ABSTRACT

A variety of machine learning tasks—e.g., matrix factorization, topic modelling, and feature allocation—can be viewed as learning the parameters of a probability distribution over bipartite graphs. Recently, a new class of models for networks, the sparse exchangeable graphs, have been introduced to resolve some important pathologies of traditional approaches to statistical network modelling; most notably, the inability to model sparsity (in the asymptotic sense). The present paper explains some practical insights arising from this work. We first show how to check if sparsity is relevant for modelling a given (fixed size) dataset by using network subsampling to identify a simple signature of sparsity. We discuss the implications of the (sparse) exchangeable subsampling theory for test–train dataset splitting; we argue common approaches can lead to biased results, and we propose a principled alternative. Finally, we study sparse exchangeable Poisson matrix factorization as a worked example. In particular, we show how to adapt mean field variational inference to the sparse exchangeable setting, allowing us to scale inference to huge datasets.

1 INTRODUCTION

Consider a dataset consisting of users, items, and links between users and items whenever a user has consumed a particular item. A common task is to recommend unconsumed items to users. Loss functions that directly optimize the quality of the recommendation tend to be intractable, which motivates learning a recommendation rule by instead minimizing some proxy. A particularly natural choice is to fit a generative model for the dataset and base recommendations on this model, e.g., by recommending items that have a high posterior probability of being ranked highly by the user. Intuitively, the quality of the recommendation depends on the quality of the model. The vast majority of relational data modelling approaches used in practice fall under the remit of the dense exchangeable (or dense graphon) framework [2, 15, 20]; models in this class are intuitive and easy to work with, but have a limited capacity to capture the structure of real-world data. In particular, they are misspecified as models for sparse data [20]. Recently, the dense exchangeable framework has been generalized to accommodate a much larger range of phenomena. This new framework is known as the sparse exchangeable (or graphex) framework [5–9, 12, 16, 17, 21–23]. By viewing relational datasets as bipartite graphs we are able to, in principle, apply the sparse exchangeable framework to generalize many existing approaches in machine learning and improve the quality of the underlying model.

This idea is widely applicable. For example, in topic modelling, we take one part of the bipartite graph to be words, the other part to be documents, and the edges indicate whether each word is included in each document. In feature allocation, one part of the graph is people, the other part is features, and the edges indicate whether each feature is possessed by each person. In recommendation, one part is users, the other part is items, and each edge (i, j) indicates that user i has consumed item j. For the sake of concreteness, we will use this user-item analogy throughout the remainder of the paper.

We call a sequence of growing bipartite graphs dense if a constant fraction of all edges are present as either (or both) the number of users or items increases, and we call a sequence sparse (or not dense) if it is not dense.

Folk wisdom holds that real-world relational datasets are sparse, and thus that the traditional modelling approach is unsatisfactory. However, sparsity is a property of a sequence of observations, and in many data analysis situations we just have a single observation at some particular size. This begs the question: does sparsity have practical relevance in this case? To answer this question, we develop a simple method for directly checking whether sparsity is relevant for a given dataset. The key idea is to use the subsampling theory for sparse exchangeable graphs [5, 23] to extract a sequence of shrinking subgraphs from the dataset; the sparsity of this sequence acts as a signature for whether sparsity needs to be accounted for in the modelling of the dataset. We use this method to show that sparsity is indeed common in real-world datasets.

Next, we treat the question of how a dataset should be split into training and testing sets. This is a subtle question in the relational data setting, and often ad hoc methods are used. In the probabilistic approach a dataset \( G_s \) is modeled as a realization of size \( s \) from a probabilistic model with parameters \( \Theta \), i.e.,

\[
G_s \mid \Theta \sim P(G_s \in \cdot \mid \Theta).
\]

The key observation is that the test and train sets should be distributed as size \( r \) and size \( s-r \) samples from a distribution with common parameter \( \Theta \); that is, the test and train sets should (marginally) come from the same distribution as the dataset. If this fails, then a model estimated using the training data will be biased for the test and full datasets. Accordingly, we must split the data using the unique subsampling scheme that has this property for the sparse exchangeable models. This leads to some complications that do not exist with more naive biased methods (e.g., holding out edges uniformly at random); we discuss how to deal with these in practice.
Our test–train split scheme is mandated when using an exchangeable generative model (which covers most generative model cases), but is also likely more broadly useful because it gives a new approach assessing relational data models, complementing existing approaches.

Finally, we treat sparse exchangeable Poisson matrix factorization as an extended worked example. The generative model we use is essentially the bipartite version of the model of [21]. The main novelty is a mean field variational inference scheme to scale inference to huge datasets. Roughly speaking, our inference scheme adapts the Poisson matrix factorization approach of [11], with some new techniques to account for the additional complication introduced by the sparse structure. Roughly, this generalizes Poisson matrix factorization to the sparse graph regime, although there are some small differences between the dense version of our model and the approach of [11]. Our hope is that the techniques we introduce can serve as a general blueprint for scalable variational inference of sparse exchangeable models.

In practice, we implement inference using TensorFlow [1]; this allows for GPU computation, resulting in very fast inference.¹ We find that accounting for sparsity carries negligible additional computational cost, which is in contrast to the MCMC approach of [8, 12, 21]. Interestingly, we find that accounting for sparsity has almost no effect on recommendation performance, even for sparse datasets. However, we do see an improvement in how well the model captures the structure of the data, e.g., the degree structure of the graph.

