Hierarchical Infinite Relational Model

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Abstract

This paper describes the hierarchical infinite relational model (HIRM), a new probabilistic generative model for noisy, sparse, and heterogeneous relational data. Given a set of relations defined over a collection of domains, the model first infers multiple non-overlapping clusters of relations using a top-level Chinese restaurant process. Within each cluster of relations, a Dirichlet process mixture is then used to partition the domain entities and model the probability distribution of relation values. The HIRM generalizes the standard infinite relational model and can be used for a variety of data analysis tasks including dependence detection, clustering, and density estimation. We present new algorithms for fully Bayesian posterior inference via Gibbs sampling. We illustrate the efficacy of the method on a density estimation benchmark of twenty object-attribute datasets with up to 18 million cells and use it to discover relational structure in real-world datasets from politics and genomics.

1 INTRODUCTION

Learning models for relational data is a widely studied problem that arises in a number of settings such as business intelligence (Chaudhuri et al., 2011), social networks (Carrión et al., 2005), bioinformatics (Rual et al., 2005), and recommendation systems (Su and Khoshgoftaar, 2009), amongst many others (Džeroski and Lavrač, 2001). In this setting, we observe attributes and interactions among a set of entities and our goal is to learn models that are useful for explaining or making predictions about the entities, their attributes, and/or their interactions. Fig. 1 shows two examples of relational systems for political and genomics data. For politics (Fig. 1a), one problem could be to discover what attributes of a particular country and interactions with other countries are likely to make it an attractive tourist hub. In genomics (Fig. 1b), our goal might be to predict what complexes a particular gene is likely to form, given information about its motifs, functions, and interactions with other genes. This paper addresses the problem of automatically learning probabilistic models for a variety of relational systems given a dataset of noisy and possibly sparse observations.

Learning probabilistic structure is an exceptionally difficult task (Daly et al., 2011). One approach to simplifying the learning problem is to posit a collection of hidden variables that both explain and decouple the relationships between observed variables. Using Bayesian nonparametrics, both the values and dimensionality of these hidden variables can be automatically inferred from data. This approach is commonly used for modeling relational data (Kemp et al., 2006; Xu et al., 2006; Roy and Teh, 2009; Sutskever et al., 2009; Kim et al., 2013; Nakano et al., 2014; Xuan et al., 2017; Fan et al., 2018): refer to Fan et al. (2020) for a recent survey on developments in the field. Our paper builds on the infinite relational model (IRM; Kemp et al., 2006; Xu et al., 2006), a widely used and flexible Bayesian nonparametric method that applies to a variety relational systems. The IRM is a cluster-based model: informally, to decide whether a binary relation \( R \) holds between a pair of entities \( i \) and \( j \), the IRM flips a coin whose weight depends on the (latent) cluster assignments of \( i \) and \( j \). A strength of the IRM, which we review in Sec. 2, is its ability to extract meaningful partitions from observational data. However, as we identify in Sec. 3, two limitations inherent to the IRM’s inductive bias make the model (i) susceptible to combinatorial over-clustering; and (ii) fail to discover certain predictive structure between dependent but non-identically distributed relations, which can both result in an inaccurate overall model of the data.

To address these limitations, this paper introduces the hierarchical infinite relational model (HIRM) in Sec. 4, a new method that combines the flexibility of the IRM with a structure learning prior that infers subsets of relations that are probably independent of one another. By allowing different relations to be explained by different partitions, the HIRM...
specifies a large hypothesis space that includes the standard IRM in addition to compact models of the data that can only be approximated by an IRM using a combinatorially large number of clusters. The evaluations in Sec. 5 show that the HIRM makes more accurate predictions and discovers more fine-grained clustering structure as compared to the IRM, while retaining a flexible framework for automatic Bayesian structure discovery in a variety of relational systems.

2 INFINITE RELATIONAL MODEL

We begin with a review of the IRM, using a slightly more general definition of “relations” than was originally described in Kemp et al. (2006) or Xu et al. (2006).

Definition 2.1. A relational system \( S \) consists of \( n \) domains \( D_1, \ldots, D_n \) and \( m \) relations \( R_1, \ldots, R_m \). Each domain \( D_i \) \((1 \leq i \leq n)\) is a countably infinite set of distinct entities \( \{e_1^i, e_2^i, \ldots\} \). Each relation \( R_k \) \((1 \leq k \leq m)\) is a map from the Cartesian product of \( t_k \) domains to an arbitrary codomain \( C_k \). The symbol \( d_{ki} \) \((1 \leq k \leq m, 1 \leq i \leq t_k)\) denotes the domain index of the \( i \)-th argument of \( R_k \).

