Inference, Learning, and Population Size: Projectivity for SRL Models

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Abstract
A subtle difference between propositional and relational data is that in many relational models, marginal probabilities depend on the population or domain size. This paper connects the dependence on population size to the classic notion of projectivity from statistical theory: Projectivity implies that relational predictions are robust with respect to changes in domain size. We discuss projectivity for a number of common SRL systems, and identify syntactic fragments that are guaranteed to yield projective models. The syntactic conditions are restrictive, which suggests that projectivity is difficult to achieve in SRL, and care must be taken when working with different domain sizes.

1 Introduction
In propositional or i.i.d. data, marginal probabilities are independent of the number of entities for which data are available. For example, if we start with a test set of 100 data points with fully observed attributes, and we are told that another 1,000 test cases are available, this information does not change a model’s predictions on the original 100, because all data points are independent. Several authors have observed that for relational data, this is not true (Lauritzen, Rinaldo, and Sadeghi 2017; Shalizi and Rinaldo 2013; Poole et al. 2014; Jain, Barthels, and Beetz 2010): additional entities, or nodes in a network, are potentially related, and therefore their mere presence can be inferentially relevant.

The dependence on domain size raises several difficulties. (1) Counter-intuitiveness: if we are interested in making predictions about the 100 members of a Facebook group, learning that Facebook has gained another 1,000 users in the last hour should not change our predictions about the group of interest, unless we have specific information about the new users. (2) Complexity of Inference: We typically learn from fairly large networks and apply the results of learning to draw inferences about relatively small sub-networks. If the presence of other nodes is relevant to the marginal probabilities associated with the sub-network of interest, inference becomes computationally challenging, as it involves a large summation over the possible states of many nodes outside the sub-network. (3) Complexity of Learning: The observed network for learning is typically embedded in a much larger network. If marginal predictions of the observed sub-network depend on the size of the embedding network, learning should not treat the sub-network as a closed world to be analyzed in isolation.

Our aim in this paper is to connect dependence on domain size with the classic concept of projectivity from statistical theory (Shalizi and Rinaldo 2013). An SRL model typically defines a family of probability distributions over relational structures, one for each domain size $n$. Projectivity requires that the distribution for size $m$ agrees with the marginal distribution obtained from any large domain $n > m$. This ensures that the distributions for different domain sizes are consistent with each other, and that predictions about a sub-network do not depend on the presence of outside nodes.

Most (if not all) SRL modeling frameworks support the construction of non-projective models, and in many cases, this is an important source of model expressivity. However, taking into consideration the significant benefits in terms of computational complexity and robustness of inference and learning results, it is worthwhile to explore projective fragments of SRL languages. After establishing the formal framework for defining and analyzing projectivity in an SRL context (Sections 2,3), we identify syntactic constraints for three prototypical SRL frameworks that ensure projectivity (Section 4). We finally take a closer look at how projectivity can justify maximum likelihood learning from observed sub-networks (Section 6).

Related Work. Several SRL works have addressed changing domain sizes. Poole et al. discuss the impact of domain size and inference 2014. Convergence of inference (Jaeger 1998) and learning (Xiang and Neville 2011) in the domain size limit has been investigated. Kuzelka et al. discuss the validity of learning from a sub-network embedded in a larger network. They focus on models that satisfy a given set of marginal probabilities, not projectivity. Statisticians have examined the projectivity of network models from the exponential family (Shalizi and Rinaldo 2013; Lauritzen, Rinaldo, and Sadeghi 2017), but have not considered other SRL models.
2 Background

The following definitions provide a framework for talking about SRL systems in general.

A relational signature $S$ contains relation symbols of varying arities. We write $r/k$ for a relation $r$ of arity $k \geq 0$. A possible world $\omega$ (for $S$) is given by a finite domain $D = \{a_1, \ldots, a_n\}$ on which extensions of the relations in $S$ are defined. We then refer to $n$ as the size of $\omega$. Moreover, we generally assume that $D = \{0, \ldots, n - 1\} =: [n]$. Then $\Omega(S,n)$ denotes the set of all possible worlds for the signature $S$ over the domain $[n]$. This can be abbreviated as $\Omega(n)$ when the signature is understood from the context.

$\omega \in \Omega(n)$ can also be identified with a truth value assignment

$$\omega : r(i) \mapsto \{\text{true}, \text{false}\}$$

for all ground atoms $r(i)$, where $r/k \in S$ and $i = (i_1, \ldots, i_k) \in [n]^k$.

We denote with $\Delta \Omega(n)$ the set of all probability distributions on $\Omega(n)$. A random relational structure model (rrsm) is a family of distributions $\{Q^{(n)}(\omega) : \omega \in \Delta \Omega(n)\}$. The term RRSM, which was first introduced in (Jaeger 2002), is intended to emphasize that this is a multi-relational generalization of the classical concept of random graph models (or random networks (Lauritzen, Rinaldo, and Sadegh 2017)).