We define the sparse exchangeable models in Section 2; this is a straightforward translation of the unipartite case. Model checking is treated in Section 3, and data splitting in Section 4. Finally, we cover sparse exchangeable Poisson matrix factorization in Section 5.

2 BIPARTITE SPARSE EXCHANGEABLE GRAPHS

A bipartite graph \( g = (V_U, V_I, E) \) where \( V_U, V_I \) are sets of vertices and \( E \subseteq V_U \times V_I \) is a set of (possibly weighted) edges. We denote the number of users as \( |V_U| = U(G) \), the number of items as \( |V_I| = I(G) \), and, abusing notation, the number of edges as \( |E| = E(G) \).

The model

The model for bipartite graphs we consider in this paper is the natural extension of the sparse exchangeable unipartite graphs of [6, 8, 22], also considered in [7, 8]. The basic structure is that each user \( U_i \) is assigned some latent features \( X_i \), each item \( I_j \) is assigned some latent features \( Y_j \), and, given the latent features, and each edge \( g_{ij} \) is drawn independently from some distribution parameterized by \( W(X_i, Y_j) \) for some function \( W \) (the graphon). For example, in rank \( K \) matrix factorization the features are \( K \)-dimensional vectors and typically \( g_{ij} \sim \text{Normal}(W(X_i, Y_j), 1) \) with \( W \) the inner product function. For concreteness, we will default to the case \( g_{ij} \in \{0, 1\} \)—understood as an indicator for edge inclusion—and \( W(X_i, Y_j) = \mathbb{P}(g_{ij} = 1 | X_i, Y_j) \) for the rest of the paper, but all of our discussion applies to the more general setting.

¹Code available at github.com/ekanshs/graphex-nnmf

The generative structure we have described thus far is common to both the dense exchangeable and sparse exchangeable models. The distinction lies in how the latent features are generated. In dense exchangeable models, these are drawn i.i.d. from some probability space. This is a seemingly natural choice, but it is the root cause of the pathological denseness of the models. In the sparse exchangeable model, the user feature space, \( (X, \eta) \), and item feature space, \((Y, \rho)\), are taken to be infinite measure spaces. The users are then drawn as a Poisson process \( \Pi_U \) with mean measure \( \eta(dx)du \) on \( X \times R_+ \), where the \( R_+ \) coordinates are interpreted as labels of the users; see Figure 1. The items \( \Pi_I \) are drawn in the analogous way. Edges are then randomly generated between users and items according to

\[
e_{ij} | \Pi_U, \Pi_I \sim \text{Bern}(W(X_i, Y_j))
\]

This samples in an infinite bipartite graph. To restrict to finite size, we include only users with labels \( U_i < s \) and items with labels \( I_j < a \); see Figure 1. We refer to \( s \) as the user-size of the graph, and \( a \) the item-size; these naturally correspond to the sample size of a dataset. This restriction results in an induced subgraph with a finite number of edges, but with an infinite number of items and users. This is resolved by excluding any point of the Poisson processes that fails to connect to any edge; that is, this model excludes users and items with degree zero.

Summarizing, sparse exchangeable graph distributions are naturally parameterized by \( \eta, \rho, W \), and the notion of sample size is given by \( s \) and \( a \). The analogous statement for the (more familiar) dense case is that dense exchangeable graph distributions are naturally parameterized by \( P, Q, W \)—where the user features are drawn i.i.d. according to distribution \( P \) and the item features according to \( Q \)—and the notion of sample size is the number of users and items in the graph.

A few remarks are in order:

We defined the sparse exchangeable models on infinite measure spaces. The same definition works on finite measure spaces, in which case the models are the dense exchangeable (i.i.d. features) models, up to some minor technical differences.

We emphasize again that the distinction between the dense and sparse models is simply how the latent features are generated; for this reason, it is relatively easy to postulate sparse analogues of machine learning models that are already used in practice.

The models used here may seem somewhat arbitrary. This is not so; these models are the natural extension of the dense exchangeable theory, and are derived from simple and natural postulates. See [6, 22] for a derivation from exchangeability, and [5] for a derivation from network subsampling invariance.

Subsampling

We make extensive use of the following scheme for sampling random subgraphs from a graph [23]:

**Definition 2.1.** Let \( p, q \in [0, 1] \). A \( (p, q) \)-sampling \( \text{Smpl}(q, p, q) \) of a bipartite graph \( g \) is a random subgraph of \( g \) given by including each user of \( g \) independently with probability \( p \) and each item of \( g \) independently with probability \( q \), and returning the induced subgraph with the isolated vertices removed.
Figure 1: Typical realization of a graphex process. The left panel represents a sample from a Poisson process on $\mathbb{R}_+^2$ restricted to $[0,s] \times \mathbb{R}_+$. The x-axis corresponds to users labels, while the y-axis corresponds to latent features. The middle panel shows a typical sample of the item Poisson process. The right panel displays a sample of edges between users and items, sampled independently according to $\mathcal{W}(x_i, y_j)$. The bottom panel displays the sampled graph, given by deleting the atoms of each Poisson process that do not connect to any edges.

This is the sampling scheme associated with sparse exchangeable graphs: If $G_{s, \alpha}$ is generated according to $\eta, \rho, \mathcal{W}$ then the subgraph $\text{Smpl}(G_{s, \alpha}, (p, q))$ is equal in distribution to $G_{ps, qa}$ generated according to $\eta, \rho, \mathcal{W}$ [23]. That is, this sampling scheme defines the relationship between the generated graphs at different sizes. In fact, this is a defining property of the (sparse) exchangeable graphs, and (sparse) exchangeability can be understood as equivalent to this invariance.