Example 2.2. Suppose system \( S \) has \( n = 4 \) domains \( D_1, D_2, D_3, D_4 \), and \( m = 3 \) relations \( R_1, R_2, R_3 \); with 
\[
R_1 : D_1 \times D_1 \to \{0, 1\}, \\
R_2 : D_1 \times D_3 \times D_4 \to \{1, 2, \ldots\}, \\
R_3 : D_2 \to (\infty, \infty).
\]
In this system, we have 
\[
t_1 = 2; \quad d_{11} = 1, d_{12} = 1; \quad C_1 = \{0, 1\}; \\
t_2 = 3; \quad d_{21} = 1, d_{22} = 3, d_{23} = 4; \quad C_2 = \{1, 2, \ldots\}; \\
t_3 = 1; \quad d_{31} = 2; \quad C_3 = (\infty, \infty).
\]
\( R_1 \) is a binary relation taking binary values, \( R_2 \) is a ternary relation taking positive integer values, and \( R_3 \) is a unary relation taking real values.

Remark 2.3. To simplify notation, for a given relation \( R : D_1 \times \cdots \times D_n \to C \) and entity indexes \( i_1, \ldots, i_n \in \mathbb{N} \), we will write \( R(i_1, \ldots, i_n) \) to mean \( R(e_{i_1}^1, \ldots, e_{i_n}^n) \).

Consider a system \( S \) with \( n \) domains and \( m \) relations. For each \( i = 1, \ldots, n \), the IRM assumes that entities \( \{e_1^i, e_2^i, \ldots\} \) in domain \( D_i \) are associated with integer cluster assignments \( \{z_1^i, z_2^i, \ldots\} \equiv z_i \). The IRM defines a joint probability distribution over cluster assignments and relation values with the following factorization structure:
\[
P(z^1, \ldots, z^n, R_1, \ldots, R_m) = \prod_{i=1}^{n} P(z^i) \prod_{k=1}^{m} P(R_k \mid z^1, \ldots, z^n).
\]

(1)

To allow the IRM to discover an arbitrary number of clusters for each domain \( D_i \), the cluster assignments \( z^i \) for the entities are given a nonparametric prior that assigns a positive probability to all possible partitions using the Chinese restaurant process (CRP; Aldous, 1985). For each \( i = 1, \ldots, n \), the cluster assignment probabilities \( P(z^i) = P(z_1^i, z_2^i, \ldots) \) in Eq. (1) are defined inductively with \( z_1^i := 1 \), and for \( l \geq 2 \)
\[
P(z_l^i = j \mid z_1^i, \ldots, z_{l-1}^i) \propto \begin{cases} n_j & \text{if } 1 \leq j \leq M \\ \gamma & \text{if } j = M + 1, \end{cases}
\]

(2)

where \( n_j := \sum_{c=1}^{l-1} 1[z_c^i = j] \) is the number of previous entities at cluster \( j \); \( M := \max\{z_1^i, \ldots, z_{l-1}^i\} \) is the number of clusters among the first \( l-1 \) entities; and \( \gamma > 0 \) is a concentration parameter. The cluster assignment vectors \( z^1, \ldots, z^n \) across the \( n \) domains are mutually independent, each drawn from a CRP (Eq. (2)). Next, for each relation \( R_k \) \((1 \leq k \leq m)\), a set of parameters \( \theta_k(j_1, \ldots, j_{t_k}) \) is used to dictate the distribution of \( R_k(i_1, \ldots, i_{t_k}) \), where \( j_1, \ldots, j_{t_k}, i_1, \ldots, i_{t_k} \in \mathbb{N} \). The value of a relation depends only the cluster assignments, i.e., \( R_k(i_1, \ldots, i_{t_k}) \) and \( R_k(i_1', \ldots, i_{t_k}') \) share the same parameter whenever
where (vertical/horizontal red lines) that is identical across all the relations. This conservative assumption by the IRM leads to a different on the surface, including:

- Systems with multiple attributes and interactions, where, for example, $D_1$ are countries, $D_2$ are attributes; and $D_3$ are interactions; so that $R_1 : D_1 \times D_2 \to \{0, 1\}$ models attributes and $R_2 : D_1 \times D_1 \times D_3 \to \{0, 1\}$ models interactions, where $R_2(i, j, k) = 1$ iff countries $e^1_i$ and $e^j_i$ perform interaction $e^k_k$.

3 LIMITATIONS OF THE IRM

We next describe two limitations in the standard IRM that arise when using the model in practice, motivating the hierarchical structure learning prior that we introduce in Sec. 4.

