Declarative Statistical Modeling with Datalog

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ABSTRACT

Formalisms for specifying general statistical models, such as probabilistic-programming languages, typically consist of two components: a specification of a stochastic process (the prior), and a specification of observations that restrict the probability space to a conditional subspace (the posterior). Use cases of such formalisms include the development of algorithms in machine learning and artificial intelligence. We propose and investigate a declarative framework for specifying statistical models on top of a database, through an appropriate extension of Datalog. By virtue of extending Datalog, our framework offers a natural integration with the database, and has a robust declarative semantics (that is, semantic independence from the algorithmic evaluation of rules, and semantic invariance under logical program transformations).

Our proposed Datalog extension provides convenient mechanisms to include common numerical probability functions; in particular, conclusions of rules may contain values drawn from such functions. The semantics of a program is a probability distribution over the possible outcomes of the input database with respect to the program; these possible outcomes are minimal solutions with respect to a related program that involves existentially quantified variables in conclusions. Observations are naturally incorporated by means of integrity constraints over the extensional and intensional relations. We focus on programs that use discrete numerical distributions, but even then the space of possible outcomes may be uncountable (as a solution can be infinite). We define a probability measure over possible outcomes by applying the known concept of cylinder sets to a probabilistic chase procedure. We show that the resulting semantics is robust under different chases. We also identify conditions guaranteeing that all possible outcomes are finite (and then the probability space is discrete). We argue that the framework we propose retains the purely declarative nature of Datalog, and allows for natural specifications of statistical models.

1. INTRODUCTION

Formalisms for specifying general statistical models are commonly used for developing machine learning and artificial intelligence algorithms for problems that involve inference under uncertainty. A substantial scientific effort has been made on developing such formalisms and corresponding system implementations. An intensively studied concept in that area is that of Probabilistic Programming \cite{Kopec2015} (PP), where the idea is that the programming language allows for building general random procedures, while the system executes the program not in the standard programming sense, but rather by means of inference. Hence, a PP system is built around a language and an inference engine (which is typically based on variants of Markov Chain Monte Carlo, most notably Metropolis-Hastings). An inference task is a probability-aware aggregate operation over all the possible worlds, such as finding the most likely possible world, or estimating the probability of an event (which is phrased over the outcome of the program). Recently, DARPA initiated the project of Probabilistic Programming for Advancing Machine Learning, aimed at advancing PP systems (with a focus on a specific collection of systems, e.g., \cite{Eliwell2016,Nichols2016}) towards facilitating the development of algorithms based on machine learning.

In probabilistic programming, a statistical model is typically phrased by means of two components. The first component is a generative process that produces a random possible world by straightforwardly following instructions with randomness, and in particular, sampling from common numerical probability functions; this gives the prior distribution. The second component allows to phrase constraints that the relevant possible worlds should satisfy, and, semantically, transforms the prior distribution into the posterior distribution—the subspace conditional on the constraints.

As an example, in supervised text classification (e.g., spam detection) the goal is to classify a text document into one of several known classes (e.g., spam/non-spam). Training data consists of a collection of documents labeled with classes, and the goal of learning is to build a model for predicting the classes of unseen documents. One common approach to this task assumes a generative process that produces random parameters for every class, and then uses these parameters to define a generator of random words in documents of the corresponding class \cite{Blei2003,Blei2006}. So, the prior distribution generates parameters and documents for each class, and the posterior is defined by the actual documents of the training data. In unsupervised text classification the goal is to cluster a given set of documents, so that different clusters correspond to different topics (which are not known in advance). Latent Dirichlet Allocation \cite{Blei2003} approaches this problem in a similar generative way as the above, with the addition that each document is associated with a distribution over topics.

While the agenda of probabilistic programming is the deployment of programming languages to developing statistical models, in this framework paper we explore this agenda from the point of view of database programming. Specifically, we propose and investigate an extension of Datalog for declarative specification of statistical models on top of a database. We believe that Datalog can be naturally extended to a language for building statistical models, since its essence is the production of new facts from known (database) facts. Of course, traditionally these facts are deterministic, and our exten-
sion enables the production of probabilistic facts that, in particular, involve numbers from available numerical distributions. And by virtue of extending Datalog, our framework offers a natural integration with the database, and has a robust declarative semantics: a program is a set of rules that is semantically invariant under transformations that retain logical equivalence. Moreover, the semantics of a program (i.e., the probability space it specifies) is fully determined by the satisfaction of rules, and does not depend on the specifics of any execution engine.

In par with languages for probabilistic programming, our proposed extension consists of two parts: a generative Datalog program that specifies a prior probability space over (finite or infinite) sets of facts that we call possible outcomes, and a definition of the posterior probability by means of observations, which come in the form of an ordinary logical constraint over the extensional and intensional relations.

The generative component of our Datalog extension provides convenient mechanisms to include conventional parameterized numerical probability functions (e.g., Poisson, geometrical, etc.). Syntactically, this extension allows to sample values in the conclusion of rules, according to specified parameterized distributions.

As an example, consider the relation Client(ssn, branch, avgVisits) that represents clients of a service provider, along with their associated branch and average number of visits (say, per month). The following distributional rule models a random number of visits for that client in the branch.

\[
\text{Visits}(c, b, \text{Poisson}[\lambda]) \leftarrow \text{Client}(c, b, \lambda) \quad (1)
\]

Note, however, that a declarative interpretation of the above rule is not straightforward. Suppose that we have another rule of the following form:

\[
\text{Visits}(c, b, \text{Poisson}[\lambda]) \leftarrow \text{PreferredClient}(c, b, \lambda) \quad (2)
\]

Then, what would be the semantics if a person is both a client and a preferred client? Do we sample twice for that person? And what if the two \(\lambda\)s of the two facts are not the same? Is sampling according to one rule considered a satisfaction of the other rule? What if we have also the following rule:

\[
\text{Visits}(c, b, \text{Poisson}[\lambda]) \leftarrow \text{Client}(c, b, \lambda), \text{Active}(b) \quad (3)
\]

From the viewpoint of Datalog syntax, Rule (3) is logically implied by Rule (1), since the premise of Rule (3) implies the premise of Rule (1). Hence, we would like the addition of Rule (3) to have no effect on the program. This means that some rule instantiations will not necessarily fire an actual sampling.

To make sense of rules such as the above, we associate with every program \(G\) an auxiliary program \(\hat{G}\), such that \(\hat{G}\) does not use distributions, but is rather an ordinary Datalog program where a rule can have an existentially quantified variable in the conclusion. Intuitively, in our example such a rule states that “if the premise holds, then there exists a fact \(\text{Visits}(c, b, x)\) where \(x\) is associated with the distribution \(\text{Poisson}\) and the parameter \(\lambda\).” In particular, if the program contains the aforementioned Rule (1), then Rule (3) has no effect; similarly, if the tuple \((c, b, \lambda)\) is in both Client and PreferredClient, then in the presence of Rule (2) the outcome does not change if one of these tuples is removed.

In this paper we focus on numerical probability distributions that are discrete (e.g., the aforementioned ones). Our framework has a natural extension to continuous distributions (e.g., Gaussian or Pareto), but our analysis requires a nontrivial generalization that we defer to future work.

When applying the program \(G\) to an input instance \(I\), the probability space is over all the minimal solutions of \(I\) w.r.t. \(\hat{G}\), such that all the numerical samples have a positive probability. To define the probabilities of a sample in this probability space, we consider two cases. In the case where all the possible outcomes are finite, we get a discrete probability distribution, and the probability of a possible outcome can be defined immediately from its content. But in general, a possible outcome can be infinite, and moreover, the set of all possible outcomes can be uncountable. Hence, in the general case we define a probability measure space. To make the case for the coherence of our definitions (i.e., our definitions yield proper probability spaces), we define a natural notion of a probabilistic chase where existential variables are produced by invoking the corresponding numerical distributions. We use cylinder sets \([6]\) to define a measure space based on a chase, and prove that this definition is robust, since one establishes the same probability measure no matter which chase is used.

**Related Work.** Our contribution is a marriage between probabilistic programming and the declarative specification of Datalog. The key features of our approach are the ability to express probabilistic models concisely and declaratively in a Datalog extension with probability distributions as first-class citizens. Existing formalisms that associate a probabilistic interpretation with logic are either not declarative (at least in the Datalog sense) or depart from the probabilistic programming paradigm (e.g., by lacking the support for numerical probability distributions). We next discuss representative related formalisms and contrast them with our work. They can be classified into three broad categories: (1) imperative specifications over logical structures, (2) logic over probabilistic databases, and (3) indirect specifications over the Herbrand base. (Some of these formalisms belong to more than one category.)

The first category includes imperative probabilistic programming languages \([13]\), such as BLOG \([31]\), that can express probability distributions over logical structures, via generative stochastic models that can draw values at random from numerical distributions, and con-
tion values of program variables on observations. In contrast with closed-universe languages such as SQL and logic programs, BLOG considers open-universe probability models that allow for uncertainty about the existence and identity of objects. Instantiations of this category also do not focus on a declarative specification, and indeed, their semantics is dependent on their particular imperative implementations. P-log is a Prolog-based language for specifying Bayesian networks. Although declarative in nature, the semantics inherently assumes a form of acyclicity that allows the rules to be executed serially. Here we are able to avoid such an assumption since our approach is based on the minimal solutions of an existential Datalog program.

