gamma Process

For $(\sigma, \tau) \in (0,1) \times \mathbb{R}_+ \cup [\infty \times \mathbb{R}_+$, let $\rho_{\sigma,\tau}$ denote the Lévy intensity measure of a Generalized Gamma process:

$$\rho_{\sigma,\tau}(\mathrm{d}\omega) = \frac{1}{\Gamma(1-\sigma)} \omega^{-1-\sigma} \exp(-\omega\tau)\mathrm{d}\omega,$$

Properties of GGP

- Pseudo-conjugacy relationship with Poisson distribution - useful for inference
- Poisson process has finite activation $\iff$ $\sigma < 0$ (model is equivalent to dense graph) - useful for interpretablity

Application: Sparse Non-Negative Matrix Factorization

Generative Model (TC16)

- Sample user features:

$$\{(x_1, u_1), \ldots\} \sim \mathrm{PP}(\rho_{\sigma_U,\tau_U} \times \mathrm{Leb}_{[0,s]}) \quad \theta_{ik} \overset{iid}{\sim} \mathrm{Gamma}(a, b)$$

- Sample item features:

$$\{(y_1, t_1), \ldots\} \sim \mathrm{PP}(\rho_{\sigma_I,\tau_I} \times \mathrm{Leb}_{[0,\alpha]}) \quad \beta_{jk} \overset{iid}{\sim} \mathrm{Gamma}(c, d)$$

- Given user features and item features:

$$e_{ij}^k | x_i, \{\theta_{ik}\}, y_j, \{\beta_{jk}\} \overset{ind}{\sim} \mathrm{Poi}(x_i y_j \theta_{ik} \beta_{jk})$$

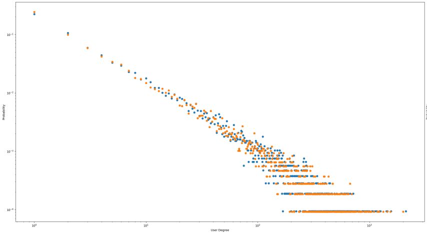
Probability of edge between user u_i and item t_j is given as $\Pr\{\sum_k e_{ij}^k > 0\}$

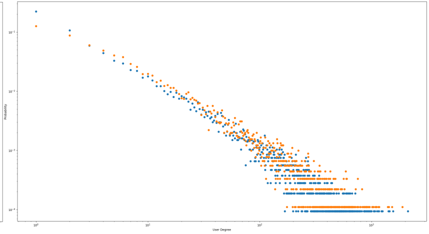
Variational Inference

- Model is defined in a way, using gamma-poisson conjugacy, complete conditionals for parameters lie in exponential family
- Use mean field approximation for the posterior distribution over parameters
- Variational distributions for all parameters are in the same exponential family as their complete conditionals
- We follow a coordinate ascent inference scheme described in [GHB14] for scaling inference
- (Forthcoming Paper for more details)

Posterior simulation

- We simulated a sparse graph of large size.
- Based on observation of a subgraph, we computed the posterior predictive distribution of the degree distribution of items for
  1. a sparse GGP prior (left figure), and
  2. a dense GGP prior (right figure).
- In both case the blue curve corresponds to the true degree distribution and the orange curve corresponds to the posterior predictive average.





Summary

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- Sampling Insights:
  - Test for sparsity
  - New train-test split for relational data
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That's all Folks!