3.1 ENFORCING SHARED DOMAIN CLUSTERINGS LEADS TO OVERFITTING

A key assumption of the IRM is that each domain $D_i$ has a single clustering $\pi^i = \{z^i_1, z^i_2, \ldots\}$ that globally dictates the partition of its entities $\{e^i_1, e^i_2, \ldots\}$. The same cluster assignments $z^i$ are used for all of relations $R_1, \ldots, R_m$ in which $D_i$ participates, which can lead to substantial over-clustering and a failure to accurately model data in the presence of structural independences between relations. Fig. 2 illustrates and discusses this limitation in further detail.

3.2 RESTRICTIONS WHEN CLUSTERING MULTIPLE RELATIONS

Kemp et al. (2006) applied the IRM to clustering multiple relations, by treating the relations themselves as entities within a new domain. More specifically, for a system with relations $R_1, \ldots, R_m$, all defined on same domain and codomain (say $D$ and $C$), the key idea is to encode the system using one higher-order relation $R' : D' \times D \to C$, where the entities of $D'$ are relations over $D$, i.e., $R'(i, j) := R_j(i)$ (for $1 \leq j \leq m, i \in D$). While an IRM for $R'$ will learn a
For each subsystem index \(i\), clusters, and relation values with the following factorization:

\[
R_i(y) = \max_{y \in \mathcal{Y}} \prod_{i=1}^{|D_i|} \gamma_{\ell i}(y_i) \tag{1}
\]

where \(\gamma_{\ell i}(y_i)\) are the cluster assignments of the relations are denoted by \(y = \{y_1, \ldots, y_m\}\). This partition induces a random number of subsystems \(S_1, \ldots, S_K\) of \(S\). For each \(\ell = 1, \ldots, K\), the relations \(R_i \mid 1 \leq i \leq m, y_i = \ell\) assigned to subsystem \(S_\ell\) are modeled jointly by an IRM (Eqs. (3)–(5)), independently of all relations assigned to another subsystem \(S_{\ell'} (\ell' \neq \ell)\). The HIRM thus defines a probability distribution over relation clusters, domain entity clusters, and relation values with the following factorization:

\[
P(y_1, \ldots, y_m, \{z^{\ell 1}, \ldots, z^{\ell n}\}_{\ell=1}^K) = P(y) \prod_{\ell=1}^K \prod_{i=1}^{|D_i|} P(z^{\ell i} | y) \prod_{k|y_k=\ell} P(R_k | z^{\ell 1}, \ldots, z^{\ell n}). \tag{6}
\]

For each subsystem index \(\ell = 1, \ldots, K\); domain index \(i = 1, \ldots, n\); relation index \(k = 1, \ldots, m\); entity indexes \(i_1, \ldots, i_{t_k}\); and cluster indexes \(j_1, \ldots, j_{t_k}\), the generative specification of the HIRM is given by the following process:

\[
\{y_1, \ldots, y_m\} \sim \text{CRP}(\gamma_0) \tag{7}
\]
\[
\{z_{1 \ell i}, z_{2 \ell i}, \ldots\} \sim \text{CRP}(\gamma_{\ell i}) \tag{8}
\]
\[
\theta_k(j_1, \ldots, j_{t_k}) \sim \tau_k(\lambda_k) \tag{9}
\]
\[
R_k(i_1, \ldots, i_{t_k}) \sim L_k(\theta_k(z_{1 \ell 1}, \ldots, z_{m \ell n})) \tag{10}
\]

where \((\gamma_0, \{\gamma_{\ell i}\}_{i=1}^n)_{\ell=1}^K, \{\lambda_k\}_{k=1}^m\) are model hyperparameters, possibly endowed with their own hyperpriors.

The HIRM generalizes and extends the IRM. First, it recovers the standard IRM when \(\gamma_0 = 0\). For \(\gamma_0 > 0\), Eq. (7) specifies a CRP partition prior over relations, where relations in the same block are modeled jointly using a standard IRM (Eqs. (8)–(10)). In Eq. (8), each domain \(D_i\) is associated with a different partition \(z_{\ell i}\) for each subsystem \(S_\ell\) in which it participates. This inductive bias allows the HIRM to express structural independences between relations and avoid modeling a Cartesian product of domain partitions when the data for (a subset of) relations in the system are not well-aligned (Sec. 3.1 and Fig. 2).

Additionally, Eq. (7) allows the HIRM to directly cluster dependent relations together, without using higher-order encodings that are limited to relations defined on the same domain as in the IRM (Sec. 3.2). Further, Eqs. (9) and (10) imply that relations \(R_k\) and \(R_{k'}\) that are clustered together in a subsystem \(S_\ell\) need not be identically distributed (resp. Fig. 3), as they each have their own parameters \(\theta_k\) and \(\theta_{k'}\), respectively. The dependence is instead modeled by the shared domain partitions \(\{z^{\ell 1}, \ldots, z^{\ell n}\}\) within subsystem \(S_\ell\). In sum, the nonparametric structure learning prior Eq. (7) retains the benefits of the standard IRM while addressing the limitations discussed in Sec. 3, all within a Bayesian nonparametric model discovery framework.

