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Bridging Weighted Rules and Graph Random Walks for Statistical Relational Models

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2 ABSTRACT

The aim of statistical relational learning is to learn statistical models from relational or graph-3 structured data. Three main statistical relational learning paradigms include weighted rule 4 learning, random walks on graphs, and tensor factorization. These paradigms have been mostly 5 developed and studied in isolation for many years, with few works attempting at understanding 6 7 the relationship among them or combining them. In this paper, we study the relationship between 8 the path ranking algorithm (PRA), one of the most well-known relational learning methods in the graph random walk paradigm, and relational logistic regression (RLR), one of the recent 9 developments in weighted rule learning. We provide a simple way to normalize relations and 10 prove that relational logistic regression using normalized relations generalizes the path ranking 11 algorithm. This result provides a better understanding of relational learning, especially for the 12 weighted rule learning and graph random walk paradigms. It opens up the possibility of using the 13 more flexible RLR rules within PRA models and even generalizing both by including normalized 14 and unnormalized relations in the same model. 15 16 Keywords: Statistical Relational Artificial Intelligence, Relational Learning, Weighted Rule Learning, Graph Random Walk, Relational

17 Logistic Regression, Path Ranking Algorithm

1 INTRODUCTION

Traditional machine learning algorithms learn mappings from a feature vector indicating categorical and 18 19 numerical features to an output prediction of some form. Statistical relational learning (Getoor and Taskar, 20 2007), or statistical relational AI (StarAI) (De Raedt et al., 2016), aims at probabilistic reasoning and learning when there are (possibly various types of) relationships among the objects. The relational models 21 developed in StarAI community have been successfully applied to several applications such as knowledge 22 graph completion (Lao et al., 2011; Nickel et al., 2012; Bordes et al., 2013; Pujara et al., 2013; Trouillon 23 et al., 2016), entity resolution (Singla and Domingos, 2006; Bhattacharya and Getoor, 2007; Pujara and 24 Getoor, 2016; Fatemi, 2017), tasks in scientific literature (Lao and Cohen, 2010b), stance classification 25 (Sridhar et al., 2015; Ebrahimi et al., 2016), question answering (Khot et al., 2015; Dries et al., 2017), etc. 26

During the past decade and more, three paradigms of statistical relational models have appeared. The first paradigm is the weighted rule learning where first-order rules are learned from data and a weight is assigned to each rule indicating a score for the rule. The main difference among these models is in the types 30 of rules they allow and their interpretation of the weights. The models in this paradigm include Problog

(De Raedt et al., 2007), Markov logic (Domingos et al., 2008), probabilistic interaction logic (Hommersom
and Lucas, 2011), probabilistic soft logic (Kimmig et al., 2012), and relational logistic regression (Kazemi

33 et al., 2014). Recent

The second paradigm is the random walk on graphs, where several random walks are performed on a graph each starting at a random node and probabilistically transitioning to neighbouring nodes. The probability of each node being the answer to a query is proportional to the probability of the random walks ending up at that node. The main difference among these models is in the way they walk on the graph and how they interpret obtained results from the walks. Examples of relational learning algorithms based on random walk on graphs include PageRank (Page et al., 1999), FactRank (Jain and Pantel, 2010), path ranking algorithm (Lao and Cohen, 2010b; Lao et al., 2011), and HeteRec (Yu et al., 2014).

The third paradigm is the tensor factorization paradigm, where for each object and relation an embedding is learned. The probability of two objects participating in a relation is a simple function of the objects' and relation's embeddings (e.g., the sum of the element-wise product of the three embeddings). The main difference among these models is in the type of embeddings and the function they use. Examples of models in this paradigm include YAGO (Nickel et al., 2012), TransE (Bordes et al., 2013), and ComplEx (Trouillon et al., 2016).

The models in each paradigm have their own advantages and disadvantages. Kimmig et al. (2015) survey the models based on weighted rule learning. Nickel et al. (2016) survey models in all paradigms for knowledge graph completion. Kazemi et al. (2017) compare several models in these paradigms for relational aggregation. None of these surveys, however, aims at understanding the relationship among these paradigms. In fact, these paradigms have been mostly developed and studied in isolation with few works aiming at understanding the relationship among them or combining them (Riedel et al., 2013; Nickel et al., 2014; Lin et al., 2015).

With several relational paradigms/models developed during the past decade and more, understanding 54 the relationship among them and pruning the ones that either do not work well or are subsets of the other 55 models is crucial. In this paper, we study the relationship between two relational learning paradigms: graph 56 random walk and weighted rule learning. In particular, we study the relationship among path ranking 57 algorithm (PRA) (Lao and Cohen, 2010b) and relational logistic regression (RLR) (Kazemi et al., 2014). 58 The former is one of the most well-known relational learning tools in graph random walk paradigm, and 59 the latter is one of the recent developments in weighted rule learning paradigm. By imposing restrictions 60 on the rules that can be included in models, we identify a subset of RLR models that we call RC-RLR. 61 Then we provide a simple way to normalize relations and prove that PRA models correspond to RC-RLR 62 models using normalized relations. Other strategies for walking randomly on the graph (e.g., data-driven 63 path finding (Lao et al., 2011)) can then be viewed as structure learning methods for RC-RLR. Our result 64 can be extended to several other weighted rule learning and graph random walk models. 65

The relationship between weighted rules and graph random walks has not been discovered before. For instance, Nickel et al. (2016) describe them as two separate classes of models for learning from relational data in their survey. Lao et al. (2011) compare their instance of PRA to a model based on weighted rules empirically, reporting their PRA model outperforms the weighted rule model, but not realizing that their PRA model could be a subset of the weighted rule model if they had normalized the relations. 71 Our result is beneficial for both graph random walk and weighted rule learning paradigms, as well as for

72 researchers working on theory and applications of statistical relational learning. Below is a list of potential

