Non-Parametric Learning of Gaifman Models

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Abstract

We consider the problem of structure learning for Gaifman models and learn relational features that can be used to derive feature representations from a knowledge base. These relational features are first-order rules that are then partially grounded and counted over local neighborhoods of a Gaifman model to obtain the feature representations. We propose a method for learning these relational features for a Gaifman model by using relational tree distances. Our empirical evaluation on real data sets demonstrates the superiority of our approach over classical rule-learning.

1 Introduction

Learning embeddings of large knowledge bases has become a necessity due to the importance of reasoning about objects, their attributes and relations in large graphs. Statistical Relational AI/Learning (StaRAI) (Raedt et al. 2016; Getoor and Taskar 2007), has the ability to learn and reason with multi-relational data in the presence of uncertainty. While specific models such as Markov Logic (Richardson and Domingos 2006), ProbLog (De Raedt, Kimmig, and Toivonen 2007) and PSL (Brocheler, Mihalkova, and Getoor 2010) (to name a few) exist, a more scalable model (Niepert 2016) was proposed recently. This work built on Gaifman’s locality theorem (Gaifman 1982; Grohe and Wöhrle 2004), which states that every first-order sentence is equivalent to a Boolean combination of sentences whose quantifiers range over local neighborhoods of the Gaifman graph. The key idea is that if one could identify effective representations from local neighborhoods (of objects or tuples of objects), one could learn machine learning models that can be used for reasoning in large graphs. This “local representation” approach was inspired by the success and scalability of convolutional neural networks (CNNs, (Goodfellow, Bengio, and Courville 2016)), specifically, the ability of CNNs to engineer complex features from locally-connected image neighborhoods.

In a similar manner, relational Gaifman models seek to identify locally-connected relational neighborhoods within knowledge bases for effective representation, learning and inference. While effective, the relational learning model recently proposed by Niepert (Niepert 2016), called Discriminative Gaifman Models, used relational features that were hand-crafted rather than learned, that is, structure learning (to use the terminology from probabilistic graphical models) was not performed.

We address this problem of structure learning for learning relational features for training the Gaifman model. We consider three different approaches. (1) As suggested by Niepert (Niepert 2016), we employ Inductive Logic Programming (ILP) (Muggleton 1991) to learn discriminative first-order rules; (2) Inspired by the success of random walks in deep relational models (Lao and Cohen 2010; Lao, Mitchell, and Cohen 2011; Kaur et al. 2017), we employ relational random walks; (3) Finally, as a novel contribution, we propose the use of paths from relational trees learned via relational one-class classification (Khot, Natarajan, and Shavlik 2014); specifically, each path from root to leaf of a relational tree can be considered a relational feature. Given these relational features, we apply traditional discriminative machine learning algorithms.

We make the following key contributions. (1) We present a method for learning relational embeddings for reasoning over large graphs. (2) We adapt a recently developed relational learning method for constructing relational features. (3) We adapt well-known relational rule learners for learning local neighborhood representations. (4) We combine these relational features with discriminative classifiers to learn discriminative Gaifman models. (5) We demonstrate that combining the more novel relational trees with a discriminative classifier is more effective in learning on large graphs compared to a standard ILP learner. (6) Our empirical evaluation reveals an important characteristic of our approach: high recall without sacrificing precision in both medical and imbalanced data sets. This is the first work on structure learning for Gaifman models.

