

Explainability in Autonomous Agents: Interpretable Models, Abstraction, and Beyond

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1 Introduction

Modern models for machine learning are paving the way for a new generation of autonomous agents. However, these agents are increasingly deployed in situations where they have to interact with human users, and in that setting, humans may need communicate their knowledge to these agents, as well as understand the internal logic of the decisions taken by the agents. Fundamentally, this boils down to the question of interpretable decision making, and whether humans can understand the inner workings of the machine learning models used in those agents. In this project, we will look at fundamental questions pertaining to the topic of interpretability and explainability, including a framework for abstraction, for defining how to interface high-level instructions and low-level modules.

2 Proposed Research

2.1 Background

Logical approaches to reasoning have dominated the fields of artificial intelligence (AI) and computing for many decades. They have resulted in expert systems that can use reasoning to make predictions and diagnose problems [19], logic programming languages that allow the user to declaratively describe the problem and trust the inference algorithm to find the answer efficiently [24], and automated (interactive) theorem proving and proof checking software that assists mathematicians in constructing correct proofs [32]. Probabilistic methods, on the other hand, have particularly flourished with the arrival of big data and access to more data in general, transforming areas such as natural language processing and pattern recognition [9].

While probabilistic models are great at handling uncertainty, their simplistic representations can be hard to interpret. On the other hand, systems based on logic have rich representations, but cannot handle uncertainty. *First-order probabilistic inference* (FOPI) (also known as *statistical relational AI*) attempts to bridge the gap between the two and suggests a range of representations¹ capable of handling probabilities as well as (parts of) first-order logic [9]. The models can be constructed manually or learned from data, and the process of computing the probability of a query—usually in the form of a random variable, possibly conditioned on other random variables—is called *inference*.

Most of these models are based either on adding probabilities to programming languages or on adding richer representational structure to probabilistic graphical models (PGMs). The former kind is called *probabilistic programming* [18] and is an active area of research with many implementations. A well-known example is *ProbLog* [30]—a language that extends the logic programming language Prolog by attaching a probability to every clause in the program. A prominent example of the latter is a *Markov logic network* (MLN) [31], which is simply a collection of first-order statements (formulas), with a weight attached to each statement.

¹We will sometimes refer to FOPI models as *probabilistic relational models*, since relations play an important part in this richer representational structure.

MLNs were proposed as a first-order generalisation of *Markov random fields*—an undirected PGM. We will use MLNs to provide concrete examples, but we do not commit ourselves to a specific FOPI model just yet.

As an area of research, FOPI is a subfield of AI and can be thought as the probabilistic cousin of automated reasoning. The problem of learning a FOPI model from data draws the attention of researchers not only from the machine learning community, but also data mining and knowledge discovery. Due to how many of the models are formulated, there is also significant overlap with research in programming languages and, specifically, logic programming.

In the last decade, we have seen applications of FOPI in a wide range of areas, ranging from toy problems in probability one might find in a textbook [12] all the way to genetics [35] and cancer research [8]. For instance, probabilistic relational structures have been integrated into recommendation systems [42] and stream mining software [4], and various FOPI models have been used to predict the remaining lifetime of hardware components [41] as well as patterns of criminal and terrorist activity [10]. Moreover, one type of probabilistic logic has been extended to explicitly deal with changes over time and has been used to model virtual spaces such as online chat rooms and massively multiplayer online games [38, 39].

2.2 Key Idea

“To investigate how first-order probabilistic models can be transformed into more abstract representations without losing (significant) detail crucial to the set of relevant queries.”

Abstraction can be broadly defined as the process (and result) of omitting detail [23]. Sometimes the omitted information is irrelevant in answering the questions we are interested in, and sometimes an abstraction provides a simplified (and approximately correct) view of a situation that originally was too complex to be reasoned about. While areas such as planning and verification have benefited from abstraction in various ways [34], research into abstraction in FOPI has just begun and awaits significant contributions [2, 21, 22].