- 73 benefits our result provides:
- It provides a clearer intuition and understanding on two relational learning paradigms thus facilitating
 further improvements of both.
- It opens up the possibility of using the more flexible RLR rules within PRA models.
- It opens up the possibility of generalizing both PRA and RLR models by using normalized and unnormalized relations in the same model.
- It sheds light on the shortcomings of graph random walk algorithms and points out potential ways to
 improve them.
- One of the claimed advantages of models based on weighted rule learning compared to other relational
 models is that they can be easily explained to a broad range of people (Nickel et al., 2016). Our result
 improves the explainability of models learned through graph random walk, by providing a weighted
 rule interpretation for them.
- It identifies a sub-class of weighted rules that can be evaluated efficiently and have a high modelling power as they have been successfully applied to several applications. The evaluation of these weighted rules can be even further improved using sampling techniques developed within graph random walk community (e.g., see Fogaras et al. (2005); Lao and Cohen (2010a); Lao et al. (2011)). Several structure learning algorithms (corresponding to random walk strategies) have been already developed for this sub-class.
- It facilitates leveraging new insights and techniques developed within each paradigm (e.g., weighted rule models that leverage deep learning techniques (Šourek et al., 2015; Kazemi and Poole, 2018), or reinforcement learning based approaches to graph walk (Das et al., 2017)) to the other paradigm.
- For those interested in the applications of relation learning, our result facilitates decision making on selecting the paradigm or the relational model to be used in their application.

2 BACKGROUND AND NOTATIONS

96 In this section, first we define some basic terminology. Then we introduce a running example which will 97 be used throughout the paper. Then we describe relational logistic regression and path ranking algorithm 98 for relational learning. While semantically identical, our descriptions of these two models may be slightly 99 different from the descriptions in the original articles as we aim at describing the two algorithms in a way 100 that simplifies our proofs.

101 2.1 Terminologies

102 Throughout the paper, we assume True is represented by 1 and False is represented by 0.

103 A population is a finite set of objects (or individuals). A logical variable (logvar) is typed with a

104 population. We represent logvars with lower-case letters. The population associated with a logvar x is Δ_x . 105 The cardinality of Δ_x is $|\Delta_x|$. For every object, we assume there exists a unique *constant* denoting that

106 object. A lower-case letter in bold represents a tuple of logvars and an upper-case letter in bold represents

- 107 a tuple of constants. An **atom** is of the form $V(t_1, \ldots, t_k)$ where V is a functor and each t_i is a logvar or
- 108 a constant. When $range(V) \in \{0, 1\}$, V is a predicate. A unary atom contains exactly one logvar and a
- 109 binary atom contains exactly two logvars. We write a substitution as $\theta = \{\langle x_1, \ldots, x_k \rangle / \langle t_1, \ldots, t_k \rangle \}$



Figure 1. (a) A relation showing citations among papers (papers on the Y axis cite papers on the X axis), (b) The relation in part (a) after row-wise count normalization.

110 where each x_i is a different logvar and each t_i is a logvar or a constant in Δ_{x_i} . A **grounding** of an atom 111 $V(x_1, \ldots, x_k)$ is a substitution $\theta = \{\langle x_1, \ldots, x_k \rangle / \langle X_1, \ldots, X_k \rangle\}$ mapping each of its logvars x_i to an 112 object in Δ_{x_i} . Given a set \mathcal{A} of atoms, we denote by $\mathcal{G}(\mathcal{A})$ the set of all possible groundings for the atoms 113 in \mathcal{A} . A **value assignment** for a set of groundings $\mathcal{G}(\mathcal{A})$ maps each grounding $V(\mathbf{X}) \in \mathcal{G}(\mathcal{A})$ to a value in 114 range(V).

115 A literal is an atom or its negation. A formula φ is a literal, a disjunction $\varphi_1 \vee \varphi_2$ of formulae or a 116 conjunction $\varphi_1 \wedge \varphi_2$ of formulae. Our formulae correspond to open formulae in negation normal form in 117 logic. An instance of a formula φ is obtained by replacing each logvar x in φ by one of the objects in Δ_x . 118 Applying a substitution $\theta = \{\langle x_1, \ldots, x_k \rangle / \langle t_1, \ldots, t_k \rangle\}$ on a formula φ (written as $\varphi \theta$) replaces each x_i 119 in φ with t_i . A weighted formula (WF) is a pair $\langle w, \varphi \rangle$ where w is a weight and φ is a formula.

A binary predicate S(x, y) can be viewed as a function whose domain is Δ_x and whose range is 2^{Δ_y} : 120 each $X \in \Delta_x$ is mapped to $\{Y : S(X, Y)\}$. Following Lao and Cohen (2010b), we consider S^{-1} as the 121 inverse of S whose domain is Δ_y and whose range is 2^{Δ_x} , such that $S^{-1}(x, y)$ holds iff S(y, x) holds. A 122 **path relation** \mathcal{PR} is of the form $x_0 \xrightarrow{\mathsf{R}_1} x_1 \xrightarrow{\mathsf{R}_2} \dots \xrightarrow{\mathsf{R}_l} x_l$ where $\mathsf{R}_1, \mathsf{R}_2, \dots, \mathsf{R}_l$ are predicates, x_0, \dots, x_l 123 are different logvars, $domain(\mathsf{R}_i) = \Delta_{x_{i-1}}$ and $range(\mathsf{R}_i) = \Delta_{x_i}$. We define $domain(\mathcal{PR}) = \Delta_{x_0}$ 124 and $range(\mathcal{PR}) = \Delta_{x_l}$. Applying a substitution $\theta = \{\langle x_1, \ldots, x_k \rangle / \langle t_1, \ldots, t_k \rangle\}$ on a path relation \mathcal{PR} 125 (written as $\mathcal{PR}\theta$) replaces each x_i in \mathcal{PR} with t_i . A weighted path relation (WPR) is a pair $\langle w, \mathcal{PR} \rangle$ 126 where w is a weight and \mathcal{PR} is a path relation. 127

128 2.2 Running Example

129 As a running example, we use the *reference recommendation* problem: finding relevant citations for a new paper. We consider three populations: the population of new papers for which relevant citations are to be 130 found, the population of existing papers whose citations are known, and the population of publication years. 131 The atoms that will be used for this problem throughout the paper are the following. WillCite(q, p) is the 132 atom to be predicted and indicates whether a query/new paper q will cite an existing paper p. $Cited(p_1, p_2)$ 133 shows whether or not an existing paper p_1 has cited another existing paper p_2 . Publn(p, y) shows that p has 134 been published in year y. ImBef (y_1, y_2) indicates that y_2 is the year immediately before y_1 . The reference 135 recommendation problem can be viewed as follows: given a query paper Q, find a subset of existing papers 136 that Q will cite (i.e. find any paper P such that WillCite(Q, P) holds). 137

138 2.3 Relational Logistic Regression

139 Relational logistic regression (Kazemi et al., 2014) defines conditional probabilities based on weighted

rules. It can be viewed as the directed analogue of logistic regression, and as the directed analogue of
Markov logic (Domingos et al., 2008).