For this paper we limit ourselves to the consideration of exchangeable RRSMs: a single distribution $Q^{(n)}$ is exchangeable, if $Q^{(n)}(\omega) = Q^{(n)}(\omega')$ whenever $\omega$ and $\omega'$ are isomorphic. An RRSM is exchangeable, when all $Q^{(n)}$ $(n \in \mathbb{N})$ are exchangeable. Exchangeability of $Q^{(n)}$ implies that $Q^{(n)}(r(i) = \text{true}) = Q^{(n)}(r(j) = \text{true})$ when $j = \pi(i)$ for some permutation $\pi$ of $[n]$.

RRSMs defined by typical SRL frameworks are necessarily exchangeable when the model specification does not make use of any constants referring to specific domain elements, and is not conditioned on a pre-defined structure on the domain. Examples of RRSMs that do not satisfy this condition are temporal models such as hidden Markov models, where the model is conditioned on a linear ordering $0 < 1 < \cdots < n - 1$ of the domain, and the marginal distributions at different timepoints $t \neq t'$ are usually different.

SRL Systems

In this section we briefly review three different SRL frameworks that can be used to define RRSMs. We do not give complete definitions of syntax and semantics for these frameworks here, but only describe their main characteristics by way of examples. The selected systems are representatives for three distinct modeling paradigms.

Relational Bayesian Networks Relational Bayesian networks (RBNs) (Jaeger 1997) are a representative of frameworks that are closely linked to directed graphical models. Other approaches in this group include probabilistic relational models (Friedman et al. 1999), Bayesian logic programs (Kersting, De Raedt, and Kramer 2000) and relational logistic regression (Kazemi et al. 2014).

An RBN associates with each relation $r \in S$ a functional expression that defines the probabilities of ground atoms $r(i)$ conditional on other ground atoms. Functional expressions can be formed by combining and nesting basic constructs, which support Boolean conditions, mixtures of distributions, and aggregation of dependencies using the central tool of combination functions.

For example, the two formulas

$$\begin{align*}
\text{red}(X) & \leftarrow 0.3 \\
\text{black}(X) & \leftarrow \text{if red}(X) : 0 \text{ else } : 0.5
\end{align*}$$

define Boolean attributes $\text{red}$ and $\text{black}$, such that no element can be both $\text{red}$ and $\text{black}$. One can then condition a binary edge relation on the colors of the nodes:

$$\begin{align*}
\text{edge}(X, Y) & \leftarrow \text{if red}(X) \& \text{red}(Y) : 0.7 \\
& \text{ else if black}(X) \& \text{black}(Y) : 0.4 \\
& \text{ else } : 0.05
\end{align*}$$

Together, the three formulas for $\text{red}$, $\text{black}$ and $\text{edge}$ represent a simple stochastic block model (Snijders and Nowicki 1997). The main expressive power of RBNs derives from combination functions that can condition a ground atom on properties of other domain entities:

$$t(X) \leftarrow \text{noisy-or}\{\text{if edge}(X, Y) \& \text{red}(Y) : 0.2 | Y\}$$

This formula makes the probability of the attribute $t$ for $X$ dependent on the number of $\text{red}$ entities $Y$ that $X$ is connected to via an $\text{edge}$. Each such entity causes $t(X)$ to be true with probability 0.2, and the different causes $Y$ are modeled as independent via the noisy-or combination function.

An RBN specification defines an RRSM, provided that for each $n$ the formulas induce an acyclic dependency structure on the atoms of $\Omega(S,n)$. The distribution $Q^{(n)}$ can then be represented by a Bayesian network whose nodes are the ground atoms $r(i)$, and where $r'(i')$ is a parent of $r(i)$, if the truth value of $r'(i')$ is needed to evaluate the probability formula for $r(i)$.

Markov Logic Networks Markov Logic networks (MLNs) (Richardson and Domingos 2006) are the multi-relational generalization of exponential random graph models (Frank and Strauss 1986). A MLN consists of a set of weighted formulas. As an example, let $S = \{\text{red}/1, \text{edge}/2\}$, and define the following two weighted formulas:

$$\begin{align*}
\phi_1(X, Y) & := \text{edge}(X, Y) \& \text{red}(X) \& \text{red}(Y) \\
\phi_2(X, Y) & := \text{edge}(X, Y) \& \text{red}(X) \& \neg \text{red}(Y)
\end{align*}$$

These two weighted formulas represent a homophily model for the $\text{red}$ attribute in a graph. Each pair $\{i, j\} \in [n]^2$ contributes a weight of $1.2 (-0.2)$ to a possible world $\omega \in \Omega(S,n)$ if $\phi_1(i, j) \& (\phi_2(i, j))$ is true in $\omega$. The probability $Q^{(n)}(\omega)$ then is the normalized sum of all weights contributed by all the weighted formulas, and all possible substitutions of domain elements for the variables in the formulas.
$Q^{(n)}$ can be represented by a Markov network whose nodes are the ground atoms $r(i)$, and where two atoms $r(i), r'(j)$ are connected by an edge if these two atoms appear jointly in a grounding of one of the weighted formulas.