Our goal is to develop new types of abstractions, find efficient algorithms for constructing an abstraction from a given model, and investigate how abstraction can be integrated into both inference and learning algorithms. Simplification and abstraction can benefit us in both efficiency and interpretability, i.e, simpler models are likely to result in faster inference, while at the same time being easier to understand by the user. Finally, the quest for abstraction algorithms is likely to lead to a better theoretical understanding of what properties can be preserved by an abstraction, what error bounds can be established when abstraction approximates the answer, and upper and lower bounds on the complexity of performing abstraction and providing the desired guarantees.

2.3 Objectives

- To further the theoretical understanding of abstraction in FOPI.
- To improve inference speed by investigating abstraction as a separate process as well as a component of inference.
- To make models learned from data simpler and more transferable.
- To increase the explainability of FOPI models.

2.4 State of the Art

2.4.1 Inference

Recall that a ProbLog program is a set of clauses, where each clause has an associated probability. The ProbLog inference rule [29, 36] for calculating the probability of an arbitrary query Q being true is

$$P(Q) = \sum_{F \models Q} \prod_{f \in F} P(f) \prod_{f \notin F} 1 - P(f).$$

Here, we are summing over all instantiations of variables (called *possible worlds*) that satisfy the query, where F denotes a set of clauses that are evaluated as true. For each world, we calculate its probability by multiplying probabilities associated with clauses or their negations. With this definition, the inference problem becomes an instance of weighted model counting [29].

Weighted model counting (WMC) is an extension of model counting, which is an extension of the *Boolean satisfiability problem* (SAT) [5]. SAT asks whether one can assign values to variables so that a given formula evaluates to true. Model counting asks to count the number of ways that can be done. Weighted model counting further extends this problem by assigning a weight to each possible world (in whatever way is appropriate for the problem) and asks for the sum of the weights corresponding to all possible worlds where the formula (or query) is true. In the case of ProbLog, the weight of a world is the product of probabilities of all literals (whether evaluated/instantiated to true or false) [29]. The WMC instance is then compiled to some type of logical circuit for efficient inference. *Knowledge compilation* [11] is the state-of-the-art inference technique for PGMs as well as many FOPI models [29].

Inference for MLNs works in a similar way. We still sum over all possible worlds where the query is true, but the probability of a world x is now defined as

$$P(x) = \frac{1}{Z} \exp \left(\sum_{i=1}^F w_i n_i(x) \right),$$

where Z is the normalising constant more commonly known as the *partition function*, F is the number of formulas in the MLN, w_i is the weight of the i th formula, and $n_i(x)$ is the number of ways that formula i can be grounded in order to satisfy world x . Here, *grounding* a formula refers to replacing each variable with a value so that the formula evaluates to true.

A commonly used inference algorithm for MLNs relies on *probabilistic theorem proving* [17, 40] which is an example of a *lifted inference* algorithm, i.e., an algorithm that attempts to work directly with variables without having to consider every possible value [28]. The underlying problem, however, is still WMC, and is solved using a combination of techniques well established in the SAT community, e.g., unit propagation and clause learning [40].

2.4.2 Abstraction

Abstraction is an important tool in human cognition and a well-studied subject in cognitive science. For example, Gentner and Hoyos [15] investigate how children learn abstract patterns from observing several objects with a common property, while Bransford and Franks [3] show how the idea conveyed by a sentence is abstracted away from the particulars of its syntactic expression.

Abstraction is also well-known in the AI community, where the main goal of abstraction is to reduce the computational complexity of a task, while ensuring that the process of abstraction itself is reasonably efficient [34]. For instance, abstraction plays a key part in modern approaches to planning, where compound tasks are used to abstract away the details of how those tasks can be implemented [14]. More specifically, abstraction is essential in developing explainable AI [1], where it has been used to create interpretable abstractions of observed behaviour [27] and model the domain knowledge of the user as an abstraction of the system, thus producing explanations that are at the level of detail corresponding to the user’s knowledge [37].

Model checking and verification benefit from abstraction as well, particularly in the area of software verification, where a complete model of the program might be too big to be handled by even the most efficient methods, in which case an abstract model could be developed. Depending on how it is created, sometimes properties of the system can be verified using the abstraction [7], while other times the abstract model might produce a false positive, i.e., signal about a possible problem where there is none. If the occurrence of a false positive is suspected, parts of the abstraction can be refined to provide the necessary level of detail, while keeping other parts as they were [6, 20].