### 4.1 POSTERIOR INFERENCE

An observed dataset \(\{r_1, \ldots, r_m\}\) for a relational system consists of a finite number of realizations of relation values, i.e., observations of random variables of the form \(R_k(i_1, \ldots, i_{t_k}) = r_k(i_1, \ldots, i_{t_k})\). For notational ease and without loss of generality, we assume that the relation values are fully observed for \(N_i \geq 1\) entities \(\{e_1, \ldots, e_{N_i}\}\) of each domain \(D_i\) \(i = 1, \ldots, n\), across all relations that it participates in (our reference implementations of the HIRM handles arbitrary index combinations with missing data).

Posterior inference in the HIRM is carried out by simulating an ergodic Markov chain that converges to the distribution obtained by conditioning Eq. (6) on the observed dataset. The chain initializes a state \(\mathcal{S}\) by sampling it from the prior (Eqs. (7)–(9)) and iterates the state using Gibbs sampling. Algorithm 1 shows one full Gibbs scan through all the variables in the state \(\mathcal{S}\). We next describe transition operators for the updates in lines 2, 8 and 15 of Algorithm 1.
Algorithm 1 MCMC Gibbs Scan for HIRM (Sketch)

**Require:** Markov chain state $S$ containing relation cluster assignments \{y_1, \ldots, y_m\}, entity cluster assignments \{z_1^i, \ldots, z_{N_1}^i\}, and parameters \{\theta_k(j_1, \ldots, j_{k_1})\}, for $1 \leq i \leq m$, $1 \leq \ell \leq K$, and $1 \leq k \leq m$; dataset $r$. 

1: for $k = 1, \ldots, m$ do 
2: resample $y_k$ given $(r, S \setminus \{y_k\})$ 
3: for $\ell = 1, \ldots, \max(y_1, \ldots, y_m)$ do 
4: $\triangleright I_\ell$ is set of domains in subsystem $S_\ell$ 
5: $I_\ell \leftarrow \{d_\ell j \mid 1 \leq k \leq m, 1 \leq j \leq t_k, y_k = \ell\}$ 
6: for $i \in I_\ell$ do 
7: for $j = 1, \ldots, N_\ell$ do 
8: resample $z_i^j$ given $(r, S \setminus \{z_i^{j,1}\})$ 
9: $\triangleright T_\ell$ is set of relations in subsystem $S_\ell$ 
10: $T_\ell \leftarrow \{k \mid 1 \leq k \leq m, y_k = \ell, (\pi_k, L_k) \text{ nonconjugate}\}$ 
11: for $k \in T_\ell$ do 
12: for $j_1 = 1, \ldots, \max(z_1^{d_1}, \ldots, z_{N_1}^{d_1})$ do 
13: $\cdots$ 
14: for $j_k = 1, \ldots, \max(z_1^{d_k}, \ldots, z_{N_k}^{d_k})$ do 
15: resample $\theta_k(j_1, \ldots, j_k)$ given $(r, S)$ 

Reampling relation cluster assignments $y_k$: This kernel uses the auxiliary Gibbs sampler (Neal, 2000, Algorithm 8). Let $C_\ell := |\{k \mid 1 \leq k \leq K, y_k = \ell\}|$ be the number of relations in $S_\ell$ and $W_{ij} := \max(z_i^j, \ldots, z_{N_\ell}^j)$ be the number of clusters for domain $D_i$ within $S_\ell (1 \leq \ell \leq K)$. 

Case 1: If $y_k$ is a singleton ($C_k > 1$), then it is resampled to take a new value $\ell \in \{1, \ldots, K\}$ with probability 

$$c_{k\ell} = \prod_{j_1 = 1}^{W_{d_1k}} \cdots \prod_{j_k = 1}^{W_{d_kk}} w_{k\ell}(j, \theta_k),$$

where $j := (j_1, \ldots, j_k)$ and 

$$c_{k\ell} := \begin{cases} 
\gamma_0/(m-1+\gamma_0) & \text{if } \ell = y_k \\
C_\ell/(m-1+\gamma_0) & \text{otherwise},
\end{cases}$$

$$w_{k\ell}(j, \theta_k) := \prod_{i \in A_{k\ell}(j)} L_k(r_k(i); \theta_k(i)).$$