3 CHECKING SPARSITY

Sparsity is a property of a sequence of graphs, but typically analysis is performed on some particular, fixed size, dataset. Accordingly, it may seem that the ability to model sparsity is not relevant for most applications in practice. We show that this intuition is incorrect: sparsely generated datasets have a readily identifiable signature. Accordingly, we can assess ahead of time whether sparse structure is present in our data, and thus whether we should incorporate sparsity into the model.

Define the edge density of a bipartite graph $g$ to be $\rho(g) = e(g)/(U(g)l(g))$. In the dense case, $\rho(G_{s, \alpha})$ is constant with respect to $s, \alpha$, but in the sparse case it decreases as either (or both) $s$ or $\alpha$ increases. Thus, if we could observe the graph process at different values of $s, \alpha$, we could observe sparsity as a change in the value of the edge density. The key insight is that $(p, q)$-sampling allows us to effectively simulate this; intuitively, this is because, marginally, a $(p, q)$-sampling is a sample of the graph at user size $ps$ and item size $qa$.

The content of the following theorem is that this intuition carries through even conditional on the observed data.

Theorem 3.1. If $(G_{s, \alpha})$ is dense then, for $p, q > 0$,

$$\lim_{s, \alpha \to \infty} \frac{\rho(\text{Smpl}(G_{s, \alpha}, (p, q)))}{\rho(G_{s, \alpha})} = 1 \text{ a.s.}$$

Proof. (Sketch) From the definition of dense, $\rho(G_{s, \alpha}) \to c$ almost surely as $\min(s, \alpha) \to \infty$, for some constant $c$. The result follows because the distributional invariance of sparse exchangeable models under $(p, q)$-sampling [5, 23] guarantees that $\rho(\text{Smpl}(G_{s, \alpha}, (p, q))) \to c$, with the same the same limit $c$. □

Accordingly, we can check if a graph is sparsely generated by plotting the edge density of subsampled graphs against the $(p, q)$-sampling levels; see Figure 2. This is theoretically sound if the model is generated according to an exchangeable model, which is a common assumption in generative modelling of relational data. Otherwise, this strategy simply provides a powerful heuristic for assessing sparsity.

4 TEST–TRAIN SPLİT

Model evaluation is a key component of data analysis. Often, this involves randomly splitting the available data into a test set and a training set. There are many seemingly natural ways to partition a bipartite graph, so some care is required in splitting the data. The choice of partitioning scheme may induce a significant sampling bias in the test and training sets, impeding evaluation and complicating model comparison. In this section we give an approach motivated by the sampling theory of sparse exchangeable graphs. This approach is the ‘right’ one for exchangeable models (including dense ones), and is also useful as complement to existing ad hoc approaches for evaluating non-generative models.

To see the difficulty with test–train splitting in the relational data setting, consider a common evaluation procedure for recommender systems: A test set is produced by holding out reviews independently at random. For each user with at least one heldout ranked item, the trained model is asked to recommend items by ranking the set of all films the user has not rated in the training data (i.e., the non-ratings and the heldout data). Then performance is scored by how highly the algorithm ranks the heldout data. Notice that this test–train split induces a degree biased sampling of the users and items; that is, we expect that a typical user in the test set consumes more items than a typical user in the training set, and that a typical item in the test set is more popular than a typical item in the training set. This means that evaluation procedures based on such a split tend to focus on the task of recommending popular items to popular users—this is often not a good proxy for the true task of interest. It is easy to modify the scheme to address this particular problem, but in general it remains a concern that any test–train scheme may induce some more subtle sampling bias.

In the generative model setting, we must choose the splitting procedure such that the parameters of the generative model can be consistently estimated from the training set. For (sparse) exchangeable models, this means partitioning via $(p, q)$-sampling. Concretely, we propose the following data splitting scheme; see Figure 3.

1. Sample $G_{\text{train}} = \text{Smpl}(G, (p, 1))$, and take $G_{\text{holdout}}$ to be the complement of $G_{\text{train}}$ in $G$

2. Sample $G_{\text{test}} = \text{Smpl}(G_{\text{holdout}}, (1, q))$ and take $G_{\text{holdout}}$ to be the complement of $G_{\text{test}}$ in $G_{\text{holdout}}$
The point of the scheme is that if $G$ is drawn as a $\alpha$ item-size, $s$ user-size sparse exchangeable graph generated according to $\eta, \rho, \lambda W$, then $G_{\text{train}}$ and $G_{\text{test}}$ are distributed as, respectively, size $p, \alpha$ and size $p_s, q_s$ graphs generated according to $\eta, \rho, \lambda W$. If we had used some other sampling scheme then, generally, the test and train sets would be distributed according to different distributions, and a model that performed well on the training set would not be expected to perform well on the test set or on fresh data.

For concreteness, we envision an estimation procedure as an algorithm that takes an observed bipartite graph $G$ and outputs estimates $\hat{\eta}, \hat{\rho}, \hat{\lambda} W$ for the model parameters, and $\hat{u}_i$ for the latent feature of each user, and $\hat{v}_j$ for the latent feature of each item. The output of the estimation procedure on $G_{\text{train}}$ includes estimates for $\hat{\lambda} W$ and for the latent features of the items in $G_{\text{train}}$. However, it does not include estimates for the latent features of the users in the test set. Indeed, $G_{\text{train}}$ does not carry information about these values. This motivates splitting the holdout set: the validation procedure should use $W, \hat{\eta}$, and $G_{\text{holdout}}$ to produce an estimate for the latent user features of the test set. This last step is possible for exchangeable random graph models because of the conditional independence structure: to estimate the latent feature of any user, it is sufficient to know $W, \eta$, and the latent features of its neighbours.