The formalisms in the second category view the generative part of the specification of a statistical model as a two-step process. In the first step, facts are being randomly generated by a mechanism external to the program. In the second step, a logic program, such as Prolog or Datalog, is evaluated over the resulting random structure. This approach has been taken by PRISM, the Independent Choice Logic, and to a large extent by probabilistic databases and their semistructured counterparts. The focus of our work, in contrast, is on a formalism that completely defines the statistical model, without referring to external processes.

One step beyond the second category and closer to our work is taken by uncertainty-aware query languages for probabilistic data such as TriQL, I-SQL, and world-set algebra. The latter two are natural analogs to SQL and relational algebra for the case of incomplete information and probabilistic data. They feature constructs such as repair-key, choice-of, possible, certain, and group-worlds-by that can construct possible worlds representing all repairs of a relation with respect to (w.r.t.) key constraints, close the possible worlds by unioning or intersecting them, or group the worlds into sets with the same results to sub-queries. World-set algebra has been extended to (world-set) Datalog, fixpoint, and while-languages to define Markov chains. While such languages cannot explicitly specify probability distributions, they may simulate a specific categorical distribution indirectly using non-trivial programs with specialized language constructs like repair-key on input tuples with weights representing samples from the distribution.

MCDB and SimSQL propose SQL extensions (with for-loops and probability distributions) coupled with Monte Carlo simulations and parallel database techniques for stochastic analytics in the database. In contrast, our work focuses on existential Datalog with recursion and probability spaces over the minimal solutions of the data w.r.t. the Datalog program. Formalisms in the third category are indirect specifications of probability spaces over the Herbrand base, which is the set of all the facts that can be obtained using the predicate symbols and the constants of the database. This category includes Markov Logic Networks (MLNs), where the logical rules are used as a compact and intuitive way of defining factors. In other words, the probability of a possible world is the product of all the numbers (factors) that are associated with the rules that the world satisfies. This approach is applied in DeepDive, where a database is used for storing relational data and extracted text, and database queries are used for defining the factors of a factor graph. We view this approach as indirect since a rule does not determine directly the distribution of values. Moreover, the semantics of rules is such that the addition of a rule that is logically equivalent to (or implied by, or indeed equal to) an existing rule changes the semantics and thus the probability distribution. A similar approach is taken by Probabilistic Soft Logic, where in each possible world every fact is associated with a weight (degree of truth).

Further formalisms in this category are probabilistic Datalog, probabilistic Datalog+/-, and probabilistic logic programming (ProbLog). In these formalisms, every rule is associated with a probability. For ProbLog, the semantics is not declarative as the rules follow a certain evaluation order; for probabilistic Datalog, the semantics is purely declarative. Both semantics are different from ours and that of the other formalisms mentioned thus far. A Datalog rule is interpreted as a rule over a probability distribution over possible worlds, and it states that, for a given grounding of the rule, the marginal probability of being true is as stated in the rule. Probabilistic Datalog+/- uses MLNs as the underlying semantics. Besides our support for numerical probability distributions, our formalism is used for defining a single probability space, which is in par with the standard practice in probabilistic programming.

As said earlier, the programs in our proposed formalism allow for recursion. As we show in the paper, the semantics is captured by Markov chains that may be infinite. Related formalisms are those of the Probabilistic Context-Free Grammar (PCFG) and the more general Recursive Markov Chain (RMC), where the probabilistic specification is by means of a finite set of transition graphs that can call one another (in the sense of method call) in a possibly recursive fashion. In database research, PCFGs and RMCs have been explored in the context of probabilistic XML. Although these formalisms do not involve numerical distributions, in future work we plan to conduct a study of the relative expressive power between them and restrictions of our framework. Moreover, we plan to study whether and how inference techniques on PCFGs and RMCs can be adapted to our framework.

**Organization.** The remainder of the paper is organized as follows. In Section 2 we give basic definitions. The syntax and semantics of generative Datalog is intro-
duced in Section 3 where we focus on the case where all solutions are finite. In Section 4 we present our adaptation of the chase. The general case of generative Datalog, where solutions can be infinite, is presented in Section 5. We complete our development in Section 6 where generative Datalog is extended with constraints (observations) to form Probabilistic-Programming Datalog (PPDL). Finally, we discuss extensions and future directions in Section 7 and conclude in Section 8.

2. PRELIMINARIES

In this section we give some preliminary definitions that we will use throughout the paper.

Schemas and instances. A (relational) schema is a collection $S$ of relation symbols, where each relation symbol $R$ is associated with an $arity$, denoted $arity(R)$, which is a natural number. An attribute of a relation symbol $R$ is any number in $\{1, \ldots, arity(R)\}$. For simplicity, we consider here only databases over real numbers; our examples may involve strings, which we assume are translatable into real numbers. A fact over a schema $S$ is an expression of the form $R(c_1, \ldots, c_n)$ where $R$ is an $n$-ary relation and $c_1, \ldots, c_n \in \mathbb{R}$. An instance $I$ over $S$ is a finite set of facts over $S$. We will denote by $R^I$ the set of all tuples $(c_1, \ldots, c_n)$ such that $R(c_1, \ldots, c_n) \in I$ is a fact of $I$.

Datalog programs. In this work we use Datalog with the option of having existential variables in the head $\exists \cdot$. Formally, an existential Datalog program, or just Datalog$^3$ program for short, is a triple $D = (E, I, \Theta)$ where: (1) $E$ is a schema, called the existential database (EDB) schema, (2) $I$ is a schema, called the intensional database (IDB) schema, and is disjoint from $E$, and (3) $\Theta$ is a finite set of Datalog$^3$ rules, i.e., first-order formulas of the form

$$\forall x \exists y (\varphi(x, y)) \leftarrow \psi(x)$$

where $\varphi(x)$ is a conjunction of atomic formulas over $E \cup I$ and $\psi(x, y)$ is an atomic formula over $I$, such that each variable in $x$ occurs in at least one atomic formula of $\varphi$. Here, by an atomic formula (or, atom) we mean an expression of the form $R(t_1, \ldots, t_n)$ where $R$ is an $n$-ary relation and $t_1, \ldots, t_n$ are either constants (i.e., real numbers) or variables. We usually omit the universal quantifiers for readability’s sake. Datalog is the fragment of Datalog$^3$ where the conclusion (left-hand side) of each rule is a single atomic formula without existential quantifiers.

Let $D = (E, I, \Theta)$ be a Datalog$^3$ program. An input instance for $D$ is an instance $I$ over $E$. A solution of $I$ w.r.t. $D$ is a possibly-infinite set $F$ of facts over $E \cup I$, such that $I \subseteq F$ and $F$ satisfies all rules in $\Theta$ (viewed as first-order sentences). A minimal solution of $I$ (w.r.t. $D$) is a solution $F$ of $I$ such that no proper subset of $F$ is a solution of $I$. The set of all, finite and infinite, minimal solutions of $I$ w.r.t. $D$ is denoted by $\text{min-sol}_D(I)$, and the set of all finite minimal solutions is denoted by $\text{min-sol}^f_D(I)$. It is a well known fact that, if $D$ is a Datalog program (that is, without existential quantifiers), then every input instance $I$ has a unique minimal solution, which is finite, and therefore $\text{min-sol}^f_D(I) = \text{min-sol}_D(I)$.

Probability spaces. We separately consider discrete and continuous probability spaces. We initially focus on the discrete case; there, a probability space is a pair $(\Omega, \pi)$, where $\Omega$ is a finite or countably infinite set, called the sample space, and $\pi : \Omega \to [0, 1]$ is such that $\sum_{o \in \Omega} \pi(o) = 1$. If $(\Omega, \pi)$ is a probability space, then $\pi$ is a probability distribution over $\Omega$. We say that $\pi$ is a numerical probability distribution if $\Omega \subseteq \mathbb{R}$. In this work we focus on discrete numerical distributions.

A parameterized probability distribution is a function $\delta : \Omega \times \mathbb{R}^k \to [0, 1]$, such that $\delta(\cdot, p) : \Omega \to [0, 1]$ is a probability distribution for all $p \in \mathbb{R}^k$. We use $\text{pardim}(\delta)$ to denote the number $k$, called the parameter dimensionality of $\delta$. For presentation’s sake, we may write $\delta(o|p)$ instead of $\delta(o, p)$. Moreover, we denote the (non-parameterized) distribution $\delta(\cdot|p)$ by $\delta[p]$. Examples of (discrete) parameterized distributions follow.

- Flip$(x|p)$: $\Omega = \{0, 1\}$ and for a parameter $p \in [0, 1]$ we have Flip$\{1|p\} = p$ and Flip$\{0|p\} = 1 - p$.
- Poisson$(x|\lambda)$: $\Omega = \mathbb{N}$, and for a parameter $\lambda \in (0, \infty)$ we have $\text{Poisson}(x|\lambda) = \lambda^x e^{-\lambda}/x!$.
- Geo$(x|p)$: $\Omega = \mathbb{N}$, and for a parameter $p \in [0, 1]$ we have $\text{Geo}(x|p) = (1 - p)^x p$.