**ProbLog** ProbLog (De Raedt, Kimmig, and Toivonen 2007) [Kimmig et al. 2011] is a representative of RRSMs that are closely linked to logic programming. Other frameworks in this class are Prism (Sato 1995) and independent choice logic (Poole 2008). A ProbLog model consists of a set of labeled facts, which are atoms with a probability label attached:

$$0.8 :: \text{red}(X) \quad (1)$$

together with background knowledge consisting of (non-probabilistic) definite clauses:

$$\text{edge}(X, Y) : - \text{red}(X), \text{red}(Y). \quad (2)$$

We note that (Kimmig et al. 2011) emphasize the use of ground atoms in the labeled facts. Since our interest is with generic, domain-independent RRSMs, we restrict attention to ProbLog models that do not contain domain constants.

The ProbLog model consisting of (1) and (2) defines the background knowledge become applicable. In our example, we can add a new relation rule2, an additional labeled fact

$$0.5 :: \text{rule}(X, Y), \quad (3)$$

and modify the background knowledge to

$$\text{edge}(X, Y) : - \text{red}(X), \text{red}(Y), \text{rule}(X, Y). \quad (4)$$

Now the resulting ProbLog model is a (partial) stochastic block model, where with probability 0.5 two red nodes are connected by an edge (and still no other than pairs of red nodes could be connected; further labeled facts and rules can be added to also model connections between non-red nodes).

## 3 Projectivity

For $Q^{(n)} \in \Delta \Omega^{(n)}$ and a subset $\{i_0, \ldots, i_{m-1}\} \subseteq [n]$ we denote with $Q^{(n)} \downarrow \{i_0, \ldots, i_{m-1}\}$ the marginal distribution on the sub-structures induced by $\{i_0, \ldots, i_{m-1}\}$, or, equivalently, the marginal distribution on the ground atoms $r(i)$ with $i \in \{i_0, \ldots, i_{m-1}\}^k$. When $Q^{(n)}$ is exchangeable, then the induced distribution is independent of the actual choice of the elements $i_h$, and we may assume that $\{i_0, \ldots, i_{m-1}\} = \{0, \ldots, m-1\}$. We therefore can limit attention to the marginalizations

$$Q^{(n)} \downarrow \{m\} \in \Delta \Omega^{(m)}. \quad (5)$$

Based on (Shalizi and Rinaldo 2013) we define several different versions of “projectivity” for probabilistic relational models. Our definitions are more restricted than the one given by Shalizi and Rinaldo (2013) in that we specifically tailor the definitions to random relational structure models. For convenience, we also include the condition of exchangeability in the following definitions, even though exchangeability and projectivity are not necessarily linked.

**Definition 3.1** A RRSM is projective, if
- every $Q^{(n)}$ is exchangeable
- for every $n$, every $m < n$: $Q^{(n)} \downarrow \{m\} = Q^{(m)}$.

**Example 3.2** A simple classical example for a projective RRSM is the Erdős-Rényi random graph model with edge probability $p$, where $S = \{e/2\}$, and for $\omega \in \Omega^{(n)}$:

$$Q^{(n)}(\omega) = p^{|e(\omega)|}(1 - p)^{n^2 - |e(\omega)|},$$

where $|e(\omega)|$ denotes the number of edges in $\omega$.

An example of a very different nature is the RRSM where for every $n$:

$$Q^{(n)} = \frac{1}{2} I_{K_n} + \frac{1}{2} I_{E_n} \quad (6)$$

where $K_n$ is the complete and $E_n$ the empty graph over $n$, and $I_{\omega}$ denotes the distribution that assigns probability one to $\omega$.

Not projective are sparse random graph models, where the edge probability is a decreasing function of the domain size $n$, e.g., $Q^{(n)}(e(i,j)) = \theta/n$ for some parameter $\theta$.

Definition 3.1 relates to a single RRSM. In the context of learning, we are initially only given a space of candidate models. The models in this space are typically characterized by a structural component, and a set of numerical parameters. In the following, we assume that the learning problem only consists of optimizing over a fixed set of numerical parameters, i.e., structure learning is outside the scope of our considerations.

Concretely, let $\Theta \subseteq \mathbb{R}^k$ be a parameter space, so that each $\theta \in \Theta$ defines a distribution $Q^{(n)}_{\theta} \in \Delta \Omega^{(n)}$. Then $\{Q^{(n)}_{\theta} \mid \theta \in \Theta, n \in \mathbb{N}\}$ is a parametric family of RRSMs.

This leads to the following definition of projectivity, which is essentially the one of (Shalizi and Rinaldo 2013).

**Definition 3.3** A parametric family of RRSMs is projective, if $\{Q^{(n)}_{\theta} \mid n \in \mathbb{N}\}$ is projective for every $\theta \in \Theta$.

We can weaken this as follows:

**Definition 3.4** A parametric family of rmss is structurally projective if
- every $Q^{(n)}_{\theta}$ is exchangeable
- for every $n$, $\theta$, and $m < n$: there exists $\theta' \in \Theta$ such that $Q^{(n)}_{\theta} \downarrow \{m\} = Q^{(m)}_{\theta'}$.