142 Let $V(\mathbf{x})$ be an atom whose probability depends on a set \mathcal{A} of atoms, ψ be a set of WFs containing only 143 atoms from \mathcal{A} , \hat{I} be a value assignment for the groundings in $\mathcal{G}(\mathcal{A})$, \mathbf{X} be an assignment of objects to \mathbf{x} , 144 and { \mathbf{x}/\mathbf{X} } be a substitution mapping logvars \mathbf{x} to objects \mathbf{X} .

Relational logistic regression (RLR) defines the probability of V(X) given \hat{I} as follows:

$$Prob_{\psi}(\mathsf{V}(\mathbf{X}) = True \mid \hat{I}) = \sigma\Big(\sum_{\langle w, \varphi \rangle \in \psi} w * \eta(\varphi\{\mathbf{x}/\mathbf{X}\}, \hat{I})\Big)$$
(1)

145 where $\eta(\varphi\{\mathbf{x}/\mathbf{X}\}, \hat{I})$ is the number of instances of $\varphi\{\mathbf{x}/\mathbf{X}\}$ that are True with respect to \hat{I} and σ is the 146 sigmoid function. RLR makes the closed-world assumption: any ground atom that has not been observed 147 to be True is False. Note that $\eta(\text{True}, \hat{I}) = 1$.

Following Kazemi et al. (2014) and Fatemi et al. (2016), we assume that formulae in WFs have no disjunction and replace conjunction with multiplication. Then atoms whose functors have a continuous range can be also allowed in formulae. For instance if a value assignment maps R(X) to 1, S(X) to 0.9 and T(X) to 0.3, then the formula R(X) * S(X) * T(X) evaluates to 1 * 0.9 * 0.3 = 0.27.

152 EXAMPLE 1. An RLR model may use the following WFs to define the conditional probability of 153 WillCite(q, p) in our running example:

154
$$WF_0:\langle w_0,\mathsf{True}
angle$$

$$WF_1: \langle w_1, \mathsf{Publn}(q, y) * \mathsf{ImBef}(y, y') * \mathsf{Publn}(p, y') \rangle$$
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$$WF_2: \langle w_2, \mathsf{Publn}(q, y) * \mathsf{Publn}(p', y) * \mathsf{Cited}(p', p) \rangle$$

 $WF_3: \langle w_3, \mathsf{Cited}(p_1, p_2) * \mathsf{Cited}(p_2, p) \rangle$

157 WF_0 is a bias. WF_1 considers existing papers that have been published a year before the query paper. A 158 positive weight for this WF indicates that papers published a year before the query paper are more likely to 159 be cited. WF_2 considers existing papers cited by the other papers published in the same year as the query 160 paper. A positive weight for this WF indicates that as the number of times a paper has been cited by the other papers published in the same year as the query paper grows, the chances of the query paper citing 161 that paper increases. WF_3 considers existing papers that have been cited by other papers that have been 162 163 themselves cited by other papers. Note that the score of the last WF only depends on the paper being cited, 164 not the paper citing.

165 Consider the citations among existing papers in Fig. 1(a) and let the publication year for all the six 166 papers be 2017. Suppose we have a query paper Q which is to be published in 2017 and we want to find 167 the probability of WillCite $(Q, Paper_2)$ according to the WFs above. Applying the substitution $\{\langle q, p \rangle /$ 168 $\langle Q, Paper_2 \rangle \}$ to the above four WFs gives the following four WFs respectively:

$$WF_0: \langle w_0, \mathsf{True} \rangle$$

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$$WF_1: \langle w_1, \mathsf{Publn}(Q, y) * \mathsf{ImBef}(y, y') * \mathsf{Publn}(Paper_2, y') \rangle$$

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$$WF_2: \langle w_2, \mathsf{Publn}(Q, y) * \mathsf{Publn}(p', y) * \mathsf{Cited}(p', Paper_2) \rangle$$
$$WF_3: \langle w_3, \mathsf{Cited}(p_1, p_2) * \mathsf{Cited}(p_2, Paper_2) \rangle$$

Then we evaluate each WF. The first one evaluates to w_0 . The second evaluates to 0 as Q is being published in 2017 and $Paper_2$ has also been published in 2017. The third WF evaluates to $w_2 * 2$ as there are 2 papers that have been published in the same year as Q and cite $Paper_2$. And the last WF evaluates to $w_3 * 4$ as $Paper_5$ and $Paper_6$ (that cite $Paper_2$) are each cited by two other papers. Therefore, the conditional probability of WillCite $(Q, Paper_2)$ is as follows:

$$\sigma(w_0 + w_2 * 2 + w_3 * 4)$$

176 2.4 Path Ranking Algorithm

177 Let V(s, e) be a target binary predicate, i.e. for a query object $S \in \Delta_s$, we would like to find the 178 probability of any $E \in e$ having the relation V with S. **Path ranking algorithm (PRA)** (Lao and Cohen, 179 2010b) defines this probability using a set of WPRs Ψ . The first logvar of each path relation in Ψ is either s 180 or a logvar other than s and e, the last logvar is always e, and the middle logvars are neither s nor e.