A concrete example given in Section 5.3.3. Figure 4 shows degree distribution samples from the approximate posterior distribution over the test sets from a model trained using the training sets, under our proposed test–train splittings scheme. This figure also plots the true degree distribution from the test–data. Note that the model fit to the training data is able to accurately predict the structure of the test data.

5 SPARSE POISSON MATRIX FACTORIZATION

We now turn to non-negative matrix factorization as an extended example. We adapt the model of [21], using the bipartite variant as a component of probabilistic matrix factorization. We emphasize that the model we present here is chosen for its simplicity, with the aim of exposing sparsity considerations as clearly as possible. The aim is not to write down the best possible model for the recommendation task we consider, and indeed there are several obvious extensions that we omit because they are essentially orthogonal to the study of sparsity.

5.1 The generative model

Let $PP(m)$ denote the distribution of a Poisson process with mean measure $m$, and $\text{Gamma}(a, b)$ denote a gamma distribution with shape $a$ and rate $b$.
5.1.1 Generalized Gamma Process. We follow the approach of [7] and its successors [8, 12, 21] based on the Generalized Gamma Process (GGP), a Poisson process with mean measure
\[ g_{\sigma, \tau}(du) = \frac{1}{\Gamma(1 - \sigma)} u^{(1+\sigma)} \exp(-\tau u) \, du, \]
for \((\sigma, \tau) \in (0, 1) \times (0, \infty) \cup (-\infty, 0] \times (0, \infty)\).

For our purposes, there are two important facts about the GGP. First, points of the GGP are equivalent to i.i.d. draws from a Gamma distribution if and only if \(\sigma < 0\). In the model defined below this means the model is dense if and only if \(\sigma_1 + \sigma_2 < 0\) [8]. This property allows for easy, interpretable comparison between sparse and dense variants of the model.

Second, the GGP admits a pseudo-conjugacy relationship with the Poisson distribution. Informally, if \(\xi = ((\theta_1, \omega_1), (\theta_2, \omega_2), \ldots)\) is a GGP with parameters \(\sigma, \tau\) and \(N\), then \(\xi \sim \text{Poi}(\lambda\omega)\) then \(\xi | N\) is equal in distribution to a point process with two independent components: One component consists of all atoms for which \(N_i = 0\), this is distributed as another GGP with parameters \(\sigma, \tau\) and \(\tau + \lambda\). The other component consists of the atoms for which \(N_i > 0\), in this case the posterior masses are distributed as Gamma\((N_i - \sigma, \tau + \lambda)\), independent of each other and of the first part of the process. Intuitively speaking, this is the posterior distribution of \(\sum_{\omega_i \in \cdot} | N_i\) of the observed weights. In the case that \(\sigma < 0\), this is the same conjugate posterior update that we would arrive at by taking \(\omega_i \sim \text{Gamma}(\sigma, \tau)\) hence the pseudo-conjugacy terminology. It is this property that makes the GGP amenable to efficient inference.

5.1.2 Sparse Poisson Matrix Model. The model assigns each item and user a \(K\) dimensional latent feature. The basic structure is:

1. Each user \(i\) is assigned a total popularity \(P_i\) and affinities \((\phi_{ik})_{k=1}^K\) to each feature dimension \(k\).
2. Each item \(j\) is assigned a total popularity \(P_j\) and affinities \((\phi_{jk})_{k=1}^K\) to each feature dimension \(k\).
3. Given the features, each edge \((i,j)\) is included independently with probability \(1 - \exp(\beta_i \phi_{ik} \phi_{jk})\).

The inclusion probability is the probability of a non-zero draw from a Poisson distribution with mean \(P_i P_j \sum_k \phi_{ik} \phi_{jk}\); this is done to allow us to exploit the GGP-Poisson pseudo-conjugacy for inference.

We present the generative model in a somewhat different form allowing for easy derivation of the inferential updates. The user parameters are:
\[ \xi = \{(\gamma_1, u_1), (\gamma_2, u_2), \ldots\} \sim \text{PP}(g_{\sigma_U, \tau_U} \times \lambda), \]
\[ \theta_{ik} \sim \text{Gamma}(a, b), \]
\[ \phi_{ik} \sim \text{Gamma}(c, d). \]
Let \(g_{ij} = 1\) indicate that edge \((u_i, t_j)\) is included in the graph (and \(g_{ij} = 0\) otherwise). The generative model for the connections is:
\[ e_{ij}^k \mid \gamma_i, \{\theta_{ik}\}_{k=1}^K, \omega_j, \{\beta_{jk}\}_{k=1}^K \sim \text{Poi}(\gamma_i \omega_j \theta_{ik} \beta_{jk}) \]
\[ g_{ij} = I[\sum_k e_{ij}^k > 0]. \]

The use of \(K\) latent edge counts per user-item pair should be viewed as an auxiliary variable technique; this idea is borrowed from [11].

5.2 Inference

The learning task has two components: inferring the parameters of \(\eta\) and \(\rho\) (noting that \(W\) is fixed), and inferring the latent feature values of the users and items.