This concept of structural projectivity corresponds to weak consistency in the sense of (Lauritzen, Rinaldo, and Sadeghi 2017) restricted to exchangeable distributions.

An example for structurally projective models are sparse random graph models with edge probabilities $\theta/n$: here we then have $Q^{(n)}_{\theta} \downarrow I = Q^{(m)}_{\theta'}$ with $\theta' = \theta m / n$.
Example 3.5 MLNs are not structurally projective: consider the MLN
\[ a(X), e(X, Y) \quad w \]

defining probability distributions \( Q_w^{(a)} \) depending on the weight parameter \( w \). Consider the conditional probability
\[
q(n, w) := Q_w^{(a)}(a(0)|\neg e(0, 0), \neg e(0, 1), \neg e(1, 0), \neg e(1, 1)).
\]

(7)

If \( w > 0 \), then \( q(n, w) \) is increasing in \( n \) (and in \( w \)). However, for \( n = 2 \), we have \( q(n, w) = 1/2 \), regardless of the value of \( w \). Thus, for a suitable combination of \( n, w \) where \( q(n, w) > 1/2 \), we cannot find a value \( w' \) such that \( Q_w^{(a)}[2] = Q_w^{(2)} \).

The lack of structural projectivity sets some limits to the approach of defining the weights in an MLN as functions of the domain size \( n \) (Jain, Barthels, and Beetz 2010) in order to compensate for the domain dependence of the model.

Example 3.6 RBNs are not structurally projective: similarly to Example 3.5 we can construct a counterexample as follows. Consider the RBN
\[
\text{edge}(X, Y) \leftarrow 0.5
\]
\[
a(X) \leftarrow \text{noisy-or} \{i \mid \text{edge}(X, Y) : \theta \mid Y \}
\]

defines probability distributions \( Q_{\phi}^{(a)} \) depending on the probability parameter \( \theta \). Defining \( q(n, \theta) \) as in (7), we obtain that \( q(2, \theta) = 0 \), regardless of \( \theta \), but \( q(n, \theta) > 0 \) for \( n \geq 3 \) and \( \theta > 0 \).

4 Projective Fragments of SRL Systems

In this section we identify for the three representative SRL frameworks introduced in Section 2 restrictions on model structure that give rise to projective models.

For the propositions stated in this section we give short proof sketches. Full proofs would need to refer to complete formal specifications of syntax and semantics of the various frameworks, which we have omitted in Section 2. Even the proof sketches we provide may appeal to some facts about the individual frameworks that were not explicitly spelled out in Section 2.

Proposition 4.1 An RBN defines a projective RRSM if it does not contain any combination functions.

Proof: [Sketch] Consider the Bayesian network representation \( B^{(n)} \) of \( Q^{(a)} \), and a parent child pair \( r'(i') \rightarrow r(i) \) in \( B^{(n)} \). If the probability for the relation \( r \) is defined without the use of combination functions, then all constants appearing in \( i' \) must also be contained in \( i \). This implies that the sub-network for the ground atoms over \([m]\) \((m \leq n)\) is an upward-closed sub-graph of \( B^{(n)} \) whose structure and probability parameters do not depend on \( n \). This means that the marginal distributions on the ground atoms over \([m]\) does not depend on \( n \).

Even though combination functions are the main source for the expressive power of RBNs, one can still encode some relevant models with the combination function free fragment. One example are the stochastic block models as shown in Section 2. Another example are temporal models such as dynamic Bayesian networks or hidden Markov models. However, as mentioned in Section 2 these models are not exchangeable, and therefore outside the scope of this paper.

Proposition 4.2 An MLN defines a projective RRSM if its formulas \( \phi_i \) satisfy the property that any two atoms appearing in \( \phi_i \) contain exactly the same variables.

Proof: [Sketch] If the condition of the proposition holds, then the Markov network representation \( M^{(n)} \) of \( Q^{(a)} \) decomposes into a system of disconnected sub-networks, where each sub-network contains ground atoms over a fixed set of domain elements, with a cardinality at most equal to the maximal arity of any \( r \in S \). The structure and parameterization of sub-networks containing only the atoms for domain elements from \([m]\) \((m \leq n)\) are the same for all \( n \), and they define a marginal distribution that is independent of the nodes contained in the other sub-networks, i.e., independent of \( n \).

Alternatively, Proposition 4.2 can also be proven by an application of Theorem 1 of (Shalizi and Rinaldo 2013). Our MLN example from Section 2 does not satisfy the restriction of Proposition 4.2. A somewhat synthetic example that satisfies the condition is
\[
\begin{align*}
\text{red}(X) \land \text{edge}(X, X) & \quad -1.5 \\
\text{edge}(X, Y) \land \text{edge}(Y, X) & \quad 0.8
\end{align*}
\]

This MLN represents a model according to which red nodes are unlikely to have self-loops, and the edge relation tends to be symmetric. It is an open question whether our projective MLN fragment contains more natural and practically relevant classes of models.

Proposition 4.3 A ProbLog model defines a projective RRSM, if all the background knowledge clauses satisfy the property that the body of the clause does not contain any variables that are not contained in the head of the clause.

