Tractable Probabilistic Reasoning Through Effective Grounding

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Abstract
Templated Statistical Relational Learning languages, such as Markov Logic Networks (MLNs) and Probabilistic Soft Logic (PSL), offer much of the expressivity of probabilistic graphical models in a compact form that is intuitive to both experienced modelers and domain experts. However, these languages have historically suffered from tractability issues stemming from the large size of the instantiated models and the complex joint inference performed over these models. Although much research has gone into improving the tractability of these languages using approximate or lifted inference, a relatively small amount of research has gone into improving tractability through efficient instantiation of these large models. In this position paper, we will draw attention to open research areas around efficiently instantiating templated probabilistic models.

1. Introduction
Templated Statistical Relational Learning languages, such as Markov Logic Networks (MLNs) (Richardson & Domingos, 2006) and Probabilistic Soft Logic (PSL) (Bach et al., 2017), offer much of the expressivity of probabilistic graphical models in a compact form that is intuitive to both experienced modelers and domain experts. However, these languages have historically suffered from tractability issues stemming from the large size of the fully instantiated models and the complex joint inference performed over these models. Although much research has gone into improving the tractability of these languages using approximate or lifted inference, a relatively small amount of research has gone into improving tractability through efficient instantiation of these large models. In this position paper, we will draw attention to open research areas around efficiently instantiating templated probabilistic models.

2. Background
2.1. SRL Templating Languages
SRL techniques combine the power of statistical inference with relational data to produce rich models with intricate constraints and dependencies (Getoor & Taskar, 2007). Modeling relational data is inherently complicated by the large number of interconnected and overlapping structural dependencies that are typically present. To make modeling relational data easier, many SRL frameworks use familiar first order logic as a compact representation of the model (Raedt et al., 2007; Riedel, 2008; Kok et al., 2009; Niu et al., 2011; Noessner et al., 2013; Magliacane et al., 2015; Poole & Mackworth, 2017; Bach et al., 2017; Alberti et al., 2017). For example, the following logical clause can be used to express the concept of transitive similarity:

\[ \text{Similar}(A, B) \land \text{Similar}(B, C) \rightarrow \text{Similar}(A, C) \]
We refer to the logical clauses that define models in these languages as rules. A rule is composed of a collection of atoms joined by logical operators. An atom consists of a predicate with constants or variables as arguments. A ground atom is an atom where all the arguments are constants. Ground atoms with a fixed value act as observed variables, while ground atoms with an unknown value are random variables. A ground rule is a rule instance that only consists of ground atoms. These ground rules act as cliques in a graphical model, typically a Markov random field (MRF). During inference these cliques are transformed into functions that assign a numeric value to the variable assignment, i.e. a potential function, the exact form of this function is chosen by the specific SRL language. Each rule is also assigned a weight that affects the penalty for not satisfying the rule. Most templated SRL languages come with the ability to either set weights manually, or learn them from data (Kok & Domingos, 2005; Singla & Domingos, 2005; Lowd & Domingos, 2007; Huynh & Mooney, 2009; 2010; Bach et al., 2013; Chou et al., 2016; Sarkhel et al., 2016; Das et al., 2016).

2.2. Probabilistic Soft Logic

Probabilistic Soft Logic (PSL) is one of the aforementioned templating SRL languages. As its underlying graphical model, PSL uses hinge-loss Markov random fields (HL-MRF), a special class of the undirected graphical model given by Definition 1. HL-MRFs are conditional distributions over real-valued atom assignments in [0, 1]. Unlike discrete MRFs where ground logical clauses are either satisfied or violated, a potential in HL-MRFs returns a continuous value that represents the potential’s distance to satisfaction. More formally:

Definition 1. Let \( \mathbf{x} = (x_1, ..., x_m) \) be a vector of known variables, \( \mathbf{y} = (y_1, ..., y_n) \) be a vector of unknown random variables, \( \mathcal{R} = (R_1, ..., R_l) \) be a set of rules, \( \mathbf{w} = (w_1, ..., w_l) \) be a set of real-valued weights each corresponding to a rule, and \( \phi = (\phi_1, ..., \phi_l) \) be a set of potentials where each potential corresponds to a rule and \( \phi_R(x_r, y_r) \) assigns the variables of this ground instance \( r \) of rule \( R \) a real-valued score. Then, a templated Markov Random Field is a probability distribution of the form:

\[
P(\mathbf{y}|\mathbf{x}) = \frac{1}{Z} \exp \left( - \sum_{R \in \mathcal{R}} \sum_{r \in R} w_R \cdot \phi_R(x_r, y_r) \right)
\]

where

\[
Z = \sum_{\mathbf{x}} \exp \left( - \sum_{R \in \mathcal{R}} \sum_{r \in R} w_R \cdot \phi_R(x_r, y_r) \right)
\]

