Static Analysis of Probabilistic Programs: An Algebraic Approach

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For my parents

Abstract

Probabilistic programs are programs that can draw random samples from probability distributions and involve random control flows. They are becoming increasingly popular and have been applied in many areas such as algorithm design, cryptographic protocols, uncertainty modeling, and statistical inference. Formal reasoning about probabilistic programs comes with unique challenges, because it is usually not tractable to obtain the exact result distributions of probabilistic programs. This thesis focuses on an algebraic approach for static analysis of probabilistic programs. The thesis first provides a brief background on measure theory and introduces an imperative arithmetic probabilistic programming language Appl with a novel hyper-graph program model. Second, the thesis presents an algebraic denotational semantics for Appl that can be instantiated with different models of nondeterminism. The thesis also develops a new model of nondeterminism that involves nondeterminacy among state transformers and presents a domain-theoretic characterization of the new model. Based on the algebraic denotational semantics, the thesis proposes a general algebraic framework PMAF for designing, implementing, and proving the correctness of static analyses of probabilistic programs. The thesis also includes a concrete static analysis—central-moment analysis for cost accumulators in probabilistic programs—and elaborates implementation strategies to improve the usability and efficiency of the analysis. There is a gap between the general PMAF framework and the central-moment analysis, in the sense that the former is based on abstraction and iterative approximation, but the latter is based on constraint solving. The thesis provides some preliminary results on bridging the gap, via the development of novel regular hyper-path expressions, which finitely represent possibly-infinite hyper-paths on control-flow hyper-graphs of probabilistic programs without nondeterminism, and DMKAT algebraic structures, which can be used to interpret regular hyper-path expressions. Future directions for extending the research covered by this thesis include developing an algebraic static-analysis framework based on DMKAT and instantiating it to perform central-moment analysis, generalizing DMKAT with support for nondeterminism and formalizing an equational axiomatization for the generalized algebraic framework, as well as applying the analysis framework developed in the thesis to the analysis and verification of statistical guarantees for Bayesian probabilistic programming.

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Chapter 1

Introduction

Probabilistic systems are becoming increasingly popular in computer science, for their capability of improving efficiency (e.g., randomized Quicksort [70]), protecting confidential information (e.g., optimal asymmetric encryption padding [12]), modeling peripheral uncertainty (e.g., airborne collision-avoidance systems [109]), and describing statistical models (e.g., probabilistic graphical models [96]). *Probabilistic programming* provides a framework for implementing and analyzing probabilistic systems, such as randomized algorithms [8], cryptographic protocols [9], cyber-physical systems [17], and machine-learning algorithms [61].

A *probabilistic program* is any program that can draw random samples from probability distributions and involve random control flows. In practice, the source of randomness is usually a *pseudo-random number generator* (e.g., the `rand()` function in C language); however, in this thesis, I focus on *true randomness*, in the sense that given an initial program state, a probabilistic program produces a *distribution* that describes the probability of its computation results. The two reasons why I assume true randomness in my development are that (i) some high-quality random number generators are shown to be sufficiently good approximations of true randomness [77], so the behavior of a program under pseudo-randomness would be conceptually close to its behavior under true randomness, and (ii) compared to pseudo-randomness, there are plenty of well-studied mathematical theories for true randomness, such as measure theory.

As the interest in probabilistic programming is increasing, there has been a corresponding increase in the study of *formal reasoning* about probabilistic programs: *What is the probability that an assertion holds after a program terminates? Is there any expression that is an invariant under expectation for a probabilistic loop? What is the expected time complexity of a program?* In general, these kinds of reasoning problems are challenging, because it is usually not tractable to compute the result distributions of probabilistic programs precisely: composing simple distributions can quickly complicate the result distribution, and randomness in the control flow can easily lead to state-space explosion. Monte-Carlo simulation [134] is a common approach to analyze probabilistic programs, but the technique does not provide formal guarantees on the accuracy of analysis results, and can sometimes be inefficient [11].

Static analysis is a longstanding area about (usually automated) techniques for analyzing and proving program properties *without* actually executing the programs. Static analysis of probabilistic programs has also received a lot of attention [19, 20, 24–29, 39, 50–52, 55, 60, 85–87, 126, 136]. In this thesis, I have conducted research on *algebraic* approaches for *compositional* static analysis of

probabilistic programs, i.e., designing and implementing static analyses based on *semantic algebra*, which consists of a space of program properties and composition operators that correspond to program constructs.

> **Thesis Statement** Algebraic static analysis helps people reason about probabilistic programs at compile time in a compositional and versatile way. Markov algebras provide a natural way to describe the algebraic structure of probabilistic programs. Based on Markov algebras, a denotational semantics for combining nondeterminism and probabilities lays the foundation for an algebraic framework for static analysis of probabilistic programs.

Denotational Semantics with Nondeterminism The first step in my development of static-analysis techniques is to provide a suitable formal semantics for probabilistic programs. Despite the fact that lots of existing work focuses on *high*-level probabilistic programs, e.g., lambda calculus [16], higher-order functions [48, 69], and recursive types [145], I observe that *low*-level features could arise naturally. For example, when developing a compiler for a probabilistic programming language [58, 128], we need a semantics for the imperative target language to prove compiler correctness. Also, static analysis of low-level code becomes desirable for verifying cross-language programs [153] and detecting security vulnerabilities [1]. There have been studies on *denotational* semantics for *well-structured* imperative programs [14, 78, 85, 98, 99, 110, 111, 126, 144], as well as *operational* semantics for *control-flow graphs* (CFGs) based on Markov chains and Markov decision processes ([27, 28, 55]). On the one hand, I prefer CFGs as program representations because they enable rich low-level features such as *unstructured* flows, e.g., those introduced by **break** and **continue**. On the other hand, from the perspective of formal reasoning, a denotational semantics (i) abstracts from details about program executions and focuses on program *effects*, and (ii) is *compositional* in the sense that the semantics of a program fragment is established from the semantics of the fragment's proper constituents.

Therefore, I devise a denotational semantics for low-level probabilistic programs with nondeterminism. This semantics is published as a standalone article at the 35^{th} Conference on the *Mathematical Foundations of Programming Semantics* [148]. In that work, I make three main contributions:

- I use *hyper-graphs* as the representation for low-level probabilistic programs with unstructured control-flow, general recursion, and nondeterminism.

- I develop a domain-theoretic characterization of a new model of nondeterminism for probabilistic programming, which involves nondeterminacy among *state transformers*, opposed to a common model that involves nondeterminacy among *program states*.

- I propose *Markov algebras* and devise an *algebraic* framework for denotational semantics. One advantage of the framework is that it can be instantiated with different models of nondeterminism. I also prove that for programs without procedure calls and nondeterminism, the resulting denotational semantics is equivalent to a standard distribution-based operational semantics.

An Algebraic Framework for Static Analysis Despite the fact that there have been many static analyses for probabilistic programs, these analyses are usually standalone developments, and it is not immediately clear how different techniques relate. For example, Claret et al. [29] propose a syntax-directed data-flow analysis to perform Bayesian inference, Chakarov and Sankaranarayanan [25] develop a martingale-based abstract interpretation to construct expectation invariants, and Sankaranarayanan et al. [136] combine symbolic execution with probabilistic volume-bound computation to estimate the probability that an assertion holds at a program point. Thus, I develop a framework, which I call *PMAF* (for Pre-Markov Algebra Framework), for designing, implementing, and proving the correctness of static analyses of probabilistic programs. The framework is published as a standalone article at the 39$^{\text{th}}$ Conference on *Programming Language Design and Implementation* [146]. Using PMAF, I can formulate and generalize several analyses that may appear to be quite different. Examples include Bayesian inference [29, 51, 52], Markov decision problem with rewards [130], and probabilistic-invariant generation [25, 86].

PMAF is based on the algebraic denotational semantics that I described earlier in this chapter. To formulate a static analysis, I introduce a new algebraic structure, called a *pre-Markov algebra*, which is equipped with operations corresponding to control-flow actions in probabilistic programs: *sequencing*, *conditional-choice*, *probabilistic-choice*, and *nondeterministic-choice*. To establish correctness, I introduce *probabilistic abstractions* between a pre-Markov algebra—which represents the abstract semantics—and the concrete semantics. This work shows how, with suitable extensions, a blending of ideas from previous work on (i) static analysis of single-procedure probabilistic programs, and (ii) interprocedural dataflow analysis of standard (non-probabilistic) programs can be used to create a framework for interprocedural analysis of probabilistic programs. In particular,

- The semantics on which PMAF is based is an interpretation of the CFGs for a program's procedures. One key idea is to treat each CFG as a *hyper-graph* rather than a standard graph.
- The abstract semantics is formulated so that the analyzer can obtain *procedure summaries*.

The main advantage of PMAF is that instead of starting from scratch to create a new analysis, one only needs to instantiate PMAF with the implementation of a new pre-Markov algebra. To establish soundness, one has to establish some well-defined algebraic properties, and can then rely on the soundness proof of the framework. To implement the analysis, one can rely on PMAF to perform sound interprocedural analysis, with respect to the provided abstraction. The PMAF implementation supplies common parts of different static analyses of probabilistic programs, e.g., efficient iteration strategies with widenings and interprocedural summarization. Moreover, improvements made to the PMAF implementation could immediately translate into improvements to *all of its instantiations*.

Central Moment Analysis for Cost Accumulators As a concrete static analysis of probabilistic programs, I study a specific yet important kind of uncertain quantity: *cost accumulators*, which are program variables that can only be incremented or decremented through the program execution and do not influence the control flow. Examples of cost accumulators include termination time [11, 26, 27, 85, 126], rewards in Markov decision processes [130], position information in control systems [10, 17, 136], and cash flow during bitcoin mining [154]. Recent work [17, 104, 124, 154] has proposed successful static-analysis approaches that leverage *aggregate* information of a cost accumulator X, such as X's *expected* value $\mathbb{E}[X]$ (i.e., X's "first moment"). The intuition why it is

beneficial to compute aggregate information—in lieu of distributions—is that aggregate measures like expectations *abstract* distributions to a single number, while still indicating nontrivial properties. Moreover, expectations are transformed by statements in a probabilistic program in a manner similar to the weakest-precondition transformation of formulas in a non-probabilistic program [111].

One important kind of aggregate information is *moments*. Whereas most previous work focused on *raw* moments (i.e., $\mathbb{E}[X^k]$ for any $k \geq 1$) I find out that *central* moments (i.e., $\mathbb{E}[(X - \mathbb{E}[X])^k]$ for any $k \geq 2$) can usually provide more information about distributions. For example, the *variance* $\mathbb{V}[X]$ (i.e., $\mathbb{E}[(X - \mathbb{E}[X])^2]$, X's "second central moment") indicates how X can deviate from its mean, the *skewness* (i.e., $\frac{\mathbb{E}[(X-\mathbb{E}[X])^3]}{(\mathbb{V}[X])^{3/2}}$, X's "third standardized moment") indicates how lopsided the distribution of X is, and the *kurtosis* (i.e., $\frac{\mathbb{E}[(X-\mathbb{E}[X])^4]}{(\mathbb{V}[X])^2}$, X's "fourth standardized moment") measures the heaviness of the tails of the distribution of X. One application of moments is to answer queries about *tail bounds*, e.g., the assertions about probabilities of the form $\mathbb{P}[X \geq d]$, via *concentration-of-measure* inequalities from probability theory [47]. With central moments, we find an opportunity to obtain more precise tail bounds of the form $\mathbb{P}[X \geq d]$, and become able to derive bounds on tail probabilities of the form $\mathbb{P}[|X - \mathbb{E}[X]| \geq d]$.

In this thesis, I have proposed and implemented the first fully automatic analysis for deriving symbolic *interval* bounds on higher central moments for cost accumulators in probabilistic programs with general recursion and continuous distributions. This analysis is published as a standalone article at the 42$^{\text{nd}}$ Conference on *Programming Language Design and Implementation* [149]. One challenge is to support *inter*procedural reasoning to reuse analysis results for procedures. My solution makes use of a "lifting" technique from the natural-language-processing community. That technique derives an algebra for second moments from an algebra for first moments [107]. I follow the *algebraic* approach and develop *moment semirings*, and use them to carry out interprocedural analysis, as well as derive a novel *frame* rule to handle procedure calls with *moment-polymorphic recursion*.

Bridging the Gap between PMAF and Moment Analysis Although I have developed a general framework PMAF for designing and implementing static analysis of probabilistic programs, my central-moment analysis tool is implemented as a standalone tool. One reason why I do not implement central-moment analysis as a PMAF abstract domain is that the underlying algorithm of PMAF is *iteration* based, i.e., the algorithm starts with an initial solution to the analysis problem and then iterates until convergence, but my central-moment analysis framework is *constraint* based, i.e., the analysis walks through the analyzed program to collect constraints and then discharges those constraints using an off-the-shelf constraint solver. PMAF has to rely on iterations because the control-flow hyper-graph for a probabilistic program usually contains loops. For non-probabilistic programs, people have been successful to sidestep iterations by using Kleene algebras, which have a Kleene-star operation that interprets loops, as the algebraic foundations of static analysis (e.g., [53, 54, 89, 92, 133, 157]). The key ideas are (i) the control-flow graph of a non-probabilistic program can be precisely encoded as a regular expression, and (ii) the Kleene-star operation can be implemented by non-iteration-based loop-summarization techniques. However, such algebraic static-analysis framework cannot directly apply to probabilistic programs: probabilistic programs are represented as control-flow *hyper*-graphs.

In this thesis, I present my current progress on developing the *Deterministic Markov-Kleene*

Algebra with Tests (DMKAT) framework. As the name suggests, I focus on deterministic probabilistic programs, which do not use nondeterministic choices. A control-flow graph of a non-probabilistic program encodes a regular set of program paths, thus it can then be expressed by a regular expression. Following the same methodology, I discover that a control-flow hyper-graph of a deterministic probabilistic program encodes a regular *hyper-path*, which is essentially a possibly-infinite tree, and develop a theory on regular hyper-paths. I then devise the novel *regular hyper-path expressions*, which serve as finite representations for possibly-infinite trees. I also present an algorithm that can construct a regular hyper-path expression from a deterministic control-flow hyper-graph.