In PRA, each path relation $\mathcal{PR} = x_0 \xrightarrow{\mathsf{R}_1} x_1 \xrightarrow{\mathsf{R}_2} \dots \xrightarrow{\mathsf{R}_l} e$ defines a distribution over the objects in 181 Δ_e . This distribution corresponds to the probability of following \mathcal{PR} and landing at each of the objects 182 in Δ_e , and is computed as follows. Firstly, a uniform distribution D_0 is considered on the objects in Δ_{x_0} , 183 corresponding to the probability of landing at each of these objects if the object is selected randomly. For 184 instance if there are α objects in Δ_{x_0} , D_0 for all objects is $\frac{1}{\alpha}$. Then, the distribution D_1 over the objects 185 in Δ_{x_1} is calculated by marginalizing over the variables in D_0 and following a random step on R₁. For 186 instance for an object $X_1 \in \Delta_{x_1}$, assume $\mathsf{R}_1(x_0, X_1)$ holds only for two objects X_0 and X'_0 in Δ_{x_0} . Also 187 assume X_0 and X'_0 have the R₁ relation with β and γ objects in x_1 respectively. Then the probability of 188 landing at X_1 is $\frac{1}{\alpha} * \frac{1}{\beta} + \frac{1}{\alpha} * \frac{1}{\gamma}$. The following distributions D_2, \ldots, D_l can be computed similarly. D_l 189 gives the probability of landing at any object in Δ_e . 190

191 Let $\theta = \{\langle s, e \rangle / \langle S, E \rangle\}$. In order to find Prob(V(S, E)), for each path relation $\mathcal{PR} \in \Psi$, PRA calculates 192 the probability of landing at *E* according to $\mathcal{PR}\theta$ (denoted by $h(\mathcal{PR}\theta)$), and calculates Prob(V(S, E)) by 193 taking the sigmoid of the weighted sum of these probabilities as follows:

$$Prob(\mathsf{V}(S, E)) = \sigma(\sum_{\langle w, \mathcal{PR} \rangle \in \Psi} w \cdot h(\mathcal{PR\theta}))$$
(2)

Algorithm 1 shows a recursive algorithm for calculating $h(\mathcal{PR})$ for a path relation \mathcal{PR} . The first 194 if statement specifies that the walk starts randomly at any object in Δ_{x_0} . $uniform(\Delta_{x_0})$ indicates a 195 uniform probability over the objects in Δ_{x_0} . This is the termination criterion of the recursion. When 196 $\mathcal{PR} = x_0 \xrightarrow{\mathsf{R}_1} x_1 \xrightarrow{\mathsf{R}_2} \dots \xrightarrow{\mathsf{R}_l} x_l$ is not empty $(l \neq 0)$, first the probability of landing at any object E'197 in the range of $\mathcal{PR}' = x_0 \xrightarrow{\mathsf{R}_1} x_1 \xrightarrow{\mathsf{R}_2} \dots \xrightarrow{\mathsf{R}_{l-1}} x_{l-1}$ is calculated using a recursive call to $h(\mathcal{PR}')$ and 198 stored in $pLand_{l-1}$. The probability of landing at any object E in range of \mathcal{PR} by randomly walking 199 on \mathcal{PR} can then be calculated as the sum of the probabilities of landing at each object E' by randomly 200 walking on \mathcal{PR}' multiplied by the probability of reaching E from E' by a random walk according to the 201 predicate R_l . The two nested for loops calculate the probability of landing at any object $E \in range(\mathcal{PR})$ 202 according to R_l . $R_l(E', E)$ indicates whether there is a link from E' to E (otherwise the probability of 203

Algorithm 1 $h(\mathcal{PR})$

Input: Relation path $\mathcal{PR} = x_0 \xrightarrow{\mathsf{R}_1} x_1 \xrightarrow{\mathsf{R}_2} \dots \xrightarrow{\mathsf{R}_l} x_l$ **Output:** Probability of landing at any object in Δ_{x_1} when starting randomly at any object in Δ_{x_0} and walking on \mathcal{PR} . 1: **if** l = 0 **then return** $uniform(\Delta_{x_0})$ 2: 3: $\mathcal{PR}' = x_0 \xrightarrow{\mathsf{R}_1} x_1 \xrightarrow{\mathsf{R}_2} \dots \xrightarrow{\mathsf{R}_{l-1}} x_{l-1}$ 4: $pLand_{l-1} = h(\mathcal{PR}')$ for $E \in range(\mathcal{PR})$ do 5: $pLand_l(E) = 0$ 6: 7: for $E' \in range(\mathcal{PR}')$ do $C_{R_l}(E') = \#E \in range(\mathcal{PR})$ s.t. $R_l(E', E) = 1$ 8: for $E \in range(\mathcal{PR})$ do 9: $pWalk(E', E) = \frac{R_l(E', E)}{C_{R_l}(E')}$ 10: $pLand_l(E) + pLand_{l-1}(E') * pWalk(E', E)$ 11: 12: return $pLand_l$

transitioning from E' to E according to R_l is 0) and C_{R_l} is a normalization constant indicating the number of possible transitions from E' according to R_l . pWalk(E', E) indicates the probability of walking from E' to E if one of the objects connected to E' through R_l is selected uniformly at random, which equals $\frac{R_l(E',E)}{C_{R_l}}$. $pLand_l$ stores the probability of landing at any object E in the range of (\mathcal{PR}) following \mathcal{PR} , and is returned as the output of the function.

EXAMPLE 2. A PRA model may use the following WPRs to define the conditional probability of WillCite(q, p) in our running example:

$$WPR_0: \langle w_0, p \rangle$$

$$WPR_1 : \left\langle w_1, q \xrightarrow{\mathsf{Publn}} y \xrightarrow{\mathsf{ImBef}} y' \xrightarrow{\mathsf{Publn}^{-1}} p \right\rangle$$
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$$WPR_{2}: \left\langle w_{2}, q \xrightarrow{\mathsf{Publn}} y \xrightarrow{\mathsf{Publn}^{-1}} p' \xrightarrow{\mathsf{Cited}} p \right\rangle$$

$$WPR_{3}: \left\langle w_{3}, p_{1} \xrightarrow{\mathsf{Cited}} p_{2} \xrightarrow{\mathsf{Cited}} p \right\rangle$$

WPR₀ is a bias, WPR₁ considers the papers published a year before the query paper, WPR₂ considers papers cited by other papers published in the same year as the query paper, and WPR₃ mimics PageRank algorithm for finding important papers in terms of citations (cf. Lao and Cohen (2010b) for more detail). Consider the citations among existing papers in Fig. 1(a) and let the publication year for all the six papers be 2017. Suppose we have a query paper Q which is to be published in 2017 and we want to find the probability of WillCite(Q, Paper₂) according to the PRA model above. Applying the substitution $\{\langle q, p \rangle /$ $\langle Q, Paper_2 \rangle\}$ to the above WPRs gives the following WPRs respectively:

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$$WPR_0 : \langle w_0, Paper_2 \rangle$$
$$WPR_1 : \left\langle w_1, Q \xrightarrow{\mathsf{Publn}} y \xrightarrow{\mathsf{ImBef}} y' \xrightarrow{\mathsf{Publn}^{-1}} Paper_2 \right\rangle$$

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$$WPR_2 : \left\langle w_2, Q \xrightarrow{\mathsf{Publn}} y \xrightarrow{\mathsf{Publn}^{-1}} p' \xrightarrow{\mathsf{Cited}} Paper_2 \right\rangle$$
$$WPR_3 : \left\langle w_3, p_1 \xrightarrow{\mathsf{Cited}} p_2 \xrightarrow{\mathsf{Cited}} Paper_2 \right\rangle$$

WPR₀ evaluates to w_0 . WPR₁ evaluates to 0. WPR₂ evaluates to $w_2 * (\frac{1}{6} * \frac{1}{4} + \frac{1}{6} * \frac{1}{2}) = w_2 * 0.125$ as for the path $y \xrightarrow{\text{Publn}^{-1}} p'$ there is $\frac{1}{6}$ probability for randomly walking to either Paper₅ or Paper₆ and then there is $\frac{1}{4}$ probability to walk randomly from Paper₅ to Paper₂ and $\frac{1}{2}$ probability to walk randomly from Paper₆ to Paper₂ according to Cited relation. WPR₃ evaluates to $w_3 * \frac{1}{6} * (\frac{1}{2} * \frac{1}{4} + \frac{1}{3} * (\frac{1}{4} + \frac{1}{2}) + \frac{1}{4} * \frac{1}{2}) \approx w_3 * 0.083$. The $\frac{1}{6}$ outside parenthesis is the probability of randomly starting at any paper, $\frac{1}{2} * \frac{1}{4}$ is the probability of transitioning from Paper₃ to Paper₅ and then to Paper₂, and so forth. Therefore, the conditional probability of WillCite(Q, Paper₂) is as follows:

$$\sigma(w_0 + w_2 * 0.125 + w_3 * 0.083)$$

3 RLR WITH NORMALIZED RELATIONS GENERALIZES PRA

In order to prove that RLR with normalized relations generalizes PRA, we first define relation chains anddescribe some of their properties.

232 3.1 Relations Chain

233 DEFINITION 1. We define a **relations chain** as a list of binary atoms $V_1(x_0, x_1), \ldots, V_m(x_{m-1}, x_m)$ 234 such that for each V_i and V_{i+1} , the second logvar of V_i is the same as the first logvar of $V_{i+1}, x_0, \ldots, x_m$ 235 are different logvars, and V_i and V_j can be the same or different predicates.

EXAMPLE 3. $V_1(x, y)$, $V_2(y, z)$ is a relations chain, and $V_1(x, y)$, $V_2(z, y)$ and $V_1(x, y)$, $V_2(y, z)$, $V_3(z, x)$ are not relations chains.

DEFINITION 2. A first-order formula corresponds to a relations chain if all its literals are binary predicates and non-negated, and there exists an ordering of the literals that is a relations chain.

EXAMPLE 4. The first-order formula $V_1(x_1, x_2) * V_2(x_3, x_1)$ corresponds to a relations chain as the order $V_2(x_3, x_1)$, $V_1(x_1, x_2)$ is a relations chain.

It follows from RLR definition that re-ordering the literals in each of its WFs does not change the distribution. For any WF whose formula corresponds to a relations chain, we assume hereafter that its literals have been re-ordered to match the order of the corresponding relations chain.

DEFINITION 3. Let V(x, y) be a target atom. *Relations chain RLR (RC-RLR)* is a subset of RLR for defining a conditional probability distribution for V(x, y) where:

- formulae of WFs correspond to relations chains,
- for each WF, the second logvar of the last atom is y,
- x may only appear as the first logvar of the first atom,
- *y* may only appear as the second logvar of the last atom.

For RLR models, in order to evaluate a formula, one may have nested loops over logvars of the formula that do not appear in the target atom, or conjoin all literals one by one and then count. WFs of RC-RLR,

Algorithm 2 $Eval(\varphi)$

Input: Formula $\varphi = \mathsf{R}_1(x_0, x_1) * \mathsf{R}_2(x_1, x_2) * \cdots * \mathsf{R}_l(x_{l-1}, x_l).$ **Output:** Evaluation of $\hat{\varphi}$. 1: **if** l = 0 **then** return $ones(|\Delta_{x_0}|)$ 2: 3: $\varphi' = \mathsf{R}_1(x_0, x_1) * \mathsf{R}_2(x_1, x_2) * \cdots * \mathsf{R}_{l-1}(x_{l-2}, x_{l-1})$ 4: $eval_{l-1} = Eval(\varphi')$ 5: for $E \in \Delta_{x_l}$ do $eval_l(E) = 0$ 6: 7: for $E' \in \Delta_{x_{l-1}}$ do for $E \in \Delta_{x_1}$ do 8: $canWalk(E', E) = R_l(E', E)$ 9: $eval_l(E) += eval_{l-1}(E') * canWalk(E', E)$ 10: 11: return eval_l

however, can be evaluated in a special way. In order to evaluate a formula in RC-RLR, starting from the end (or beginning), the effect of each literal can be calculated and then the literal can be removed from the formula. Algorithm 2 indicates how a formula corresponding to a relations chain can be evaluated. This evaluation grows with the product of the number of literals in the formula and the number of observed data which makes it highly scalable.