Proof: [Sketch] If the stated property holds, then a proof for a ground atom \( r(i) \) can only contain ground atoms \( r'(i') \) with \( i' \subseteq i \). The probability that \( r(i) \) is provable when \( i \subseteq [m] \) then only depends on the probabilities of ground labeled facts with arguments from \([m]\). The joint distribution of these ground facts is independent of \( n \).

The ProbLog example of Section 2 satisfies the condition of Proposition 4.3.

Discussion

Our conditions for the projective RBN and ProbLog structures are very similar, and it seems that both fragments support more or less the same types of models. The projectivity conditions are essentially limitations on probabilistic dependencies. For the frameworks that (implicitly) encode a directed sampling process for possible worlds (RBN, ProbLog), the limit on the dependency is that when a
ground atom \( r(i) \) is sampled, its distribution cannot depend on ground atoms containing elements other than included in \( i \). However, \( r(i) \), in turn, may influence the sampling probabilities of other atoms containing elements not in \( i \). As a consequence, both in the RBN and the ProbLog model of Section \( 2 \) the value of \( r(i) \) influences the probability for \( \text{edge}(i, j) \), and as a result, the two variables \( r(i), \text{edge}(i, j) \) are not independent.

Due to the undirected nature of MLNs, one there cannot impose an “upstream only” limitation on probabilistic dependencies. As a result, the restriction imposed in Proposition \( 4.2 \) implies that when a model defines two random variables \( r(i), \text{edge}(i, j) \) \((i ≠ j)\), these must be independent.

5 Projectivity and Inference
In an inference scenario, we are given an RRSM \( \{Q(n) \mid n ∈ \mathbb{N}\} \), a domain of size \( n \), and a query, for which the sake of concreteness we assume to be of the form

\[
P(r(i) \mid (−)r_1(i_1), \ldots, (−)r_h(i_h)) = ?,
\]

where the \((−)r_j(i_j)\) are observed evidence literals. Let \( I := \cup_{j=1}^h i_j \), and \( m := |I| \). To answer the query, all we need is the marginal distribution \( Q^{(n)} \bigg| I \). If the model is projective, then this marginal is equivalent to \( Q^{(m)} \), and independent of \( n \). In practice this means, that when inference is performed by grounding the relational model over a concrete domain, that we here only need to ground the model over the domain that contains exactly the entities mentioned in the query.

Apart from the clear computational advantages that projectivity affords, it also leads to robustness with regard to domains that are only incompletely known or observed: in many cases it can be difficult to specify exactly the size of the domain in which our observed entities \( I \) “live”. (what is the domain of a person’s social network?)? Here projectivity means that our inferences are not impacted by missing or imprecise information about the domain.

6 Projectivity and Learning
In a learning setting, we are interested in estimating the parameter \( θ \) for a given parametric family of RRSMs. We assume that the training data consists of one or several observed possible worlds, in the latter case possibly worlds of varying sizes. Like [Xiang and Neville 2011] and [Kuzelka et al. 2018] we mostly focus on the scenario where the training data consists of a single possible world \( ω ∈ Ω^{(m)} \), and we estimate \( θ \) by maximizing the likelihood

\[
L(θ|ω) = Q_θ^{(m)}(ω).
\]

For simplicity we here restrict attention to pure maximum likelihood inference, but our considerations are also pertinent for penalized likelihood or Bayesian inference approaches.

For this learning problems, too, the dependence on the domain size \( n \) is an important concern. Consider, for example, the problem of learning a model for an evolving (social) network. Is the model we learn today, while the network is of size \( m \), still a good model when the network has evolved to size \( n > m \)? Moreover, the data from which we learn may not be complete, and not contain the data about all the entities that are actually present in the relational domain. Then we try to learn a model for a domain of size \( n \), from data corresponding to a domain of smaller size \( m < n \) [Kuzelka et al. 2018].

The general question we want to address, therefore, is the following: let \( θ^* ∈ Θ \) be the parameter estimate we obtain by maximizing \( Q_θ^{(n)} \) for some \( ω ∈ Ω^{(m)} \). Let \( ω' ∈ Ω^{(n)} \) such that \( ω' ↓ I = ω \) for some \( I ⊂ [n] \) of size \( m \), and \( θ^{**} \) the estimate obtained by maximizing \( Q_θ^{(n)}(ω') \). What can we say about the relationship between \( θ^* \) and \( θ^{**} \)?

To obtain more precise statements of this overall question, we first consider the scenario where we do not know \( ω' \), but we do know \( ω' \)'s size \( n \). Then, given the partial observation \( ω \), we can maximize likelihood in the appropriate space \( \{Q_θ^{(n)} \mid θ ∈ Θ\} \) via the marginal likelihood function

\[
ML^{(n)}(θ|ω) := Q_θ^{(n)}(\{ω' ∈ Ω^{(n)} : ω' ↓ [m] = ω\}) \tag{9}
\]

The following then is immediate:

**Proposition 6.1** If the parametric family \( \{Q_θ^{(n)} \mid θ ∈ Θ, n ∈ \mathbb{N}\} \) is projective, then the likelihood functions \( Q_θ^{(n)} \) and \( Q_θ^{(m)} \) are identical.