Kleene algebras can be used to interpret regular expressions; following the same methodology, I develop a new family of algebras, namely the DMKATs, to interpret regular hyper-path expressions. It turns out that DMKATs are suitable for expressing concrete semantics: I demonstrate two DMKATs for a relational interpretation (non-probabilisitic) and a distribution-transformer interpretation (probabilistic), respectively. I also prove that the hyper-path model is sound for any valid DMKAT model, in the sense that if two regular hyper-path expressions correspond to the same hyper-path, then their interpretations under a DMKAT are also the same. Based on DMKATs, I sketch some possibilities to develop a non-iteration-based static-analysis framework for probabilistic programs, and discuss how the framework would work do derive invariants on the moments of program variables.

1.1 Thesis Organization

Chapter 2 provides necessary background for understanding this thesis. It first reviews standard notions from measure theory. Then, it introduces an imperative probabilistic programming language Appl that I use in this thesis, and a basic program execution model for the language.

Chapter 3 presents a *denotational* semantics for Appl with a novel *nondeterminism-first* resolution. This chapter develops a domain-theoretic characterization of nondeterminism-first and proposes an algebraic denotation semantics for probabilistic programs.

Chapter 4 designs an algebraic analysis framework, called PMAF, for designing, implementing, and proving the correctness of static analyses of probabilistic programs. The framework is based the algebraic denotational semantics presented in Chapter 3. This chapter also includes three instantiations of PMAF to solve different analysis problems.

Chapter 5 develops a novel static analysis for deriving symbolic interval bounds on higher *central moments* for *cost accumulators* in probabilistic programs. The analysis is based on a novel algebraic structure called *moment semirings*. This chapter proves the soundness of the moment-bound analysis with respect to a Markov-chain cost semantics. This chapter also discusses some implementation strategies to improve the usability and efficiency of the central-moment analysis.

Chapter 6 focuses on probabilistic programs without nondeterminism and proposes a generalization of PMAF, which is presented in Chapter 4, to support non-iteration-based analysis algorithms. The new framework in based on a new family of algebras called DMKATs, which can be used to interpret novel regular hyper-path expressions that encodes control-flow hyper graphs. The ultimate goal is to develop an algebraic abstract domain to carry out the central-moment analysis in Chapter 5.

Chapter 7 gives concluding remarks.

1.2 Publications

This thesis contains work that was published in three different articles:

1. Di Wang, Jan Hoffmann, and Thomas Reps. 2019. A Denotational Semantics for Low-Level Probabilistic Programs with Nondeterminism. In *the 35th Conference on the Mathematical Foundations of Programming Semantics (MFPS'19)*. Chapter 3 presents the denotational semantics.

2. Di Wang, Jan Hoffmann, and Thomas Reps. 2018. PMAF: An Algebraic Framework for Static Analysis of Probabilistic Programs. In *the 39th Conference on Programming Language Design and Implementation (PLDI'18)*. Chapter 4 presents the algebraic framework.

3. Di Wang, Jan Hoffmann, and Thomas Reps. 2021. Central Moment Analysis for Cost Accumulators in Probabilistic Programs. In *the 42nd Conference on Programming Language Design and Implementation (PLDI'21)*. Chapter 5 presents the central moment analysis.

For the second and third articles, we also submitted implementations and data as research artifacts [147, 151]) and they were validated by the Artificial Evaluation Committees.

Chapter 2

Setting the Stage: An Imperative Probabilistic Programming Language

In this thesis, I use an imperative arithmetic probabilistic programming language APPL that supports unstructured control-flow, general recursion, and nondeterminism, where program variables have numeric values. I use the following notational conventions. Natural numbers $\mathbb{N}$ *exclude* 0, i.e., $\mathbb{N} \stackrel{\text{def}}{=} \{1, 2, 3, \cdots\} \subseteq \mathbb{Z}^+ \stackrel{\text{def}}{=} \{0, 1, 2, \cdots\}$. Reals, nonnegative reals, and extended nonnegative reals are denoted by $\mathbb{R}$, $\mathbb{R}^+$, and $\mathbb{R}^+_\infty$, respectively. Let $\mathbb{2}$ denote the set of Boolean values, i.e., $\mathbb{2} \stackrel{\text{def}}{=} \{\top, \bot\}$. The *Iverson brackets* $[\cdot]$ are defined by $[\varphi] = 1$ if φ is true and otherwise $[\varphi] = 0$. Finite partial maps from A to B can be represented by finite sets of bindings, e.g., $\{a_1 \mapsto b_1, a_2 \mapsto b_2, \cdots, a_n \mapsto b_n\}$. Updating an existing binding of x in a finite map f to v is denoted by $f[x \mapsto v]$.

2.1 Preliminaries on Measure Theory

This section reviews the following standard notions from measure theory: measurable spaces, measurable functions, random variables, probability measures, expectations, and kernels. Interested readers can refer to textbooks in the literature [15, 155] for more details about measure theory.

A *measurable space* is a pair $(S, \mathcal{S})$, where S is a nonempty set, and $\mathcal{S}$ is a σ-algebra on S, i.e., a family of subsets of S that contains $\emptyset$ and is closed under complements and countable unions. The smallest σ-algebra that contains a family $\mathcal{A}$ of subsets of S is said to be *generated* by $\mathcal{A}$, denoted by $\sigma(\mathcal{A})$. Every topological space (S, τ) (i.e., $\tau \subseteq \wp(S)$ is a collection of open sets that is closed under arbitrary unions and finite intersections) admits a *Borel σ-algebra*, given by $\sigma(\tau)$. This gives canonical σ-algebras on $\mathbb{R}$, $\mathbb{Q}$, $\mathbb{N}$, etc.

Example 2.1. One of the most important σ-algebras is the Borel σ-algebra on $\mathbb{R}$, and it is a standard shorthand to denote this σ-algebra by $\mathcal{B}$. Elements of $\mathcal{B}$ can be very complex, so people have come up with simpler constructions for $\mathcal{B}$, e.g., $\mathcal{B} = \sigma(\{(-\infty, x] \mid x \in \mathbb{R}\})$.

A *measure* μ on a measurable space $(S, \mathcal{S})$ is a mapping from $\mathcal{S}$ to $\mathbb{R}^+_\infty$ such that (i) $\mu(\emptyset) = 0$, and (ii) for all pairwise-disjoint $\{A_n\}_{n\in\mathbb{N}}$ in $\mathcal{S}$, it holds that $\mu(\bigcup_{n\in\mathbb{N}} A_n) = \sum_{n\in\mathbb{N}} \mu(A_n)$. The triple $(S, \mathcal{S}, \mu)$ is called a *measure space*. A measure μ is called a *probability* (resp., *sub-probability*)

measure, if $\mu(S) = 1$ (resp., $\mu(S) \leq 1$). We denote the collection of probability measures on $(S, \mathcal{S})$ by $\mathbb{D}(S, \mathcal{S})$. The set of sub-probability measures on $(S, \mathcal{S})$ with the pointwise order forms an *ω-complete partial order* (ω-cpo), i.e., every ω-chain of sub-probability measures $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_n \leq \cdots$ has a supremum that is also a sub-probability measure. The *zero measure* $\mathbf{0}$ is defined as $\lambda A.0$. For each $x \in S$, the *Dirac measure* $\delta(x)$ is defined as $\lambda A.[x \in A]$, i.e., a point measure on x. For measures μ and ν, we write $\mu + \nu$ for the measure $\lambda A.\mu(A) + \nu(A)$. For a measure μ and a scalar $c \geq 0$, we write $c \cdot \mu$ for the measure $\lambda A.c \cdot \mu(A)$.

Example 2.2. The Lebesgue measure Leb *on* $(\mathbb{R}, \mathcal{B})$ *makes precise the concept of* length *of a measurable subset of* $\mathbb{R}$. Leb *is defined as the unique measure such that for any A that can be written as a finite union $A = (a_1, b_1] \cup \cdots \cup (a_m, b_m]$ where $m \in \mathbb{N}$ and $a_1 \leq b_1 \leq \cdots \leq a_m \leq b_m$, it holds that* $\text{Leb}(A) = \sum_{i=1}^{m}(b_i - a_i)$.

The counting measure *is commonly used on a measurable space $(S, \mathcal{S})$ where S is finite or countable. The measure μ is defined by $\mu \stackrel{\text{def}}{=} \lambda A.|A|$, where $|A|$ denotes the cardinality of the set A, with the understanding that $\mu(A) = \infty$ if A is an infinite set.*

Lemma 2.3. *The set of sub-probability measures on a measurable space $(S, \mathcal{S})$, ordered pointwise, forms an ω-cpo.*

Proof. Let $\{\mu_n\}_{n\in\mathbb{N}}$ be an ω-chain of sub-probability measures on $(S, \mathcal{S})$. Let $\mu \stackrel{\text{def}}{=} \lambda A. \lim_{n\to\infty} \mu_n(A)$ be the pointwise limit of $\{\mu_n\}_{n\in\mathbb{N}}$. Then μ is a set function from $\mathcal{S}$ to the unit interval $[0, 1]$, and $\mu(\emptyset) = \lim_{n\to\infty} \mu_n(\emptyset) = 0$.

Fix a pairwise-disjoint $\{A_m\}_{m\in\mathbb{N}}$ in $\mathcal{S}$. We conclude the proof by

$$\begin{aligned}
\mu\left(\bigcup\nolimits_{m\in\mathbb{N}} A_m\right) &= \lim_{n\to\infty} \mu_n\left(\bigcup\nolimits_{m\in\mathbb{N}} A_m\right) = \sup_{n\in\mathbb{N}} \mu_n\left(\bigcup\nolimits_{m\in\mathbb{N}} A_m\right) \\
&= \sup_{n\in\mathbb{N}} \sum_{m=1}^{\infty} \mu_n(A_m) \\
&= \sup_{n\in\mathbb{N}} \sup_{k\in\mathbb{N}} \sum_{m=1}^{k} \mu_n(A_m) = \sup_{k\in\mathbb{N}} \sup_{n\in\mathbb{N}} \sum_{m=1}^{k} \mu_n(A_m) \\
&\quad \dagger\ \{\mu_n(A_m)\}_{n\in\mathbb{N}} \text{ is an } \omega\text{-chain for any } m = 1, \cdots, k\ \dagger \\
&= \sup_{k\in\mathbb{N}} \sum_{m=1}^{k} \sup_{n\in\mathbb{N}} \mu_n(A_m) = \sup_{k\in\mathbb{N}} \sum_{m=1}^{k} \mu(A_m) = \sum_{m=1}^{\infty} \mu(A_m).
\end{aligned}$$

□

A function $f : S \to T$, where $(S, \mathcal{S})$ and $(T, \mathcal{T})$ are measurable spaces, is said to be $(\mathcal{S}, \mathcal{T})$-*measurable*, if $f^{-1}(B) \in \mathcal{S}$ for each $B \in \mathcal{T}$. If $T = \mathbb{R}$, we tacitly assume that the Borel σ-algebra $\mathcal{B}$ is defined on $\mathbb{R}$, and we simply say f is *measurable*, or f is a *random variable*. Measurable functions form a vector space, and products and maxima preserve measurability; that is, for any measurable functions f_1, f_2 and real numbers c_1, c_2, the functions $(c_1 \cdot f_1 + c_2 \cdot f_2)$, $(f_1 \cdot f_2)$, and $\max(f_1, f_2)$ are also measurable.

Example 2.4. Consider an experiment where one tosses a coin infinitely often. We can take $\Omega \stackrel{\text{def}}{=} \{\mathsf{H}, \mathsf{T}\}^{\mathbb{N}}$, so an element ω of Ω is a coin-toss sequence $\omega = \{\omega_n\}_{n\in\mathbb{N}}$, where $\omega_n \in \{\mathsf{H}, \mathsf{T}\}$. We

now define a σ-algebra $\mathcal{F}$ on Ω as

$$\mathcal{F} \stackrel{\text{def}}{=} \sigma(\{\{\omega \in \Omega \mid \omega_n = \mathscr{C}\} \mid \mathscr{C} \in \{\mathsf{H}, \mathsf{T}\}, n \in \mathbb{N}\}),$$

which allows us to reason about events such as "the n-th toss shows heads." Then for any $n \in \mathbb{N}$, $X_n \stackrel{\text{def}}{=} \lambda\omega.[\omega_n = \mathsf{H}]$ is a random variable on the measurable space $(\Omega, \mathcal{F})$. Because measurable functions form a vector space, the number of heads in first n tosses $S_n \stackrel{\text{def}}{=} \sum_{i=1}^{n} X_i$ is also a random variable.

LEMMA 2.5. *Let $\{f_n\}_{n\in\mathbb{N}}$ be an ω-chain of nonnegative measurable functions on a measurable space $(S, \mathcal{S})$, i.e., $f_n : S \to \mathbb{R}^+_\infty$ for all $n \in \mathbb{N}$. Then the pointwise limit of $\{f_n\}_{n\in\mathbb{N}}$ is also measurable.*

PROOF. Let $f \stackrel{\text{def}}{=} \lambda x. \lim_{n\to\infty} f_n(x)$. Fix a measurable subset B of $\mathbb{R}^+_\infty$. It is sufficient to consider B with the form $[0, c]$ for some $c \in \mathbb{R}^+_\infty$ (the class of such intervals generates the Borel σ-algebra on $\mathbb{R}^+_\infty$) and show that $f^{-1}(B) \in \mathcal{S}$. Indeed, we have

$$f^{-1}(B) = \{x \in S \mid f(x) \le c\} = \{x \in S \mid \lim_{n\to\infty} f_n(x) \le c\} = \bigcap_{n\in\mathbb{N}} f_n^{-1}(B),$$

which is a measurable set because f_n is measurable for all $n \in \mathbb{N}$ and measurable sets are closed under countable intersections. □

The *integral* of a measurable function f on $A \in \mathcal{S}$ with respect to a measure μ on $(S, \mathcal{S})$ is defined following Lebesgue's theory and is denoted by $\mu(f; A)$, $\int_A f d\mu$, or $\int_A f(x)\mu(dx)$. If μ is a probability measure, we call the integral as the *expectation* of f, written $\mathbb{E}_{x\sim\mu}[f; A]$, or simply $\mathbb{E}[f; A]$ when the scope is clear in the context. If $A = S$, we tacitly omit A from the notations. For each $A \in \mathcal{S}$, it holds that $\mu(f; A) = \mu(f \cdot \mathrm{I}_A)$, where $\mathrm{I}_A \stackrel{\text{def}}{=} \lambda x.[x \in A]$ is the indicator function for A. If f is nonnegative, then $\mu(f)$ is well-defined with the understanding that the integral can be infinite. If $\mu(|f|) < \infty$, then f is said to be *integrable*, written $f \in \mathcal{L}^1(S, \mathcal{S}, \mu)$, and its integral is well-defined and $\mu(f) = \mu(f^+) - \mu(f^-)$, where $f^+ \stackrel{\text{def}}{=} \lambda x. \max(f(x), 0)$ and $f^- \stackrel{\text{def}}{=} \lambda x. \max(-f(x), 0)$. Integration is *linear*, in the sense that for any $c, d \in \mathbb{R}$ and integrable functions f, g, the function $(c \cdot f + d \cdot g)$ is integrable and $\mu(c \cdot f + d \cdot g) = c \cdot \mu(f) + d \cdot \mu(g)$.