5.2.1 Global parameters. The sparse model requires us to set hyperparameters that are not relevant in the dense setting; namely, the GGP parameters \(\sigma_U\) and \(\sigma_U\), and the sizes \(s\) and \(\alpha\). We use the general estimation strategy of [19]. This provides a consistent estimator \(\hat{\sigma}_U\) for \(\sigma_U\) as a function of the degrees of the users in the dataset. Namely, for a graph \(g\) where each user \(i\) has degree \(d_i\),
\[ \hat{\sigma}_U = \frac{\log(U(g)) - \log(2^\alpha - d_i)}{\log 2}. \]

The estimator for \(\sigma_1\) is the obvious analogue.

It can also be shown that, for some slowly growing function \(C_\alpha\) of \(\alpha\) (e.g., \(C_\alpha = O(\log \log \alpha)\)),
\[ \log U(G_{\alpha}, \sigma_U) \sim (\sigma_U) \log e(G_{\alpha}, \sigma_U) = C_\alpha + (1 - \sigma_U) \log(s) + o_s(1), \]
see [9] for a derivation of the asymptotics in the (harder) unipartite case; the bipartite case is a straightforward adaption. We can estimate \(C_\alpha\), which depends on the model, by treating it as a constant with respect to \(\alpha\), and estimating this constant by simulating data (with known user size) from the model. We then set the user size by subbing \(\hat{\sigma}_U\) for \(\sigma_U\), throwing away the \(o_s(1)\) term, and solving for \(s\). We also use the analogous strategy for setting \(\alpha\).

We use an empirical Bayes type procedure, fixing these hyperparameters to their estimated values, and using a more sophisticated approach to estimating the posterior distribution of the latent features.
5.2.2 Latent features. We adopt a mean field variational inference (VI) approach, approximating the true posterior distribution over the parameters by a fully factorized distribution. See [4] for a review of variational inference. Namely, main challenge here is that the likelihood has no closed form expression—it can’t be readily differentiated, or even evaluated—and it is computationally expensive to draw samples from. This disallows most general purpose variational inference algorithms.

The solution is that we have parameterized the model such that the complete conditional distribution of each variable is (approximately) an exponential family distribution—we demonstrate this below, and discuss the required approximations (Section 5.2.3). Complete conditional distributions are the conditional distributions given the data and all other variables. The significance of this property is that it allows us to read off a Coordinate Ascent Variational Inference scheme (CAVI) automatically [10, 14]. It is rather remarkable that this works: CAVI was developed for conjugate Bayesian models with i.i.d. observations, but in the sparse graph case there is no possible independent prior on the user weights or item weights that would reproduce the model. Nevertheless, the pseudo-conjugacy of the GGP suffices for efficient inference.

Broadly, the structure of the resulting algorithm is that each variable (e.g., \( \theta_{ik} \)) gets a parameterized approximating distribution (e.g., \( q(\theta_{ik} \in \cdot \mid \phi_{ik}) \)), and the algorithm learns the parameters by iteratively updating them given all other parameters. Complete conditionals in exponential family form allow us to read off the form of \( q \) and the parameter updates.

5.2.3 Complete Conditionals. Most of the results presented here are readily derived by ordinary conjugate update manipulations in combination with the generalized gamma process–Poisson pseudo-conjugacy; additionally, a detailed treatment of the unipartite case is given in [21].

Let \( e_{ij}^k = \sum_j e_{ij}^k \) and \( e_i = \sum_k e_{ik}^k \), and let \( \rho_k^* = \sum_i e_i = \gamma_i \theta_{ik} 1[u_i < s] \). Intuitively speaking, \( \rho_k^* \) is the total mass of type \( k \) belonging to user atoms that have failed to connect to any items; this turns out to be a sufficient statistic for user atoms that do not connect to any items. We also need the analogous definitions for the items, writing \( \rho_k^* \) for the total mass of type \( k \) belonging to item atoms that have failed to connect to any users. Then,

\[
\theta_{ik} \mid \xi, \zeta, \beta, e \sim \text{Gamma}(\alpha + \xi, b + \gamma_i(\sum_{j \in \psi_i} \omega_j \beta_{jk} + \rho_k^*)), \\
\beta_{jk} \mid \xi, \zeta, \theta, e \sim \text{Gamma}(c + \epsilon_j, d + \omega_j(\sum_{i \in \psi_j} \gamma_i \theta_{ik} + \mu_k^*)).
\]

The GGP weights for atoms that connect to at least 1 edge:

\[
\gamma_i \mid \zeta, \theta, \beta, e \sim \text{Gamma}(\alpha_i + e_i, \tau_i + \sum_k \theta_{ik} (\sum_{j \in \psi_i} \omega_j \beta_{jk} + \rho_k^*)), \\
\omega_j \mid \zeta, \theta, \beta, e \sim \text{Gamma}(\alpha_j + e_j, \tau_j + \sum_k \beta_{jk} (\sum_{i \in \psi_j} \gamma_i \theta_{ik} + \mu_k^*)).
\]

Notice that in the case \( \sigma_U < 0 \), the complete conditional for \( \gamma_i \) corresponds to a Gamma\((-\alpha_i, \tau_i\)) prior distribution. However, in the case that \( \sigma_U > 0 \), there is no independent prior on \( \gamma_i \) that could have given rise to this posterior.