Eq. (11) is the conditional probability from the CRP prior (Eq. 2), and in Eq. (13) the symbol 

$$A_{k\ell}(j) := \{i \mid z_{i}^{d_1} = j_1, \ldots, z_{j_k}^{d_k} = j_k\}$$

(14) 

denotes the set of entity indexes $i := (i_1, \ldots, i_k)$ for domains $(d_1, \ldots, d_k)$ that are assigned to cluster $j$ of subsystem $S_\ell$ (where $1 \leq k \leq m; 1 \leq \ell \leq M; 1 \leq j_1 \leq W_{d_1}, \ldots; 1 \leq j_k \leq W_{d_k}$). Note that if $(\pi_k, L_k)$ is a conjugate pair, the parameters $\theta_k$ can be analytically integrated out, and Eq. (13) becomes 

$$w_{k\ell}(j) := \int_\theta \left[ \prod_{i \in A_{k\ell}(j)} L_k(r_k(i); \theta) \right] \pi_k(\theta; \lambda_k) d\theta.$$ 

Case 2: If $y_k$ is not a singleton ($C_k > 1$), then 

1. For domain indexes $i = 1, \ldots, n$, draw cluster assignments for a fresh entity partition, i.e.,

$$z_{i}^{K+1,1}, \ldots, z_{N_\ell}^{K+1,1} \sim \text{CRP}(\gamma),$$

$$W_{K+1,1} := \max(\{z_1^{K+1,1}, \ldots, z_{N_\ell}^{K+1,1}\})$$

2. Draw parameters $\theta_k(j_1, \ldots, j_k)$ for relation indexes $k = 1, \ldots, m$ and cluster indexes $j_1 = 1, \ldots, W_{K+1, d_1}; \ldots; j_k = 1, \ldots, W_{K+1, d_k}$. 

Next, resample $y_k$ to take a new value $\ell \in \{1, \ldots, K + 1\}$ using the same terms in Eqs. (11)–(13) from the previous case, except that the CRP weight $c_{k\ell}$ in Eq. (12) is instead 

$$c_{k\ell} := \begin{cases} 
(C_\ell - 1)/(m-1+\gamma_0) & \text{if } \ell = y_k \\
C_\ell/(m-1+\gamma_0) & \text{if } \ell \neq y_k, \ell \leq K \\
\gamma_0/(m-1+\gamma_0) & \text{if } \ell = K + 1.
\end{cases}$$

Resampling entity cluster assignments $z_i^{j,1}$: Within each subsystem $S_\ell$, the entity cluster assignments are transitioned using the collapsed Gibbs sampler (Neal, 2000, Alg. 3). Alternatively, the split-merge algorithm can be used (Jain and Neal, 2004). Xu et al. (2007) discuss additional sampling-based and variational approaches for these variables.

Resampling cluster parameters $\theta_k(j_1, \ldots, j_k)$: Sample $\theta_k(j_1, \ldots, j_k)$ from a proposal distribution (e.g., the prior $\pi_k(\lambda_k)$ or Gaussian drift $N(\theta_k(i), \sigma_k(i))$) and accept the move according to the Metropolis-Hastings probability 

$$\min \left( 1, \frac{\pi_k(\theta_k(j_1, \ldots, j_k); \lambda_k) w_{k\ell}(j, \theta_k(j)) q_k(\theta_k(j_1, \ldots, j_k); \theta_k(j))}{\pi_k(\theta_k(j_1, \ldots, j_k); \lambda_k) w_{k\ell}(j, \theta_k(j)) q_k(\theta_k(j_1, \ldots, j_k); \theta_k(j))} \right).$$

where is $w_{k\ell}$ (Eq. 13) is the data likelihood for cluster $j$. 

5 EVALUATION

We implemented a prototype of the HIRM\(^1\) and evaluated it in three settings: solving density estimation tasks in object-attribute data; discovering relational structure in political data; and learning relationships between gene properties. 

5.1 OBJECT-ATTRIBUTE BENCHMARKS

We assessed the predictive performance of the HIRM on a benchmark of 20 object-attribute datasets (Gens and Domingos, 2013) and compared the results to two Bayesian non-parametric baselines. In Table 1, the first four columns