In Section 7 we will discuss the extension of our framework to models that have an unbounded number of parameters, and to continuous distributions.

3. GENERATIVE DATALOG

A Datalog program without existential quantifiers specifies how to obtain a solution from an input EDB instance by producing the set of inferred IDB facts. In this section we present generative Datalog programs, which specify how to infer a distribution over possible outcomes given an input EDB instance.

3.1 Syntax

We first define the syntax of a generative Datalog program, which we call a GDatalog$^\Delta$ program.

**Definition 3.1 (GDatalog$^\Delta$).** Let $\Delta$ be a finite set of parametrized numerical distributions.

1. A $\Delta$-term is a term of the form $\delta[p_1, \ldots, p_k]$ where $\delta \in \Delta$ is a parametrized distribution with $\text{pardim}(\delta) = k$, and $p_1, \ldots, p_k$ are variables and/or constants.

2. A $\Delta$-atom in a schema $S$ is an atomic formula $R(t_1, \ldots, t_n)$ with $R \in S$ an $n$-ary relation, such that exactly one term $t_i$ (1 $\leq i \leq n$) is a $\Delta$-term,
1. Earthquake(c, Flip(0.01)) ← City(c, r)
2. Unit(h, c) ← Home(h, c)
3. Unit(b, c) ← Business(b, c)
4. Burglary(x, c, Flip[r]) ← Unit(x, c), City(c, r)
5. Trig(x, Flip[0.6]) ← Unit(x, c), Earthquake(c, 1)
6. Trig(x, Flip[0.9]) ← Burglary(x, c, 1)
7. Alarm(x) ← Trig(x, 1)

Figure 1: An example GDatalog[∆] program \( \mathcal{G} \)

and all other \( t_j \) are constants and/or variables.

3. A GDatalog[∆] rule over a pair of disjoint schemas \( \mathcal{E} \) and \( \mathcal{I} \) is a first-order sentence of the form \( \forall x(\psi(x)) \) where \( \phi(x) \) is a conjunction of atoms in \( \mathcal{E} \cup \mathcal{I} \) and \( \psi(x) \) is either an atom in \( \mathcal{I} \) or a \( \Delta \)-atom in \( \mathcal{I} \).

4. A GDatalog[∆] program is a triple \( \mathcal{G} = (\mathcal{E}, \mathcal{I}, \Theta) \), where \( \mathcal{E} \) and \( \mathcal{I} \) are disjoint schemas and \( \Theta \) is a finite set of GDatalog[∆] rules over \( \mathcal{E} \) and \( \mathcal{I} \).

Example 3.2. Our example is based on the burglar example of Pearl [36] that has been frequently used for illustrating probabilistic programming (e.g., [35]). Consider the EDB schema \( \mathcal{E} \) consisting of the following relations: House(h, c) represents houses h and their location cities c, Business(b, c) represents businesses b and their location cities c, City(c, r) represents cities c and their associated burglary rates r, and AlarmOn(x, y) represents units (houses or businesses) x where the alarm is on. Figure 2 shows an instance \( I \) over this schema. Now consider the GDatalog[∆] program \( \mathcal{G} = (\mathcal{E}, \mathcal{I}, \Theta) \) of Figure 1. Here, \( \Delta \) consists of only one distribution, namely Flip. The first rule above, intuitively states that, for every fact of the form City(c, r), there must be a fact Earthquake(c, y) where y is drawn from the Flip (Bernoulli) distribution with the parameter 0.01.

3.2 Possible Outcomes

To define the possible outcomes of a GDatalog[∆] program, we associate to each GDatalog[∆] program \( \mathcal{G} = (\mathcal{E}, \mathcal{I}, \Theta) \) a corresponding Datalog\(^3\) program \( \mathcal{G} = (\mathcal{E}, \mathcal{I}^\Delta, \Theta^\Delta) \). The possible outcomes of an input instance \( I \) w.r.t. \( \mathcal{G} \) will then be minimal solutions of \( I \) w.r.t. \( \mathcal{G} \). Next, we describe \( \mathcal{I}^\Delta \) and \( \Theta^\Delta \).

The schema \( \mathcal{I}^\Delta \) extends \( \mathcal{I} \) with the following additional relation symbols: whenever a rule in \( \Theta \) contains a \( \Delta \)-atom of the form \( R(. . . , \delta[i], . . .) \), and \( i \leq \text{arity}(R) \) is the argument position at which the \( \delta \)-term in question occurs, then we add to \( \mathcal{I}^\Delta \) a corresponding relation symbol \( R^\Delta_i \), whose arity is \( \text{arity}(R) + \text{pardim}(\delta) \). These relation symbols \( R^\Delta_i \) are called the directational relation symbols of \( \mathcal{I}^\Delta \), and the other relation symbols of \( \mathcal{I}^\Delta \).

Figure 2: The Datalog\(^3\) program \( \mathcal{G} \) for the GDatalog[∆] program \( \mathcal{G} \) of Figure 1

\( \mathcal{I}^\Delta \) (namely, those of \( \mathcal{I} \)) are referred to as the ordinary relation symbols. Intuitively, a fact in \( R^\Delta_i \) asserts the existence of a tuple in \( R \) and a sequence of parameters, such that the \( i \)-th element of the tuple is sampled from \( \delta \) using the parameters.

The set \( \Theta^\Delta \) contains three kinds of rules:

(i) All Datalog rules from \( \Theta \) that contain no \( \Delta \)-terms;  
(ii) The rule \( \exists y R^\Delta_i(t, y, t', p) \leftarrow \phi(x) \) for every rule of the form \( R(t, \delta[p], t') \leftarrow \phi(x) \) in \( \Theta \), where \( i \) is the position of \( \delta[p] \) in \( R(t, \delta[p], t') \);  
(iii) The rule \( \forall x, p(R(x) \leftarrow R^\Delta_i(x, p)) \) for every distributional relation symbol \( R^\Delta_i \in \mathcal{I}^\Delta \).

Note that in (ii), \( t \) and \( t' \) are the terms that occur before and after the \( \Delta \)-term \( \delta[p] \), respectively. A rule in (iii) states that every fact in \( R^\Delta_i \) should be reflected in the relation \( R \).

Example 3.3. The GDatalog[∆] program \( \mathcal{G} \) given in Example 3.2 gives rise to the corresponding Datalog\(^3\) program \( \mathcal{G} \) of Figure 2. As an example of (ii), rule 6 of Figure 1 is replaced with rule 6 of Figure 2. Rules 8–10 of Figure 2 are examples of (iii).

A possible outcome is defined as follows.

Definition 3.4 (Possible Outcome). Let \( I \) be an input instance for a GDatalog[∆] program \( \mathcal{G} \). A possible outcome for \( I \) w.r.t. \( \mathcal{G} \) is a minimal solution \( F \) of \( I \) w.r.t. \( \mathcal{G} \), such that \( \delta[b[p]] \geq 0 \) for every distributional fact \( R^\Delta_i(a, b, c, p) \in F \) with \( b \) in the \( i \)-th position.

We denote the set of all possible outcomes of \( I \) w.r.t. \( \mathcal{G} \) by \( \Omega^\mathcal{G}(I) \), and we denote the set of all finite possible outcomes by \( \Omega^\mathcal{G}_{\text{fin}}(I) \).

The following proposition provides an insight into the possible outcomes of an instance, and will reappear later on in our study of the chase. For any distributional relation \( R^\Delta_i \in \Theta^\Delta \), the functional dependency associated to \( R^\Delta_i \) is the functional dependency...
3.3 Finiteness and Weak Acyclicity

Our presentation first focuses on the case where all possible outcomes for the GDatalog[∆] program are finite. Before we proceed to defining the semantics of such a GDatalog[∆] program, we present the notion of weak acyclicity for a GDatalog[∆] program, as a natural syntactic property that guarantees finiteness of all possible outcomes. This draws on the notion of weak acyclicity for Datalog²³ [18]. Consider any GDatalog[∆] program \( G = (F, I, \Theta) \). A position of \( I \) is a pair \((R, i)\) where \( R \in \mathcal{I} \) and \( i \) is an attribute of \( R \). The dependency graph of \( G \) is the directed graph that has the attributes of \( \mathcal{I} \) as the nodes, and the following edges:

- A normal edge \((R, i) \rightarrow (S, j)\) whenever there is a rule \( \psi(x) \leftarrow \varphi(x) \) and a variable \( x \) at position \((R, i) \) in \( \varphi(x) \), and at position \((S, j)\) in \( \psi(x) \).
- A special edge \((R, i) \rightarrow^* (S, j)\) whenever there is a rule of the form

\[
S(t_1, \ldots, t_{j-1}, \delta(p), t_{j+1}, \ldots, t_n) \leftarrow \varphi(x)
\]

and an exported variable at position \((R, i) \) in \( \varphi(x) \). By an exported variable, we mean a variable that appears in both the premise and the conclusion.

We say that \( G \) is weakly acyclic if no cycle in the dependency graph of \( G \) contains a special edge.