Even in the context of a projective family, however, learning from \( ω \) that is a sub-sample of the “true” world \( ω' \), usually is problematic: the use of the marginal likelihood function \( Q_θ^{(n)} \) only is justified, when the data in \( ω \) is *missing at random* [Rubin 1976]. This will be the case when \( ω \) is the induced sub-structure of \( ω' \) uniformly, randomly selected elements from the domain \([n]\) of \( ω' \) (induced subgraph sampling [Kolaczyk 2009] Chapter 5). However, a more realistic scenario for observing a substructure of a possible world \( ω' \) is by mechanisms such as traceroute or snowball sampling [Kolaczyk 2009] Chapter 5). When \( ω \) is observed through such a mechanism, then \( Q_θ^{(n)} \) is not an appropriate likelihood function.

**Projectivity and Maximum Likelihood Learning**
In the following, we make the idealized assumption that \( ω ∈ Ω^{(m)} \) was observed through induced subgraph sampling from a larger world \( ω' ∈ Ω^{(n)} \). In conjunction with projectivity, the use of \( Q_θ^{(n)} \) then is justified, giving us the parameter estimate \( θ^* \). Can we derive some guarantees for the quality of \( θ^* \) as an approximation of the estimate \( θ^{**} \) one would obtain by maximizing \( Q_θ^{(n)}(ω') \)?

Clearly, for any specific pair \( ω, ω' \), no guarantees can be given, because \( ω \) could be a very un-representative substructure of \( ω' \). We therefore can only ask whether such guarantees can be given in expectation, where expectation is with respect to induced subgraph sampling of \( ω \) from \( ω' \).

This question still has two distinct precise formalizations, expressed by the following two equalities:

\[
E_ω[\arg \max_θ \log L^{(m)}(θ|ω)] = \arg \max_θ \log L^{(n)}(θ|ω') \tag{10}
\]
\[
\arg \max_θ E_ω[\log L^{(m)}(θ|ω)] = \arg \max_θ \log L^{(n)}(θ|ω') \tag{11}
\]
We here turn to the log-likelihood, because the expectation in the left-hand side expression of (11) is more meaningful when applied to the log-likelihood. For all other expressions in (10) and (11) the application of the log makes no difference. In cases where the log-likelihood functions need not have a unique maximum, the \( \arg \max_\theta \) should be read as returning the set of all maxima.

Condition (10) basically says that estimating \( \theta \) from an \( m \)-element induced substructure of \( \omega' \) is an unbiased estimator for the estimate one would have obtained from \( \omega' \). Condition (11) essentially expresses a statistical consistency property: if one takes repeated size \( m \) samples \( \omega_1, \ldots, \omega_N \), and maximizes the sample log-likelihood \( \frac{1}{N} \sum_{i=1}^{N} \log L^{(m)}(\theta|\omega_i) \) then, for large \( N \), this will become equivalent to maximizing \( L^{(n)}(\theta|\omega') \). We note though, that (11) alone does not directly guarantee this consistency. Additional regularity conditions on the likelihood function will be needed.

The following is a cautionary example that shows that even for projective models, neither (10) nor (11) need hold.

**Example 6.2** Consider the following RBN:

\[
\begin{align*}
\text{red}(X) & \leftarrow \theta \quad (12) \\
\text{edge}(X, Y) & \leftarrow \theta \quad (13)
\end{align*}
\]

In this RBN there is a common parameter \( \theta \) that denotes both the probability for the attribute \( a/1 \), and the edge relation \( \text{edge}/2 \). This form of parameter sharing by different probability formulas is supported by RBNs and their learning tools, even though it seems to be of limited use in practice. This RBN clearly is projective.

Now consider the possible world \( \omega' \in \Omega^{(n)} \) where \( a(i) \) is true for \( i = 0, \ldots, n/2 \), and false for \( i = n/2, \ldots, n-1 \), and where \( \text{edge}(i, j) \) is false for all \( i, j \). Let \( m = 2 \). A random \( \omega \in \Omega^{(2)} \) drawn from \( \omega' \) then is with equal probability one of the 4 worlds with \( (0,0), (1,1), (0,1), (1,0) \) and no edges. Writing \( l \theta \) for \( \log \theta \), and \( l \bar{\theta} \) for \( \log(1 - \theta) \), we obtain the expected log-likelihood:

\[
E_\omega [\log L^{(2)}(\theta|\omega)] = \frac{1}{4} ((4l \bar{\theta} + 2l \theta) + 2(4l \bar{\bar{\theta}} + l \theta + l \bar{\theta}) + (4l \bar{\bar{\bar{\theta}}} + 2l \bar{\theta}))
\]

where the recurring first term \( 4l \bar{\theta} \) accounts for the absence of the four possible edges (including possible self-loops) in all possible sampled worlds. Maximizing this gives

\[
\theta^* = \arg \max_\theta E_\omega [\log L^{(2)}(\theta|\omega)] = 1/6.
\]