Next, the auxiliary variables:

\[
(e_{ij}^1, \ldots, e_{ij}^K) \mid \theta, \beta, \xi, \zeta, [g_{ij} = 1] \\
\sim \text{tPoi}(\gamma_i(\theta_{i1} \beta_{1j}, \ldots, \gamma_i \theta_{iK} \beta_{Kj})),
\]

where tPoi(\( \lambda_1, \ldots, \lambda_K \)) is the K-dimensional truncated Poisson distribution defined by the following scheme. For drawing a sample \((N_1, \ldots, N_K)\): Draw \( N \sim \text{Po}(\sum_k \lambda_k) \) conditional on \( N > 0 \), and then draw \((N_1, \ldots, N_K) \mid N \sim \text{Multi}(\lambda_1/\sum_k \lambda_k, \ldots, \lambda_K/\sum_k \lambda_k)\), see [21].

The complete conditional of \((\mu_i^*, \ldots, \rho_k^*)\) is not available in closed form. However, using point process techniques, we can derive the conditional expectation and variance, see Appendix A. We find that \( \text{var}(\mu_i^* \mid \zeta, \beta, e) \approx \mathbb{E}[\mu_i^* \mid \zeta, \beta, e] \) in the large data regime. This motivates the approximation \( \mathbb{P}(\mu_i^* \in \cdot \mid \zeta, \beta, e) \approx \delta_{\mathbb{E}[\mu_i^* \mid \zeta, \beta, e]} \).

That is, we simply ignore the variability. This approximation works well in practice when used as an input to our inference procedure.

The expectation of the complete conditional is given by:

\[
\mathbb{E}[\mu_i^* \mid \zeta, \beta, e] = s\mathbb{E} \left[ \frac{\theta_{i1}^*}{\tau_U + \sum_k \theta_{ik}^* \sum_j \omega_j \beta_{jk}} \mid \zeta, \beta, e \right]
\]

for \( \mu_i^* \simiid \text{Gamma}(a, b) \); this is easy to approximate with Monte Carlo sampling.

We also use the analogous approximation for the complete conditional of \((\rho_i^*, \ldots, \rho_k^*)\).

5.3 Empirical study

This section covers an empirical comparison of dense and sparse exchangeable Poisson matrix factorization. The main takeaways are:

1. The inference algorithm works well. Our algorithm is able to accurately recover the structure of simulated data, suggesting that the various approximations involved in our inference scheme are valid in practice.
2. The sparse model does a better job recovering the graph structure of sparse data, including real world data.
3. However, despite this, there is no appreciable difference in recommendation performance between the sparse and dense models.

5.3.1 Datasets. We consider the following datasets:

1. **Simulated Dataset**: A sample from the model generated according to the following parameters: \( \sigma_U = \alpha = 0.2, \tau_U = \tau_I = 1.0, a = b = c = d = 0.1, s = \alpha = 1200.0 \). Dataset consists of 9.7M edges with 40,565 users and 40,768 items.
2. **Netflix**: Consists of ratings that users have assigned to movies. In our experiment, we treat this as a simple graph by including an edge in the graph whenever user has rated a movie. The resulting dataset consists of 480,189 users, 17,770 movies (items), and 100M ratings (edges).
3. **Echonest**: The Echonest taste profile dataset [3] is a music dataset with 1,019,318 users, 384,546 songs (items) and 48M entries where each entry is the number of times a user played a song. We treat this as a simple graph by including an edge whenever user played a song.
5.3.2 Hyperparameters. For the sparse models, we set the sparsity parameters \(\sigma_U\) and \(\sigma_I\), and the sizes \(s\) and \(a\), according to the estimation scheme described above. For dense models, we set \(\sigma_U = \sigma_I = -0.1\) (and \(s = a = 0\)). Empirically, we find that the performance of the dense model is robust to the choice of \(\sigma_U\) and \(\sigma_I\), the analogous observation was also made in [11].

For all experiments, we set \(\tau_I = \tau_T = 1.0, a = c = b = d = 0.1\) and \(K = 30\). Model performance is somewhat dependent on these parameter choices, but our conclusions seem to hold generally.

5.3.3 Data splitting and posterior predictive model. We partition each dataset \(G\) into \(G_{\text{train}}, G_{\text{test}}\), and \(G_{\text{holdout}}\) according to the scheme described in Section 4, taking \(p = q = 0.2\). We now specialize the discussion of Section 4 to the sparse exchangeable Poisson matrix factorization model.

To evaluate the quality of our model, we would like to find the posterior predictive distribution of the test set given \(G_{\text{train}}\) and \(G_{\text{holdout}}\); i.e., \(P(G_{\text{test}} \in \cdot \mid G_{\text{train}}, G_{\text{holdout}})\). We could then, e.g., recommend items to users in the test set by recommending those items such that \(P(e_{ij} = 1 \mid G_{\text{train}}, G_{\text{holdout}})\) is large.

Letting \(\Theta = \{\sigma_U, \sigma_I, \xi, \zeta, \theta, \beta\}\) denote the parameters of the model, the posterior predictive on the test data has the form:

\[
P(G_{\text{test}} \in \cdot \mid \Theta)P(\Theta \mid G_{\text{train}}, G_{\text{holdout}})d\Theta. \tag{5.1}
\]

Running our inference algorithm on \(G_{\text{test}}\) returns a distribution \(q(\sigma_U, \sigma_I, \xi_{\text{test}}, \zeta, \theta_{\text{test}}, \beta)\) that approximates \(P(\Theta \mid G_{\text{test}})\)—the subscript on the user parameters denotes restriction to only those users that are included in the training set. Intuitively speaking, we would like to approximate \(P(\Theta \mid G_{\text{train}}, G_{\text{holdout}}) \approx q(\Theta)\).