**Theorem 3.6.** If a GDatalog[∆] program \( G \) is weakly acyclic, then \( \Omega_{G}(I) = \Omega_{G}^f(I) \) for all input instances \( I \).

\[ R^I_i : \{1, \ldots, \text{arity}(R^I_i) \} \rightarrow i, \text{expressing that the} \]
\[ \text{i-th attribute is functionally determined by the rest.} \]

**Proposition 3.5.** Let \( I \) be any input instance for a GDatalog[∆] instance \( G \). Then every possible outcome in \( \Omega_{G}(I) \) satisfies all functional dependencies associated to distributional relations.

The proof of Proposition 3.5 is easy: if an instance \( J \) violates the functional dependency associated to a distributional relation \( R^I_i \), then one of the two facts involved in the violation can be removed, showing that \( J \) is, in fact, not a minimal solution w.r.t. \( G \).

### 3.4 Probabilistic Semantics

Intuitively, the semantics of a GDatalog[∆] program is a function that maps every input instance \( I \) to a probability distribution over \( \Omega_{G}(I) \). We now make this precise. Let \( G \) be a GDatalog[∆] program, let \( I \) be an input for \( G \). Again, we first consider the case where an input instance \( I \) only has finite possible outcomes (i.e., \( \Omega_{G}(I) = \Omega_{G}^f(I) \)). Observe that, when all possible outcomes of \( I \) are finite, the set \( \Omega_{G}(I) \) is countable, since we assume that all of our numerical distributions are discrete. In this case, we can define a discrete probability distribution over the possible outcomes of \( I \) w.r.t. \( G \). We denote this probability distribution by \( Pr_{G,I} \).

For a distributional fact \( f = R^I_i(a_1, \ldots, a_n, p) \), we define the weight of \( f \) (notation: \( \text{weight}(f) \)) to be \( \delta(a_1|p) \). For an ordinary (non-distributional) fact \( f \), we set \( \text{weight}(f) = 1 \). For a finite set \( F \) of facts, we denote by \( P(F) \) the product of the weights of all the facts in \( F \).

\[
P(F) = \prod_{f \in F} \text{weight}(f)
\]

The probability assigned to a possible outcome \( J \in \Omega_{G}^f(I) \), denoted \( Pr_{G,I}(J) \), is simply \( P(J) \). If a possible outcome \( J \) does not contain any distributional facts, then \( Pr_{G,I}(J) = 1 \) by definition.
EXAMPLE 3.7. (continued) Let $J$ be the instance that consists of all of the relations in Figures 3 and 4. Then $J$ is a possible outcome of $I$ w.r.t. $G$. For convenience in the case of distributional relation symbols, we have added the weight of each fact to the corresponding row as the rightmost attribute. This weight is not part of our model (since it can be inferred from the rest of the attributes). For presentation’s sake, the sampled values are under the attribute name draw (while attribute names are again external to our formal model). $Pr_{G,I}(J)$ is the product of all of the numbers in the columns titled “$w(f)$,” that is, 0.01 $\times$ 0.99 $\times$ 0.03 $\times$ \ldots $\times$ 0.4. □

The following theorem states that $Pr_{G,I}$ is indeed a probability space over all the possible outcomes.

**Theorem 3.8.** Let $G$ be a GDatalog[$\Delta$] program, and $I$ an input instance for $G$, such that $\Omega_I(G) = \Omega^G_I(I)$. Then $Pr_{G,I}$ is a discrete probability function over $\Omega^G_I(I)$.

We prove Theorem 3.8 in Section 4 In Section 5 we consider the general case, and in particular the generalization of Theorem 3.8 where not all possible outcomes are guaranteed to be finite. There, if one considers only the (countable set of all) finite possible outcomes, then the sum of probabilities is not necessarily one. But still:

**Theorem 3.9.** Let $G$ be a GDatalog[$\Delta$] program, and $I$ an input for $G$. Then $\sum_{J \in \Omega^G_I(I)} Pr_{G,I}(J) \leq 1$.

We conclude this section with some comments. First, we note that the restriction of a conclusion of a rule to include a single $\Delta$-term significantly simplifies the presentation, but does not reduce the expressive power. In particular, we could simulate multiple $\Delta$-terms in the conclusion using a collection of predicates and rules. For example, if one wishes to have conclusion where a person gets both a random height and a random weight (possibly with shared parameters), then she can do so by deriving PersonHeight$(p, h)$ and PersonWeight$(p, w)$ separately, and using the rule PersonHW$(p, h, w) \leftarrow$ PersonHeight$(p, h)$, PersonWeight$(p, w)$. We also highlight the fact that our framework can easily simulate the probabilistic database model of independent tuples with probabilities mentioned in the database, using the Flip distribution, as follows. Suppose that we have the EDB relation $R(x, p)$ where $p$ represents the probability of every tuple. Then we can obtain the corresponding probabilistic relation $R'$ using the rules $S(x, Flip[p]) \leftarrow R(x, p)$ and $R'(x) \leftarrow S(x, 1)$. Finally, we note that a disjunctive Datalog rule, where the conclusion can be a disjunction of atoms, can be simulated by our model (with probabilities ignored): If the conclusion has $n$ disjuncts, then we construct a distributional rule with a probability distribution over $\{1, \ldots, n\}$, and additional $n$ deterministic rules corresponding to the atoms.

4. CHASING GENERATIVE PROGRAMS

The chase [328] is a classic technique used for reasoning about tuple-generating dependencies and equality-generating dependencies. In the special case of full tuple-generating dependencies, which are syntactically isomorphic to Datalog rules, the chase is closely related to a (tuple-at-a-time version of) the naive bottom-up evaluation strategy for Datalog program (cf. [2]). In this section, we present a suitable variant of the chase for generative Datalog programs, and analyze some of its properties. The goal of that is twofold. First, as we will show, the chase provides an intuitive executional counterpart of the declarative semantics in Section 3. Second, we use the chase to prove Theorems 3.8 and 3.9.

We note that, although the notions and results could arguably be phrased in terms of a probabilistic extension of bottom-up Datalog evaluation strategy, the fact that a GDatalog[$\Delta$] rule can create new values makes it more convenient to phrase them in terms of a suitable adaptation of the chase procedure.

To simplify the notation in this section, we fix a GDatalog[$\Delta$] program $G = (\mathbb{E}, \mathcal{I}, \Theta)$. Let $\hat{G} = (\mathbb{E}, \mathcal{I}^{\Delta}, \Theta^{\Delta})$ be the associated Datalog$^{\Delta}$ program.

We define the notions of chase step and chase tree.

**Chase step.** Consider an instance $J$, a rule $\tau \in \Theta^{\Delta}$ of the form $\psi(x) \leftarrow \varphi(x)$, and a tuple $a$ such that $\varphi(a)$ is satisfied in $J$ but $\psi(a)$ is not satisfied in $J$. If $\psi(x)$ is a distributional atom of the form $\exists yR^b_i(t, y, t', p)$, then $\psi$ being “not satisfied” is interpreted in the logical sense (regardless of probabilities): there is no $y$ such that the tuple $(t, y, t', p)$ is in $R^b_i$. In that case, let $J'$ be the set of all instances $J_h$ obtained by extending $J$ with $\psi(a)$ for a specific value $b$ of the existential variable $y$, such that $\delta(b|p) > 0$. Furthermore, let $\pi$ be the discrete probability distribution over $J$ that assigns to $J_h$ the probability mass $\delta(b|p)$. If $\psi(x)$ is an ordinary atom without existential quantifiers, $J$ is simply defined as $\{J'\}$, where $J'$ extends $J$ with the facts in $\psi(a)$, and $\pi(J') = 1$. Then, we say that $J \xrightarrow{\tau(a)} (J', \pi)$ is a valid chase step.

**Chase tree.** Let $I$ be an input instance for $G$. A chase tree for $I$ w.r.t. $G$ is a possibly infinite tree, whose nodes are labeled by instances over $\mathbb{E} \cup \mathcal{I}$, and whose edges are labeled by a real number $r \in [0, 1]$ such that

1. The root is labeled by $I$;

2. For each non-leaf node labeled $J$, if $J$ is the set of labels of the children of the node, and if $\pi$ is the map assigning to each $J' \in J$ the label of the edge from $J$ to $J'$, then $J \xrightarrow{\tau(a)} (J', \pi)$ is a valid chase step for some rule $\tau \in \Theta^{\Delta}$ and tuple $a$.

3. For each leaf node labeled $J$, there does not ex-
ist a valid chase step of the form $J \xrightarrow{\tau(n)} (\mathcal{J}, \pi)$. In other words, the tree cannot be extended to a larger chase tree.

We denote by $L(v)$ the label (instance) of the node $v$. Each instance $L(v)$ of a node of $v$ of a chase tree is said to be an intermediate instance w.r.t. that chase tree. A chase tree is said to be injective if no intermediate instance is the label of more than one node; that is, for $v_1 \neq v_2$ we have $L(v_1) \neq L(v_2)$. As we will see shortly, due to the specific construction of $\Theta^\Delta$, every chase tree turns out to be injective.

Properties of the chase. We now state some properties of our chase procedure.

**Proposition 4.1.** Let $I$ be any input instance, and consider any chase tree for $I$ w.r.t. $\mathcal{G}$. Then every intermediate instance satisfies all functional dependencies associated to distributional relations.