Probabilistic abstractions have been used in the context of software verification, where probabilities can help the verification algorithm choose which part of the abstract model needs to be refined [43]. Meanwhile,

in the probabilistic programming community, abstractions have been used to determine the required number of Monte Carlo samples in order to compute a probability within a required level of precision [26].

However, only recently has the general case of abstraction for FOPI models been formalised, and the work is mostly limited to defining several key properties that an abstraction may have and showing how those properties interact with each other [2]. While the work on probabilistic programming considers specific examples of abstractions [22] and presents an algorithm for performing predicate abstraction [21], significant work is required to achieve the full generality outlined in this proposal.

2.5 Our Solution

While some theoretical groundwork for abstraction in FOPI has recently been developed by Belle [2], there are many questions left to be answered:

1. How to efficiently create an abstraction of an already-existing model?
2. When is the correct time to stop? What is the right balance between simplicity and information?
3. What makes one abstraction preferable to another?
4. How to incorporate abstraction steps into learning a model from data?
5. How to provide guarantees about an abstraction? For example, we may want to bound the error of an answer to any query, or to ensure that all answers remain exact for a selected set of queries.

In order to answer these questions and develop the required algorithms and techniques, we can draw inspiration from the theory of abstraction for reasoning in formal systems developed by Giunchiglia and Walsh [16] and recent work on abstraction for structural equation models [33]. In particular, an abstraction is often defined as a transformation of the representation into a different form. One way to create such a transformation is via a composition of atomic operations. For example:

- In some cases, $a \rightarrow b$ and $b \rightarrow c$ can be simplified to $a \rightarrow c$.
- If a statement S is true with high probability, perhaps that probability can be rounded up to 1, eliminating the need to consider the case where S is false.
- If a statement is true for all values of a variable, barring a few exceptions, perhaps the exceptions can be discarded.

Consider a specific query Q . Applying such an abstraction rule may or may not change the answer to Q , depending on whether the removed information is relevant to the query. Even if the answer becomes less precise, it might be an acceptable approximation, given that the error is bounded to a reasonable degree. Either way, the abstraction can reduce the search space the inference algorithm has to explore in order to produce an answer.

It becomes clear that it is important to consider creating abstractions with respect to a specific set of queries. Question 5 can then be answered by considering how each abstraction rule affects different types of queries. Sometimes we may get a reasonable numerical upper bound on the error, while other times it may be too time-consuming (or impossible) to bound the error to any reasonable degree, forcing us to reject the abstraction rule altogether.

Thus, we will develop a comprehensive list of abstraction rules (transformations) and define a way to categorise all queries answerable by a FOPI model such that we could answer the following set of questions for each abstraction rule:

- What types of queries can no longer be answered exactly after applying the abstraction rule?
- What is the error bound? Can it be calculated in constant time?
- What is the complexity of applying the abstraction?

Questions 2 and 3 delve deeper into how an abstraction algorithm could work. If the set of rules is extensive enough, any model might eventually be oversimplified into something trivial. We need to measure two things: the amount of (relevant) information preserved by an abstraction, and the complexity of the model. The two metrics would provide a systematic way to answer both questions, while being easily adaptable to different needs (e.g., how much precision are we willing to sacrifice? What queries do we want to support?).

Lastly, we will integrate abstraction steps into both inference and learning algorithms, resulting in faster inference as well as simpler and more robust models.

2.6 Innovative Aspects

We aim to innovate by expanding the idea of abstraction in AI to new domains as well as enhancing both inference and learning of probabilistic relational models.

Abstraction in AI The work on abstraction so far has focused almost exclusively on deterministic systems. We will extend previous work to target rich probabilistic models, resulting in new theoretical ideas and definitions as well as algorithms for transforming models into their abstractions.

FOPI As FOPI subsumes both probabilistic inference (often $\#P$ -complete) and logical inference (NP-complete) [31], it is unlikely that a useful variation of FOPI can ever be tractable. Thus, improvements in inference speed are highly desirable. We will integrate abstraction steps into inference algorithms, making the algorithm recognise opportunities to reduce the complexity of the model before continuing the search. This is likely to yield significant benefits to inference speed.