2 Background and Related Work

A grounding of a predicate with logical variables \(x_1, \ldots, x_k\) is a substitution \(\{<x_1, \ldots, x_k>/X_1, \ldots, X_k\}\) mapping each of its variables to a constant in the population of that variable. A knowledge base \(B\) consists of (1) a finite domain

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A Gaifman neighborhood can be thought of as representing \( \text{DDI} \). Given entities (drugs, enzymes, transporters) and relations between them, the underlying machine-learning task is to predict if two drugs interact. The dotted line represents the second-order proximity between nodes. The interpretation is that nodes with shared neighbors are more likely to be similar and more likely to have a link between them. Discriminative Gaifman Models (DGMs, Niepert et al. 2016) are relational models that can exploit structural features of a local neighborhood of a knowledge base. These structural features are aggregated from locally-sampled neighborhoods, and the aggregation is based on the Gaifman locality theorem (Gaifman 1982) stated as: Every first-order sentence is logically equivalent to a Boolean combination of basic \( r \)-local sentences. An \( r \)-local sentence is of the form \( \exists x_1 \ldots \exists x_k \left( \wedge_{1 \leq i < j \leq k} d(x_i, x_j) > 2r \right) \land \wedge_{1 \leq i \leq j} \varphi(x_i) \), where \( r, j \geq 1 \) and \( \varphi \) is an \( r \)-local first order formula. In simpler terms, the locality theorem states that only a small part of a given structure is relevant for evaluating a query statement and thus a global structure search is not required. For example, if querying about the drug \( d_1 \) in Figure 1, a search within the 1-neighborhood of \( e_1 \) (say), that is \( \{t_1, e_1\} \) is more relevant than searching through the complete graph which can be greatly computationally inefficient. Another way to look at the theorem is: a \( r \)-order rule is true if it is true in the local \( r \)-neighborhoods of a given graph.

Discriminative Gaifman Models: The Gaifman graph \( G \), also known as the primal graph, of a knowledge base \( B \) is an undirected graph, where the nodes are the entities \( e \in D \). \( G \) contains edges joining two nodes only if the entities \( a \) and \( b \) corresponding to those nodes are present in a relation together \( R(a, \ldots, b, \ldots) \in B \). \( G \) can be used to easily identify co-occurrences (or lack thereof) among every pair of entities in \( B \). Furthermore, cliques in \( G \) group entities that co-occur pairwise through shared relationships, and such cliques capture the local structure of a knowledge base. We illustrate this in Figure 1 which shows a knowledge-base fragment and the corresponding Gaifman graph for drug-drug interaction (DDI). Given entities (drugs, enzymes, transporters) and relations between them, the underlying machine-learning task is to predict if two drugs interact. The dotted line represents the target predicate, and identifying it is link prediction.

The distance \( d(a, b) \) between two nodes \((a, b) \in G\) is the minimum number of hops required to reach node \( b \) from node \( a \). For example, in Fig. 1, \( d(d_1, t_1) = 1 \) and \( d(d_2, d_3) = 2 \). The \( r \)-neighborhood of a node \( a \in G \) is the set of all nodes that are at most a distance \( r \) from \( a \) in the Gaifman graph: \( N^r_a = \{ \bar{a} \in G \mid d(a, \bar{a}) \leq r \} \). For example, \( N_1(d_1) = \{t_1, e_1\} \) and \( N_2(d_3) = \{t_1, e_1, d_2, d_3\} \). Figure 2 shows the 1 and 2-neighborhood of a node (colored red) in a given Gaifman model. When a first-order rule/clause \( \varphi(x) \) is relativized by the neighborhood of the free variable \( x \), the resulting first-order rule \( \psi_{N^r_a(x)}(\varphi) \) is called \( r \)-local. A Gaifman neighborhood can be thought of as representing second-order proximity between nodes. The interpretation is that nodes with shared neighbors are more likely to be similar and more likely to have a link between them. Discriminative Gaifman Models (DGMs, Niepert et al. 2016) are relational models that can exploit structural features of a local neighborhood of a knowledge base. These structural features are aggregated from locally-sampled neighborhoods, and the aggregation is based on the Gaifman locality theorem (Gaifman 1982) stated as: Every first-order sentence is logically equivalent to a Boolean combination of basic \( r \)-local sentences. An \( r \)-local sentence is of the form \( \exists x_1 \ldots \exists x_k \left( \wedge_{1 \leq i < j \leq k} d(x_i, x_j) > 2r \right) \land \wedge_{1 \leq i \leq j} \varphi(x_i) \), where \( r, j \geq 1 \) and \( \varphi \) is an \( r \)-local first order formula. In simpler terms, the locality theorem states that only a small part of a given structure is relevant for evaluating a query statement and thus a global structure search is not required. For example, if querying about the drug \( d_1 \) in Figure 1, a search within the 1-neighborhood of \( e_1 \) (say), that is \( \{t_1, e_1\} \) is more relevant than searching through the complete graph which can be greatly computationally inefficient. Another way to look at the theorem is: a \( r \)-order rule is true if it is true in the local \( r \)-neighborhoods of a given graph.