**Proposition 4.2.** Every chase tree w.r.t. $\mathcal{G}$ is injective.

We denote by leaves($T$) the set of leaves of a chase tree $T$, and we denote by $L$ (leaves($T$)) the set $\{L(v) \mid v \in$ leaves($T$)$\}$.

**Theorem 4.3.** Let $T$ be a chase tree for an input instance $I$ w.r.t. $\mathcal{G}$. The following hold.

1. Every intermediate instance is a subset of some possible outcome in $\Omega_\mathcal{G}(I)$.
2. If $T$ does not have infinite directed paths, then $L$(leaves($T$)) $= \Omega^\mathcal{G}_I(I)$.

This theorem is a special case of a more general result, Theorem 5.3, which we prove later.

### 4.1 Proof of Theorems 3.8 and 3.9

By construction, for every node of a chase tree $T$, the weights of the edges that emanate from the node in question sum up to one. We can associate to each intermediate instance $L(v)$ a weight, namely the product of the edge labels on the path from the root to $v$. This weight is well defined, since $T$ is injective. We can then consider a random walk over the tree, where the probabilities are given by the edge labels. Then, for a node $v$, the weight of $L(v)$ is equal to the probability of visiting $v$ in this random world. From Theorem 4.3, we conclude that, if all the possible outcomes are finite, then $T$ does not have any infinite paths, and moreover, the random walk defines a probability distribution over the labels of the leaves, which are the possible outcomes. This is precisely the probability distribution of Theorem 3.8. Moreover, in the general case, $\Sigma_{T \in \mathcal{G}^\mathcal{F}(I)} \Pr_{\mathcal{G}, I}(J)$ is the probability that the random walk terminates (at a leaf), and hence, Theorem 3.9 follows from the fact that this probability (as is any probability) is a number between zero and one.

### 5. Infinite Possible Outcomes

In the general case of a GDatolog[$\Delta$] program, possible outcomes may be infinite, and moreover, the space of possible outcomes may be uncountable.

**Example 5.1.** We now discuss examples that show what would happen if we straightforwardly extended our current definition of the probability $\Pr_{\mathcal{G}, I}(J)$ of possible outcomes $J$ to infinite possible outcomes (where, in the case where $J$ is infinite, $\Pr_{\mathcal{G}, I}(J)$ would be the limit of an infinite product of weights).

Consider the GDatolog[$\Delta$] program defined by the rule $R(y, \delta[y]) \leftarrow Q(x, y)$ where $\delta$ is a probability distribution with one parameter $p$ and such that $\delta(z|p)$ is equal to 1 if $z = 2p$ and 0 otherwise. Then, $I = \{R(0,1)\}$ has no finite possible outcome. In fact, $I$ has exactly one infinite possible outcome: $\{R(0,1)\} \cup \{R^\mathcal{F}_2(2^i, 2^{i+1}) \mid i \geq 0\} \cup \{R^\mathcal{F}_2(2^i, 2^{i+1}) \mid i \geq 0\}$.

Now consider the previous program extended with the rule $R(0, \text{Flip}[0.5]) \leftarrow Q(x)$, and consider the input instance $I' = \{Q(0)\}$. Then, $I'$ has one finite possible outcome $J = \{Q(0), R(0,0), R^\mathcal{F}_2(0,0,0.5)\}$ with $\Pr_{\mathcal{G}, I'}(J) = 0.5$, and another infinite possible outcome $J' = \{R(0,1), R^\mathcal{F}_2(0,1,0.5)\} \cup \{R^\mathcal{F}_2(2^i, 2^{i+1}, 2^i) \mid i \geq 0\} \cup \{R^\mathcal{F}_2(2^i, 2^{i+1}) \mid i \geq 0\}$ with $\Pr_{\mathcal{G}, I'}(J') = 0.5$.

Next, consider the GDatolog[$\Delta$] program defined by $R(y, \delta'[y]) \leftarrow Q(x, y)$, where $\delta'$ is a probability distribution with one parameter $p$, and $\delta'(z|p)$ is equal to 0.5 if $z \in \{2p, 2p+1\}$ and 0 otherwise. Then, for $I = \{R(0,1)\}$, every possible outcome is infinite, and would have the probability 0.

Now consider the previous program extended with the rule $R(0, \text{Flip}[0.5]) \leftarrow Q(x)$, and consider again the input instance $I' = \{Q(0)\}$. Then $I'$ would have exactly one possible outcome $J$ with $\Pr_{\mathcal{G}, I'}(J) > 0$, namely $J = \{Q(0), R(0,0), R^\mathcal{F}_2(0,0,0.5), R^\mathcal{F}_2(0,0,0)\}$ where $\Pr_{\mathcal{G}, I'}(J) = 0.25$.

### 5.1 Generalization of Probabilistic Semantics

To generalize our framework, we need to consider probability spaces over uncountable domains; those are defined by means of measure spaces, which are defined as follows.

Let $\Omega$ be a set. A $\sigma$-algebra over $\Omega$ is a collection $\mathcal{F}$ of subsets of $\Omega$, such that $\mathcal{F}$ contains $\Omega$ and is closed under complement and countable unions. (Implied properties include that $\mathcal{F}$ contains the empty set, and that $\mathcal{F}$ is closed under countable intersections.) If $\mathcal{F}'$ is a nonempty collection of subsets of $\Omega$, then the closure of $\mathcal{F}'$ under complement and countable unions is a $\sigma$-algebra, and it is said to be generated by $\mathcal{F}'$.

A probability measure space is a triple $(\Omega, \mathcal{F}, \pi)$, where: (1) $\Omega$ is a set, called the sample space. (2) $\mathcal{F}$ is a $\sigma$-algebra over $\Omega$, and (3) $\pi : \mathcal{F} \rightarrow [0, 1]$, called a probability measure, is such that $\pi(\Omega) = 1$, and $\pi(\bigcup E) = \sum e \in E \pi(e)$ for every countable set $E$ of pairwise-disjoint measurable sets.
Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, and let $I$ be an input for $\mathcal{G}$. We say that a sequence $f = (f_1, \ldots, f_n)$ of facts is a derivation (w.r.t. $I$) if for all $i = 1, \ldots, n$, the fact $f_i$ is the result of applying some rule of $\mathcal{G}$ that is not satisfied in $I \cup \{f_1, \ldots, f_{i-1}\}$ (in the case of applying a rule with a $\Delta$-atom in the head, choosing a value randomly). If $f_1, \ldots, f_n$ is a derivation, then the set $\{f_1, \ldots, f_n\}$ is a derivation set. Hence, a finite set $F$ of facts is a derivation set if and only if $I \cup F$ is an intermediate instance in some chase tree.

Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, let $I$ be an input for $\mathcal{G}$, and let $F$ be a set of facts. We denote by $\Omega^F_G(I)$ the set of all the possible outcomes $J \subseteq \Omega_G(I)$ such that $F \subseteq J$. The following theorem states how we determine the measure space defined by a GDatalog[$\Delta$] program.

**Theorem 5.2.** Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, and let $I$ be an input for $\mathcal{G}$. There exists a unique probability measure space $(\Omega, \mathcal{F}, \pi)$, denoted $\mu_G$, that satisfies all of the following.

1. $\Omega = \Omega_G(I)$;
2. The $\sigma$-algebra $(\Omega, \mathcal{F})$ is generated from the sets of the form $\Omega^F_G(I)$ where $F$ is finite;
3. $\pi(\Omega^F_G(I)) = \mathbf{P}(F)$ for every derivation set $F$.

Moreover, if $J$ is a finite possible outcome, then $\pi(J) = \mathbf{P}(F)$.

Observe that the items (i) and (ii) of Theorem 5.2 describe the unique properties of the probability measure space. The proof will be given in the next section. The last part of the theorem states that our discrete and continuous probability definitions coincide on finite possible outcomes; this is a simple consequence of item (ii), since for a finite possible outcome $J$, the set $F = J \setminus I$ is such that $\Omega^F_G(I) = \{J\}$, and $F$ is itself a derivation set (e.g., due to Theorem 4.3).

### 5.2 Measure Spaces by Infinite Chase

We prove Theorem 5.2 by defining and investigating measure spaces that are defined in terms of the chase. Consider a GDatalog[$\Delta$] program $\mathcal{G}$ and an input $I$ for $\mathcal{G}$. A maximal path of a chase tree $T$ is a path $P$ that starts with the root, and either ends in a leaf or is infinite. Observe that the labels (instances) along a maximal path form a chain (w.r.t. the set-containment partial order). A maximal path $P$ of a chase tree is fair if whenever the premise of a rule is satisfied by some tuple in some intermediate instance on $P$, then the conclusion of the rule is satisfied for the same tuple in some intermediate instance on $P$. A chase tree $T$ is fair (or has the fairness property) if every maximal path is fair. Note that every finite chase tree is fair. We will restrict attention to fair chase trees. Fairness is a classic notion in the study of infinite computations; moreover, fair chase trees can easily be constructed, for examples, by maintaining a queue of “active rule firings” (cf. any textbook on term rewriting systems or lambda calculus).

Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, let $I$ be an input for $\mathcal{G}$, and let $T$ be a chase tree. We denote by $\text{paths}(T)$ the set of all the maximal paths of $T$. (Note that $\text{paths}(T)$ may be uncountably infinite.) For $P \in \text{paths}(T)$, we denote by $\cup P$ the union of the (chain of) labels $L(v)$ along $P$. The following generalizes Theorem 1.3.

**Theorem 5.3.** Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, let $I$ be an input for $\mathcal{G}$, and $T$ a fair chase tree. The mapping $P \rightarrow \cup P$ is a bijection between $\text{paths}(T)$ and $\Omega_G(I)$.

### 5.3 Chase Measures

Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, let $I$ be an input for $\mathcal{G}$, and let $T$ be a chase tree. Our goal is to define a probability measure over $\Omega_G(I)$. Given Theorem 5.3, we can do that by defining a probability measure over $\text{paths}(T)$. A random path in $\text{paths}(T)$ can be viewed as a Markov chain that is defined by a random walk over $T$, starting from the root. A measure space for such a Markov chain is defined by means of cylinderification [6]. Let $v$ be a node of $T$. The $v$-cylinder of $T$, denoted $C_v^T$, is a subset of $\text{paths}(T)$ that consists of all the maximal paths that contain $v$. A cylinder of $T$ is a subset of $\text{paths}(T)$ that forms a $v$-cylinder for some node $v$. We denote by $C(T)$ the set of all the cylinders of $T$.

Recall that $L(v)$ is a finite set of facts, and observe that $\mathbf{P}(L(v))$ is the product of the weights along the path from the root to $v$. The following theorem is a special case of a classic result on Markov chains (cf. [6]).

**Theorem 5.4.** Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, let $I$ be an input for $\mathcal{G}$, and let $T$ be a chase tree. There exists a unique probability measure $(\Omega, \mathcal{F}, \pi)$ that satisfies all of the following.

1. $\Omega = \text{paths}(T)$.
2. $(\Omega, \mathcal{F})$ is the $\sigma$-algebra generated from $C(T)$.
3. $\pi(C_v^T) = \mathbf{P}(L(v))$ for all nodes $v$ of $T$.

Theorems 5.3 and 5.4 suggest the following definition.

**Definition 5.5 (Chase Probability Measure).** Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, let $I$ be an input for $\mathcal{G}$, let $T$ be a chase tree, and let $(\Omega, \mathcal{F}, \pi)$ be the probability measure of Theorem 5.4. The probability measure $\mu_T$ over $\Omega_G(I)$ is the one obtained from $(\Omega, \mathcal{F}, \pi)$ by replacing every maximal path $P$ with the possible outcome $\cup P$.

Next, we prove that the probability measure space represented by a chase tree is independent of the specific chase tree of choice. For that, we need some notation and a lemma. Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, let $I$ be an input for $\mathcal{G}$, let $T$ be a chase tree, and let $v$ be a node of $T$. We denote by $\cup \bigcup C_v^T$ the set $\{\cup P \mid P \in C_v^T\}$. The following lemma is a consequence of Propositions 1.1 and 5.3.
Lemma 5.6. Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, let $I$ be an input for $\mathcal{G}$, and let $T$ be a fair chase tree. Let $v$ be a node of $T$ and $F = L(v)$. Then $\cup C_v^T = \Omega_{\mathcal{G}}^{F_c}(I)$; that is, $\cup C_v^T$ is the set $\{ J \in \Omega_{\mathcal{G}}(I) \mid L(v) \subseteq J \}$.

Using Lemma 5.6 we can prove the following theorem.

Theorem 5.7. Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, let $I$ be an input for $\mathcal{G}$, and let $T$ and $T'$ be two fair chase trees. Then $\mu_T = \mu_{T'}$.

5.4 Proof of Theorem 5.2

We can now prove Theorem 5.2. Let $\mathcal{G}$ be a GDatalog[$\Delta$] program, let $I$ be an input for $\mathcal{G}$, and let $T$ be a fair chase tree for $I$ w.r.t. $\mathcal{G}$. Let $\mu_T = (\Omega_{\mathcal{G}}(I), \mathcal{F}_T, \pi_T)$ be the probability measure on $\Omega_{\mathcal{G}}(I)$ associated to $T$, as defined in Definition 5.3.

Lemma 5.8. The $\sigma$-algebra $(\Omega_{\mathcal{G}}(I), \mathcal{F}_T)$ is generated by the sets of the form $\Omega_{\mathcal{G}}^{F_c}(I)$, where $F$ is finite.

Proof. Let $(\Omega_{\mathcal{G}}(I), \mathcal{F})$ be the $\sigma$-algebra generated from the sets $\Omega_{\mathcal{G}}^{F_c}(I)$. We will show that every $\Omega_{\mathcal{G}}^{F_c}(I)$ is in $\mathcal{F}_T$, and that every $\cup C_v^T$ is in $\mathcal{F}$. The second claim is due to Lemma 5.4 so we will prove the first. So, let $\Omega_{\mathcal{G}}^{F_c}(I)$ be given. Due to Lemma 5.7, the set $\Omega_{\mathcal{G}}^{F_c}(I)$ is the countable union $\cup_{u \in U}(\cup C_u^T)$ where $U$ is the set of all the nodes $u$ such that $F \subseteq u$. Hence, $\Omega_{\mathcal{G}}^{F_c}(I) \in \mathcal{F}_T$. □

Lemma 5.9. For every derivation set $F$ we have $\pi_T(\Omega_{\mathcal{G}}^{F_c}(I)) = \text{P}(F)$.

Proof. Let $F$ be a derivation set. Due to Theorem 5.2 it suffices to prove that for some chase tree $T$ it is the case that $\pi_T(\Omega_{\mathcal{G}}^{F_c}(I)) = \text{P}(F)$. But since $F$ is a derivation set, we can craft a chase tree $T'$ that has a node $v$ with $L(v) = F$. Then we have that $\pi_T(\Omega_{\mathcal{G}}^{F_c}(I))$ is the product of the weights along the path to $v$, which is exactly $\text{P}(F)$. □

Lemma 5.10. Let $\mu = (\Omega, \mathcal{F}, \pi)$ be any probability space that satisfies (i)–(iii) of Theorem 5.3. Then $\mu_T = \mu_{\pi_T}$.

Proof. Let $\mu_T = (\Omega_{\mathcal{G}}(I), \mathcal{F}_T, \pi_T)$. Due to Lemma 5.8 we have that $\mathcal{F} = \mathcal{F}_T$. So it is left to prove that $\pi = \pi_T$. Due to Lemmas 5.2 and 5.8 we have that $\pi$ agrees with $\pi_T$ on the cylinder sets of $T$. Due to Theorems 5.3 and 5.4 we get that $\pi$ must be equal to $\pi_T$ due to the uniqueness of $\pi_T$. □

The above lemmas show that $\mu_T = (\Omega_{\mathcal{G}}(I), \mathcal{F}_T, \pi_T)$ is a probability measure space that satisfies (i) and (ii) of Theorem 5.2 and moreover, that no other probability measure space satisfies (i) and (ii).

6. PROBABILISTIC-PROGRAMMING DATALOG

To complete our framework, we define probabilistic-programming Datalog, PPDL for short, wherein a program augments a generative Datalog program with constraints; these constraints unify the traditional integrity constraints of databases and the traditional observations of probabilistic programming.

Definition 6.1 (PPDL[$\Delta$]). Let $\Delta$ be a finite set of parametrized numerical distributions. A PPDL[$\Delta$] program is a quadruple $(\mathcal{E}, \mathcal{I}, \Theta, \Phi)$, where $(\mathcal{E}, \mathcal{I}, \Theta)$ is a GDatalog[$\Delta$] program and $\Phi$ is a finite set of logical constraints over $\mathcal{E} \cup \mathcal{I}$.

Example 6.2. Consider again Example 3.2. Suppose that we have the EDB relations ReportHAlarm and ReportBAlarm that represent reported home and business alarms, respectively. We obtain from the program in the example a PPDL[$\Delta$]-program by adding the following constraints.

1. ReportHAlarm($h$) $\rightarrow$ Alarm($h$)

2. ReportBAlarm($b$) $\rightarrow$ Alarm($b$)

Note that we use right (in contrast to left) arrows to distinguish constraints from ordinary Datalog rules. □

The semantics of a PPDL[$\Delta$] program is the posterior distribution over the corresponding GDatalog[$\Delta$] program, conditioned on the satisfaction of the constraint. A formal definition follows.

Let $\mathcal{P} = (\mathcal{E}, \mathcal{I}, \Theta, \Phi)$ be a PPDL[$\Delta$] program, and let $\mathcal{G}$ be the GDatalog[$\Delta$] program $(\mathcal{E}, \mathcal{I}, \Theta)$. An input instance for $\mathcal{P}$ is an input instance $I$ for $\mathcal{G}$. We say that $I$ is a legal input instance for $\mathcal{P}$ if $\{ J \in \Omega_{\mathcal{G}}(I) \mid J \models \Phi \}$ is a measurable set in the probability space $\mu_{\mathcal{G}, I}$, and moreover, its measure is nonzero. Intuitively, an input instance $I$ is legal if it is consistent with the observations (i.e., with the conjunction of the constraints in $\Phi$), given $\mathcal{G}$. The semantics of a PPDL[$\Delta$] program is defined as follows.