Statistical relational learning Abstraction can also be integrated into learning a FOPI model from data. This is likely to make the model more understandable to the user as well as increase the transferability of the model to previously unseen data.

3 Methodology

3.1 Comparative Survey of FOPI Models (WP1)

As there is no consensus over the quality and capabilities of various FOPI models, we will develop a list of problems that can be used to compare and challenge state-of-the-art inference algorithms for various representations. We will draw inspiration from problems that already exist in the literature and have been used to propose new approaches, e.g., the classic ‘a friend of a smoker is likely to be a smoker’ example commonly used to introduce FOPI representations [9, 11, 31, 40] and the urn-and-balls scenario that requires handling uncertainty about the number of objects and their identities [25]. These and other example problems will allow us to compare modern FOPI models in terms of what complexities of the problem can be represented in a reasonable way, and efficiency of inference (both empirical and in terms of computational complexity).

Deliverable: a report with a list of problems, indication of which representations are able to solve each problem, the computational complexity of each solution, and plots comparing the performance of different models for each problem.

3.2 Abstraction Rules and Their Properties (WP2)

Developing a list of abstraction rules (transformations) that can be composed to achieve any (even a trivial) abstraction is an important step in our proposal. While some examples have already been mentioned here and more can be found in previous work [2, 16, 22, 34], our aim is to develop a complete list of abstraction rules that are able to simplify individual snippets of first-order logic, their probabilities, and interactions

among two or more snippets. After constructing such a list, we will investigate whether (or to what extent) it satisfies several key properties (the first three as defined by Belle [2]):

Soundness Do events that were possible before the abstraction stay possible?

Completeness Were events that are possible after applying the abstraction possible before?

Exactness Are all computable probabilities in the abstraction equal to the corresponding probabilities before the abstraction was applied?

Commutativity Can the order of two transformations be changed without changing the result?

Thoroughness Is the list of abstraction rules extensive enough to simplify any model into a trivial one? It is unlikely that we would do so in practice, but the list should be rich enough to support that.

Deliverables: a report detailing a list of abstraction rules, their properties, and the required proofs as described above.

3.3 Applying Abstraction Rules in Practice (WP3)

We will build on the work produced in the previous WP to bring the theory closer to a useful implementation. Specifically, we will decide on a particular internal representation for our chosen FOPI model in order to achieve efficient application of abstraction rules. We will implement algorithms for applying each rule, consider their computational complexity, and detail our findings in a report with pseudocode snippets and investigations into the efficiency of applying each transformation. **Deliverables:** a working implementation featuring internal data structures, some example problems, and algorithms for applying abstraction rules; a report describing our findings.

3.4 Ensuring a Sufficient Level of Precision (WP4)

While knowing which abstraction rules are exact is useful, we would also like to ensure that non-exact rules maintain a sufficient level of precision. For each such rule, we will describe what queries can no longer be answered exactly after applying the rule. Then, we will construct algorithms to bound the error caused by the rule, and investigate their performance in terms of computational complexity as well as empirical studies. **Deliverables:** a report detailing how non-exactness affects classes of queries, implementation of error-bounding algorithms, their theoretical and empirical analysis.

3.5 Greedy Algorithms (WP5)

At this point, we can reason about applying multiple abstraction rules in sequence. We will aim to answer two key questions:

- How to choose which abstraction rule should be applied first?
- When is the correct time to stop simplifying things?

Exploring different answers to these questions will result in a set of abstraction algorithms. As we expect most abstraction rules to commute with one another, making the order the rules are applied in immaterial, we will focus on *greedy* algorithms, where we choose which abstraction rule should be applied on a model based solely on the current state of the model.

Each algorithm will take a model, a description of a set of queries that need to be supported, and an indication of how much loss in precision (if any) the user is willing to tolerate. We will explore a variety of heuristics that establish preferences over which abstraction rule should be applied first as well as termination conditions. For instance, we could always pick an abstraction rule that results in a model with highest entropy (similar ideas have been very successful in reinforcement learning [44]), or prefer rules that have little effect on

precision. While a natural termination condition could be an inability to apply an abstraction rule without losing too much precision, the process could also be terminated because either the loss in precision or the expected running time of applying the abstraction is too high for the predicted benefits in inference speed. **Deliverables:** implementations of the algorithms as well as one or more papers detailing the reasoning behind design decisions, observed empirical performance, and the differences in inference speed before and after running each algorithm.