Given this definition, MAP inference is achieved by maximizing the sum of weighted potentials in the model:

\[
\arg \max_{\mathbf{y}} \sum_{R \in \mathcal{R}} \sum_{r \in R} w_R \cdot \phi_R(x_r, y_r)
\]

Furthermore, in an HL-MRF the potential function, \( \phi \), is always a linear combination of the variables involved in the potential. This means that each potential is not just continuous, but also convex. These convex potentials makes MAP inference on an HL-MRF a convex optimization problem. Framing inference as a convex optimization problem allows PSL to provide an exact solution to continuous problems and an approximate answer to discrete (MAX SAT) problems with rounding guarantees (Bach et al., 2015).

The continuous nature of the HL-MRF allows PSL to scale beyond what was previously feasible for SRL frameworks. Solving MAP inference as a convex optimization problem makes inference in PSL linear time with respect to the number of ground rules. This fast inference has allowed PSL to solve problems with tens of millions of ground rules in minutes (Kouki et al., 2018). PSL has also been shown to outperform industrial interior point methods (Bach et al., 2017) as well as existing MLN implementations (Pujara et al., 2013; Augustine & Getoor, 2018).

The expressive modeling and tractability of PSL has lead it to be used in many types of problems such as image classification (Gridach et al., 2017; Aditya et al., 2018a), scene understanding (Aditya et al., 2018b), activity recognition (London et al., 2013), natural language processing (Beltagy et al., 2014; Deng & Wiebe, 2015; Ebrahimi et al., 2016; Wang & Ku, 2016), bioinformatics (Sridhar et al., 2016), recommender systems (Kouki et al., 2015; Lalithsena et al., 2017), diagnosis of physical systems (Chen et al., 2014), knowledge bases (Pujara et al., 2015; Pujara & Getoor, 2016; Embar et al., 2018), and information retrieval (Alshukaili et al., 2016; Platanios et al., 2017).

2.3. Grounding

Grounding is the process of instantiating each ground rule given a rule template and the data. Grounding is generally approached in one of two ways: top-down or bottom-up. Top-down grounding starts with the rules and employs nested loops to perform replacements over all the variables (Kok et al., 2009). It is simple and easy to implement, but slow. Alternatively, bottom-up grounding works in two phases (Niu et al., 2011). First, a database query is issued that finds all the assignments of constants to variables for a specific rule. As an example, variable assignments for the transitive similarity rule from Section 2.1 can be computed by the following SQL query:
SELECT
S1. argument1 AS A,
S1. argument2 AS B,
S2. argument2 AS C
FROM
Similar S1,
Similar S2,
Similar S3
WHERE
S1. argument1 = S3. argument1
AND S1. argument2 = S2. argument1
AND S2. argument2 = S3. argument2

We will refer to these queries for variable assignment as *grounding queries*. After executing a grounding query, bottom-up grounding instantiates each returned variable assignment into a ground rule. As a result of finding variable assignments using a relational database, grounding leverages the huge amount of work done by the RDBMS community in query optimization, fast relational joins, and memory management. Bottom-up grounding has shown significant improvements over top-down grounding, but comes at the cost of more complex systems (Niu et al., 2011; Augustine & Getoor, 2018). For the remainder of this paper, we will only be discussing bottom-up grounding.

### 3. Opportunities for Improving Grounding

All of the templated SRL frameworks discussed thus far are severely impacted by grounding time. Grounding is difficult because the number of ground rules can quickly become intractable. Seemingly innocuous rule templates can hide a polynomial number of instantiations. Once again, consider the case of transitive similarity:

\[
\text{Similar}(A, B) \land \text{Similar}(B, C) \rightarrow \text{Similar}(A, C)
\]

This pattern is simple and is seen in many practical problem domains. However, the number of ground rules instantiated by this rule is cubic in the size of the input data. When applying this rule in a social networking context where each variable represents a user, even a modest social network of 1,000 users generates a ground model of a billion ground rules. Rules like these allow for expressive and interdependent models, but present a significant systems challenge to efficiently ground.