Example 2.6. Recall the coin-toss experiment in Example 2.4. If the tossed coin is fair, we can assign a probability measure μ on the measurable space $(\Omega, \mathcal{F})$ such that

$$\mu(\{\omega \in \Omega \mid \omega_n = \mathscr{C}\}) = \frac{1}{2}, \quad \forall \mathscr{C} \in \{\mathsf{H}, \mathsf{T}\}, n \in \mathbb{N}.$$

Then the expectation of the random variable X_n for any n is $\mathbb{E}[X_n] = \sum_{\mathscr{C}\in\{\mathsf{H},\mathsf{T}\}} \frac{1}{2} \cdot [\mathscr{C} = \mathsf{H}] = \frac{1}{2}$ and by linearity, we obtain that for any n, the expectation of S_n is $\mathbb{E}[S_n] = \sum_{i=1}^{n} \mathbb{E}[X_i] = \frac{1}{2}n$.

A *kernel* from a measurable space $(S, \mathcal{S})$ to another $(T, \mathcal{T})$ is a mapping from $S \times \mathcal{T}$ to $\mathbb{R}^+_\infty$ such that (i) for each $x \in S$, the set function $\lambda B.\kappa(x, B)$ is a measure on $(T, \mathcal{T})$, and (ii) for each $B \in \mathcal{T}$, the function $\lambda x.\kappa(x, B)$ is measurable. We sometimes also use the curried version of kernels with the signature $(S \to \mathcal{T} \to \mathbb{R}^+_\infty)$. We write $\kappa : (S, \mathcal{S}) \rightsquigarrow (T, \mathcal{T})$ to declare that κ is a kernel from $(S, \mathcal{S})$ to $(T, \mathcal{T})$. Intuitively, kernels describe measure transformers from one measurable space to another. A kernel κ is called a *probability* (resp., *sub-probability*) kernel, if

$\kappa(x,T) = 1$ (resp., $\kappa(x,T) \leq 1$) for all $x \in S$. We denote the collection of probability kernels from $(S,\mathcal{S})$ to $(T,\mathcal{T})$ by $\mathbb{K}((S,\mathcal{S}),(T,\mathcal{T}))$. If the two measurable spaces coincide, we simply write $\mathbb{K}(S,\mathcal{S})$. The set of sub-probability kernels from $(S,\mathcal{S})$ to $(T,\mathcal{T})$ with the pointwise order forms an ω-cpo. We can *push-forward* a measure μ on $(S,\mathcal{S})$ to a measure on $(T,\mathcal{T})$ through a kernel $\kappa : (S,\mathcal{S}) \rightsquigarrow (T,\mathcal{T})$ by integration: $\mu \gg\!= \kappa \stackrel{\text{def}}{=} \lambda B. \int_S \kappa(x,B) \cdot \mu(dx)$. We can also *compose* $\kappa_1 : (S_0,\mathcal{S}_0) \rightsquigarrow (S_1,\mathcal{S}_1)$ and $\kappa_2 : (S_1,\mathcal{S}_1) \rightsquigarrow (S_2,\mathcal{S}_2)$ to get their composition kernel by integration: $\kappa_1 \fatsemi \kappa_2 \stackrel{\text{def}}{=} \lambda(x,B). \int_{S_1} \kappa_1(x,dy) \cdot \kappa_2(y,B)$.

Example 2.7. As explained by Kozen [99], for a measurable space $(S,\mathcal{S})$ where S is finite or countable, a probability kernel $\kappa \in \mathbb{K}(S,\mathcal{S})$ has a representation as a Markov transition matrix M_κ, in which each entry $M_\kappa(x,x')$ for a pair of elements $(x,x') \in S \times S$ gives the probability that x transitions to x' under the kernel κ, and for any $x \in S$ and $A \in \mathcal{S}$, it holds that $\kappa(x,A) = \sum_{x' \in A} M_\kappa(x,x')$.

Lemma 2.8. *The set of sub-probability kernels from a measurable space $(S,\mathcal{S})$ to another $(T,\mathcal{T})$, ordered pointwise, forms an ω-cpo.*

Proof. Let $\{\kappa_n\}_{n\in\mathbb{N}}$ be an ω-chain of sub-probability kernels from $(S,\mathcal{S})$ to $(T,\mathcal{T})$. Let $\kappa \stackrel{\text{def}}{=} \lambda(x,B). \lim_{n\to\infty} \kappa_n(x,B)$ be the pointwise limit of $\{\kappa_n\}_{n\in\mathbb{N}}$. For each $x \in S$, the sequence $\{\lambda B.\kappa_n(x,B)\}_{n\in\mathbb{N}}$ forms an ω-chain of sub-probability measures on $(T,\mathcal{T})$, thus by Lemma 2.3 the set function $\lambda B.\kappa(x,B)$ is also a sub-probability measure. For each $B \in \mathcal{T}$, the sequence $\{\lambda x.\kappa_n(x,B)\}_{n\in\mathbb{N}}$ forms an ω-chain of nonnegative measurable functions, thus by Lemma 2.8 the function $\lambda x.\kappa(x,B)$ is also a measurable function. Thus we conclude that κ is a sub-probability kernel. □

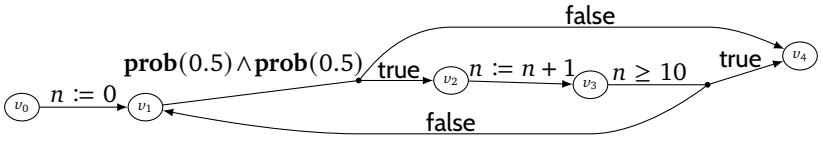
The *product* of two measurable spaces $(S_1,\mathcal{S}_1)$ and $(S_1,\mathcal{S}_2)$ is defined as $(S_1,\mathcal{S}_1) \otimes (S_2,\mathcal{S}_2) \stackrel{\text{def}}{=} (S_1 \times S_2, \mathcal{S}_1 \otimes \mathcal{S}_2)$, where $\mathcal{S}_1 \otimes \mathcal{S}_2$ is the smallest σ-algebra that makes coordinate maps measurable, i.e., $\sigma(\{\pi_1^{-1}(A_1) \mid A_1 \in \mathcal{S}_1\} \cup \{\pi_2^{-1}(A_2) \mid A_2 \in \mathcal{S}_2\}))$, where π_i is the i-th coordinate map.

2.2 A Hyper-Graph Program Model

In contrast to program models—such as standard control-flow graphs (CFGs)—for deterministic programming languages, I use *control-flow hyper-graphs* (CFHGs) to model probabilistic programs. Hyper-graphs consist of *hyper-edges*, each of which connects one source node and possibly several destination nodes. For example, probabilistic choices are represented by weighted hyper-edges with *two* destinations. Nondeterminism is then represented by multiple hyper-edges starting in the same node. The interpretation of hyper-edges is also different from standard edges. If the CFHG were treated as a standard graph, the subpaths from each successor of a branching node would be reasoned about *independently*. In contrast, the hyper-graph approach interprets a probabilistic-choice hyper-edge with probability p as a function $\lambda a.\lambda b.(a \ {}_p\!\oplus\ b)$, where ${}_p\!\oplus$ is an operation that weights the subpaths through the two successors by p and $(1-p)$. In other words, we do not reason about subpaths starting from a node *individually*, instead we reason about these subpaths *jointly* as a probability distribution. If a node has two outgoing probabilistic-choice hyper-edges, it represents two "worlds" of subpaths, each of which carries a probability distribution with respect to the probabilistic choice made in this "world."

```
n := 0;
while prob(0.5) ∧ prob(0.5) do
  n := n + 1;
  if n ≥ 10 then break
  else continue
  fi
od
```

(a)



(b)

Fig. 2.1: (a) An example of probabilistic programs; (b) The corresponding CFHG.

To define CFHGs of probabilistic programs, I adopt a common approach for standard CFGs in which the nodes represent program locations, and edges labeled with instructions describe transitions among program locations (e.g., [54, 106, 123]). Instead of standard directed graphs, I make use of *hyper-graphs* [59].

Definition 2.9. A *hyper-graph* H is a quadruple $(V, E, v^{\mathsf{entry}}, v^{\mathsf{exit}})$, where V is a finite set of nodes, E is a set of hyper-edges, $v^{\mathsf{entry}} \in V$ is a distinguished *entry node*, and $v^{\mathsf{exit}} \in V$ is a distinguished *exit node*. A *hyper-edge* is an ordered pair (x, Y), where $x \in V$ is a node and $Y \subseteq V$ is an ordered, nonempty set of nodes. For a hyper-edge $e = (x, Y)$ in E, we use $src(e)$ to denote x and $Dst(e)$ to denote Y. Following the terminology from graphs, we say that e is an *outgoing edge* of x and an *incoming edge* of each of the nodes $y \in Y$. We assume v^{entry} does not have incoming edges, and v^{exit} has no outgoing edges.

Definition 2.10. A *probabilistic program* contains a finite set of procedures $\{H_i\}_{1 \le i \le n}$, where each procedure $H_i = (V_i, E_i, v_i^{\mathsf{entry}}, v_i^{\mathsf{exit}})$ is a *control-flow hyper-graph* (CFHG) in which each node except v_i^{exit} has *at least* one outgoing hyper-edge, and v_i^{exit} has no outgoing hyper-edges. Define $V \stackrel{\text{def}}{=} \bigcup_{1 \le i \le n} V_i$. To assign meanings to probabilistic programs modulo *data actions* Act and *deterministic conditions* Cond that *can* be probabilistic, we associate with each hyper-edge $e \in E = \bigcup_{1 \le i \le n} E_i$ a *control-flow action* $Ctrl(e)$ that has one of the following three forms:

$$\begin{aligned} \mathsf{Ctrl} ::= {} & seq[\mathsf{act}], \text{ where } \mathsf{act} \in \mathsf{Act} \\ \mid {} & cond[\varphi], \text{ where } \varphi \in \mathsf{Cond} \\ \mid {} & call[i \to j], \text{ where } 1 \le i, j \le n \end{aligned}$$

where the number of destination nodes $|Dst(e)|$ of a hyper-edge e is 1 if $Ctrl(e)$ is $seq[\mathsf{act}]$ or $call[i \to j]$, and 2 otherwise.

Example 2.11. Fig. 2.1(b) shows the CFHG of the program in Fig. 2.1(a), where v_0 is the entry and v_4 is the exit. The hyper-edge $(v_2, \{v_3\})$ is associated with a sequencing action $seq[n := n + 1]$, while $(v_1, \{v_2, v_4\})$ is assigned a deterministic-choice action $cond[\mathbf{prob}(0.5) \wedge \mathbf{prob}(0.5)]$, i.e., an event where two coin flips both show heads.

Note that **break**, **continue** (and also **goto**) are not data actions, and are encoded directly as edges in CFHGs in a standard way. The grammar below defines data actions Act and deterministic

conditions Cond for APPL, where $p \in [0,1]$, $a, b, c \in \mathbb{R}$, $a < b$, and $n \in \mathbb{N}$.

$$\begin{aligned} \mathsf{Act} &::= x := e \mid x \sim D \mid \mathbf{observe}(\varphi) \mid \mathbf{skip} \\ \varphi \in \mathsf{Cond} &::= \top \mid \neg\varphi \mid \varphi_1 \wedge \varphi_2 \mid e_1 \le e_2 \mid \mathbf{prob}(p) \\ e \in \mathsf{Exp} &::= x \mid c \mid e_1 + e_2 \mid e_1 \times e_2 \mid \cdots \\ D \in \mathsf{Dist} &::= \textsc{Binomial}(n, p) \mid \textsc{Uniform}(a, b) \mid \cdots \end{aligned}$$

Dist stands for a collection of primitive probability distributions. For example, $\textsc{Binomial}(n, p)$ with $n \in \mathbb{N}$ and $p \in [0,1]$ describes the distribution of the number of successes in n independent experiments, each of which succeeds with probability p; $\textsc{Uniform}(a, b)$ represents a uniform distribution on the interval $[a, b]$. Each distribution D is associated with a probability measure $\mu_D \in \mathbb{D}(\mathbb{R})$. For example, the probability measure for $\textsc{Uniform}(a, b)$ is the integration of its density function $\mu_{\textsc{Uniform}(a,b)}(A) \stackrel{\text{def}}{=} \int_A \frac{[a \le x \le b]}{b-a} dx$.

2.3 A Distribution-Based Small-Step Operational Semantics

The next step is to define an operational semantics for APPL based on CFHGs. I adapt Borgström et al. [16]'s distribution-based small-step operational semantics for lambda calculus to the hypergraph setting, while suppressing the features of multiple procedures and nondeterminism for now. In Chapter 3, I will develop a denotational semantics that supports multiple procedures and nondeterminism, and justify the denotational semantics by proving an equivalence result with respect to the small-step operational semantics that I develop in this section.

Three components are used to define the operational semantics:

- A measurable space $(\Omega, \mathcal{F})$ on program states. For APPL, we define $\Omega \stackrel{\text{def}}{=} \mathsf{Var} \to \mathbb{R}$, i.e., a set of partial maps from a finite set of program variables to their values, and $\mathcal{F}$ be the Borel σ-algebra on the finite-dimensional space Ω.

- A (sub-)probability kernel $[\![\mathsf{act}]\!]$ on program states for each data action act. Intuitively, $[\![\mathsf{act}]\!](\omega, F)$ is the probability that the action act, starting in state $\omega \in \Omega$, halts in a state that satisfies $F \in \mathcal{F}$.

- A $[0,1]$-valued measurable function $[\![\varphi]\!]$ from program states for each deterministic condition φ. Intuitively, $[\![\varphi]\!](\omega)$ is the probability that the condition φ holds in state $\omega \in \Omega$.