3.6 Abstraction During Inference (WP6)

There is no reason to limit abstraction to the intermediate stage between constructing (or learning) a model and performing inference. Thus, we will investigate how the state-of-the-art inference algorithm for our chosen FOPI model can benefit from performing abstraction steps throughout its execution. For example, a common way to compute a conditional probability $P(Q \mid E)$ inside a model Δ using WMC is by calculating the WMC of $\Delta \wedge Q \wedge E$ and $\Delta \wedge E$ separately, and then dividing one by the other [5]. It is likely that the two computations would benefit from different abstractions. **Deliverables:** an implementation of a new inference algorithm with abstraction, and a report describing its design and performance.

3.7 Abstraction in Learning (WP7)

A learned model is, in a way, an abstraction of the training data. Performing abstraction afterwards is suboptimal, since the algorithm would attempt to stay close to the learned model rather than the underlying data itself. While learning algorithms already measure goodness of fit, the measure will have to be combined with a meaningful measure of simplicity in order to provide a reasonable balance between the two. The abstraction rules themselves will need to be rethought in the context of data, as abstraction ought not to be added at the end as an extra step, but rather a fully integrated part of the learning process that concerns itself primarily with a meaningful and accurate representation of data. The abstraction ideas developed in previous work packages will help ensure that the learned models are both more explainable and transferable to new kinds of data. **Deliverables:** an implementation of a learning algorithm with integrated abstraction, and a report describing the rationale for its design as well as observed performance.

3.8 Dissemination (WP8)

We will make the implementations of abstraction, inference, and learning algorithms (as well as the newly constructed test data) publicly available in a repository. A website dedicated to the project will provide a coherent view of all developments as they are being implemented and written. We will aim to produce a series of papers detailing both theoretical contributions and empirical results in journals and conferences such as JAIR, UAI, IJCAI, AAAI, NeurIPS, etc. **Deliverables:** project website, code repository, dissemination activities.

4 Measurable Outcomes

- A set of problems delineating the differences amongst various representations as well as guiding future research efforts (WP1).
- Demonstrated increase in exact and approximate inference speed (WP6).
- Demonstrated improvement in models learned from data in terms of simplicity and transferability without (significant) loss in precision (WP7).

5 Risks

Creating a new algorithm always carries a risk that the algorithm may not perform well compared to what has already been achieved. Fortunately, previous work, which features a very limited version of abstraction, shows promising results in terms of reduction in inference speed [21]. We are confident that we can observe similarly successful results with a much broader range of abstractions. In any case, the project will result in valuable theoretical contributions regardless of how well the ideas perform in practice.

Another risk is related to integrating abstraction into inference. Namely, it might take too much time to create the abstraction compared to the time saved during inference. Even if this turns out to be the case, the developed abstraction algorithms would still be useful for models that are constructed once and used to perform many inferences. However, the observed reductions in inference speed seem to reduce the complexity of the task [21], while at least some abstraction rules can definitely be implemented in linear time. This suggests that with a big enough model the gains in inference speed should eventually overtake the time taken to construct the abstraction.

6 Impact and National Importance

National Importance Our proposal covers an EPSRC growth area for statistics and applied probability as well as several maintenance areas such as AI technologies, logic and combinatorics, and theoretical computer science. Furthermore, our work will contribute to areas such as big data (as more scalable inference will allow expressive probabilistic models to be used with more data) as well as other scientific disciplines (as both abstraction and richness of representation are important topics in social sciences and medicine). Moreover, abstraction for FOPI models is a new yet promising research area [21] which is likely to see many major developments.

Impact The survey will highlight the weaknesses of current approaches and direct future research towards open problems. Furthermore, many of the basic ideas behind abstraction for a particular model are likely to be transferable to many others, perhaps even inspiring a unifying theory behind all representations. Moreover, making the models more efficient and explainable should also make them more attractive to a larger user base, both academic and industrial.

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