When l = 0, the formula corresponds to True and evaluates to 1 for any $X_0 \in x_0$. Therefore, in 258 this case the algorithm returns a vector of ones of size $|\Delta_{x_0}|$. Otherwise, the algorithm first evaluates 259 $\varphi' = \mathsf{R}_1(x_0, x_1) * \mathsf{R}_2(x_1, x_2) * \cdots * \mathsf{R}_{l-1}(x_{l-2}, x_{l-1})$ using a recursive call to the Eval function. The 260 resulting vector is stored in $eval_{l-1}$ such that for a $E' \in \Delta_{x_{l-1}}$, $eval_{l-1}[E']$ indicates the result of evaluating 261 $\varphi' = \mathsf{R}_1(x_0, x_1) * \mathsf{R}_2(x_1, x_2) * \cdots * \mathsf{R}_{l-1}(x_{l-2}, E')$. Then in order to evaluate φ for some $E \in \Delta_{x_l}$, we sum 262 $eval_{l-1}[E']$ s for any $E' \in \Delta_{x_{l-1}}$ such that $R_l(E', E)$ holds. canWalk in the algorithm is 1 if $R_l(E', E)$ 263 holds and 0 otherwise, and $eval_l(E) + eval_{l-1}(E') * canWalk(E', E)$ adds $eval_{l-1}[E']$ to $eval_l[E]$ if 264 canWalk is 1. 265

266 **PROPOSITION 1.** Algorithm 2 is correct.

PROOF. Let $\varphi = \mathsf{R}_1(x_0, x_1) * \mathsf{R}_2(x_1, x_2) * \cdots * \mathsf{R}_l(x_{l-1}, x_l) * \mathsf{eval}_l(x_l)$ ($\mathsf{eval}_l(x_l)$ can be initialized to a vector of ones at the beginning of the algorithm). Since by definition of relations chain x_l only appears in R_l and $\mathsf{eval}_l(x_l)$, for any $X_{l-1} \in \Delta_{x_{l-1}}$ we can evaluate $\mathsf{eval}_{l-1}(X_{l-1}) = \sum_{X_l \in \Delta_{x_l}} \mathsf{R}_l(X_{l-1}, X_l) * \mathsf{eval}_l(X_l)$ separately and replace $\mathsf{R}_l(x_{l-1}, x_l) * \mathsf{eval}_l(x_l)$ with $\mathsf{eval}_{l-1}(x_{l-1})$ thus getting $\varphi' = \mathsf{R}_1(x_0, x_1) * \mathsf{R}_2(x_1, x_2) *$ $\cdots * \mathsf{R}_{l-1}(x_{l-2}, x_{l-1}) * \mathsf{eval}_{l-1}(x_{l-1})$. The same procedure can compute φ' .

272 3.2 From PRA to Relation Chains

273 PROPOSITION 2. A path relation corresponds to a relations chain.

PROOF. Let $\mathcal{PR} = x_0 \xrightarrow{\mathsf{R}_1} x_1 \xrightarrow{\mathsf{R}_2} \dots \xrightarrow{\mathsf{R}_l} x_l$ be a path relation. We create a relation atom $\mathsf{R}_i(x_{i-1}, x_i)$ for any sub-path $x_{i-1} \xrightarrow{\mathsf{R}_i} x_i$ resulting in relations $\mathsf{R}_1(x_0, x_1), \mathsf{R}_2(x_1, x_2), \dots, \mathsf{R}_l(x_{l-1}, x_l)$. By definition of path relations, the second logvar of any relation R_i is the same as the first logvar of the next relation. Since by definition the logvars in a path relation are different, the second logvar of any relation R_i is only equivalent to the first logvar of the next relation. EXAMPLE 5. Consider the path relation $q \xrightarrow{\text{Publn}} y \xrightarrow{\text{Publn}^{-1}} p' \xrightarrow{\text{Cited}} p$ from Example 2. This path relation corresponds to a relations chain with atoms Publn(q, y), $\text{Publn}^{-1}(y, p')$ and Cited(p', p).

281 3.3 Row-Wise Count Normalization

Having a binary predicate V(x, y) and a set of pairs of objects for which V holds, one may consider the 282 283 importance of these pairs to be different. For instance, if a paper has cited only 20 papers, the importance of these citations may be more than the importance of citations for a paper citing 100 papers. One way to take 284 the importance of the pairs into account is to normalize the relations. A simple way to normalize a relation 285 is to normalize it by row-wise counts. For some $X \in \Delta_x$, let α represent the number of $Y' \in \Delta_u$ such 286 that V(X, Y') holds. When $\alpha \neq 0$, instead of considering V(X, Y) = 1 for a pair $\langle X, Y \rangle$, we normalize 287 it to $V(X,Y) = \frac{1}{\alpha}$. After this normalization, the citations of a paper with 20 citations are 5 times more 288 important than the citations of a paper with 100 citations overall. Note that when $\alpha = 0$, we do not change 289 any values. We refer to this normalization method as row-wise count (RWC) normalization. Fig. 1(b) show 290 the result of applying RWC normalization to the relation in Fig. 1(a). Note that there may be several other 291 ways to normalize a relation; here we introduced RWC because, as we will see in the upcoming sections, it 292 is the normalization method used in PRA. 293

294 3.4 Main Theorem

295 THEOREM 1. Any PRA model is equivalent to an RC-RLR model with RWC normalization.

PROOF. Let $\Psi = \{ \langle w_0, \mathcal{PR}_0 \rangle, \dots, \langle w_k, \mathcal{PR}_k \rangle \}$ represent a set of WPRs used by a PRA model. We 296 proved in Proposition 2 that any path relation \mathcal{PR}_i in Ψ corresponds to a relations chain. By multiplying 297 the relations in the relation chain, one gets a formula φ_i for each \mathcal{PR}_i and this formula is by construction 298 guaranteed to correspond to a relations chain. We construct an RC-RLR model whose WFs are ψ = 299 $\{\langle v_0, \varphi_0 \rangle, \dots, \langle v_k, \varphi_k \rangle\}$. Given that the relations (and their order) used in \mathcal{PR}_i and φ_i are the same for any 300 *i*, the only differences between the evaluation of \mathcal{PR}_i and φ_i according to Algorithm 1 and Algorithm 2 301 are: 1- Algorithm 1 divides $R_l(E', E)$ by $C_{R_l}(E')$ while Algorithm 2 does not, and 2- in the termination 302 condition, Algorithm 1 returns a uniform distribution over objects in Δ_{x_0} while Algorithm 2 returns a 303 vector of ones of size $|\Delta_{x_0}|$. Dividing $R_l(E', E)$ by $C_{R_l}(E')$ is equivalent to RWC normalization and the 304 difference in the constant value of the function in the termination condition gets absorbed in the weights 305 that are multiplied to each path relation or formula. Therefore, the RC-RLR model with WFs ψ is identical 306 to the PRA model with WPRs Ψ after normalizing the relations using RWC. 307