\(^1\)Reference implementations of the HIRM in C++ and Python are available at [https://github.com/probcomp/hierarchical-irm](https://github.com/probcomp/hierarchical-irm).
summarize the dataset statistics (16–1556 columns, 2000–330212 rows). The last three columns show the test log-likelihood from the HIRM, IRM (Kemp et al., 2006; Xu et al., 2006), and Dirichlet process mixture model (DPMM; Lo, 1984). As in Kemp et al. (2006), the IRM encodes object-attribute data using one binary relation \( R : \text{Attr} \times \text{Obj} \rightarrow \{0,1\} \). The HIRM encodes each dataset using \( N_{\text{cols}} \) unary relations \( \{R_i : \text{Obj} \rightarrow \{0,1\} \mid i \in \text{Attr}\} \) with structure learning (Eq. (7)) over the dependence between the attributes. The DPMM uses the same encoding as the HIRM but without structure learning (i.e., all attributes are modeled jointly). Dots indicate significantly worse values than the HIRM (\( p = 0.05 \), Mann–Whitney U test on the \( N_{\text{test}} \) predictions from each model). Table 1 shows that the HIRM consistently outperforms these baselines—it is significantly better in 17 cases and worse in zero cases. Fig. 4 shows a plot of runtime vs. held-in data log score for two runs of the HIRM and IRM on four of the benchmarks. Despite using a structure learning prior, the runtime of the HIRM matches or outperforms the IRM; in fact, the HIRM often infers simpler partitions within the independent subsystems, which can improve both the runtime scaling and model fit.

To further assess the density estimation results, we compared the HIRM test log-likelihood to those obtained from probabilistic deep learning baselines for object-attribute data: LearnSPN (Gens and Domingos, 2013) and RAT-SPN (Pe-

Table 2: Summary of no. of wins, ties, and losses of HIRM on benchmarks from Table 1, compared to two Bayesian nonparametric baselines and two probabilistic deep learning baselines.

| Dataset | \( N_{\text{cols}} \) | \( N_{\text{train}} \) | \( N_{\text{test}} \) | HIRM | IRM | DPMM | LearnSPN | RAT-SPN |
|---------|-----------------|-----------------|-----------------|----------|----------|--------|----------|--------|
| BBC | 16 | 18338 | 3236 | -0.06 | -0.01 | -0.01 | -0.01 | -0.01 |
| MSNIBC | 17 | 330212 | 58265 | -0.19 | -0.27 | -0.22 | -0.22 | -0.22 |
| KDDcup 2000 | 64 | 199999 | 34955 | -0.13 | -0.12 | -0.13 | -0.13 | -0.13 |
| Plants | 69 | 19733 | 3482 | -13.75 | -14.23 | -13.81 | -13.81 | -13.81 |
| Audio | 100 | 17000 | 3000 | -39.99 | -40.34 | -40.02 | -40.02 | -40.02 |
| Jester | 100 | 10000 | 4110 | -52.91 | -52.96 | -52.92 | -52.92 | -52.92 |
| Netflix | 100 | 3500 | 3000 | -56.96 | -57.48 | -56.96 | -56.96 | -56.96 |
| Accidents | 111 | 14458 | 2551 | -33.85 | -39.43 | -38.93 | -38.93 | -38.93 |
| Retail | 135 | 24979 | 4408 | -10.90 | -10.99 | -10.92 | -10.92 | -10.92 |
| Pumsb-star | 163 | 13897 | 2452 | -32.77 | -38.95 | -38.02 | -38.02 | -38.02 |
| DNA | 180 | 2000 | 1186 | -87.65 | -93.44 | -97.62 | -97.62 | -97.62 |
| Kosarok | 190 | 37825 | 6675 | -10.91 | -10.99 | -10.95 | -10.95 | -10.95 |
| MSWeb | 294 | 62191 | 5000 | -10.23 | -11.20 | -10.26 | -10.26 | -10.26 |
| Book | 500 | 9859 | 1739 | -34.43 | -34.52 | -34.76 | -34.76 | -34.76 |
| EachMovie | 500 | 5526 | 391 | -52.23 | -52.09 | -54.86 | -54.86 | -54.86 |
| WebKB | 839 | 3361 | 838 | -156.67 | -157.27 | -158.26 | -158.26 | -158.26 |
| Reuters-52 | 889 | 7560 | 1540 | -90.22 | -90.06 | -89.34 | -89.34 | -89.34 |
| 20 Newsgroup | 910 | 15057 | 3764 | -153.52 | -156.46 | -153.95 | -153.95 | -153.95 |
| BBC | 1058 | 1895 | 330 | -253.36 | -253.86 | -254.59 | -254.59 | -254.59 |
| Ad | 1556 | 2788 | 491 | -45.19 | -46.17 | -52.40 | -52.40 | -52.40 |

* indicates significantly worse than HIRM (\( p = 0.05 \), Mann–Whitney U test).
Indonesia, Jordan, Burma, India, Israel, Egypt, Poland, USSR, UK, USA, Brazil

Neutral

Allies

Exports

Netherlands

Indonesia

Poland

Burma

Jordan

Egypt

India

Israel

China

USSR

Brazil

Netherlands

USA

UK

and UK, who in turn translate books from the USSR. Fig. 5d represents a subsystem of relations in which the USA is a clear outlier due to its unusually high number of immigrants and foreign students: the HIRM has inferred that these interactions are independent of the fact that China and Russia, for example, are geopolitical rivals of the USA (Fig. 5b). Fig. 5e contains sparse relations such as “Attack Embassy” and “Sever Relations”, which form a subsystem with one country cluster and a small probability for the hostile event.