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Relational and Structure Learning: One of the most important tasks in relational learning is that of link prediction which determines whether a relation (link) exists between entities based on the given relational database. Taskar et al. (Taskar et al. 2004) use template graphical models. Martinez et al. (Martinez, Berzas, and Cubero 2017) and Hasan et al. (Al Hasan and Zaki 2011) present a comprehensive survey on link prediction problems in complex networks and social networks respectively. Graph neural networks (H<formula>arada, Akita, and others 2018</formula>), metric-learning (Chuan, Ali, and Ji 2009) have been extensively surveyed recently; see for instance, Nickel et al. (Nickel et al. 2016), Wang et al. (Wang et al. 2017) and Cai et al. (Cai, Zheng, and Chang 2018). In general, Gaifman models tend to scale better than many such approaches to higher-arity relations and target-query complexity (Niepert 2016) owing to their local view and incorporation of count-based features.
3 Learning Discriminative Gaifman models

Given: A knowledge base $\mathcal{B}$, facts $F_\mathcal{B}$, and its corresponding Gaifman graph $G$; 
Output: A DGM $\mathcal{M}$ that is trained for a particular link prediction task $T$; 
To Do: Construct a set of relational features $\Phi$, and train a discriminative learner to predict $T$.

Our approach, Learning Gaifman Embeddings (LGE), (1) constructs rules $\Phi$ that form the base set of relational features; (2) instantiates rules and performs counting based on task $T$ to construct propositional features $\mathcal{F}$; and finally, (3) learns a discriminative classifier with $\mathcal{F}$ (Figure 3).

3.1 Learning Relational Rules

Given a knowledge base $\mathcal{B}$, the Gaifman graph $G$ is obtained by instantiating the entities that are connected by an edge type (relation) together in the form $R(e_1, e_2)$, that is, relation$(type_1, type_2)$. The relation (link) to be predicted, defined by the target predicate, forms the set of positive examples. We make the closed-world assumption, that is, unobserved edges in the graphs are negative examples. Each relational example also has facts associated with it, which are the ground predicates in $\mathcal{B}$ that describe relational example, its attributes and relationships. All such facts are denoted $F_\mathcal{B}$.

Features via Relational Rule Learning. Our first solution is inspired by Niepert (Niepert 2016), who suggested the use of an Inductive Logic Programming (ILP) style learning method. This method learns a set of discriminative Horn clauses (implications of the form if <condition> then <consequence>). Specifically, we use an ILP system called WILL (Walker T. 2009) to learn the relational feature$^2$. WILL first selects an example from the set of all examples and then finds a clause (rule) that best covers the examples. The best covering is the most general clause that maximizes the difference between the number of positive and negative examples covered$^2$. Each best covering clause becomes a relational rule in our model. The examples covered by the clause are then removed and the process is repeated till a stopping criterion is satisfied; for example, we have extracted a maximum number of rules/ clauses. Note that when a stopping criterion requires $n$ rules to be extracted, it is sometimes possible to extract $m < n$ rules that cover the examples adequately.