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The difficulty is that \(q\) does not carry any information about the users in the test set. To resolve this, we introduce a new approximation:

\[
P(\sigma_U, \sigma_I, \xi_{\text{test}}, \zeta, \theta_{\text{test}}, \beta \mid G_{\text{holdout}}) 
\approx q'(\xi_{\text{test}}, \theta_{\text{test}})q(\sigma_U, \sigma_I, \zeta, \beta).
\]

That is, we approximate the posterior distribution of parameters given \(G_{\text{holdout}}\) as a factorized distribution consisting of the approximate posterior over the sparsity and item parameters (already learned from the training data), and a new approximating distribution \(q'\) over the user parameters. We take \(q'\) in the same family as we would use for mean-field variational inference on \(G_{\text{holdout}}\) and fit it by minimizing the variational loss between \(P(\sigma_U, \sigma_I, \xi_{\text{test}}, \zeta, \theta_{\text{test}}, \beta \mid G_{\text{holdout}})\) and the distribution \(q'(\xi_{\text{test}}, \theta_{\text{test}})q(\sigma_U, \sigma_I, \zeta, \beta)\). In practice, this is achieved by running our coordinate ascent variational inference scheme using \(G_{\text{holdout}}\) as the dataset, and fixing \(q(\sigma_U, \sigma_I, \zeta, \beta)\) to the distribution learned on the training set.

In summary, we take

\[
P(\sigma_U, \sigma_I, \xi_{\text{test}}, \zeta, \theta_{\text{test}}, \beta \mid G_{\text{train}}, G_{\text{holdout}}) 
\approx \delta_{\tilde{\theta}_U, \tilde{\theta}_I}q'(\xi_{\text{test}})q(\theta_{\text{test}})q(\zeta)q(\beta).
\]

The posterior predictive distribution for the test set is then computed by substituting this approximation into (5.1).

There is one remaining subtlety: we must also set the sample sizes \(N_{\text{test}}\) and \(q_{\text{test}}\) for the posterior predictive distribution for the test set. It follows from the structure of the test–train split that \(N_{\text{test}} = pN_{\text{train}}\) and that \(q_{\text{test}} = q_{\text{train}}\).

5.3.4 Posterior Predictive Checks. We now assess the quality of the approximate posterior distribution for the test data. In principle, the performance depends on three separate levels of approximation:

1. whether an exchangeable model is appropriate (i.e., can the distribution on the test data be estimated in an unbiased way from the training data)
2. whether Poisson matrix factorization a suitable model, and
3. whether the various approximations used in the inference are sound

We assess the quality by drawing samples from the posterior predictive distribution (over the test set) and comparing summary statistics between these samples and the true test data.

Figure 4 plots the degree distributions of the posterior samples from dense and sparse models against test datasets. Table 1 gives simple summary statistic for the posterior draws. The model does a good job predicting the structure of the test data. For datasets that appear genuinely sparse—e.g., Echonest or Wikipedia—the predictive performance of the sparse models seems better. The sparse model generates a large number of (low degree) vertices that are present in the actual data, but that are missed by the dense model. \(\hat{\sigma}\) estimated on the sparse model samples are closer to \(\hat{\sigma}\) estimates on the actual data. This can be interpreted as meaning either that the sparse models do a better job of capturing degree heterogeneity—recall \(\hat{\sigma}\) is a function of the degree distribution—or simply that the sparse models do a better job of predicting sparsity in the data. It is an interesting fact that even dense Poisson matrix factorization is able to predict some degree of sparsity in the data, although it biases towards increased density.

5.3.5 Recommendation Task. For each user in the test set, we recommend a list of items in the test set. To generate recommendations for each user \(i\), we rank the items according to the values of

| Simulated Data | Netflix | Echonest | Wikipedia |
|---------------|---------|----------|-----------|
| Train Set:    | Test Set: | Test Set: | Test Set: |
| V1: Sparse Model | 5,029 | 94,083 | 199,635 | 5,914 |
| Dense Model | 4,319 | 92,560 | 189,971 | 5,895 |
| Test Set: | 5,285 | 3,628 | 59,270 | 19,558 |
| V2: Sparse Model | 4,906 | 3,812 | 56,272 | 15,085 |
| Dense Model | 4,474 | 3,647 | 51,151 | 14,226 |
| Test Data: | 374,458 | 4,306,108 | 1,385,036 | 812,208 |
| Dense Model | 374,375 | 4,312,407 | 1,375,401 | 814,144 |
| Simulated Data | Test Set: | Test Set: | Test Set: |
| \(\xi, \sigma_I\) | Sparse Model | 0.2252 (0.2298) | (0.0122 (0.0005)) | (0.1671 (0.2555)) |
| Dense Model | 0.1428 (0.2044) | (0.0564 (0.0071)) | (0.1876 (0.2830)) |
| \(\sigma_U\) | 0.1510 (0.0515) | (0.0551 (0.0069)) | (0.1744 (0.2170)) |
| \(\kappa\) | 0.0097 (0.0086) | (0.0071 (0.0061)) |

Table 1: Posterior Predictive Checks. We compare samples from the approximate posterior predictive for the test data given the training data to the actual test data. The sparse models do a moderately better job predicting the structure of the test set when the dataset is sparse.
The main insights from this paper are: First, sparsity has a signature that can be easily recognized in fixed size datasets, and sparse behaviour occurs in real-world data. Second, the (common) assumption that the data is generated according to an exchangeable model implies a unique correct scheme for splitting the data into train and test sets, and this splitting procedure can be adapted as a component of practical model evaluation procedures. Finally, it is possible to scale inference for sparse exchangeable models to very large datasets.