In contrast to the HIRM, the IRM cannot detect subsystem structure of this form since it uses a single country partition for all interactions, which is an inaccurate explanation of the data in light of the widely varying interaction patterns in the subsystems (Figs. 5b–5e) discovered by the HIRM.

5.3 GENOMIC PROPERTIES

Our third application of the HIRM is to structure discovery in a widely used dataset of yeast genomes (Cheng et al., 2002). Fig. 1b shows a diagram of the relational system. There are nine domains: the GENE domain has 1,243 unique identifiers and the remaining domains represent gene properties. There is one binary relation between GENE and each of the eight other domains, as well as one binary relation (Interact) on GENE. A single gene is typically involved in multiple relations with the COMPLEX, PHENOTYPE, CLASS, MOTIF, and FUNCTION domains, but has only one value for ESSENTIAL and CHROMOSOME. Table 3 shows an example record for gene G235131: some characteristics of this gene are that the CLASS is missing, it forms two COMPLEX, has

| Countries (Domain) | Indonesia, Jordan, Burma, India, Israel, Egypt, Poland, USSR, UK, USA, Brazil |
|-------------------|--------------------------------------------------------------------------------|
| Attributes (Unary Relations) | Area, Telephone Users, Communist, Literacy, Protests, Purges, Democracy, ... |
| Interactions (Binary Relations) | Exports, Enemies, Allies, Economic Aid, Book Translations, Treaties, Tourism, ... |
two Function; there are five observed Phenotype; and it interacts with 11 other genes (three of which are listed).

Table 3: Example Gene

| Field          | Value                  |
|----------------|------------------------|
| GENE           | G235131                |
| ESSENTIAL      | Non-Essential          |
| CLASS          | ?                      |
| COMPLEX        | Histone Acetyltransferase |
| PHENOTYPE      | Auxotrophies           |
| CHROMOSOME     | PS00633                |
| FUNCTION       | Transcription          |
| LOCALIZATION   | Nucleus                |
| Interactions   | G234980, G235780, G235278, ... |

Table 4: Example gene posterior co-clustering probabilities in each of the two contexts shown in Fig. 6a.

| GENE 1 | GENE 2 | Co-clustering probability within subsystem containing | Pattern |
|--------|--------|--------------------------------------------------------|---------|
| G235131| G235278| 0.98                                                   | 0.87    |
| G235131| G239017| 0.52                                                   | 0.47    |
| G235131| G236063| 0.03                                                   | 0.13    |
| G235131| G235388| 0.83                                                   | 0.27    |
| G235131| G240065| 0.03                                                   | 0.68    |

U = Unlikely 0–0.33; M = Medium 0.33–0.66; L = Likely 0.66–1

to an unknown CLASS, the HIRM is still able to compute its co-clustering probabilities within this context by using observations of its other properties (i.e., relation values) that are inferred to be predictive of the missing value.

We next computed posterior co-clustering probabilities for domains that represent gene properties. In Fig. 6b, the HIRM infers a likely cluster of localization entities that includes cell wall, extracellular, integral membrane, and lipid particles, whereas cytoplasm and nucleus are inferred as probable singletons. Fig. 6c shows co-clustering probabilities for CLASS, which reflect a probable cluster (cyclins, tubulins, adaptins, ... ) embedded within a larger more noisy cluster, as well as singletons such as transcription factor and polymerases. These heatmaps show quantitative estimates of posterior uncertainty in the partition structures detected by the HIRM, which cannot be captured using inference approaches such as approximate maximum likelihood or maximum a posteriori estimation and highlight a key benefit of using fully Bayesian sampling approaches (Sec. 4.1) for probabilistic structure learning in complex domains.

6 RELATED WORK

Several variations of the standard IRM have been introduced in the literature on nonparametric relational Bayesian mod-
els (Ishiguro et al., 2012; Ohama et al., 2013; Jonas and Kording, 2015; Briercliffe, 2016). Our method is distinguished by being the first hierarchical extension that uses a nonparametric structure learning prior over the relations themselves to improve modeling capacity and address shortcomings of the IRM identified in Sec. 3, which include combinatorial over-clustering and failing to detect relationships between dependent but non-identically distributed relations. These limitations have not been addressed by previous variations of the IRM. A key advantage of our hierarchical approach is that it can be composed with several IRM variants that address other shortcomings of the standard IRM, including (i) the subset IRM (Ishiguro et al., 2012), which detects and filters out irrelevant observations in the case of extreme sparsity; and (ii) the logistic regression IRM (Jonas and Kording, 2015), which improves predictive accuracy for semi-supervised tasks that specify one or more target variables as well as exogenous (non-probabilistic) predictor variables.