Features via Relational Random Walks. Relational data is often represented using a graph that defines a domain’s schema; in such a representation, a relation $R(e_1, e_2)$ is a predicate edge between two entity type nodes: $e_1, e_2$. A relational random walk (RW) through a graph is a chain of such edges corresponding to a conjunction of predicates. For a random walk to be semantically sound, we should ensure that the input type (domain) of the $i+1$-th predicate is the same as the output type (range) of the $i$-th predicate. An example relational random walk from the drug-discovery domain is:

\[
\text{Interacts}(d_0,d_3) \iff \text{TargetInhib}(d_0,t_0) \land \text{TargetInhib}(t_0,d_1) \land \text{TransporterSubstr}(d_1,t_2) \land \text{TransporterInhib}(t_2,d_3).
\]

This is a semantically sound random walk as it is possible to chain the second argument of each predicate to the first argument of the succeeding predicate. This random walk also contains inverse predicates (prefixed by an underscore, such as _Transporter). Inverse predicates are distinct from their corresponding predicates as their arguments are reversed. Thus, this relational random walk chains the first variable $d_0$ in the target predicate Interacts($d_0, d_3$) with the second variable $d_3$. The chain represents a relational feature and constitutes a random local structure of the form:

\[
d_0 \xrightarrow{\text{TargetInhibitor}} t_0 \xrightarrow{\text{TargetInhibitor}} \cdots \xrightarrow{\text{TransporterInhib}} d_3.
\]

Thus, to construct a relational random walk, only the schema describing the knowledge base is required. We adapt path-constrained random walks (PCRW, (Lao and Cohen 2010)) to construct relational random walks. The algorithm starts at the first entity in the target relation, and makes a walk over the (parameterized) graph to end at the second entity present in the target relation. One limitation of PCRW is that the random walks are only performed over binary relations. However, since we employ a predicate representation, we generalize and learn with arbitrary $n$-ary relations.

Features via Relational One-Class Classification (re-IoCC) Features. A common issue in many real-world relational domains, especially knowledge bases, is that only “positive” instances of a relation are annotated, while “negative” instances are not explicitly identified. This is because the number of instances where the relation does not hold is very large, and annotation can be prohibitively expensive. Learning with highly imbalanced data sets requires reasoning over just the positive instances, commonly referred to as one-class classification. Intuitively, if we can construct a relational one-class classifier describing the positive examples, then rules characterizing this classifier are essentially features that describe positive examples. One-class classification typically requires a distance measure to characterize the density of the positive class. While, for standard vector and matrix data, many different distance measures exist, the issue is far more challenging for relational data, and depends on the underlying representation of the classifier.

Suppose we use an off-the-shelf learner to learn relational trees (Blockeel and Raedt 1998) to describe each class in the data. Such relational trees form a decision-list of relational rules. These trees can then be used to compute the relational distance between a pair of examples $x_1$ and $x_2$:

\[
d(x_1, x_2) = \begin{cases} 
0, & \text{LCA}(x_1, x_2) \text{ is leaf;} \\
\exp(-\lambda \cdot \text{depth}(\text{LCA}(x_1, x_2))), & \text{otherwise,}
\end{cases}
\]

where LCA refers to the least common ancestor of the examples $x_1$ and $x_2$. Figure 4 shows examples $x_1 \equiv \text{advisedBy(Tom, Mary)}$ and $x_2 \equiv \ldots$
The distance function can then be used to compute the density estimate for a new relational example \( z \) as a weighted combination of the individual tree-level distances:

\[
D(z) = \sum_i \beta_i d_i(z)
\]

where \( \beta_i \) is the weight of the \( i \)th tree and \( \sum \beta_i = 1, \beta_i \geq 0 \). The non-parametric function \( D(\cdot, \cdot) \) is a relational distance measure learned on the data.