Definition 6.3. Let $\mathcal{P} = (\mathcal{E}, \mathcal{I}, \Theta, \Phi)$ be a PPDL[$\Delta$] program, and let $\mathcal{G}$ be the GDatalog[$\Delta$] program $(\mathcal{E}, \mathcal{I}, \Theta)$. Let $I$ be a legal input instance for $\mathcal{P}$, and let $\mu_{\mathcal{G}, I} = (\Omega_{\mathcal{G}}(I), \mathcal{F}_I, \pi_{\mathcal{G}, I})$. The probability space defined by $\mathcal{P}$ and $I$, denoted $\mu_{\mathcal{P}, I}$, is the triple $(\Omega_{\mathcal{P}}(I), \mathcal{F}_I, \pi_{\mathcal{P}})$ where:

- $\Omega_{\mathcal{P}}(I) = \{ J \in \Omega_{\mathcal{G}}(I) \mid J \models \Phi \}$
- $\mathcal{F}_I = \{ S \cap \Omega_{\mathcal{P}}(I) \mid S \in \mathcal{F}_I \}$
- $\pi_{\mathcal{P}}(S) = \pi_{\mathcal{G}}(S)/\pi_{\mathcal{G}}(\Omega_{\mathcal{P}}(I))$ for every $S \in \mathcal{F}_I$.

In other words, $\mu_{\mathcal{P}, I}$ is $\mu_{\mathcal{G}, I}$ conditioned on $\Phi$.

Example 6.4. Continuing Example 3.2, the semantics of this program is the posterior probability distribution for the prior of Example 3.2 under the conditions that the alarm is on whenever it is reported.

1. The restriction of the language of constraints to a fragment with tractability (or other goodness) properties is beyond the scope of this paper.
Then, one can ask various queries over the probability space defined, for example, the probability of the fact Earthquake(Napa, 1). Observe that, with negation, we could also phrase the condition that an alarm is off unless reported.

We note that a traditional integrity constraint on the input (e.g., there are no \( x, c_1 \) and \( c_2 \) such that both \( \text{Home}(x, c_1) \) and \( \text{Business}(x, c_2) \) hold) can be viewed as a constraint in \( \Phi \) that holds with either probability 0 (and then the input is illegal) or with probability 1 (and then the prior \( \mu_{\Phi, I} \) is the same as the posterior \( \mu_{P, I} \)).

An important direction for future work is to establish tractable conditions that guarantee that a given input is legal. Also, an interesting problem is to detect conditions under which the chase is a self conjugate \(^{[39]} \). That is, the probability space \( \mu_{P, I} \) is captured by a chase procedure without backtracking.

### 7. Extensions and Future Work

Our ultimate goal is to design a language for probabilistic programming that possesses the inherent declarative and logical nature of Datalog. To that end, extensions are required. In this section we discuss some of the important future directions and challenges to pursue. We focus on the semantic aspects of expressive power. (An obvious aspect for future work is a practical implementation, e.g., corresponding sampling techniques.)

#### 7.1 Unbounded Number of Parameters

It is often the case that the probability distributions have a large number of parameters. A simple example is the categorical distribution where a single member of a finite domain of items is to be selected, each item with its own probability. In that case, the domain can be very large, and moreover, it can be determined dynamically from the database content and be unknown to the static program. To support such distributions, one can associate the distribution with a relation symbol in a schema, and here we illustrate it for the case of a categorical distribution.

Let \( R \) be a relation symbol. A categorical distribution over \( R \) is associated with two attributes \( i \) and \( j \) of \( R \) that determine dynamic parameters: \( i \) represents a possible value, and \( j \) represents its probability. In addition, the distribution is associated with a tuple \( g \) of attributes of \( R \) that split \( R \) into groups with the semantics of SQL's GROUP BY. We denote this distribution by \( \text{Cat}^R(i, j; g)(x; q) \), where \( g \) and \( q \) have the same length. Given a relation \( R^I \) over \( R \) and parameters \( q \), let \( R^*_g \) be the sub-relation of \( R^I \) that have the values in the attributes vector \( g \) equal to \( q \). Suppose that the facts of \( R^*_g \) are \( f_1, \ldots, f_n \). We assume that \( f_k[j] \in [0, 1] \) for all \( k = 1, \ldots, n \), and moreover, that \( \sum_{k=1}^n f_k[j] = 1 \). Then we define \( \text{Cat}^R(i, j; g)(x; q) = s \), where \( s \) is the sum of \( f_k[j] \) over all \( k \in \{1, \ldots, n\} \) with \( f_k[i] = x \).

As an example, consider the relation \( \text{Cor}(w, e, q) \) that provides, for every English word \( w \), a distribution over the possible misspelled words \( w_e \); hence, the fact \( \text{Cor}(w, e, q) \) means that \( w_e \) is misspelled into \( w \) with probability \( q \). In our notation, this distribution will be captured by the notation \( \text{Cat}^{\text{Cor}}(2; 3; 1)(w, e, w) \). Hence, the following program contains, for each document, the set of words that the document can contain by replacing each word with a corresponding correction. The relation \( \text{Doc}(d, i, w) \) denotes that document \( d \) has the word \( w \) as its \( i \)th token. The relation \( \text{CDoc} \) is the same as \( \text{Doc} \), except that each word is replaced with a random correction.

\[
\text{CDoc}(d, i, \text{Cat}^{\text{Cor}}(2; 3; 1)(w_e; w)) \leftarrow \text{Doc}(d, i; w)
\]

7.3 Continuous Distributions

A natural and important extension is to support multivariate distributions, which are distributions with a support in \( \mathbb{R}^k \) for \( k > 1 \). Examples of popular such distributions are multinomial, Dirichlet, and multivariate Gaussian distribution. When \( k \) is fixed, one can replace our single distributional term with multiple such terms. But when \( k \) is unbounded, such a distribution should be supported as an aggregate operation that implies in a set of facts (rather than a single one).

#### 7.3 Continuous Distributions
A natural extension of our framework is the support of continuous probability distributions (e.g., continuous uniform, Pareto, Gaussian, Dirichlet, etc.). This is a very important extension, as such distributions are highly popular in defining statistical models. Syntactically, this extension is straightforward: we just need to include these distributions in $\Delta$. Likewise, extending the probabilistic chase is also straightforward.

The challenge, though, is with the semantic analysis, and in particular, with the definition of the probability space implied by the chase. When a chase step involves a continuous numeric distribution, such as $U(0,1)$ (the uniform distribution between 0 and 1), then no chase step is measurable, and hence, we can no longer talk about the probability of a step or the probability of a cylinder set (but we can talk about the density of those). Note that our definition of the measure space in Section is inherently based on the assumption that the set of possible outcomes that contains a given finite set of facts is measurable. But to support continuous distribution, the definition of measurable sets will need to be based on sets of paths. We refer this to future work, and we believe that our current framework will naturally extend to continuous distributions.

8. CONCLUDING REMARKS

We proposed and investigated a declarative framework for specifying statistical models in the context of a database, based on an extension of Datalog with numerical distributions. The framework differs from traditional probabilistic programming languages not only due to the tight integration with a database, but also because of its fully declarative rule-based language: the interpretation of a program is independent under transformations (such as reordering or duplication of rules) that preserve the first-order semantics. This was achieved by treating a GDatalog$[\Delta]$ program as a Datalog program with existentially quantified variables in the conclusion, and using the minimal solutions as the sample space of a (discrete or continuous) probability distribution. Using a suitable notion of chase that we introduced, we established that the resulting probability distributions are well-defined and robust.

This work is done as part of the effort to extend the LogicBlox database and its Datalog-based data management language LogiQL, to support the specification of statistical models. Through its purely declarative rule-based syntax, such an extension of LogiQL allows for natural specifications of statistical models. Moreover, there is a rich literature on (extensions of) Datalog, and we expect that, through our framework, techniques and insights from this active research area can be put to use to advance the state of the art in probabilistic programming.

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APPENDIX

A. ADDITIONAL PROOFS

A.1 Proof of Theorem 3.6
Theorem 3.6. If a GDatalog[Δ] program G is weakly acyclic, then \( \Omega_G(I) = \Omega^P_G(I) \) for all input instances I.

Proof. It is easy to show that if G is weakly acyclic in our sense, then P is weakly acyclic according to the classic definition of weak acyclicity given in [18]. We then apply the following result (restated here to match our notation), which was established in [20]: if a Datalog program D is weakly acyclic, then there is a polynomial p(\( I \)) (depending only on D) such that for every input instance I and for every solution J of I w.r.t. D, there is a solution J′ of I w.r.t. D with \( |J′| \leq p(|I|) \). In particular, all J ∈ min-sol(D) are finite and have size at most p(|I|).

A.2 Proof of Proposition 4.1

Proposition 4.1. Let I be any input instance, and consider any chase tree for I w.r.t. G. Then every intermediate instance satisfies all functional dependencies associated to distributional relations.