EXAMPLE 6. Consider the PRA model in Example 2. For the four WPRs in that model, we create the following corresponding WFs for an RC-RLR model by multiplying the relations in the path relations:

 $\langle v_0, \mathsf{True} \rangle$

- 310 $\langle v_1, \mathsf{Publn}(q, y_1) * \mathsf{ImBef}(y_1, y_2) * \mathsf{Publn}^{-1}(y_2, p) \rangle$
- 311 $\langle v_2, \mathsf{Publn}(q, y_1) * \mathsf{Publn}^{-1}(y_1, p') * \mathsf{Cited}(y_1, p) \rangle$

312
$$\langle v_3, \mathsf{Cited}(p_1, p_2) * \mathsf{Cited}(p_2, p) \rangle$$

Consider computing WillCite $(Q, Paper_2)$ according to an RC-RLR model with the above WFs, where all existing papers and Q have been published in 2017 and the relations have been normalized using RWC normalization (e.g., as in Fig. 1(b) for relation Cited). Then the first formula evaluates to v_0 . The second

WF evaluates to 0. The third WF evaluates to $v_2 * \frac{1}{6} * (\frac{1}{4} + \frac{1}{2})$ as the values in relation Publn⁻¹ have been normalized to $\frac{1}{6}$ for year 2017 and the values in relation Cited have been normalized to $\frac{1}{4}$ and $\frac{1}{2}$ for *Paper*₅ 316 317 and $Paper_6$ as in Fig. 1(b). The last WF evaluates to $v_3 * (\frac{1}{2} * \frac{1}{4} + \frac{1}{3} * (\frac{1}{4} + \frac{1}{2}) + \frac{1}{4} * \frac{1}{2})$. The $\frac{1}{2} * \frac{1}{4}$ comes from Cited($Paper_3$, $Paper_5$) * Cited($Paper_5$, $Paper_2$), $\frac{1}{3} * (\frac{1}{4} + \frac{1}{2})$ comes from Cited($Paper_4$, $Paper_5$) * 318 319 Cited(Paper_5, Paper_2) and Cited(Paper_4, Paper_6) * Cited(Paper_6, Paper_2) and $\frac{1}{4} * \frac{1}{2}$ comes from 320 321 $Cited(Paper_5, Paper_6) * Cited(Paper_6, Paper_2)$. As it can be viewed from Example 2, after creating the 322 equivalent RC-RLR model and normalizing the relations using RWC normalization, all WPRs evaluate to the same value as their corresponding WF, except the last WF. The $\frac{1}{6}$ before the parenthesis in Example 2 323 is missing when evaluating the last WF. This $\frac{1}{6}$, however, is a constant independent of the query (it is the 324 constant value of the uniform distribution in the if statement corresponding to the termination criteria in 325 Algorithm 1). Assuming $v_3 = w_3 * \frac{1}{6}$ and all other v_i s are the same as w_i s, the conditional probability of 326 $Cited(Q, Paper_2)$ according to the RC-RLR model above will be the same as the PRA model in Example 2. 327

328 3.5 From Random Walk Strategies to Structure Learning

The restrictions imposed on the formulae by path relations in PRA reduces the number of possible formulae to be considered in a model compared to RLR models. However, there may still be many possible path relations and considering all possible path relations for a PRA model may not be practical.

Lao and Cohen (2010b) allow the random walk to follow any path, but restrict the maximum number of steps. In particular, they only allow for path relations whose length is less than some l. The value of l can be selected based on the number of objects, relations, available hardware, and the amount of time one can afford for learning/inference. This strategy automatically gives a (very simple) structure learning algorithm for RC-RLR by considering only formulae whose number of relations are less than l.

Lao et al. (2011) follow a more sophisticated approach for limiting the number of path relations. Besides 337 limiting the maximum length of the path relations to l, Lao et al. (2011) impose two more restrictions: 338 for any path relation to be included, 1- the probability of reaching the target objects must be non-zero 339 for at least a fraction α of the training query objects, and 2- it should at least retrieve one target object 340 in the training set. During parameter learning, they impose a Laplacian prior on their weights to further 341 reduce the number of path relations. In an experiment on knowledge completion for NELL (Carlson et al., 342 2010), they show that these two restrictions plus the Laplacian prior reduce the number of possible path 343 relations by almost 99.6 and 99.99 percents when l = 3 and l = 4 respectively. Therefore, their random 344 walk strategy is capable of taking more steps (i.e. selecting a larger value for l) and capture features that 345 require longer chains of relations. This random walk strategy is called *data-driven path finding*. 346

Both restrictions in data-driven path finding can be easily verified for RC-RLR formulae and the set of possible formulae can be restricted accordingly. Furthermore, during parameter learning, a Laplacian prior can be imposed on the weights of the weighted formulae. RC-RLR models learned in this way corresponds to PRA models learned using data-driven path finding. Therefore, data-driven path finding can be also considered as a structure learning algorithm for RC-RLR. With the same reasoning, several other random walk strategies can be considered as structure learning algorithms for RC-RLR, and vice versa. This allows for faster development of the two paradigms by leveraging ideas developed in each community in the other.

4 PRA VS. RLR

An advantage of PRA models over RLR models is their efficiency: there is a smaller search space for WFs and all WFs can be evaluated efficiently. Such efficiency makes PRA scale to larger domains where models based on weighted rule learning such as RLR often have scalability issues. It also allows PRA models to
scale to and capture features that require longer chains of relations. However, the efficiency comes at the
cost of losing modelling power. In the following subsections, we discuss such costs.