The splitting criteria used in classification is inversely related to the density of the labeled example \( E \), which can be used as a relational feature. The splitting criteria is the squared error over the examples and the goal is to minimize squared error in each node as shown in equation (2):

\[
\min \sum_{y \in \mathcal{Y}} \left[ I(z) - E(z \notin \text{class}) - \sum_{x, j \in \mathcal{X}} \alpha_j \beta_i d_i(x, z) \right]^2 + \sum_{y \in \mathcal{Y}} \left[ I(z) - E(z \notin \text{class}) - \sum_{x, j \in \mathcal{X}} \alpha_j \beta_i d_i(x, z) \right]^2
\]

(2)

\( I(z) \) is the indicator function and returns 1 if \( z \) is an unlabeled example or 0 otherwise. Also, \( x_l \) and \( x_r \) are the examples that take the left and right branch respectively. A greedy search approach is employed for tree learning, thereby providing a non-parametric approach for learning these relational trees. Algorithm 1 shows our structure learning method for DGMs using relOCC.

**Procedure 1 Structure Learning using relOCC**

**Input:** fact base \( F_s \), positive ex. pos, negative ex. neg

1. function LearnGaifmanStruct(\( F_s \), pos, neg)
2. for every \( x_1, x_2 \) in pos do
3. Calculate \( d(x_1, x_2) \) according to equation 1
4. \( D(x_1, x_2) = \sum_i \beta_i d_i(x_1, x_2) \) Compute weighted distance between \( x_1, x_2 \)
5. end for
6. for a given new unlabeled example \( z \) do
7. \( E(z \notin \text{class}) = \sum_j \alpha_j D(x_j, z) \) Calculate the density estimate
8. end for
9. Learn the tree \( T \) iteratively by minimizing equation 2
10. return LeftBranch(T)
11. end function

### 3.2 Feature Construction

Once extracted, relational rules are instantiated (grounded) to obtain graphs \( G_{pos} \) and \( G_{neg} \). While several _feature..._
**Procedure 2** Learning Embeddings from Discriminative Gaifman Models; **Input:** target query $q$, knowledge base $B$, positives pos, negatives neg; **Params:** depth $r$, size $k$ and number of Gaifman neighborhoods $w$

1: \textbf{function} LGE($q$, $B$, pos, neg)  
2: \hspace{1em} $\mathcal{G} =$ MakeGaifmanGraph($B$) \hspace{0.5em} \triangleright \text{construct Gaifman graph from facts}$
3: \hspace{1em} $F_0 =$ MakeFactBase($B$)  
4: \hspace{1em} $\Phi =$ LearnGaifmanStruct($F_0$, pos, neg) \hspace{0.5em} \triangleright \text{extract relational features (section 3.1)}$
5: \hspace{1em} G_{pos}, G_{neg} =$ Ground($\Phi$, $F_0$, pos) \hspace{0.5em} \triangleright \text{ground positive and negative examples}$
6: \hspace{1em} $T_0^{pos}, T_0^{neg} =$ GetQueryTuples($q$, $F_0$) \hspace{0.5em} \triangleright \text{all tuples satisfying } q \in F_0, (pos), -q \in F_0, (neg)$
7: \hspace{1em} for every $t$ in $T_0^{pos}$ do  
8: \hspace{2em} $\mathcal{N} =$ GenerateNeighborhoods($t$, $r$, $k$) \hspace{0.5em} \triangleright \text{generate } w \text{ neighborhoods of depth } r \text{ and size } k$
9: \hspace{1em} for every $\varphi$ in $\Phi$ do  
10: \hspace{2em} $\theta = \varphi/t$ \hspace{0.5em} \triangleright \text{substitute query tuple } t \text{ in feature } \varphi$
11: \hspace{2em} $x^p = $ Count($\theta, N, G_{pos}$) \hspace{0.5em} \triangleright \text{count groundings satisfied in the neighborhoods}$
12: \hspace{1em} end for
13: \hspace{1em} $x^p = [\ldots, x_1^p, \ldots, x_{|\Phi|}^p]$ \hspace{0.5em} \triangleright \text{embedding for tuple } t$
14: \hspace{1em} end for
15: \hspace{1em} for every $t$ in $T_0^{neg}$ do  
16: \hspace{2em} $\mathcal{N} =$ GenerateNeighbors($t$, $r$, $k$) \hspace{0.5em} \triangleright \text{generate } w \text{ neighborhoods of depth } r \text{ and size } k$
17: \hspace{1em} for every $\varphi$ in $\Phi$ do  
18: \hspace{2em} $\theta = \varphi/t$ \hspace{0.5em} \triangleright \text{substitute query tuple } t \text{ in feature } \varphi$
19: \hspace{2em} $x^e = $ Count($\theta, N, G_{neg}$) \hspace{0.5em} \triangleright \text{count groundings satisfied in the neighborhoods}$
20: \hspace{1em} end for
21: \hspace{1em} $x^e = [\ldots, x_1^e, \ldots, x_{|\Phi|}^e]$ \hspace{0.5em} \triangleright \text{embedding for tuple } t$
22: \hspace{1em} end for
23: \hspace{1em} return $\mathcal{F} = \{x^p, \{x^e\}_\Phi\}$ \hspace{0.5em} \triangleright \text{return embeddings}$
24: \hspace{1em} end function$