Proof. The proof proceeds by induction on the distance from the root of the chase tree. Suppose that in a chase step J \( \rightarrow \pi(a) \) (J, π), some J′ ∈ J contains two \( R^k_i \)-facts that are identical except for the i-th attribute. Then either J already contains both atoms, in which case we can apply our induction hypothesis, or J′ is obtained by extending J with one of the two facts in question, in which case, it is easy to see that the conclusion of τ was already satisfied for the tuple a, which is not possible in case of a valid chase step.

A.3 Proof of Proposition 4.2

Proposition 4.2. Every chase tree w.r.t. G is injective.

Proof. For the sake of a contradiction, assume that two nodes n1 and n2 in a chase tree are labeled by the same instance J. Let n0 be the node that is the least common ancestor of n1 and n2 in the tree, and let n′ 1 and n′ 2 be the children of n0 that are ancestors of n1 and n2, respectively. By construction, n′ 1 and n′ 2 are labeled with distinct instances \( J_1 \neq J_2 \), respectively. Consider the rule τ = \( \psi(x) \leftarrow \varphi(x) \) and tuple a constituting the chase step applied at node n0. Since n0 has more than one child, \( \psi(x) \) must be a distributional atom, say \( \exists y R^k_i(t, y, t', p) \). Then each \( J_k \) (k = 1, 2) contains an \( R^k_i \)-fact. Moreover, the two \( R^k_i \)-facts in question differ in the choice of value for the variable y, and are otherwise identical. Due to the monotonic nature of the chase, both atoms must belong J, and hence, J′ violates the functional dependency of Proposition 4.1. Hence, we have reached a contradiction.

A.4 Proof of Theorem 5.3

Theorem 5.3. Let G be a GDatalog[Δ] program, I an input for G, and T a fair chase tree. The mapping \( P \to \cup P \) is a bijection between \( \text{paths}(T) \) and \( \Omega_G(I) \).

Proof. We first prove that every \( \cup P \) is in \( \Omega_G(I) \). Let \( P \in \text{paths}(T) \) be given. We need to show that \( \cup P \in \Omega_G(I) \). By definition it is the case that every distributional fact of \( \cup P \) has a nonzero probability. It is also clear that \( \cup P \) is consistent, due to the fairness property of T. Hence, it suffices to prove that \( \cup P \) is a minimal solution, that is, no proper subset of \( \cup P \) is a solution. So, let K be a strict subset of \( \cup P \) and suppose, by way of contradiction, that K is also a solution. Let \( (J, J′) \) be the first edge in \( P \) such that \( \cup P \) contains a fact that is not in K. Now, consider the chase step that leads from J to J′. Let f be the unique fact in \( J′ \setminus J \). Then \( J \subseteq K \) and \( f \in J′ \setminus K \). The selected rule τ in this step cannot be deterministic, or otherwise K must contain f as well. Hence, it is a distributional rule, and f has the form \( R^k_i(a[p]) \). But then, K satisfies this rule, and hence, K must include a fact \( f′ = R^k_i(a′[p]) \), where a′ differs from a only in the ith element. And since some node in \( \cup P \) contains both f and f′, we get a violation of the fd of Proposition 4.1. Hence, a contraction.

Next, we prove that every possible outcome J in \( \Omega_G(I) \) is equal to \( \cup P \) for some \( P \in \text{paths}(T) \). Let such \( J \) be given. We build the path P inductively, as follows. We start with the root, and upon every node v we select the next edge to be one that leads to a subset K of J; note that K must exist since J resolves the rule violated in \( L(v) \) by some fact, and that fact must be in one of the children of v. Now, \( \cup P \) is consistent since T is fair, and \( \cup P \subseteq J \) by construction. And since J is a minimal solution, we get that \( \cup P \) is in fact equal to J.

Finally, we need to prove that if \( \cup P_1 = \cup P_2 \) then \( P_1 = P_2 \). We will prove the contrapositive statement. Suppose that \( P_1, P_2 \in \text{paths}(T) \) are such that \( P_1 \neq P_2 \). The two paths agree on the root. Let J be the first node in the paths such that the two paths disagree on the outgoing edge of J. Suppose that P1 has the edge from J to J1 and P2 has an edge from J to J2. Then J1 ∪ J2 have a pair of facts that violate the functional dependency of Proposition 4.1, and in particular, \( J_1 \not\subseteq \cup P_2 \). We conclude that \( \cup P_1 = \cup P_2 \), as claimed.

A.5 Proof of Theorem 5.7

Theorem 5.7. Let G be a GDatalog[Δ] program, let I be an input for G, and let T and T′ be two fair chase trees. Then \( \mu_T = \mu_{T′} \).

Proof. Let \( \mu_T = (\Omega, F, \pi) \) and \( \mu_{T′} = (\Omega′, F′, \pi′) \). We need to prove that \( \Omega = \Omega′ \), \( F = F′ \) and \( \pi = \pi′ \). We have \( \Omega = \Omega′ \) due to Theorem 5.3. To prove that \( F = F′ \), it suffices to prove that every \( \cup C^T_{\sigma} \) is in \( F′ \) and \( \cup C^{T′}_{\sigma} \) is in \( F \) (since both \( \sigma \)-algebras are generated by the cylinders). And due to symmetry, it suffices to prove that \( C^T_{\sigma} \) is in \( F′ \). So, let \( \nu′ \) be a node of \( T′ \). Recall that \( L(\nu′) \) is a set of facts. Due to Lemma 5.6 we have that \( \cup C^T_{\sigma} \) precisely the set of all possible outcomes J in \( \Omega_G(I) \) such that \( L(\nu′) \subseteq J \). Let U be the set of all the nodes of u of P with \( L(\nu′) \subseteq L(u) \). Then, due
to Theorem 5.3 we have that \( \cup C_{v'}^{T'} = \cup_{w \in U}(\cup C_{v}^{T}) \). Observe that \( U \) is countable, since \( T \) has only a countable number of nodes (as every node is identified by a finite path from the root). Moreover, \((\Omega, \mathcal{F})\) is a closed under countable unions, and therefore, \( \cup_{w \in U}(\cup C_{v}^{T}) \) is in \( \mathcal{F} \).

It remains to prove that \( \pi = \pi' \). By now we know that the \( \sigma \)-algebras \((\Omega, \mathcal{F})\) and \((\Omega', \mathcal{F}')\) are the same. Due to Theorem 5.3 every measure space over \((\Omega, \mathcal{F})\) can be translated into a measure space over the cylinder algebra of \( T \) and \( T' \). So, due to the uniqueness property of Theorem 5.3 it suffices to prove that every \( \cup C_{v'}^{T'} \) has the same probability in \( \mu_{T'} \) and \( \mu_{T'} \). That is, \( \pi(\cup C_{v'}^{T'}) = \mathbb{P}(L(v')) \). We do so next. We assume that \( v' \) is not the root of \( T' \), or otherwise the claim is straightforward. Let \( U \) be the set of all the nodes \( u \) in \( T \) with the property that \( L(v') \subseteq L(u) \) but \( L(v') \not\subseteq L(p) \) for the parent \( p \) of \( u \). Due to Lemma 5.6 we have the following:

\[
\pi(\cup C_{v'}^{T'}) = \sum_{u \in U} \mathbb{P}(L(u))
\]

Let \( E \) be the set of all the edges \( (v_1, u_1) \) of \( T \), such that \( L(u_1) \setminus L(v_1) \) consists of a node in \( v' \). Let \( Q \) be the set of all the paths from the root of \( T \) to nodes in \( U \). Due to Proposition 4.1 we have that every two paths \( P_1 \) and \( P_2 \) in \( Q \) and edges \( (v_1, u_1) \) and \( (v_2, u_2) \) in \( P_1 \) and \( P_2 \), respectively, if both edges are in \( E \) and \( v_1 = v_2 \), then \( u_1 = u_2 \). Let \( T'' \) be the tree that is obtained from \( T \) by considering every edge \( (v_1, u_1) \) in \( E \), changing its weight to 1, and changing the weights of remaining \( (v_1, u'_1) \) emanating from \( v_1 \) to 0. Then we have the following for every node \( u \in U \):

\[
\mathbb{P}(u) = w_{T''}(u) \cdot \mathbb{P}(L(v'))
\]

where \( w_{T''}(u) \) is the product of the weights along the path from the root of \( T'' \) to \( u \). Combining (5) and (6), we get the following.

\[
\pi(\cup C_{v'}^{T'}) = \mathbb{P}(L(v')) \cdot \sum_{u \in U} w_{T''}(u)
\]

Let \( p = \sum_{u \in U} w_{T''}(u) \). We need to prove that \( p = 1 \). Observe that \( p \) is the probability of visiting a node of \( U \) in a random walk over \( T'' \) (with the probabilities defined by the weights). Equivalently, \( p \) is the probability that random walk over \( T'' \) eventually sees all of the facts in \( v' \). But due to the construction of \( T'' \), every rule violation that arises due to facts in both \( L(v') \) and any node of \( T'' \) is deterministically resolved exactly as in \( L(v') \). Moreover, since \( L(v') \) is obtained from a chase derivation (i.e., \( L(v') \) is a derivation set), solving all such rules repeatedly results in the containment of \( L(v') \). Finally, since \( T'' \) is fair (because \( T \) is fair), we get that every random walk over \( T'' \) eventually sees all of the facts in \( L(v') \). Hence, \( p = 1 \), as claimed. \( \square \)