The log-likelihood function induced by \( \omega' \) is

\[
\log L^{(n)}(\theta|\omega') = n^2 l \bar{\theta} + (n/2) l \theta + (n/2) l \bar{\theta}
\]

which is maximized by

\[
\theta^{**} = \arg \max_\theta \log L^{(n)}(\theta|\omega') = \frac{n/2}{n^2 + n} = \frac{1}{2(n+1)}
\]

Thus, (11) does not hold. We also compute

\[
E_\omega [\arg \max_\theta \log L^{(2)}(\theta|\omega)] = \frac{1}{4} \left( \frac{1}{3} + \frac{1}{6} + \frac{1}{6} + 0 \right) = \frac{1}{6},
\]

and see that (10) also fails (in general, other than in this example, the left-hand sides of (10) and (11) need not be identical).

Finally, now suppose that the two formulas (12) and (13) each are defined by distinct parameters \( \theta_1 \) and \( \theta_2 \) respectively. Then the likelihood function (14) becomes

\[
\frac{1}{4}l((4l \bar{\theta}_1 + 2l \theta_1) + 2(4l \bar{\bar{\theta}}_2 + l \theta_1 + l \bar{\theta}_1) + (4l \bar{\bar{\bar{\theta}}} + 2l \bar{\theta}_1)),
\]

and (15) turns into

\[
n^2 l \bar{\theta}_1 + (n/2) l \theta_1 + (n/2) l \bar{\theta}_1,
\]

both of which are maximized by \( \theta_1 = 0 \) and \( \theta_1 = 1/2 \).

We now proceed to establish conditions under which (11) is guaranteed to hold. We first restrict attention to models where the sufficient statistics for \( Q^{(n)}_\theta(\omega) \) are given by induced substructure counts, defined next.

**Definition 6.3** Let \( \omega \in \Omega^{(n)} \) and \( k \leq n \). Let \( \tilde{\omega} \in \Omega^{(k)} \). The ordered substructure count of \( \tilde{\omega} \) in \( \omega \) is defined as

\[
| \{ i : \omega \downarrow i \equiv \tilde{\omega} \}_i | := C_{\omega}(\tilde{\omega})
\]

where

- \( i = (i_0, \ldots, i_{k-1}) \) ranges over the \( \frac{n!}{(n-k)!} \) tuples of \( k \) distinct elements from \([n]\)
- \( \omega \downarrow i \) is the sub-structure induced by \( i \) in \( \omega \)
- \( \equiv \) stands for isomorphism under the mapping \( i_j \mapsto j \)

We refer to this as ordered substructure count, because it corresponds to taking an ordered sample of \( k \) elements from \( \omega \), and matching the induced substructure against \( \tilde{\omega} \) under the unique mapping \( i_j \mapsto j \) defined by the order of \( i \). The ordered substructure counts are closely related to the “Model B” of (Kuzelka et al., 2018) for defining the probability of a formula, and homomorphism densities for the convergence analysis of graph sequences (Borgs \( \eta \) \( \equiv \)).

Collecting all ordered substructure counts for worlds \( \tilde{\omega} \) up to size \( k \), we obtain:

**Definition 6.4** The complete \( k \)-count statistics of \( \omega \) is the set

\[
C_k(\omega) := \cup_{1 \leq \ell \leq k} \{ C_{\omega}(\tilde{\omega}) \mid \tilde{\omega} \in \Omega^{(\ell)} \}
\]

Clearly, there is redundancy in the complete \( k \)-count statistics, since the substructure counts for worlds of size \( l < k \) can be derived from the substructure counts for the worlds of size \( k \). However, it is convenient to also directly include the counts for smaller substructures explicitly in our statistics. The following definition describes a special case of statistical sufficiency, which is suitable in our context.

**Definition 6.5** Let \( k \geq 1 \). A parametric family of RRSMSs is determined by \( k \)-count statistics, if for all \( n \), \( Q^{(n)}_\theta(\omega) \) depends on \( \omega \) only as a function of \( C_k(\omega) \).

It is straightforward that \( k \)-count statistics are sufficient for MLNs that contain at most \( k \) variables in each formula. For RBNs, \( k \)-count statistics are not sufficient in general, but they are sufficient for the restricted class of projective RBNs identified in Section 4. For ProbLog the situation is a bit more involved, as discussed in Example 6.10 below.
As a first step to exploit determination by \(k\)-count statistics to ensure (11), we note that induced substructure sampling provides an unbiased estimator for the ordered substructure counts of \(\omega'\) (normalized to substructure frequencies):

**Lemma 6.6** Let \(\omega' \in \Omega^{(n)}, \; k \leq m \leq n\), and \(\tilde{\omega} \in \Omega^{(k)}\). Then
\[
E_{\omega'} \left[ \frac{(m - k)!}{m!} C_{\omega'}(\omega) \right] = \frac{(n - k)!}{n!} C_{\omega'}(\omega'),
\]
where the expectation is with respect to induced substructure sampling from \(\omega'\) of worlds \(\omega \in \Omega^{(m)}\).