If the grounding satisfies the relational feature and since CytochromeP4502C9 is present in the Gaifman neighborhood of Pravastatin (as well as Simvastatin), the count of the relational feature is increased by 1. Thus, for every query variable $q$ we obtain a propositional feature $f_i = [f_1, \ldots, f_{|\Phi|}]$ of length $|\Phi|$:  
$$f_i = \begin{cases} |\psi^{N_r(q)}(q)|, & \text{if } q(e_1, e_2) \text{ partially grounds } \Phi, \\ 0, & \text{otherwise.} \end{cases}$$

Recall that $\psi$ refers to the relativized first-order formula, and consequently $\psi^{N_r(q)}(q)$ is the $r$-local formula for a neighborhood $N$ of depth $r$. Thus, we count the number of entities in the satisfied grounded features that are also satisfied in the neighborhood structure of the Gaifman graph.

**Procedure 2** presents our method, LGE for extracting embeddings from DGMs. In [Line 2–3]: we build the initial Gaifman graph $\mathcal{G}$. In [Line 4]: we learn the relational features from one of the methods defined in [3.1] which are then grounded using both the positive and negative examples [Line 5]: in addition, tuples of the positive and negative examples are also obtained [Line 6]. For both positive ($T_0^{pos}$) and negative tuples ($T_0^{neg}$), the neighborhood of each entity in the tuple is obtained, and each relational feature is partially grounded with the entities $\in t$ [Line 8, 16]. GenerateNeighborhoods [Niepert 2016] generates entity neighborhoods for a tuple $t \in T_0$. Neighborhood generation relies on three parameters: (1) $r$, the depth of neighborhood when counting, (2) $k$, the number of neighbors to sample, and (3) $w$, the number of neighborhoods to be generated. For each entity in tuple $t$, all neighbors at a maximum distance of $r$ form the neighborhood (Fig. 2: the outer region). This process is repeated until we obtain $w$ neighborhoods for each training example. For example, if $r = 1, w = 5$ and $k = 10$ and we have 10 relational features ($|\Phi| = 10$), we obtain 50 propositional examples with 10 features by looking at 1-neighbors for each entity. The Count function [Line 11, 19] counts how many entities in the neighborhood of each query satisfy the partially-grounded relational features. Each such count becomes a propositional feature. In this manner, we can construct a propositionalized data set of $k \times w$ positive examples and $k \times w$ negative examples.

**Learning a Discriminative Model:** After learning the propositional features, any standard classifier can be used for link prediction. In our experiments, we employ gradient-boosting [Friedman 2001] and logistic regression. Results using more algorithms are given in the Appendix. The classification algorithm itself is not a key contribution of our work and as we demonstrate empirically next, a standard classifier suffices for learning an effective discriminative model.