Fig. 2.2 shows an interpretation of the data actions and deterministic conditions given in §2.2, where $\omega(e)$ evaluates expression e in state ω. If φ does not contain any probabilistic choices $\mathbf{prob}(p)$, then $[\![\varphi]\!](\omega)$ is either 0 or 1. Intuitively, $[\![\varphi]\!](\omega)$ is the probability that φ is true in the state ω, with respect to a probability space specified by all the $\mathbf{prob}(p)$'s in φ. Then the probability of $(\varphi_1 \wedge \varphi_2)$ is defined as the product of the individual probabilities of φ_1 and φ_2, because φ_1 and φ_2 are interpreted with respect to probabilistic choices in φ_1 and φ_2, respectively, and these two sets of choices are disjoint, thus independent.

Suppose that $P = (V, E, v^{\mathsf{entry}}, v^{\mathsf{exit}})$ is a single-procedure probabilistic program without nondeterminism, i.e., each node in P except v^{exit} is associated with *exactly* one hyper-edge. The *program configurations* $T = V \times \Omega$ are pairs of the form $\langle v, \omega \rangle$, where $v \in V$ is a node in the CFHG, and

$[\![x := e]\!] \stackrel{\text{def}}{=} \lambda\omega.\ \delta(\omega[x \mapsto \omega(e)])$	$[\![\top]\!] \stackrel{\text{def}}{=} \lambda\omega.\ 1$
$[\![x \sim D]\!] \stackrel{\text{def}}{=} \lambda\omega.\ \mu_D \gg\!= \lambda v.\ \delta(\omega[x \mapsto v])$	$[\![\neg\varphi]\!] \stackrel{\text{def}}{=} \lambda\omega.\ 1 - [\![\varphi]\!](\omega)$
$[\![\textbf{observe}(\varphi)]\!] \stackrel{\text{def}}{=} \lambda\omega.\ [\![\varphi]\!](\omega) \cdot \delta(\omega)$	$[\![\varphi_1 \wedge \varphi_2]\!] \stackrel{\text{def}}{=} \lambda\omega.\ [\![\varphi_1]\!](\omega) \cdot [\![\varphi_2]\!](\omega)$
$[\![\textbf{skip}]\!] \stackrel{\text{def}}{=} \lambda\omega.\ \delta(\omega)$	$[\![e_1 \le e_2]\!] \stackrel{\text{def}}{=} \lambda\omega.\ [\omega(e_1) \le \omega(e_2)]$
	$[\![\textbf{prob}(p)]\!] \stackrel{\text{def}}{=} \lambda\omega.\ p$

Fig. 2.2: An interpretation of data actions and deterministic conditions.

$$\begin{aligned}
&\langle v, \omega\rangle \longrightarrow \lambda A.\ [\![\mathsf{act}]\!](\omega, \{\omega' \mid \langle u, \omega'\rangle \in A\}) \\
&\qquad \text{where } e = (v, \{u\}) \in E, Ctrl(e) = seq[\mathsf{act}] \\
&\langle v, \omega\rangle \longrightarrow [\![\varphi]\!](\omega) \cdot \delta(\langle u_1, \omega\rangle) + (1 - [\![\varphi]\!](\omega)) \cdot \delta(\langle u_2, \omega\rangle) \\
&\qquad \text{where } e = (v, \{u_1, u_2\}) \in E, Ctrl(e) = cond[\varphi]
\end{aligned}$$

Fig. 2.3: The one-step evaluation relation.

$\omega \in \Omega$ is a program state. I then use the product measurable space $(V, \wp(V)) \otimes (\Omega, \mathcal{F})$ to construct a measurable space of program configurations, where $\wp(\cdot)$ is the powerset operator.

I define *one-step evaluation* as a relation $\langle v, \omega\rangle \longrightarrow \mu$ between configurations $\langle v, \omega\rangle$ and sub-probability measures μ on configurations, as shown in Fig. 2.3.

Example 2.12. For the program in Fig. 2.1, some one-step evaluations are $\langle v_0, \{n \mapsto 233\}\rangle \longrightarrow \delta(\langle v_1, \{n \mapsto 0\}\rangle)$, $\langle v_1, \{n \mapsto 1\}\rangle \longrightarrow 0.25 \cdot \delta(\langle v_2, \{n \mapsto 1\}\rangle) + 0.75 \cdot \delta(\langle v_4, \{n \mapsto 1\}\rangle)$, *and* $\langle v_3, n \mapsto 9\rangle \longrightarrow \delta(\langle v_1, \{n \mapsto 9\}\rangle)$.

Lemma 2.13. *The one-step evaluation relation* $\longrightarrow$ *defines a sub-probability kernel on program configurations.*

Proof. The evaluation relation $\longrightarrow$ can be seen as a function $\stackrel{\wedge}{\longrightarrow}$ defined as follows:

$$\stackrel{\wedge}{\longrightarrow}(\langle v, \omega\rangle, A) \stackrel{\text{def}}{=} \begin{cases} \mu(A) & \text{if } \langle v, \omega\rangle \longrightarrow \mu, \\ 0 & \text{otherwise.} \end{cases}$$

- For any $\langle v, \omega\rangle$, it is obvious that $\lambda A.\stackrel{\wedge}{\longrightarrow}(\langle v, \omega\rangle, A)$ is a sub-probability measure.
- For any measurable A, we want to show that the function $f \stackrel{\text{def}}{=} \lambda\langle v, \omega\rangle.\stackrel{\wedge}{\longrightarrow}(\langle v, \omega\rangle, A)$ is measurable. It is sufficient to show that for any measurable set $B \in \mathcal{B}$ of real numbers, the set $f^{-1}(B)$ is a measurable set of configurations. Observe that $f^{-1}(B)$ equals $\bigcup_{v \in V}(f^{-1}(B) \cap (\{v\} \times \Omega))$. Because V is a finite set, it is sufficient to show that for any $v \in V$, the set $f^{-1}(B) \cap (\{v\} \times \Omega)$ is measurable. If $v = v^{\mathsf{exit}}$, we have

$$f^{-1}(B) \cap (\{v^{\mathsf{exit}}\} \times \Omega) = \begin{cases} \{v^{\mathsf{exit}}\} \times \Omega & \text{if } 0 \in B, \\ \emptyset & \text{otherwise,} \end{cases}$$

$$\begin{aligned}
\langle v, \omega\rangle &\longrightarrow_0 \mathbf{0} && \\
\langle v^{\mathsf{exit}}, \omega\rangle &\longrightarrow_n \delta(\omega) && \text{if } n > 0 \\
\langle v, \omega\rangle &\longrightarrow_{n+1} \lambda F. \int_{\mathrm{supp}(\mu)} \mu(d\tau) \cdot \mu'_\tau(F) && \text{where} \langle v, \omega\rangle \longrightarrow \mu \\
& && \text{and } \tau \longrightarrow_n \mu'_\tau \text{ for any } \tau \in \mathrm{supp}(\mu)
\end{aligned}$$

Fig. 2.4: The step-indexed evaluation relation.

thus the set is measurable. If $v \neq v^{\mathsf{exit}}$, we proceed by a case analysis on the hyper-edge whose source is v.

– If $e = (v, \{u\}) \in E$ and $Ctrl(e) = seq[\mathsf{act}]$, we have

$$\begin{aligned}
f^{-1}(B) \cap (\{v\} \times \Omega) &= \{v\} \times \{\omega \mid [\![\mathsf{act}]\!](\omega, \{\omega' \mid \langle u, \omega'\rangle \in A\}) \in B\} \\
&= \{v\} \times (\lambda\omega.[\![\mathsf{act}]\!](\omega, \{\omega' \mid \langle u, \omega'\rangle \in A\}))^{-1}(B).
\end{aligned}$$

Because $[\![\mathsf{act}]\!]$ is a kernel, we conclude that the set is measurable.

– If $e = (v, \{u_1, u_2\}) \in E$ and $Ctrl(e) = cond[\varphi]$, we consider B with the form $(-\infty, c]$ for some $c \in \mathbb{R}$. (This is sufficient because the class of such intervals generates $\mathcal{B}$.) If $c < 0$ (resp., $c > 1$), we know the set $f^{-1}((-\infty, c]) \cap (\{v\} \times \Omega)$ equals $\emptyset$ (resp., $\{v\} \times \Omega$), thus measurable. Otherwise, when $c \in [0, 1]$, we have $f^{-1}((-\infty, c]) \cap (\{v\} \times \Omega) =$

$$\bigcup_{q \in \mathbb{Q}} (\{\langle v, \omega\rangle \mid \langle u_1, \omega\rangle \in A \wedge [\![\varphi]\!](\omega) \leq q\} \cap \{\langle v, \omega\rangle \mid \langle u_2, \omega\rangle \in A \wedge (1 - [\![\varphi]\!](\omega)) \leq c - q\}),$$

and if we define $F_1 \stackrel{\text{def}}{=} \{\omega \mid \langle u_1, \omega\rangle \in A\}$ and $F_2 \stackrel{\text{def}}{=} \{\omega \mid \langle u_2, \omega\rangle \in A\}$, the set equals

$$\bigcup_{q \in \mathbb{Q}} (\{v\} \times ([\![\varphi]\!]^{-1}((-\infty, q]) \cap F_1))) \cap (\{v\} \times ([\![\varphi]\!]^{-1}([1 - c + q, \infty)) \cap F_2))).$$

Because $\mathbb{Q}$ is a countable set, $[\![\varphi]\!]$ is a measurable function, and measurable sets are closed under countable unions and intersections, we conclude that the set above is measurable.

□

I now define *step-indexed evaluation* as the family of n-indexed relations $\langle v, \omega\rangle \longrightarrow_n \mu$ between configurations $\langle v, \omega\rangle$ and sub-probability measures μ on program states inductively, as shown in Fig. 2.4.

Example 2.14. For the program in Fig. 2.1, some step-indexed evaluations are $\langle v_4, \{n \mapsto 10\}\rangle \longrightarrow_1 \delta(\{n \mapsto 10\})$, $\langle v_1, \{n \mapsto 0\}\rangle \longrightarrow_2 0.75 \cdot \delta(\{n \mapsto 0\})$, *and* $\langle v_1, \{n \mapsto 0\}\rangle \longrightarrow_5 0.75 \cdot \delta(\{n \mapsto 0\}) + 0.1875 \cdot \delta(\{n \mapsto 1\})$.

LEMMA 2.15. *The step-indexed evaluation relation* $\longrightarrow_n$ *defines a sub-probability kernel from program configurations to program states for any* $n \in \mathbb{Z}^+$. *Moreover, if* $\langle v, \omega\rangle \longrightarrow_n \mu_1$, $\langle v, \omega\rangle \longrightarrow_m \mu_2$, *and* $n \leq m$, *then* $\mu_1 \leq \mu_2$ *pointwise.*

Proof. By induction on n.

- $\longrightarrow_0$ can be seen as the everywhere-zero function $\xrightarrow{\hat{}}_0$, which is obviously a kernel.
- $\longrightarrow_{n+1}$ can be seen as the function defined as follows:

$$\xrightarrow{\hat{}}_{n+1}(\langle v, \omega\rangle, F) \stackrel{\text{def}}{=} \begin{cases} 1 & \text{if } v = v^{\mathsf{exit}} \wedge \omega \in F, \\ 0 & \text{if } v = v^{\mathsf{exit}} \wedge \omega \notin F, \\ \displaystyle\int_{\mathrm{supp}(\mu)} \xrightarrow{\hat{}}_n(\tau, F) \cdot \mu(d\tau) & \text{if } \langle v, \omega\rangle \longrightarrow \mu. \end{cases}$$

  - For any $\langle v, \omega\rangle$, it is obvious that $\lambda F.\xrightarrow{\hat{}}_{n+1}(\langle v, \omega\rangle, F)$ is a sub-probability measure.
  - For any measurable F, we want to show that the function $f \stackrel{\text{def}}{=} \lambda\langle v, \omega\rangle.\xrightarrow{\hat{}}_{n+1}(\langle v, \omega\rangle, F)$ is measurable. It is sufficient to show that for any measurable set $B \in \mathcal{B}$ of real numbers, the set $f^{-1}(B)$ is a measurable set of states. Observe that $f^{-1}(B)$ equals

$$(f^{-1}(B) \cap (\{v^{\mathsf{exit}}\} \times \Omega)) \cup (f^{-1}(B) \cap ((V \setminus \{v^{\mathsf{exit}}\}) \times \Omega)).$$

    We proceed by showing both operands of the set union above are measurable.
    * We have

$$f^{-1}(B) \cap (\{v^{\mathsf{exit}}\} \times \Omega) = \{v^{\mathsf{exit}}\} \times \{\omega \mid \delta(\omega)(F) \in B\} = \{v^{\mathsf{exit}}\} \times \mathrm{I}_F^{-1}(B),$$

      where $\mathrm{I}_F \stackrel{\text{def}}{=} \lambda\omega.[\omega \in F]$ is the indicator function of F, which is measurable. We then conclude that the set $f^{-1}(B) \cap (\{v^{\mathsf{exit}}\} \times \Omega)$ is measurable.
    * We have

$$\begin{aligned} & f^{-1}(B) \cap ((V \setminus \{v^{\mathsf{exit}}\}) \times \Omega) \\ &= \{\langle v, \omega\rangle \mid v \neq v^{\mathsf{exit}}, \int \xrightarrow{\hat{}}_n(\tau, F) \cdot \xrightarrow{\hat{}}(\langle v, \omega\rangle, d\tau) \in B\} \\ &= \{\langle v, \omega\rangle \mid v \neq v^{\mathsf{exit}}, (\xrightarrow{\hat{}} \fatsemi \xrightarrow{\hat{}}_n)(\langle v, \omega\rangle, F) \in B\} \\ &= ((V \setminus \{v^{\mathsf{exit}}\}) \times \Omega) \cap (\lambda\langle v, \omega\rangle.(\xrightarrow{\hat{}} \fatsemi \xrightarrow{\hat{}}_n)(\langle v, \omega\rangle, F))^{-1}(B), \end{aligned}$$

      where $\fatsemi$ is the kernel-composition operator. Because the composition of two kernels is also a kernel, we conclude that the set $f^{-1}(B) \cap ((V \setminus \{v^{\mathsf{exit}}\}) \times \Omega)$ is measurable.

Meanwhile, we want to show that $\xrightarrow{\hat{}}_{n+1} \geq \xrightarrow{\hat{}}_n$ pointwise. We proceed by induction on n. If $n = 0$, then the inequality holds obviously. For $n > 0$, let us consider any $v \in V$, $\omega \in \Omega$, and $F \in \mathcal{F}$, and proceed by a case analysis.