Next, we consider a particular form of the likelihood function determined by \(k\)-count statistics:

**Definition 6.7** We say that the log-likelihood function is linear and separable in the \(k\)-count statistics, if for \(\omega \in \Omega^{(m)}\):
\[
\log L^{(m)}(\theta | \omega) = \sum_{l=1}^{k} c(m, l) \sum_{\omega' \in \Omega^{(l)}} C_{\omega'}(\omega) \cdot f_{\omega}(\theta[\tilde{\omega}])
\]
where
- \(c(m, l)\) is a constant depending only on \(m\) and \(l\)
- \(f_{\omega}(\theta[\tilde{\omega}])\) is a function of a subset of parameters \(\theta[\tilde{\omega}] \subseteq \theta\), such that the following separability property holds: if \(\omega \in \Omega^{(l)}, \tilde{\omega} \in \Omega^{(l')}\) with \(l \neq l'\), then \(\theta[\tilde{\omega}] \cap \theta[\tilde{\omega}'] = \emptyset\).

**Proposition 6.8** If the likelihood function is linear and separable in the \(k\)-count statistics, then (11) holds.

**Proof:** Due to the separability condition, the maximization of \(\log L^{(m)}\) can be divided into \(k\) independent maximization problems of the functions
\[
\log L^{(m)}_1(\theta | \omega) := c(n, l) \sum_{\omega' \in \Omega^{(l)}} C_{\omega'}(\omega) \cdot f_{\omega}(\theta[\tilde{\omega}]),
\]
for disjoint sets of parameters \(\theta[l] := \cup_{\omega \in \Omega^{(l)}} \theta[\tilde{\omega}]\).

Then with Lemma 6.6
\[
E_{\omega} \left[ \log L^{(m)}_1(\theta | \omega) \right] = \sum_{\omega' \in \Omega^{(l)}} E_{\omega'} \left[ \frac{(m - l)!}{m!} C_{\omega'}(\omega) \cdot f_{\omega}(\theta[\tilde{\omega}]) \right] = c(n, l) \sum_{\omega' \in \Omega^{(l)}} \frac{(n - l)!}{n!} C_{\omega'}(\omega) \cdot f_{\omega}(\theta[\tilde{\omega}]) = \frac{c(m, l) m! (n - l)!}{c(n, l) (m - l)! n!} \log L^{(n)}_1(\theta | \omega'),
\]
from which (11) follows. \(\square\)

**Directed Model Examples**

For ProbLog and RBNs we have to consider two different scenarios: the first scenario is that all relations that appear in the model are also observed in the possible worlds \(\omega\) that constitute our training data. Under complete observability, (11) holds in both models as follows.

**Example 6.9** Using Proposition 6.8 we can show that (11) holds for RBNs without combining functions, under the following two additional conditions:

(i) \(m \geq k\), where \(k\) is the largest arity of relations in the underlying signature \(S\);

(ii) the RBN does not contain multiple occurrences of the same parameter.

Condition (i) in conjunction with the restriction to the projective fragment ensures that the model is determined by \(k\)-count statistics. Condition (ii) ensures the separability property.

Related to the previous example is Schulte’s 2011 pseudolikelihood function for first-order Bayesian networks, which also satisfies the conditions of Definition 6.7.

**Example 6.10** Under complete observability, parameter learning for ProbLog becomes trivial, since the maximum likelihood parameters for the labeled facts are just obtained as the empirical frequencies with which groundings of the relations in the labeled facts are true. In particular, then the likelihood function is determined by \(k\)-count statistics, with \(k\) the maximal arity of any relation in labeled facts, and (11) trivially holds, even without the restriction to projective ProbLog.

However, more realistically, the ProbLog model will contain also some synthetic, unobserved relations, as shown in (3) and (4). In that case, the likelihood function induced by a possible world \(\omega\) for the observable relations becomes a sum of products of parameters, which does not decompose as (16).

**7 Conclusion**

The domain-size dependence of marginal probabilities is a property that causes difficulties for both inference and learning. This dependence has been examined in statistical theory using the concept of a projective family of distributions, whose inferences do not depend on domain size. This paper considered whether common SRL models define projective families. The paper gives sufficient conditions on the model structures for three different types of SRL frameworks that ensure projectivity. The conditions are quite restrictive, which is evidence that projectivity is difficult to achieve in SRL models. For learning, we examined conditions under which maximum likelihood parameter estimation is valid when it is applied to an observed sub-network drawn from a larger network of known size.

We believe that the projectivity of SRL models is an important and fruitful topic for future research. Open questions include the following. (1) Are there examples of domains for which our MLN projectivity condition is natural (all atoms in a formula share the same first-order variables)? (2) For RBNs, are there conditions on combining rules (rather than model structure) that ensure projectivity? For example, under which conditions does the combining rule average define projective models? (3) Do our learning results for maximum likelihood learning carry over to learning with pseudolikelihood functions? (4) Are suitable fragments of relational dependency networks projective (Neville and Jensen 2007)?
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