Other approaches to relational modeling include relational extensions of Bayesian networks (Heckerman et al., 2004; Koller and Pfeffer, 1997; Friedman et al., 1999) and Markov random fields (Taskar et al., 2002; Richardson and Domingos, 2006). While these approaches are typically more expressible than the models we consider here, they inherit traditional challenges of structure learning and model selection for directed models (Daly et al., 2011) (e.g., there is a super-exponential number of graphs to consider (Robinson, 1977)); and can require tuning evaluation measures, clause construction operators, or search strategies (Kok and Domingos, 2005) for undirected models. We instead build on Bayesian nonparametric relational models (Fan et al., 2020) that (i) use latent variables to provide a layer of indirectness and simplify the learning problem as compared to searching over arbitrary graphical structures; and (ii) can be learned using principled algorithms for Bayesian inference.

Deep generative models have also been developed for relational data (Kipf and Welling, 2016; Mehta et al., 2019; Fan et al., 2019; Qu et al., 2019). These methods either typically assume that there is one binary adjacency matrix being modeled (i.e., a random graph relation) or work in a semi-supervised setting of predicting labels. In contrast, we aim to discover generative models for datasets with richer relational schemas than a single binary matrix (e.g., Fig. 1) and operate in a fully unsupervised setting without assuming beforehand that there are specific labels to predict. This approach allows us in Sec. 5.1 to make predictions using inferred joint probabilities for up to 1556 variables, and in Secs. 5.2 and 5.3 to automatically model sparse and noisy systems with multiple entities, attributes, and interactions.

Using the Chinese restaurant process as a structure learning prior (Eq. (7)) has been considered in other settings, including non-relational tabular data (Mansinghka et al., 2016), multivariate time series (Saad and Mansinghka, 2018), topic modeling (Blei et al., 2010), and computer vision (Salakhutdinov et al., 2013), among others. The same insight of using an outer CRP to partition relations (used in this work to extend the IRM) can also be applied to other models that handle relational systems with multiple relations, such as the Mondrian process (Roy and Teh, 2009). More broadly, it would be particularly fruitful to investigate a representation theorem for the ergodic distributions of a relational system modeled by an HIRM within the framework of exchangeable random structures from Orbanz and Roy (2015).

In addition to the IRM, several other Bayesian nonparametric models are special cases of the HIRM, including the infinite hidden relational model (Xu et al., 2006), infinite mixture model (Rasmussen, 2000), Dirichlet process mixture model (Lo, 1984), and Cross-Categorization (Mansinghka et al., 2016). By generalizing the likelihood term in Eq. (10) to include regression on relation values that are endogenous to the system, the HIRM could be further extended to express a relational variant of Dirichlet process mixtures of generalized linear models (Hannah et al., 2011).

Finally, as a domain-general model for relational data, the HIRM can be used to extend previous methods for automatic Bayesian modeling of non-relational tabular data that synthesize probabilistic programs in domain-specific languages (Saad et al., 2019). Expressing the HIRM in probabilistic programming languages would simplify several end-user workflows for data analysis tasks such as imputation, outlier detection, dependence detection, and search (Saad and Mansinghka, 2016, 2017; Saad et al., 2017), as well as enable fast exact inference (Saad et al., 2021) for the broad range of probabilistic queries that the HIRM can handle.

7 CONCLUSION

This paper has presented the hierarchical infinite relational model (HIRM), a new method for discovering probabilistic structure in relational data. A key insight in our approach is to use a nonparametric prior that divides a system of relations into independent subsystems, each to be learned using a separate infinite relational model. This Bayesian nonparametric approach to structure learning generalizes the standard infinite relational model (Kemp et al., 2006) and addresses several limitations in its inductive biases.

While methods based on the IRM, such as the HIRM, specify relatively simple probabilistic theories for relational systems as compared to other approaches that specify more complex theories (Muggleton and de Raedt, 1994; Getoor et al., 2007), our evaluations illustrate the efficacy of our approach on density estimation tasks and show that it can discover meaningful structure in real-world politics and genomics datasets. The results also underscore the benefit of principled and fully Bayesian structure learning for inferring probable independences, which can improve scalability, interpretability, uncertainty characterization, and model fit.
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