**4 Experiments**

We consider 5 real-world novel relational data sets of varying domains (Table 1) in our empirical evaluation of feature generation using random walks, ILP and relOCC. We aim to answer the following questions: Q1: How do different feature selection strategies compare across diverse domains from different applications? Q2: Does choice of the discriminative algorithm impact the performance? Q3: How do different feature selection strategies impact performance in domains
Table 1: Evaluation domains and their properties.

| Data set      | #Entities | #Relations | #Pos | #Neg | #RW rules | #ILP rules | #relOCC rules |
|---------------|-----------|------------|------|------|-----------|------------|---------------|
| DDI           | 355       | 15         | 2832 | 3188 | 68        | 36         | 25            |
| PPI           | 797       | 7          | 1915 | 1915 | 42        | 5          | 15            |
| NELL Sports   | 4147      | 6          | 300  | 600  | 36        | 15         | 13            |
| Financial NLP | 650       | 7          | 186  | 1029 | 222       | 6          | 25            |
| ICML Co-Author| 558       | 5          | 155  | 6498 | 7         | 15         | 7             |

Table 2: Results for the relational domains. Note that the first three data sets are relatively balanced and the last two are unbalanced. Thus, we do not report Accuracy and AUC-ROC and instead report AUC-PR for the last 2 data sets.

| Data set     | Methods | Accuracy | Recall | F1   | AUC-ROC | AUC-PR |
|--------------|---------|----------|--------|------|---------|--------|
|              |         | LR       | GB     | LR   | GB      | LR     | GB     |
| DDI          | RW      | 0.657    | 0.669  | 0.564| 0.602   | 0.647  | 0.662  |
|              | ILP     | 0.696    | 0.744  | 0.592| 0.729   | 0.684  | 0.767  |
|              | relOCC  | 0.860    | **0.897** | 0.864| **0.901** | 0.864  | **0.902** |
|              | MLN-Boost | 0.711  | 0.504  | 0.618| 0.798   |         |        |
| PPI          | RW      | 0.700    | **0.785** | 0.661| 0.767   | 0.699  | **0.785** |
|              | ILP     | 0.613    | 0.661  | 0.506| 0.620   | 0.613  | 0.661  |
|              | relOCC  | 0.727    | 0.733  | 0.785| **0.789** | 0.727  | 0.733  |
|              | MLN-Boost | 0.649  | 0.453  | 0.571| 0.743   |         |        |
| NELL Sports  | RW      | 0.783    | 0.822  | 0.569| 0.689   | 0.696  | 0.762  |
|              | ILP     | 0.782    | 0.824  | 0.578| 0.699   | 0.699  | 0.769  |
|              | relOCC  | 0.793    | **0.833** | 0.597| 0.714   | 0.708  | 0.778  |
|              | MLN-Boost | 0.822  | 0.533  | 0.667| **0.894** |         |        |
| Financial NLP| RW      | 0.0      | 0.0    | 0.0  | 0.0     | 0.168  | 0.168  |
|              | ILP     | 0.068    | 0.633  | 0.112| 0.727   | 0.200  | 0.603  |
|              | relOCC  | 0.788    | **0.800** | 0.882| **0.889** | 0.826  | **0.833** |
|              | MLN-Boost | 0.764  | 0.757  | 0.807|         |         |        |
| ICML Co-Author| RW      | 0.0      | 0.0    | 0.0  | 0.0     | 0.023  | 0.023  |
|              | ILP     | 0.272    | 0.339  | 0.427| 0.506   | 0.289  | 0.356  |
|              | relOCC  | 0.346    | **0.386** | 0.517| **0.557** | 0.370  | **0.40**  |
|              | MLN-Boost | 0.326  | 0.214  | 0.210|         |         |        |

with high class imbalance? Q4: What are effects of Gaifman locality parameters \( r \), \( w \) and \( k \)? Q5: How does our method compare with state-of-the art probabilistic ILP systems?