- If $v = v^{\mathsf{exit}}$ and $\omega \in F$, then $\xrightarrow{\hat{}}_{n+1}(\langle v, \omega\rangle, F) = \xrightarrow{\hat{}}_n(\langle v, \omega\rangle, F) = 1$.
- If $v = v^{\mathsf{exit}}$ and $\omega \notin F$, then $\xrightarrow{\hat{}}_{n+1}(\langle v, \omega\rangle, F) = \xrightarrow{\hat{}}_n(\langle v, \omega\rangle, F) = 0$.
- Otherwise, suppose that $\langle v, \omega\rangle \longrightarrow \mu$, then

$$\xrightarrow{\hat{}}_{n+1}(\langle v, \omega\rangle, F) = \int_{\mathrm{supp}(\mu)} \xrightarrow{\hat{}}_n(\tau)(F) \cdot \mu(d\tau),$$

$$\xrightarrow{\hat{}}_n(\langle v, \omega\rangle, F) = \int_{\mathrm{supp}(\mu)} \xrightarrow{\hat{}}_{n-1}(\tau, F) \cdot \mu(d\tau).$$

By the induction hypothesis, we know that $\xrightarrow{\hat{}}_{n-1} \leq \xrightarrow{\hat{}}_{n}$ pointwise, and the measure μ can be seen as a nonnegative function, thus $\xrightarrow{\hat{}}_{n}(\langle v, \omega\rangle, F) \leq \xrightarrow{\hat{}}_{n+1}(\langle v, \omega\rangle, F)$.

□

For the program $P = (V, E, v^{\mathsf{entry}}, v^{\mathsf{exit}})$, by Lemma 2.15, I define its semantics as $[\![P]\!]_{\mathsf{os}}(\omega, F) \stackrel{\text{def}}{=} \sup_{n\in\mathbb{Z}^+}\{\mu(F) \mid \langle v^{\mathsf{entry}}, \omega\rangle \longrightarrow_n \mu\}$.

Example 2.16. For the program P in Fig. 2.1, the sub-probability measure $\lambda F.[\![P]\!]_{\mathsf{os}}(\omega, F)$ for any initial state ω that contains the program variable n is given by $\sum_{k=0}^{9}(0.75 \times 0.25^k) \cdot \delta(\omega[n \mapsto k]) + 0.000000953674316406 25 \cdot \delta(\omega[n \mapsto 10])$.

Lemma 2.17. *For any program P, $[\![P]\!]_{\mathsf{os}}$ defines a sub-probability kernel on program states.*

Proof. By definition, we have $[\![P]\!]_{\mathsf{os}} = \sup_{n\in\mathbb{Z}^+} \xrightarrow{\hat{}}_{n}$. Then we can conclude by the fact that the set of sub-probability kernels forms an ω-cpo. □

In general, the measure $\lambda F.[\![P]\!]_{\mathsf{os}}(\omega, F)$ that describes the evaluation results of a program P with an initial state ω is *not* always a probability measure. In the case that *P diverges* with some positive probability p from the initial state ω, the measure $\lambda F.[\![P]\!]_{\mathsf{os}}(\omega, F)$ is a sub-probability measure that satisfies $[\![P]\!]_{\mathsf{os}}(\omega, \Omega) = 1 - p$, i.e., the probabilities of the resulting states "sum up" to $(1 - p)$.

Chapter 3

A Denotational Semantics for Probabilistic Programs with Nondeterminism-First Resolution

In §2.3, I have shown how nondeterminism-free, single-procedure probabilistic programs execute *operationally*. In this chapter, I focus on developing a *denotational* semantics, which concentrates on the *effects* of programs and abstracts from how the program executes. This characterization of denotational semantics is beneficial for *rigorous reasoning* about programs, such as static analysis and model checking, because one usually only cares whether programs satisfy certain properties, e.g., if they terminate on all possible inputs. Even better, a denotational semantics is often *compositional*—that is, the property of a whole program can be established from properties of its proper constituents. In other words, one can develop *local*—and thus *scalable*—reasoning techniques based on a denotational semantics. In contrast, the operational semantics in §2.3 is not compositional—it takes into account the whole program P to define $[\![P]\!]_{\mathsf{os}}$.

Another benefit of a denotational semantics is that it is often easier to extend than an operational one. As an example, let me briefly compare the complexity of adding procedure calls and nondeterminism to an operational semantics versus a denotational semantics. To support multiple procedures and procedure calls in the semantics proposed in §2.3, one needs to introduce a notion of *stacks* to keep track of procedure calls, as done by previous work [51, 52, 126]. Then the program configurations become triples of call stacks, control-flow-graph nodes, and program states. As a consequence, the one-step and step-indexed evaluation relations in Figures 2.3 and 2.4 would become more complex. However, such an extension is almost trivial for a denotational semantics. Suppose we are able to *compose* semantic objects, e.g, $[\![C_1; C_2]\!]_{\mathsf{ds}} = [\![C_2]\!]_{\mathsf{ds}} \circ [\![C_1]\!]_{\mathsf{ds}}$, where C_1, C_2 are program fragments, $\circ$ denotes a composition operation, and $[\![C]\!]_{\mathsf{ds}}$ gives the denotation of C. For example, consider that C_1 is a procedure call **call** Q, where Q is a procedure. Because we can obtain the denotation $[\![Q]\!]_{\mathsf{ds}}$ of Q, we can interpret $[\![\textbf{call } Q; C_2]\!]_{\mathsf{ds}}$ merely as $[\![C_2]\!]_{\mathsf{ds}} \circ [\![Q]\!]_{\mathsf{ds}}$. By this means we do not need to reason about stacks explicitly.

Another important programming feature is nondeterminism. For operational semantics of probabilistic programs, nondeterminism is often formalized using the notion of a *scheduler*, which resolves a nondeterministic choice from the computation that leads up to it (e.g., [27, 28, 55]). When the scheduler is fixed, a program can be executed deterministically (as shown in §2.3). To

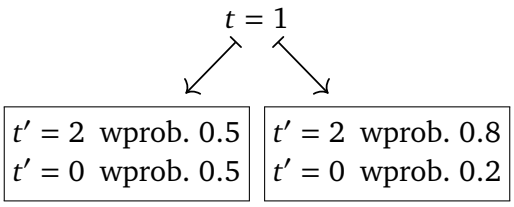


Fig. 3.1: An example where ⋆ resolved *after* t is given. A box represents a probability distribution.

reason about nondeterministic programs with respect to an operational semantics, one needs to take all possible schedulers into consideration. However, if one only cares about the effects of a program, it is possible to sidestep these schedulers by switching to a denotational semantics. For example, let C_1, C_2 be two program fragments and $[\![C_1]\!]_{\mathsf{ds}}$, $[\![C_2]\!]_{\mathsf{ds}}$ be their denotations, which could be maps from initial states to a collection of possible final states. Then the denotation $[\![\textbf{if } \star \textbf{ then } C_1 \textbf{ else } C_2 \textbf{ fi}]\!]_{\mathsf{ds}}$ of a nondeterministic-choice between C_1 and C_2 could be something like $\lambda\omega.[\![C_1]\!]_{\mathsf{ds}}(\omega) \cup [\![C_2]\!]_{\mathsf{ds}}(\omega)$. Note that this approach does not need to consider schedulers explicitly.

Some high-level decision choices about *nondeterminism* arise when I develop a denotational semantics for Appl. Nondeterminism itself is an important feature from two perspectives: (i) it arises naturally from probabilistic models, such as the agent for a Markov decision process [13], or the unknown input distribution for modeling *fault tolerance* [87], and (ii) it is required by the common paradigm of *abstraction* and *refinement*[1] on programs [46, 111]. While nondeterminism has been well studied for standard programming languages, the combination of probabilities and nondeterminism turns out to be tricky. One substantial question is *when* the nondeterminism is resolved. A well-studied model for nondeterminism in probabilistic programming is to resolve program inputs *prior to* nondeterminism [45, 110, 111, 115, 116, 144]. This model follows a commonplace principle of semantics research that represents a nondeterministic function as a set-valued function that maps an input to a collection of possible outputs, i.e., an element in $X \to \wp(X)$, where X is a program state space and $\wp(\cdot)$ is the powerset operator. However, it is sometimes desirable to resolve nondeterminism *prior to* program inputs, i.e., a nondeterministic program should represent a collection of elements in $\wp(X \to X)$. For example, one may want to show for every refined version of a nondeterministic program with each nondeterministic choice replaced by a conditional, its behavior on all *inputs* are indistinguishable. I call the common model *nondeterminism-last* and the other *nondeterminism-first*.

Example 3.1. Consider the following program P where ⋆ represents nondeterminism.

$$\textbf{if } \star \textbf{ then } t \coloneqq t + 1 \textbf{ else } t \coloneqq t - 1 \textbf{ fi}$$

Fig. 3.1 illustrates the nondeterminism-last model: given an input $t = 1$, ⋆ is resolved as $\textbf{prob}(0.5)$ *in the left box, whereas it is resolved as* $\textbf{prob}(0.8)$ *in the right box. Fig. 3.2 then demonstrates the novel nondeterminism-first model: ⋆ is resolved prior to the input, i.e., each resolution leads to a function that maps an input to a probability distribution.*

In §3.2, I present a domain-theoretic study of nondeterminism-first for probabilistic programs with a *countable* state space. Technically, I propose a notion of *generalized convexity* (*g-convexity*, for

[1] Abstraction enables reasoning about a program through its high-level specifications, and refinement allows stepwise software development, where programs are "refined" from specifications to low-level implementations.

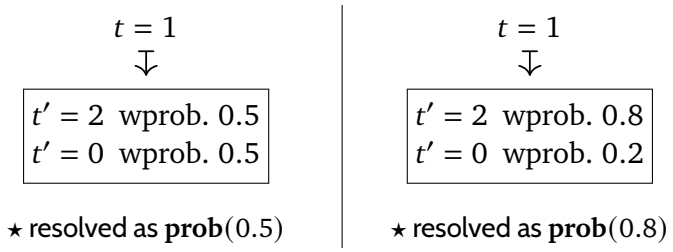


Fig. 3.2: An example where ⋆ resolved *before* t is given. A box represents a probability distribution.

$$\textbf{if} \star \ \textbf{then} \quad \textbf{if prob}(1/2) \ \textbf{then} \ t := 0 \ \textbf{else} \ t := 1 \ \textbf{fi}$$
$$\textbf{else} \quad \textbf{if prob}(1/3) \ \textbf{then} \ t := 0 \ \textbf{else} \ t := 1 \ \textbf{fi} \quad \textbf{fi}$$

Fig. 3.3: A nondeterministic, probabilistic program.

short), which expresses that a set of *state transformers* is stable under refinements (while standard convexity describes that a set of *states* is stable under refinements), as well as devise a g-convex *powerdomain* that characterizes expressible semantic objects.

To achieve my ultimate goal of developing a denotational semantics, instead of restricting myself to one specific model for nondeterminism, I propose a general *algebraic* denotational semantics in §3.3, which can be instantiated with different treatments of nondeterminism. The semantics is algebraic in the sense that it performs reasoning in some space of program states and state transformers, while the transformers should obey some algebraic laws. For instance, the program command **skip** should be interpreted as the *identity* element for sequencing in an algebra of program-state transformers. In addition, the algebraic approach is a good fit for static analysis of probabilistic programs.

The *algebraic* approach I take in this thesis is challenging in the setting of probabilistic programming. In contrast, for standard, non-probabilistic programming languages, it is almost trivial to derive a low-level denotational semantics *once* one has a semantics for well-structured programs at hand. The trick is to first define the semantic operations as a *Kleene algebra* [33, 93, 97, 100], which admits an *extend* operation, used for sequencing, a *combine* operation, used for branching, and a *closure* operation, used for looping; then extract from the CFG a *regular expression* that captures all execution paths by Tarjan [142]'s path-expression algorithm; and finally use the Kleene algebra to *reinterpret* the regular expression to obtain the semantics for the CFG. However, this approach fails when both probabilities and nondeterminism come into the picture. Consider the probabilistic program with a *nondeterministic* choice ⋆ in Fig. 3.3. The program is intended to draw a random value t from either a fair coin flip or a biased one. If one adopts the path-expression approach, one ends up with a regular expression that describes a *single* collection of four program executions: (i) $t := 0$ with probability $1/2$, (ii) $t := 1$ with probability $1/2$, (iii) $t := 0$ with probability $1/3$, and (iv) $t := 1$ with probability $2/3$. The collection does *not* describe the intended meaning, and does *not* even form a well-defined probability distribution—all the probabilities sum up to 2 instead of 1. Intuitively, the path-expression approach fails for probabilistic programs because it can only express the semantics as a collection of executions with probabilities, whereas probabilistic programs actually specify collections of *distributions* over executions.

3.1 A Summary of Existing Domain-Theoretic Developments

To present the technical development of nondeterminism-first for probabilistic programs with a *countable* state space, I will use a simplified notion of sub-probability measures. Let X be a nonempty countable set. A *distribution* on X is a function $\Delta : X \to [0,1]$ such that $\sum_{x \in X} \Delta(x) \leq 1$, and the *Dirac distribution* $\delta(x)$ for some $x \in X$ is defined as $\lambda x'.\ [x = x']$. The set of all distributions on X is denoted by $\underline{\mathcal{D}}(X)$.

My development of models for nondeterminism makes great use of existing domain-theoretic studies of powerdomains, thus in this section, I present a brief summary of them. I review some standard notions from domain theory [2, 74, 114], as well as some results on probabilistic powerdomains [82, 83] and nondeterministic powerdomains [45, 110, 111, 115, 116, 144].

3.1.1 Background from Domain Theory

Let P be a nonempty set with a partial order $\sqsubseteq$, i.e., a *poset*. The *lower closure* of a subset A is defined as $\downarrow A \stackrel{\text{def}}{=} \{x \in P \mid \exists a \in A : x \sqsubseteq a\}$. The *upper closure* of a subset A is defined as $\uparrow A \stackrel{\text{def}}{=} \{x \in P \mid \exists a \in A : a \sqsubseteq x\}$. A subset A satisfying $\downarrow A = A$ is called a *lower set*. A subset A satisfying $\uparrow A = A$ is called an *upper set*. If all elements of P are above a single element $x \in P$, then x is called the *least element*, denoted commonly by $\bot$. A function $f : P \to Q$ between two posets P and Q is *monotone* if for all $x, y \in P$ such that $x \sqsubseteq y$, it holds that $f(x) \sqsubseteq f(y)$. A subset A of P is *directed* if it is nonempty and each pair of elements in A has an upper bound in A. If A is totally ordered and isomorphic to natural numbers, then A is called an *ω-chain*. If a directed set A has a supremum, then it is denoted by $\bigsqcup^{\uparrow} A$.