359 4.1 Shortcomings of Relations Chains

Since PRA models restrict themselves to relations chains of a certain type, they lose the chance to leverage 360 many other WFs. As an example, in order to predict $Cites(p_1, p_2)$ for the reference recommendation task, 361 suppose we would like to recommend papers published a year before the target paper that have been cited 362 by the papers published in the same year as the target paper. Such a feature requires the following formula: 363 $\mathsf{Publn}(p_1, y) * \mathsf{Before}(y, y') * \mathsf{Publn}(p_2, y') * \mathsf{Cites}(p', p_2) * \mathsf{Publn}(p', y)$. It is straightforward to verify that 364 this formula cannot be included in RC-RLR (and consequently in PRA) as p_2 (the second logvar of the 365 target atom) is appearing twice in the formula, thus violating the last condition in Definition 3. While 366 restricting the formulae to the ones that correspond to relations chain may speed up learning and reasoning, 367 it reduces the space of features that can be included in a relational learning model, thus potentially 368 decreasing accuracy. 369

370 4.2 Non-binary Atoms

371 One issue with PRA models is the difficulty in including unary atoms in such models. As an example, suppose in Example 2 we would like to treat conference papers and journal papers differently. For an 372 373 RLR model, this can be easily done by including Conference(p) or Journal(p) as an extra atom in the 374 formulae. For PRA, however, this cannot be done. The way unary atoms are currently handled in PRA models is through isA and isA⁻¹ relations (Lao et al., 2011). For instance, a path relation may contain 375 paper \xrightarrow{isA} type, but the only next predicate that can be applied to this path is isA^{-1} giving the other papers 376 with the same type as the paper in the left of the arrow. This is, however, limiting and does not allow for, 377 e.g., treating conference and journal papers differently. 378

Atoms with more than two logvars are another issue for PRA models since they restrict their models to binary atoms. While any relation with more than two arguments can be converted into several binary atoms, the random walk strategies used for PRA models (and the probabilities for making these random steps) make it unclear how atoms with more than two logvars can be leveraged in PRA models.

383 4.3 Continuous Atoms

For any sub-path $x \xrightarrow{\mathsf{R}} y$ in a path relation of a PRA model, R typically has a range $\{0,1\}$: for any 384 object $X \in \Delta_x$, this sub-path gives the objects in Δ_y participating in relation R with X. PRA models can 385 be extended to handle some forms of continuous atoms. For instance for the reference recommendation 386 problem, suppose we have an atom Sim(p, p') indicating a measure of similarity between the titles of two 387 papers. The higher the Sim(p, p'), the more similar the titles of the two papers. A sensible WF for an RLR 388 model predicting Cites (p_1, p_2) may be Sim $(p_1, p') *$ Cites (p', p_2) . In order to extend PRA models to be able 389 to leverage such continuous atoms, one has to change line 8 in Algorithm 1 to sum the values of $R_l(E', E)$ 390 391 instead of counting how many times the relation holds.

For many types of continuous atoms, however, it is not straightforward to extend PRA models to leverage them. As an example, suppose we have an atom Temperature(r, d) showing the temperature of a region in a specific date. It is not clear how a random walk step can be made based on this atom as the temperature can, e.g., be positive or negative.

396 4.4 Relational Normalization

Normalizing the relations is often ignored in models based on weighted rule learning. For the most part, this ignorance may be because several of these models cannot handle continuous atoms. Given that PRA is a special form of weighted rule learning models such as RLR with RWC normalization, not normalizing the relations may be the reason why in Lao et al. (2011)'s experiments, PRA outperforms the weighted rule learning method FOIL (Quinlan, 1990) for link prediction in NELL (Carlson et al., 2010).

402 The type of normalization used in PRA (RWC) may not be the best option in many applications. As an example, suppose for the reference recommendation task we want to find papers similar to the query 403 paper in terms of the words they use. Let $Contains^{-1}(w, p)$ show the relation for words in each paper. It 404 is well-known in information retrieval that words do not have equal importances and a normalization of 405 Contains⁻¹(w, p) is necessary to take such importance into account. PRA models consider the importance 406 of each word W as $Score_1(W) = \frac{1}{f(W)}$, where f(W) is the number of papers containing the word W 407 (see e.g., (Lao and Cohen, 2010b)). However, it has been well-known in information retrieval community 408 for several decades, and information theoretically justified more than a decade ago (Robertson, 2004), 409 that $Score_2(W) = log(\frac{\#papers}{f(W)})$ provides a better importance score. Most TF-IDF (Salton and Buckley, 410 1988) based information retrieval algorithms currently rely on $Score_2$. It is straightforward to include 411 the latter score in an RLR model: one only has to multiply the formulae using word information by 412 $Score_2(W)$, without normalizing the Contains⁻¹(w, p) relation (see, e.g., (Fatemi, 2017)). However, it is 413 not straightforward how such a score can be incorporated into PRA models as they do not include unary or 414 continuous atoms. 415

416 4.5 Evaluating Formulae

Evaluating the formulae in models based on weighted rule learning is known to be expensive, especially for relations with lower sparsities and for longer formulae. In practice, approximations are typically used for scaling the evaluations. Since formulae in RC-RLR correspond to path relations, these formulae can be approximated efficiently using sampling techniques developed within graph random walk community such as fingerprinting (Fogaras et al., 2005; Lao and Cohen, 2010a), weighted particle filtering (Lao and Cohen, 2010a), and low-variance sampling (Lao et al., 2011), without noticeably affecting the accuracy. Extending sampling ideas to other formulae is an interesting future direction.

5 CONCLUSION

424 With abundance of relational and graph data, statistical relational learning has gained great amounts of 425 attention. Three main relational learning paradigms have been developed during the past decade and more: 426 weighted rule learning, graph random walk, and tensor factorization. These paradigms have been mostly 427 developed and studied in isolation with few works aiming at understanding the relationship among them or combining them. In this paper, we studied the relationship between two relational learning paradigms: 428 weighted rule learning and graph random walk. In particular, we studied the relationship between relational 429 430 logistic regression (RLR), one of the recent developments in weighted rule learning paradigm, and path 431 ranking algorithm (PRA), one of the most well-known algorithms in graph random walk paradigm. Our main contribution was to prove that PRA models correspond to a subset of RLR models after row-wise 432 433 count normalization. We discussed the advantages this proof provides for both paradigms as well as for 434 statistical relational AI community in general. Our result sheds light on several issues with both paradigms and possible ways to improve them. 435

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