**REFERENCES**

[1] Martin Abadi, Ashish Agarwal, Paul Barham, Eugene Brevdo, Zhifeng Chen, Craig Citro, Greg S. Corrado, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Ian Goodfellow, Andrew Harp, Geoffrey Irving, Michael Isard, Yangqing Jia, Rafal Jozefowicz, Lukasz Kaiser, Manjunath Kudlur, Josh Levyberg, Dan Mané, Rajat Monga, Sherry Moore, Derek Murray, Chris Olah, Mike Schuster, Jonathon Shlens, Benoit Steiner, Ilya Sutskever, Kunal Talwar, Paul Tucker, Vincent Vanhoucke, Vijay Vasudevan, Fernanda Viégas, Oriol Vinyals, Pete Warden, Martin Wattenberg, Martin Wicke, Yuan Yu, and Xiaoqiang Zheng. 2015. TensorFlow: Large-Scale Machine Learning on Heterogeneous Systems. (2015). https://www.tensorflow.org/. Software available from tensorflow.org.

[2] David J. Aldous. 1981. Representations for partially exchangeable arrays of random variables. *J. Multivariate Anal. 11, 4* (1981), 581–598. https://doi.org/10.1016/0047-259X(81)90099-3

[3] Thierry Bertin-Mahieux, Daniel P.W. Ellis, Brian Whitman, and Paul Lamere. 2011. The Million Song Dataset. In Proceedings of the 12th International Conference on Music Information Retrieval (ISMIR 2011).

[4] D. M. Blei, A. Kucukelbir, and J. D. McAuliffe. 2016. Variational Inference: A Review for Statisticians. *arXiv e-prints* (Jan. 2016). arXiv:stat.CO/1601.00670

[5] C. Borgs, J. T. Chayes, H. Cohn, and N. Holden. 2016. Sparse exchangeable graphs and their limits via graphon processes. *arXiv e-prints* (1 2016). arXiv:math.PR/1601.07134

[6] Francois Caron. 2012. Bayesian nonparametric models for bipartite graphs. In Advances in Neural Information Processing Systems 25, F. Pereira, C. J. C. Burges, L. Bottou, and K. Q. Weinberger (Eds.). Curran Associates, Inc., 2051–2059. http://papers.nips.cc/paper/4837-bayesian-nonparametric-models-for-bipartite-graphs.pdf

[7] François Caron and Emily B. Fox. 2017. Sparse graphs using exchangeable random measures. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 79, 5 (2017), 1295–1366. https://doi.org/10.1111/rssb.12333

[8] François Caron and Judith Rousseau. 2017. On sparsity and power-law properties of graphs based on exchangeable point processes. *arXiv preprint arXiv:1708.03120* (2017).

[9] Zoubin Ghahramani and Matthew J. Beal. 2001. Propagation algorithms for variational Bayesian learning. In *Advances in neural information processing systems*. 507–513.
Thus, "connects to no edges" may be viewed as a marking of the random set of atoms that fail to connect to any edges is a point process. It then follows that the random set of atoms that fail to connect to any edges is a point process. Hence, the random set of atoms that fail to connect to any edges is a point process.

A COMPLETE CONDITIONAL FOR LEFTOVER MASS

Here we sketch the computation for the complete conditional mean and variance of the total leftover item masses \( \mu_{i}^{0}, \ldots, \mu_{K}^{0} \).

We may view \( \{(y_{i}, \theta_{i1}, \ldots, \theta_{iK})\} \) as a Poisson process on \( \mathbb{R}_{+} \times \mathbb{R}_{+}^{K} \) with mean measure

\[
s_{\gamma_{\mathcal{A}}, \tau_{\mathcal{C}}}(dy)F(d\theta_{1}, \ldots, d\theta_{K}),
\]

where \( F(d\theta_{1}, \ldots, d\theta_{K}) = \prod_{k} \text{Gamma}(\theta_{k}; a, b) \). This follows by projecting the GGP on \( \mathbb{R}_{+} \times [0, s) \) onto the feature space, and viewing \( \{(y_{i}, \theta_{i1}, \ldots, \theta_{iK})\} \) as a marking.

Conditional on \( \zeta \) and \( \beta \), each atom \( \{(y_{i}, \theta_{i1}, \ldots, \theta_{iK})\} \) of this process connects to 0 edges independently with probability

\[
\exp(-\gamma_{i} \sum_{k} \theta_{ik} \sum_{j} \omega_{ij} \beta_{jk}).
\]

Thus, "connects to no edges" may be viewed as a marking of the point process. It then follows that the random set of atoms that fail to connect to any edges is a point process \( \{(y_{i}^{*}, \theta_{i1}^{*}, \ldots, \theta_{iK}^{*})\} \) with mean measure

\[
s_{\gamma_{\mathcal{A}}, \tau_{\mathcal{C}}}(dy^{*})F(d\theta_{1}^{*}, \ldots, d\theta_{K}^{*}) \exp(-\gamma^{*} \sum_{k} \theta_{ik}^{*} \sum_{j} \omega_{ij} \beta_{jk}).
\]

Notice that \( \mu_{i}^{*} = \sum_{j} y_{i}^{*} \theta_{ij}^{*} \) for each \( k \). The claimed result then follows by Campbell’s theorem and some algebraic manipulation.