A poset D is called *directed complete* or a dcpo if each directed subset A of D has a supremum $\bigsqcup^{\uparrow} A$ in D. A function $f : D \to E$ between two dcpos D and E is *Scott-continuous* if it is monotone and preserves directed suprema, i.e., $f(\bigsqcup^{\uparrow} A) = \bigsqcup^{\uparrow} f(A)$ for all directed subsets A of D. We denote the set of Scott-continuous functions from D to E, ordered pointwise, by $[D \to E]$. If both D and E have a least element, we say a function $f \in [D \to E]$ is *strict* if f preserves the least element. We denote the set of strict functions from D to E by $[D \xrightarrow{\bot!} E]$.

Example 3.2. The natural numbers $\mathbb{N}$ with the usual order does not *form a dcpo, because $\mathbb{N}$ itself as a directed set does* not *have a supremum in $\mathbb{N}$. One way to complete $\mathbb{N}$ is to add a distinguished top element ω such that $n \sqsubseteq \omega$ for all $n \in \mathbb{N}$.*

Let D be a dcpo. For two elements x, y of D, we say that x *approximates* y, denoted by $x \ll y$, if for all directed subsets A of D, it holds that $y \sqsubseteq \bigsqcup^{\uparrow} A$ implies $x \sqsubseteq a$ for some $a \in A$. We define $\twoheaddownarrow A \stackrel{\text{def}}{=} \{x \in D \mid \exists a \in A : x \ll a\}$ and $\twoheaduparrow A \stackrel{\text{def}}{=} \{x \in D \mid \exists a \in A : a \ll x\}$. A dcpo D is called *continuous* if for every element x of D, the set $\twoheaddownarrow x$ is directed and $x = \bigsqcup^{\uparrow} \twoheaddownarrow x$. A subset B of a dcpo D is said to be a *basis* for D, if for every element x of D, the set $\twoheaddownarrow x \cap B$ is directed and $x = \bigsqcup^{\uparrow}(\twoheaddownarrow x \cap B)$. Every continuous dcpo then obviously has a basis.

Example 3.3. The unit interval $[0,1]$ with the usual order forms a continuous dcpo, where the order of approximation $x \ll y$ is given by the usual number order $x < y$. The rational numbers $\mathbb{Q} \cap [0,1]$ can be seen as a basis for the unit interval.

Let D be a dcpo. A subset A is *Scott-closed* if A is a lower set and is closed under directed suprema. The complement $D \setminus A$ of a Scott-closed subset A is called *Scott-open*. These Scott-open subsets form the *Scott-topology* on D. The *closure* of a subset A is the smallest Scott-closed set containing A as a subset, denoted by $\overline{A}$.

Let X be a topological space whose open sets are denoted by $O(X)$. A *cover* C of a subset A of X is a collection of subsets whose union contains A as a subset. A *sub-cover* of C is a subset of C that still covers A. The cover C is called an *open-cover* if each of its members is an open set. A subset A is *compact* if every open-cover of A contains a finite sub-cover. A subset A is *saturated* if A is an intersection of its neighborhoods (i.e., A's open supersets). The *saturation* of a subset A is the intersection of its neighborhoods. In dcpo's equipped with the Scott-topology, saturated sets are precisely the upper sets, and the saturation of a subset A is given by $\uparrow A$.

Let D be a dcpo. A nonempty subset of D is said to be a *lens* if it is the intersection of a Scott-closed subset and a Scott-compact saturated subset. Lenses are always Scott-compact, and a canonical representation for a lens L is given by $\overline{L} \cap \uparrow L$. On lenses we can define the *Egli-Miler ordering* $\sqsubseteq_{EM}$, by $L_1 \sqsubseteq_{EM} L_2$ iff $L_1 \subseteq \downarrow L_2$ and $L_2 \subseteq \uparrow L_1$.

A continuous dcpo D is called *coherent* if, with the Scott topology, the intersection of any two Scott-compact saturated subsets is also Scott-compact. The *Lawson-topology* on a dcpo D is generated by Scott-open sets and sets of the form $D \setminus \uparrow x$ with $x \in D$. The Lawson-topology on a coherent dcpo is compact. Lenses are always Lawson-closed sets; thus, in a coherent dcpo, lenses are always Lawson-compact sets.

I am going to use the following theorems in my technical development.

Proposition 3.4 (Kleene fixed-point theorem). *Suppose $(D, \sqsubseteq)$ is a dcpo with a least element $\bot$, and let $f : D \to D$ be a Scott-continuous function. Then f has a least fixed point which is the supremum of the ascending Kleene chain of f (i.e., the ω-chain $\bot \sqsubseteq f(\bot) \sqsubseteq f(f(\bot)) \sqsubseteq \cdots \sqsubseteq f^n(\bot) \sqsubseteq \cdots$), denoted by $\mathrm{lfp}^{\sqsubseteq}_{\bot} f$.*

Proposition 3.5 (Cor. of [74, Hofmann-Mislove theorem]). *Let X be a sober space, i.e., a T_0-space where every nonempty closed set is either the closure of a point or the union of two proper closed subsets. The intersection of a filtered family $\{A_i\}_{i \in \mathcal{I}}$ (i.e., the intersection of any two subsets is in the family) of nonempty compact saturated subsets is compact and nonempty. In addition, if such a filtered intersection is contained in an open set U, it holds that $A_i \subseteq U$ for some $i \in \mathcal{I}$. Specifically, continuous dcpos equipped with the Scott-topology and coherent dcpos equipped with the Lawson-topology are sober.*

3.1.2 Probabilistic Powerdomains

Jones and Plotkin [83]'s pioneer work on probabilistic powerdomains extends the complete partially ordered sets, which are pervasively used in computer science, to model probabilistic computations. Let X be a nonempty countable set. We say that the set of all distributions on X, denoted by $\underline{\mathcal{D}}(X)$, is a *probabilistic powerdomain* over X. Distributions are ordered pointwise, i.e., $\Delta_1 \sqsubseteq_D \Delta_2 \stackrel{\text{def}}{=} \forall x \in X : \Delta_1(x) \leq \Delta_2(x)$. We define the *probabilistic-choice* of distributions Δ_1, Δ_2 with respect to a weight $p \in [0, 1]$, written $\Delta_1 \,{}_p\!\oplus\, \Delta_2$, as $p \cdot \Delta_1 + (1 - p) \cdot \Delta_2$. The operation ${}_p\!\oplus$ corresponds to the program construct "**if prob**(p) **then** $\cdots$ **else** $\cdots$ **fi**."

The following theorems provide a characterization of the probabilistic powerdomains.

Proposition 3.6 ([82, 83, 110, 144]). *The poset $(\underline{\mathcal{D}}(X), \sqsubseteq_D)$ forms a coherent dcpo with a countable basis $\{\sum_{i=1}^{n} r_i \cdot \delta(x_i) \mid n \in \mathbb{Z}^+ \wedge r_i \in \mathbb{Q}^+ \wedge \sum_{i=1}^{n} r_i \leq 1 \wedge x_i \in X\}$. It admits a least element $\bot_D \stackrel{\text{def}}{=} \lambda x.0$. Moreover, ${}_p\oplus$ is Scott-continuous for all $p \in [0,1]$.*

Proposition 3.7 ([82, 144]). *Every function $f : X \to \underline{\mathcal{D}}(X)$ can be lifted to a unique Scott-continuous linear (in the sense that it preserves probabilistic-choice) map $\widehat{f} : \underline{\mathcal{D}}(X) \to \underline{\mathcal{D}}(X)$.*

3.1.3 Nondeterministic Powerdomains

When nondeterminism comes into the picture, as I discussed at the beginning of this chapter, existing studies usually resolve program inputs *prior to* nondeterminism [45, 84, 110, 111, 115, 116, 144]. I call such a model *nondeterminism-last*, which interprets nondeterministic functions as maps from inputs to sets of outputs. Let X be a nonempty countable set. A subset A of $\underline{\mathcal{D}}(X)$ is called *convex* if for all $\Delta_1, \Delta_2 \in A$ and all $p \in [0,1]$, we have $\Delta_1 \,{}_p\oplus\, \Delta_2 \in A$. The *convex hull* of an arbitrary subset A is the smallest convex set containing A as a subset, denoted by $conv(A)$. The convexity condition ensures that from the perspective of programming, nondeterministic choices can always be *refined* by probabilistic choices. The *convex powerdomain* $\mathcal{P}\underline{\mathcal{D}}(X)$ over the probabilistic powerdomain $\underline{\mathcal{D}}(X)$ is then defined as convex *lenses* in $\underline{\mathcal{D}}(X)$—nonempty subsets of $\underline{\mathcal{D}}(X)$ each of which is the intersection of a Scott-closed subset and a Scott-compact saturated subset—with the *Egli-Milner order* $A \sqsubseteq_P B \stackrel{\text{def}}{=} A \subseteq {\downarrow}B \wedge {\uparrow}A \supseteq B$.

The following theorems provide a characterization of the convex powerdomains.

Proposition 3.8 ([110, 144]). *The poset $(\mathcal{P}\underline{\mathcal{D}}(X), \sqsubseteq_P)$ forms a coherent dcpo. It admits a least element $\bot_P \stackrel{\text{def}}{=} \{\bot_D\}$. For $r_1, r_2 \in [0,1]$ satisfying $r_1 + r_2 \leq 1$, we define $r_1 \cdot A + r_2 \cdot B \stackrel{\text{def}}{=} \overline{C} \cap {\uparrow}C$ where C is $\{r_1 \cdot \Delta_1 + r_2 \cdot \Delta_2 \mid \Delta_1 \in A \wedge \Delta_2 \in B\}$. Then the probabilistic-choice operation is lifted to a Scott-continuous operation as $A \,{}_p\oplus_P\, B \stackrel{\text{def}}{=} p \cdot A + (1-p) \cdot B$. Moreover, it carries a Scott-continuous semilattice operation, called* formal union*, defined as $A \uplus_P B \stackrel{\text{def}}{=} \overline{C} \cap {\uparrow}C$ where C is $conv(A \cup B)$.*

The formal-union operation $\uplus$ corresponds to the program construct "**if** $\star$ **then** $\cdots$ **else** $\cdots$ **fi**" for nondeterministic choices.

Proposition 3.9 ([144]). *Every function $g : X \to \mathcal{P}\underline{\mathcal{D}}(X)$ can be lifted to a unique Scott-continuous linear (in the sense that it preserves lifted probabilistic-choice) map $\widehat{\widehat{g}} : \mathcal{P}\underline{\mathcal{D}}(X) \to \mathcal{P}\underline{\mathcal{D}}(X)$ preserving formal unions.*

Example 3.10. Consider the following program P where $\star$ can be refined by any deterministic condition involving the program variable t:

$$\textbf{if } \star \textbf{ then } t := t+1 \textbf{ else } t := t-1 \textbf{ fi}$$

and we want to assign a denotation to it from $X \to \mathcal{P}\underline{\mathcal{D}}(X)$, where the state space $X = \mathbb{Q}$ represents the value of t. Fix an input $t \in \mathbb{Q}$. The data actions $t := t+1$ and $t := t-1$ then take the input to singletons $\{\delta(t+1)\}$ and $\{\delta(t-1)\}$, respectively, in the powerdomain $\mathcal{P}\underline{\mathcal{D}}(\mathbb{Q})$. Thus the nondeterministic-choice is interpreted as $\{\delta(t+1)\} \uplus_P \{\delta(t-1)\}$, which is $\{r \cdot \delta(t+1) + (1-r) \cdot \delta(t-1) \mid r \in [0,1]\}$, for a given $t \in \mathbb{Q}$.

3.2 Nondeterminism-First

In this section, I develop a new model of nondeterminism—the *nondeterminism-first* approach, which resolves nondeterministic choices *prior to* program inputs—in a domain-theoretic way. This model is inspired by reasoning about a program's behavior on different inputs (as mentioned in the beginning of this chapter), which requires nondeterministic functions to be treated as a family of *transformers* (i.e., an element of $\wp(X \to X)$) instead of a set-valued map (i.e., an element of $X \to \wp(X)$). As will be shown in this section, with nondeterminism-first, $t := t + 1$ and $t := t - 1$ are assigned semantic objects $\{\lambda t.\ \delta(t+1)\}$ and $\{\lambda t.\ \delta(t-1)\}$, respectively.

I first introduce a simplified notion of *kernels* on a countable state space, then propose a new notion of *generalized convexity* (*g-convexity*, for short), and finally develop a powerdomain for nondeterminism-first.

3.2.1 A Powerdomain for Sub-Probability Kernels

Let X be a nonempty countable set. A function $\kappa : X \to \underline{\mathcal{D}}(X)$ is called a *(sub-probability) kernel*. Intuitively, a kernel maps an input state to a distribution over output states. The set of all such kernels is denoted by $\underline{\mathcal{K}}(X) \stackrel{\text{def}}{=} X \to \underline{\mathcal{D}}(X)$. Kernels are ordered pointwise, i.e., $\kappa_1 \sqsubseteq_K \kappa_2 \stackrel{\text{def}}{=} \forall x \in X : \kappa_1(x) \sqsubseteq_D \kappa_2(x)$.

THEOREM 3.11. *The poset $(\underline{\mathcal{K}}(X), \sqsubseteq_K)$ forms a coherent dcpo, with $\bot_K \stackrel{\text{def}}{=} \lambda x.\bot_D$ as its least element.*

PROOF. We equip X with the discrete topology. We then define $X_\bot = X \cup \{\bot\}$ with a distinguished least element $\bot$ and thus $X_\bot$ is a flat domain. Then $X_\bot$ is a bounded-complete domain.[2] The Scott-compact subsets of $X_\bot$ are precisely finite subsets of X and all subsets that contain $\bot$. Thus $X_\bot$ is coherent. By [2, Ex. 4.3.11.14], we know that $X_\bot$ is an FS-domain.[3]

By Proposition 3.6 we know that $\underline{\mathcal{D}}(X)$ is coherent. Moreover, $\underline{\mathcal{D}}(X)$ is also bounded-complete. Thus, by [2, Ex. 4.3.11.14], $\underline{\mathcal{D}}(X)$ is an FS-domain. By [2, Thm. 4.2.11], we know that $[X_\bot \to \underline{\mathcal{D}}(X)]$ is an FS-domain.