To illustrate the impact of different grounding decisions, we have rerun the “End-to-End Performance” experiment from (Augustine & Getoor, 2018). The experiment is a simple SRL model implemented in Tuffy and PSL on increasingly larger instances of a synthetic dataset. In addition to Tuffy and the same version of PSL, we have included a version of PSL with naive implementations of the containing query discussed in Section 3.3 and grounding query sharing discussed in Section 3.4. Figure 3 shows the result of this experiment. Grounding in Tuffy quickly becomes intractable for this model once the number of ground rules exceeds one million. Both versions of PSL scale with the number of ground rules approximately linearly. However, the version of PSL with the grounding improvements runs about twice as fast as the unmodified PSL. As illustrated by this experiment, there is significant room for improvement in the space of grounding. In the rest of this section, we will cover several different opportunities for improving grounding for templated SRL languages.

#### 3.1. Exposing Sparse Structure in Data

As previously discussed, the number of ground rules generated from grounding can quickly become prohibitively large. Blocking (Papadakis et al., 2016) can be used to limit the size of the ground model. Blocks work by using problem specific heuristics to eliminate infeasible ground rules. In templated SRL languages, these blocks can be included in the model by incorporating them as data and including them in the rules as predicates. Then during grounding, potentials with components outside of the block will not be included in the ground model. Injecting these sparse structures into the data can limit the overall size of the model.

For example, consider the transitive similarity pattern applied to friendship prediction in a social network. We can include a block in this rule which enforces the requirement that for people to be friends they must have been members of the same social group:

\[
\text{InGroup}(A, G) \land \text{InGroup}(B, G) \land \text{InGroup}(C, G) \land \text{Friends}(A, B) \land \text{Friends}(B, C) \rightarrow \text{Friends}(A, C)
\]

Augustine & Getoor (2018) have shown large reductions in grounding time by having the modeler explicitly mark blocks in the data. However, there are two obvious places for improvement here. The first is to achieve the grounding performance of explicitly marking blocks without requiring
the modeler to actually mark them. The second, and more interesting, would be to discover sparse components in the data without the user needing to introduce them. Automatically discovering sparse components would allow the user to focus on modeling tasks without needing to worry about performance tweaks.

3.2. Improving the Performance of Ground Rule Validation Functions

In the grounding process, each configuration of variables returned from the database is checked to see if it constitutes a valid ground rule. A ground rule is valid if it is not trivial and it conforms to the semantics of the specific SRL framework. Where a trivial ground rule is one whose potential value is fixed and unchangeable regardless of the value assigned to any random variables:

$$\forall y, \phi_R(x_r, y_r) = c$$

Removing trivial ground rules at the grounding phase improves performance in the later inference phase by not wasting resources on potentials with a fixed value.

The function that validates a ground rule may be as simple as just checking if the ground rule is trivial, as is the case in the Alchemy framework (Kok et al., 2009). Tuffy, which performs partial groundings of the MRF, has a more sophisticated validation function that checks to make sure only the appropriate portions of the MRF are grounded (Domingos & Lowd, 2009). PSL enforces more language semantics in the validation function; such as requiring that every generated inference target has been explicitly defined in the input data and ensuring that legal values are returned from user-defined functional predicates (predicates where the user can write custom code to evaluate ground atoms) (Bach et al., 2017). Extensions to the different frameworks’ validation functions have been proposed to improve performance by reducing the size of the set of ground rules which pass validation. Glass & Barker (2012) and Beltagy et al. (2014) modified the Alchemy and PSL validation functions, respectively, by introducing a “relevance” score for each ground rule and only validating the ground rules with the highest score. Beltagy & Mooney (2014) used a custom validation function to enforce a stricter closed-world assumption.