Data sets: Drug-Drug interactions (DDI): This data set consists of 78 drugs obtained from DrugBank and the target is the interaction relation between the drug entities. Protein-Protein interactions (PPI): This data set is obtained from Alchemy. The target is interaction relation between two protein entities. NELL Sports: was generated by the Never Ending Language Learner (NELL) consisting of information about players and teams and the task is to predict whether a team plays a particular sport i.e. teamplayssport. Financial NLP: is obtained by extracting information from SEC Form S-1 documents, which were scraped and converted into relational format and the target relation is sentenceContainsTarget between sentence and word entities. ICML Co-Author: is obtained by mining publication data from ICML 2018; the target is the CoAuthor relation between persons.

Results: Table also shows the number of relational rules learned by different techniques. Table present the results for all the relational domains, after 5-fold cross validation, with logistic regression (LR) and gradient boosting (GB).

All experiments were run on a 64-bit Intel(R) Xeon(R) CPU E5-2630 v3 server with parameter values \( r=1 \), \( k=10 \) and \( w=5 \).

To answer Q1, we note that relOCC outperform ILP and relational RWs across a majority of the domains. This is expected since relOCC considers the density of the positive and negative examples separately, allowing the features it generates to discriminate better. In answer to Q2, results in Table show that choice of classifier does not make much difference in the final performance after learning relational rules, though the performance of GB is almost always higher than LR. The ICML CoAuthor (neg-to-pos ratio of 42:1) and Financial NLP (neg-to-pos ratio of 6:1) are highly imbalanced; consequently, we report AUC-PR. In both domains, AUC-PR for relOCC outperforms the other rule-construction methods by a large margin. Random walk rules, in particular, cause all the examples to be classified as negative, and results in recall and F1-score of 0 in both the domains. Thus, to answer Q3: different feature selection strategies do affect the performance in highly-imbalanced domains. To answer Q4, figure shows the effects of varying \( r \) (depth of neighborhoods), \( k \) (number of neighbors) and \( w \) (number of neighborhoods) on the DDI data set. Generally, \( k \) does not affect performance significantly, but increasing \( r \) causes recall report to drop sharply. This is because, with \( r = 1 \), entities in the query
neighboring neighborhood are more tightly coupled with entities in the query variables. Another important takeaway is that the rules learned using relOCC exhibit high clinically-relevant recall ($\approx 1$) on medical data sets: DDI and PPI. This has considerable implications for bioinformatics domains as recall is the most important metric; this is because a false negative (such as a misdiagnosis) results in much more serious consequences (Dhami et al. 2018) than a false positive. Finally, from figure 5 (right), we note that varying $r$ and $k$ does not change the run time. However, increasing $w$ increases the run time since the size of the neighborhood graph to be searched increases. To answer Q5, we also compare our method to two probabilistic ILP systems, MLN-Boost (Khot et al. 2011) and Tuffy (Niu et al. 2011). Table 2 shows that our method outperforms MLN-Boost by a significant margin. We also note that Tuffy could not handle the amount of data that we have used in our learning framework and thus could not learn the structure. Instead, used the ILP rules that we learned, and tried learning the weights but Tuffy could not complete training after a few hours. Thus, we sampled 10% data from all the data sets and the results for the same are presented in figure 6. In case of limited number of samples as well, our method is significantly better than the PILP system.

5 Conclusion
We considered the problem of full model learning of discriminative Gaifman models. Our algorithm first constructs a set of rules, identifies the appropriate instantiations and finally counts the number of groundings per rule. These become the raw features based on which one could train a discriminative classifier. Our work provides a method of constructing relational embeddings in an effective manner that can be combined with a scalable local model. Given the increasing importance of local neighborhoods in graph data, automatic learning of these neighborhoods is an important direction and contribution. One possible future direction could be employing more graph based embedding methods that can integrate with Gaifman’s locality principle. Evaluating on more databases and knowledge graphs is an interesting direction.

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References
[Al Hasan and Zaki 2011] Al Hasan, M., and Zaki, M. J. 2011. A survey of link prediction in social networks. In Social network data analytics.
[Blockeel and Raedt 1998] Blockeel, H., and Raedt, L. D. 1998. Top-down induction of first-order logical decision trees. Artificial Intelligence.