Let $s \stackrel{\text{def}}{=} \lambda f.f$ and $r \stackrel{\text{def}}{=} \lambda g.\lambda x.\textbf{if } x = \bot \textbf{ then } \bot_D \textbf{ else } g(x)$. Then $s : [X_\bot \xrightarrow{\bot!} \underline{\mathcal{D}}(X)] \to [X_\bot \to \underline{\mathcal{D}}(X)]$, $r : [X_\bot \to \underline{\mathcal{D}}(X)] \to [X_\bot \xrightarrow{\bot!} \underline{\mathcal{D}}(X)]$, and $r \circ s$ is the identity on $[X_\bot \xrightarrow{\bot!} \underline{\mathcal{D}}(X)]$, where $[A \xrightarrow{\bot!} B]$ stands for Scott-continuous functions from a dcpo A to a dcpo B that preserve the least element. Hence $[X_\bot \xrightarrow{\bot!} \underline{\mathcal{D}}(X)]$ is a retract of $[X_\bot \to \underline{\mathcal{D}}(X)]$. By [2, Prop. 4.2.12], we know that $[X_\bot \xrightarrow{\bot!} \underline{\mathcal{D}}(X)]$ is also an FS-domain.

For any f in $[X \to \underline{\mathcal{D}}(X)]$, we define a unique function $g \stackrel{\text{def}}{=} \lambda x.\textbf{if } x = \bot \textbf{ then } \bot_D \textbf{ else } f(x)$. For any g in $[X_\bot \xrightarrow{\bot!} \underline{\mathcal{D}}(X)]$, we define a unique function $f \stackrel{\text{def}}{=} \lambda x.g(x)$. Thus $[X \to \underline{\mathcal{D}}(X)]$ is homeomorphic to $[X_\bot \xrightarrow{\bot!} \underline{\mathcal{D}}(X)]$, and we know that $[X \to \underline{\mathcal{D}}(X)]$ is also an FS-domain. By [2,

[2] A continuous dcpo D with a least element is said to be a *bounded-complete* domain, if each bounded pair of elements of D has a supremum.

[3] A dcpo D with a least element is said to be an *FS-domain*, if there exists a directed set $\{f_i\}_{i\in I}$ of Scott-continuous functions on D, where each f_i is *finitely separated from the identity on D*, i.e., there exists a finite set M_i such that for any $x \in D$ there is $m \in M_i$ with $f_i(x) \sqsubseteq m \sqsubseteq x$, and $\bigsqcup^{\uparrow}_{i\in I} f_i$ is the identity map on D.

Thm. 4.2.18], we know that $[X \to \underline{\mathcal{D}}(X)]$ is coherent. Because the topology on X is discrete, $[X \to \underline{\mathcal{D}}(X)]$ is precisely $X \to \underline{\mathcal{D}}(X)$. Thus we conclude that $\underline{\mathcal{K}}(X)$ is coherent. □

Let $\mathbb{W}(X) \stackrel{\text{def}}{=} X \to [0,1]$ be the set of functions from X to the unit interval $[0,1]$. We denote the pointwise comparison by $\dot{\leq}$ and the constant function by $\dot{r}$ for any $r \in [0,1]$. If κ is a kernel and $\phi \in \mathbb{W}(X)$, we write $\phi \cdot \kappa$ for the kernel $\lambda x.\phi(x) \cdot \kappa(x)$. If κ_1, κ_2 are kernels and $\phi_1, \phi_2 \in \mathbb{W}(X)$ such that $\phi_1 + \phi_2 \dot{\leq} \dot{1}$, we write $\phi_1 \cdot \kappa_1 + \phi_2 \cdot \kappa_2$ for the kernel $\lambda x.\ \phi_1(x) \cdot \kappa_1(x) + \phi_2(x) \cdot \kappa_2(x)$. More generally, if $\{\kappa_i\}_{i\in\mathbb{N}}$ is a sequence of kernels, and $\{\phi_i\}_{i\in\mathbb{N}}$ is a sequence of functions in $\mathbb{W}(X)$ such that $\sum_{i=1}^{\infty} \phi_i \dot{\leq} \dot{1}$, we write $\sum_{i=1}^{\infty} \phi_i \cdot \kappa_i$ for the kernel $\bigsqcup^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \phi_i \cdot \kappa_i$. Then we define *conditional-choice* of kernels κ_1, κ_2 conditioning on a function $\phi \in \mathbb{W}(X)$ as $\kappa_1 \,{}_{\phi}\!\diamond\, \kappa_2 \stackrel{\text{def}}{=} \phi \cdot \kappa_1 + (\dot{1} - \phi) \cdot \kappa_2$. We define the *composition* of kernels κ_1, κ_2 as $\kappa_1 \otimes \kappa_2 \stackrel{\text{def}}{=} \lambda x.\ \lambda x''.\ \sum_{x'\in X} \kappa_1(x)(x') \cdot \kappa_2(x')(x'')$.

LEMMA 3.12.

1. *The conditional-choice operation* ${}_{\phi}\!\diamond$ *is Scott-continuous for all* $\phi \in \mathbb{W}(X)$.
2. *The composition operation* $\otimes$ *is Scott-continuous.*

PROOF.

1. Monotonicity is obvious. It then suffices to show that for all directed set $A \subseteq \underline{\mathcal{K}}(X)$, $\phi \cdot (\bigsqcup^{\uparrow} A) = \bigsqcup^{\uparrow}_{\kappa\in A} \phi \cdot \kappa$. Let $\kappa' \stackrel{\text{def}}{=} \bigsqcup^{\uparrow} A$. We conclude the proof by
$$\Big\rfloor^{\uparrow}_{\kappa\in A} \phi(x) \cdot \kappa(x) = \phi(x) \cdot \Big\rfloor^{\uparrow}_{\kappa\in A} \kappa(x) = \phi(x) \cdot (\Big\rfloor^{\uparrow} A)(x) = \phi(x) \cdot \kappa'(x),$$
for any $x \in X$.

2. Monotonicity is obvious. We proceed with a discussion of the left and right continuity.
Left-Scott-continuity. For all directed set $A \subseteq \underline{\mathcal{K}}(X)$ and all $\rho \in \underline{\mathcal{K}}(X)$, we want to show that $(\bigsqcup^{\uparrow} A) \otimes \rho = \bigsqcup^{\uparrow}_{\kappa\in A} \kappa \otimes \rho$. Let $\kappa' \stackrel{\text{def}}{=} \bigsqcup^{\uparrow} A$. Then it is sufficient to show that for all x and x'' in X, it holds that
$$\sum_{x'\in X} \kappa'(x)(x')\rho(x')(x'') = \Big\rfloor^{\uparrow}_{\kappa\in A} \sum_{x'\in X} \kappa(x)(x')\rho(x')(x''). \tag{3.1}$$
Because A is directed and $\underline{\mathcal{K}}(X)$ is ordered pointwise, the set $\{\kappa(x) \mid \kappa \in A\}$ is also directed in $\underline{\mathcal{D}}(X)$. By [83, Thm. 3.3] , the right-hand-side of (3.1) equals $\sum_{x'\in X} (\bigsqcup^{\uparrow}_{\kappa\in A} \kappa(x))(x')\rho(x')(x'')$. We conclude the proof by $\kappa'(x) = \bigsqcup^{\uparrow}_{\kappa\in A} \kappa(x)$ by the definition of κ'.
Right-Scott-continuity. For all directed set $A \subseteq \underline{\mathcal{K}}(X)$ and all $\rho \in \underline{\mathcal{K}}(X)$, we want to show that $\rho \otimes (\bigsqcup^{\uparrow} A) = \bigsqcup^{\uparrow}_{\kappa\in A} \rho \otimes \kappa$. Let $\kappa' \stackrel{\text{def}}{=} \bigsqcup^{\uparrow} A$. Then it is sufficient to show that for all x and x'' in X, it holds that
$$\sum_{x'\in X} \rho(x)(x')\kappa'(x')(x'') = \Big\rfloor^{\uparrow}_{\kappa\in A} \sum_{x'\in X} \rho(x)(x')\kappa(x')(x''). \tag{3.2}$$
Because A is directed and $\underline{\mathcal{K}}(X)$ as well as $\underline{\mathcal{D}}(X)$ are ordered pointwise, the set $\{\lambda x'.\kappa(x')(x'') \mid \kappa \in A\}$ is directed and bounded. By [83, Thm. 3.1], the right-hand-side of (3.2) equals $\sum_{x'\in X} \rho(x)(x')(\bigsqcup^{\uparrow}_{\kappa\in A} \lambda x'.\kappa(x')(x''))(x')$. We conclude the proof by the fact $\lambda x'.\kappa'(x')(x'') = \bigsqcup^{\uparrow}_{\kappa\in A} \lambda x'.\kappa(x')(x'')$ from the definition of κ'.

□

3.2.2 Generalized Convexity

As shown in §3.1.3, nondeterminism-*last* is captured by convex sets of distributions. However, a more complicated notion of convexity is needed to develop nondeterminism-*first* semantics over kernels. Let X be a nonempty countable set. Every semantic object should be closed under the conditional-choice ${}_{\phi}\Diamond$ for every function $\phi \in \mathbb{W}(X)$. The operation ${}_{\phi}\Diamond$ corresponds to the program construct "**if** ϕ **then** $\cdots$ **else** $\cdots$ **fi**." Recall that the definition $\kappa_1 \,{}_{\phi}\Diamond\, \kappa_2 \stackrel{\text{def}}{=} \phi \cdot \kappa_1 + (\dot{1} - \phi) \cdot \kappa_2$ is similar to a convex combination, except that the coefficients might not only be constants, but can also depend on the state. I formalize the idea by defining a notion of *g-convexity*.

Definition 3.13. A subset A of $\underline{\mathcal{K}}(X)$ is called *g-convex*, if for all sequences $\{\kappa_i\}_{i\in\mathbb{N}} \subseteq A$ and $\{\phi_i\}_{i\in\mathbb{N}} \subseteq \mathbb{W}(X)$ such that $\sum_{i=1}^{\infty} \phi_i = \dot{1}$, it holds that $\sum_{i=1}^{\infty} \phi_i \cdot \kappa_i$ is contained in A.

I now show that some domain-theoretic operations preserve g-convexity.

Lemma 3.14. *Let A be a g-convex subset of $\underline{\mathcal{K}}(X)$. Then*

1. *The saturation $\uparrow A$ and the lower closure $\downarrow A$ are g-convex.*
2. *The closure $\overline{A}$ is g-convex.*

Proof.

1. Straightforward by the fact that for any $\{\phi_i\}_{i\in\mathbb{N}} \subseteq \mathbb{W}(X)$, and any $\{\kappa_i\}_{i\in\mathbb{N}} \subseteq \underline{\mathcal{K}}(X)$, $\{\rho_i\}_{i\in\mathbb{N}} \subseteq \underline{\mathcal{K}}(X)$ satisfying that $\kappa_i \sqsubseteq_K \rho_i$ for all $i \in \mathbb{Z}^+$, it holds that $\sum_{i=0}^{\infty} \phi_i \cdot \kappa_i \sqsubseteq_K \sum_{i=0}^{\infty} \phi_i \cdot \rho_i$.
2. The Scott-closure of A can be obtained by $\overline{A} = \{\bigsqcup^{\uparrow} B \mid B \subseteq \downarrow A, B \text{ directed}\}$ [144]. For any $\{\kappa_i\}_{i\in\mathbb{N}} \subseteq \overline{A}$, there are directed subsets B_i of $\downarrow A$ such that $\kappa_i = \bigsqcup^{\uparrow} B_i$ for all $i \in \mathbb{N}$. For any $\{\phi_i\}_{i\in\mathbb{N}} \subseteq \mathbb{W}(X)$ such that $\sum_{i=1}^{\infty} \phi_i = \dot{1}$, we have

$$\begin{aligned}
\sum_{i=1}^{\infty} \phi_i \cdot \kappa_i &= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \phi_i \cdot \kappa_i \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \phi_i \cdot \left(\bigsqcup\nolimits^{\uparrow} B_i\right) \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \bigsqcup\nolimits^{\uparrow}_{\rho_i\in B_i} \phi_i \cdot \rho_i \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \bigsqcup\nolimits^{\uparrow}_{\forall i \rho_i\in B_i} \sum_{i=1}^{n} \phi_i \cdot \rho_i \\
&= \bigsqcup\nolimits^{\uparrow}_{\forall i \rho_i\in B_i} \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \phi_i \cdot \rho_i \\
&= \bigsqcup\nolimits^{\uparrow}_{\forall i \rho_i\in B_i} \sum_{i=1}^{\infty} \phi_i \cdot \rho_i,
\end{aligned}$$

   where $\sum_{i=1}^{\infty} \phi_i \cdot \rho_i$ is indeed contained in $\downarrow A$ by its g-convexity and hence $\{\sum_{i=1}^{\infty} \phi_i \cdot \rho_i \mid \forall i : \rho_i \in B_i\}$ is a directed subset of $\downarrow A$, thus $\sum_{i=1}^{\infty} \phi_i \cdot \kappa_i$ is contained in $\overline{A}$.

□

The *g-convex hull* of a subset A of $\underline{\mathcal{K}}(X)$ is the smallest g-convex set containing A as a subset, denoted by $gconv(A)$. Intuitively, $gconv(A)$ enriches A to become a reasonable semantic object that is closed under arbitrary conditional-choice.

Below are some properties of the $gconv(\cdot)$ operator.