These validation functions have been shown to be critical to scaling (Singla & Domingos, 2006), but there has been little research in how to evaluate them most effectively. Augustine & Getoor (2018) showed that there was a substantial trade-off between validating ground rules in the database (via additions to the WHERE clause in the grounding query) or in the application layer (via iteration through the results returned from the grounding query). In Augustine & Getoor’s experiments, datasets with less than 85% trivial ground rules benefited from executing these validation functions in the application layer rather than in the database. This threshold raised to 95% when execution of the validation functions was parallelized over more than one core. Potential areas for research around effective use of these validation queries include: hybrid validation functions that are split between the database and application layers, domain-independent relevance scores (generalizations of (Glass & Barker, 2012) and (Beltagy et al., 2014)), and parallel execution of validation functions.

3.3. Exploring the Database-Memory Trade-off

Early grounding techniques for SRL were primarily centered around top-down grounding. These techniques were simple and fully resided in memory. As the need for more performant grounding rose, bottom-up grounding came into favor. More and more computation was pushed into the database. However, there is more room for research in the trade-off between grounding time spent in the database and grounding time spent in memory. Tuffy has already achieved much success through a hybrid memory/database inference infrastructure (Niu et al., 2011). A similar approach to grounding could prove beneficial.

One way to exploit this trade-off would be to use simpler grounding queries that may return larger result sets in exchange for faster query execution. As previously discussed, the results of the grounding query are filtered through a validation function which removes spurious variable configurations. Because of this validation function, it is possible to substitute the grounding query with one that returns a superset of results. As long as the optimized query is safe (i.e., every variable appears in a positive atom) (Garcia-Molina et al., 2008), then the validation function will invalidate any spurious variable configurations returned by the grounding query. So instead of executing the base query, any containing query can be invoked. A query $q_1$ contains another query $q_2$ if $q_2$ produces only answers that $q_1$ also produces (Garcia-Molina et al., 2008). Because the validation functions make it possible to use queries that return larger result sets than the base grounding query, we can explore the trade-off between query size and total grounding time. More query results means more variable configurations that need to be validated, however the executed query can be simpler and contain fewer joins.

3.4. Reuse of Grounding Results

For large and/or complex models, the grounding query itself can take much more time than instantiating the results into ground rules. In addition, models often have rules that share many atoms. Once again, consider the transitive similarity example:

$$\text{Similar}(A, B) \land \text{Similar}(B, C) \rightarrow \text{Similar}(A, C)$$
A natural complement to this rule would be to negate several of the atoms:

\[ \text{Similar}(A, B) \land \text{Similar}(B, C) \implies \text{Similar}(A, C) \]

These rules are semantically quite different, but almost identical in the eyes of the first phase in bottom-up grounding where the task is to collect the combinations of constants that map to the variables in the rule. These rules share all the same variables and atoms. In cases like these, it could be possible to reuse the results of a grounding query to ground multiple rules.

When explored together with the modified grounding queries discussed in Section 3.3, the opportunities to expand grounding queries becomes much more available. Each rule can have multiple possible grounding queries (any query that contains the original query). When the collection of all rules in a model are considered together, it is possible to choose a combination of grounding queries where each individual query is not the fastest available, but the collection of queries maximize the number of rules grounded per query. For example, consider the following two rules from our social networking example:

\[
\begin{align*}
\text{InGroup}(A, G) \land \text{InGroup}(B, G) \land \text{InGroup}(C, G) \\
& \land \text{Friends}(A, B) \land \text{Friends}(B, C) \\
& \implies \text{Friends}(A, C)
\end{align*}
\]

\[
\begin{align*}
\text{InGroup}(A, G) \land \text{InGroup}(B, G) \land \text{InGroup}(C, G) \\
& \land \text{Similar}(A, B) \land \text{Similar}(B, C) \\
& \implies \text{Similar}(A, C)
\end{align*}
\]

Both rules could be grounding by using a grounding query that covers these atoms:

\[
\begin{align*}
\text{InGroup}(A, G) \land \text{InGroup}(B, G) \land \text{InGroup}(C, G)
\end{align*}
\]

4. Conclusion

Templated SRL languages have proven to be expressive and powerful tools for creating complex probabilistic models. To improve tractability, much research has gone into inference and lifting, but there are many research opportunities left in the area of grounding. In this paper, we discussed several potential areas of research pertaining to grounding for templated SRL languages. We have also illustrated through a simple experiment the performance gains a more intelligent grounding strategy can offer. Although our examples have been made concrete using PSL, the grounding tactics discussed here are general and applicable to any templated SRL language. Addressing the bottleneck of grounding breaks one of the barriers keeping templated SRL languages from being tractable.

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