LEMMA 3.15. *Suppose that A and B are g-convex subsets of $\underline{\mathcal{K}}(X)$. Then $\{\kappa \ {}_\phi\Diamond\ \rho \mid \kappa \in A \wedge \rho \in B\}$ is g-convex for all functions $\phi \in \mathbb{W}(X)$.*

PROOF. Let $\{\eta_i\}_{i\in\mathbb{N}}$ be any sequence in $\{\kappa \ {}_\phi\Diamond\ \rho \mid \kappa \in A \wedge \rho \in B\}$, and $\eta_i = \kappa_i \ {}_\phi\Diamond\ \rho_i$ such that $\kappa_i \in A, \rho_i \in B$ for all $i \in \mathbb{N}$. For any $\{\psi_i\}_{i\in\mathbb{N}} \subseteq \mathbb{W}(X)$ such that $\sum_{i=1}^{\infty} \psi_i = \dot{1}$, we have

$$
\begin{aligned}
\sum_{i=1}^{\infty} \psi_i \cdot \eta_i &= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \psi_i \cdot \eta_i \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \psi_i \cdot (\kappa_i \ {}_\phi\Diamond\ \rho_i) \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \psi_i \cdot (\phi \cdot \kappa_i + (\dot{1} - \phi) \cdot \rho_i) \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} ((\psi_i\phi) \cdot \kappa_i + (\psi_i - \psi_i\phi) \cdot \rho_i) \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \left(\sum_{i=1}^{n} (\psi_i\phi) \cdot \kappa_i + \sum_{i=1}^{n} (\psi_i - \psi_i\phi) \cdot \rho_i \right) \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} (\psi_i\phi) \cdot \kappa_i + \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} (\psi_i - \psi_i\phi) \cdot \rho_i \\
&= \phi \cdot \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \psi_i \cdot \kappa_i + (\dot{1} - \phi) \cdot \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \psi_i \cdot \rho_i \\
&= \left(\sum_{i=1}^{\infty} \psi_i \cdot \kappa_i \right) \ {}_\phi\Diamond\ \left(\sum_{i=1}^{\infty} \psi_i \cdot \rho_i \right).
\end{aligned}
$$

Because A and B are g-convex, we know that $\sum_{i=0}^{\infty} \psi_i \cdot \kappa_i \in A$ and $\sum_{i=1}^{\infty} \psi_i \cdot \rho_i \in B$. Hence $\sum_{i=1}^{\infty} \psi_i \cdot \eta_i$ is contained in $\{\kappa \ {}_\phi\Diamond\ \rho \mid \kappa \in A \wedge \rho \in B\}$. □

COROLLARY 3.16. *If A and B are g-convex, then $gconv(A \cup B)$ is given by $\{\kappa_1 \ {}_\phi\Diamond\ \kappa_2 \mid \kappa_1 \in A \wedge \kappa_2 \in B \wedge \phi \in \mathbb{W}(X)\}$.*

PROOF. It is straightforward to show that $gconv(A \cup B)$ is a superset of $\{\kappa_1 \ {}_\phi\Diamond\ \kappa_2 \mid \kappa_1 \in A \wedge \kappa_2 \in B \wedge \phi \in \mathbb{W}(X)\}$. Then it suffices to show this set is indeed g-convex. We conclude the proof by Lemma 3.15. □

For a finite subset F of $\underline{\mathcal{K}}(X)$, as an immediate corollary of Corollary 3.16, by a simple induction we know that $gconv(F) = \{\sum_{\kappa\in F} \phi_\kappa \cdot \kappa \mid \{\phi_\kappa\}_{\kappa\in F} \subseteq \mathbb{W}(X) \wedge \sum_{\kappa\in F} \phi_\kappa = \dot{1}\}$.

LEMMA 3.17. *For an arbitrary $A \subseteq \mathcal{K}(X)$, it holds that*

$$
gconv(A) = \left\{ \sum_{i=1}^{\infty} \phi_i \cdot \kappa_i \mid \{\kappa_i\}_{i\in\mathbb{N}} \subseteq A \wedge \{\phi_i\}_{i\in\mathbb{N}} \subseteq \mathbb{W}(X) \wedge \sum_{i=1}^{\infty} \phi_i = \dot{1} \right\}. \tag{3.3}
$$

Proof. It is straightforward to show that $gconv(A)$ is a superset of the right-hand-side of (3.3). Then we want to show the right-hand-side is indeed g-convex, which indicates the desired equality by the definition of $gconv(A)$.

Suppose $\{\kappa_i\}_{i\in\mathbb{N}}$ is a sequence in the right-hand-side of (3.3). Then for all $i \in \mathbb{N}$, there exist $\{\kappa_{i,j}\}_{j\in\mathbb{N}} \subseteq A$ and $\{\phi_{i,j}\}_{j\in\mathbb{N}}$ such that $\sum_{j=1}^{\infty} \phi_{i,j} = \dot{1}$ and $\kappa_i = \sum_{j=1}^{\infty} \phi_{i,j} \cdot \kappa_{i,j}$. It is sufficient to show that for all $\{\phi_i\}_{i\in\mathbb{N}}$, the kernel $\sum_{i=1}^{\infty} \phi_i \cdot \kappa_i$ is contained in the right-hand-side of (3.3). We have

$$\begin{aligned}
\sum_{i=1}^{\infty} \phi_i \cdot \kappa_i &= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \phi_i \cdot \kappa_i \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \phi_i \cdot \sum_{j=1}^{\infty} \phi_{i,j} \cdot \kappa_{i,j} \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \phi_i \cdot \bigsqcup\nolimits^{\uparrow}_{m\in\mathbb{Z}^+} \sum_{j=1}^{m} \phi_{i,j} \cdot \kappa_{i,j} \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+,m\in\mathbb{Z}^+} \sum_{1\le i\le n,1\le j\le m} (\phi_i\phi_{i,j}) \cdot \kappa_{i,j}.
\end{aligned}$$

Let $\theta : \mathbb{N}\times\mathbb{N} \to \mathbb{N}$ be an arbitrary bijection. Let $\rho_k \overset{\text{def}}{=} \kappa_{i,j}$ and $\psi_k \overset{\text{def}}{=} \phi_i\phi_{i,j}$ such that $(i,j) = \theta^{-1}(k)$. Then $\sum_{k=1}^{\infty} \psi_k = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \psi_{\theta(i,j)} = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} \phi_i\phi_{i,j} = \sum_{i=1}^{\infty} \phi_i \sum_{j=1}^{\infty} \phi_{i,j} = \sum_{i=1}^{\infty} \phi_i \cdot \dot{1} = \sum_{i=1}^{\infty} \phi_i = \dot{1}$. We now have

$$\begin{aligned}
\bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+,m\in\mathbb{Z}^+} \sum_{1\le i\le n,1\le j\le m} (\phi_i\phi_{i,j}) \cdot \kappa_{i,j} &= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+,m\in\mathbb{Z}^+} \sum_{1\le i\le n,1\le j\le m} \psi_{\theta(i,j)} \cdot \rho_{\theta(i,j)} \\
&= \bigsqcup\nolimits^{\uparrow}_{l\in\mathbb{Z}^+} \sum_{k=1}^{l} \psi_k \cdot \rho_k \\
&= \sum_{k=1}^{\infty} \psi_l \cdot \rho_l,
\end{aligned}$$

which is indeed contained in the right-hand-side of (3.3). The second last equation of the derivation above is established as follows:

- To show $\bigsqcup^{\uparrow}_{n\in\mathbb{Z}^+,m\in\mathbb{Z}^+} \sum_{1\le i\le n,1\le j\le m} \psi_{\theta(i,j)} \cdot \rho_{\theta(i,j)} \sqsubseteq_K \bigsqcup^{\uparrow}_{l\in\mathbb{Z}^+} \sum_{k=1}^{l} \psi_k \cdot \rho_k$: Fix $n_o \in \mathbb{Z}^+$ and $m_o \in \mathbb{Z}^+$. Let $l_o \overset{\text{def}}{=} \max_{1\le i\le n_o,1\le j\le m_o} \theta(i,j)$. Then we conclude by $\sum_{1\le i\le n_o,1\le j\le m_o} \psi_{\theta(i,j)} \cdot \rho_{\theta(i,j)} \sqsubseteq_K \sum_{k=1}^{l_o} \psi_k \cdot \rho_k$.
- To show $\bigsqcup^{\uparrow}_{l\in\mathbb{Z}^+} \sum_{k=1}^{l} \psi_k \cdot \rho_k \sqsubseteq_K \bigsqcup^{\uparrow}_{n\in\mathbb{Z}^+,m\in\mathbb{Z}^+} \sum_{1\le i\le n,1\le j\le m} \psi_{\theta(i,j)} \cdot \rho_{\theta(i,j)}$: Fix $l_o \in \mathbb{Z}^+$. Let $n_o \overset{\text{def}}{=} \max_{1\le k\le l_o} \theta^{-1}(k).\mathbf{fst}$ and $m_o \overset{\text{def}}{=} \max_{1\le k\le l_o} \theta^{-1}(k).\mathbf{snd}$. Then we conclude by $\sum_{k=1}^{l_o} \psi_k \cdot \rho_k \sqsubseteq_K \sum_{1\le i\le n_o,1\le j\le m_o} \psi_{\theta(i,j)} \cdot \rho_{\theta(i,j)}$.

□

Lemma 3.18.

1. *For an arbitrary $A \subseteq \underline{\mathcal{K}}(X)$, it holds that $\overline{gconv(A)} = \overline{gconv\left(\overline{A}\right)}$.*

2. *If $\{A_i\}_{i\in\mathcal{I}}$ is a directed collection of Scott-closed subsets of $\underline{\mathcal{K}}(X)$ ordered by set inclusion, then* $\overline{gconv\left(\bigcup_{i\in\mathcal{I}} A_i\right)} = \overline{\bigcup_{i\in\mathcal{I}} \overline{gconv(A_i)}}$.

Proof.

1. The $\subseteq$-direction is straightforward. For the $\supseteq$-direction, we have

$$gconv\left(\overline{A}\right) = \left\{\sum_{i=1}^{\infty} \phi_i \cdot \kappa_i \mid \{\kappa_i\}_{i\in\mathbb{N}} \subseteq \overline{A} \wedge \{\phi_i\}_{i\in\mathbb{N}} \subseteq \mathbb{W}(X) \wedge \sum_{i=1}^{\infty} \phi_i = \dot{1}\right\}$$

by Lemma 3.17 and $\overline{A} = \{\bigsqcup^{\uparrow} B \mid B \subseteq {\downarrow}A, B \text{ directed}\}$ [144]. Let $\kappa \stackrel{\text{def}}{=} \sum_{i=1}^{\infty} \phi_i \cdot \kappa_i$ be an element of $gconv\left(\overline{A}\right)$ where $\{\kappa_i\}_{i\in\mathbb{N}} \subseteq \overline{A}$. Then for all $i \in \mathbb{N}$, there exists a directed $B_i \subseteq {\downarrow}A$ satisfying $\kappa_i = \bigsqcup^{\uparrow} B_i$. Then we have

$$\begin{aligned}
\sum_{i=1}^{\infty} \phi_i \cdot \kappa_i &= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \phi_i \cdot \kappa_i \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \phi_i \cdot \bigsqcup^{\uparrow} B_i \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \bigsqcup\nolimits^{\uparrow}_{\rho_i\in B_i} (\phi_i \cdot \rho_i) \\
&= \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \bigsqcup\nolimits^{\uparrow}_{\forall i:\rho_i\in B_i} \sum_{i=1}^{n} \phi_i \cdot \rho_i \\
&= \bigsqcup\nolimits^{\uparrow}_{\forall i:\rho_i\in B_i} \bigsqcup\nolimits^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{i=1}^{n} \phi_i \cdot \rho_i \\
&= \bigsqcup\nolimits^{\uparrow}_{\forall i:\rho_i\in B_i} \sum_{i=1}^{\infty} \phi_i \cdot \rho_i.
\end{aligned}$$

Because $\rho_i \in B_i \subseteq {\downarrow}A$, there exists $\eta_i \in A$ satisfying $\rho_i \sqsubseteq_K \eta_i$ for all $i \in \mathbb{N}$, and thus $\sum_{i=1}^{\infty} \phi_i \cdot \eta_i \in gconv(A)$. We also know that $\sum_{i=1}^{\infty} \phi_i \cdot \rho_i \sqsubseteq_K \sum_{i=1}^{\infty} \phi_i \cdot \eta_i$, thus $\sum_{i=1}^{\infty} \phi_i \cdot \rho_i \in {\downarrow}gconv(A)$. Therefore $\sum_{i=1}^{\infty} \phi_i \cdot \kappa_i \in \overline{gconv(A)}$. By $gconv\left(\overline{A}\right) \subseteq \overline{gconv(A)}$ we conclude that $\overline{gconv\left(\overline{A}\right)} \subseteq \overline{gconv(A)}$.

2. For the $\supseteq$-direction, we have

$$\begin{aligned}
& \forall i \in \mathcal{I} : gconv\left(\bigcup\nolimits_{i\in\mathcal{I}} A_i\right) \supseteq gconv(A_i) \\
\Longrightarrow\ & \forall i \in \mathcal{I} : \overline{gconv\left(\bigcup\nolimits_{i\in\mathcal{I}} A_i\right)} \supseteq \overline{gconv(A_i)} \\
\Longrightarrow\ & \overline{gconv\left(\bigcup\nolimits_{i\in\mathcal{I}} A_i\right)} \supseteq \bigcup\nolimits_{i\in\mathcal{I}} \overline{gconv(A_i)} \\
\Longrightarrow\ & \overline{gconv\left(\bigcup\nolimits_{i\in\mathcal{I}} A_i\right)} \supseteq \overline{\bigcup\nolimits_{i\in\mathcal{I}} \overline{gconv(A_i)}}.
\end{aligned}$$

For the $\subseteq$-direction, we know that

$$gconv\left(\bigcup_{i\in\mathcal{I}} A_i\right) = \left\{\sum_{j=1}^{\infty} \phi_j \cdot \kappa_j \mid \{\kappa_j\}_{j\in\mathbb{N}} \subseteq \bigcup_{i\in\mathcal{I}} A_i \wedge \{\phi_j\}_{j\in\mathbb{N}} \subseteq \mathbb{W}(X) \wedge \sum_{j=1}^{\infty} \phi_j = \dot{1}\right\},$$

by Lemma 3.17. Let $\kappa \stackrel{\text{def}}{=} \sum_{j=1}^{\infty} \phi_j \cdot \kappa_j$ be an element of $gconv\left(\bigcup_{i\in\mathcal{I}} A_i\right)$ where $\{\kappa_j\}_{j\in\mathbb{Z}^+} \subseteq \bigcup_{i\in\mathcal{I}} A_i$. For all $n \in \mathbb{Z}^+$, because $\{A_i\}_{i\in\mathcal{I}}$ is directed, there exists $A_{o(n)}$ satisfying $\{\kappa_1, \cdots, \kappa_n\} \subseteq A_{o(n)}$. Thus $\sum_{j=1}^{n} \phi_j \cdot \kappa_j \in \overline{gconv\left(A_{o(n)}\right)}$. By the definition of Scott-closure, we know that $\bigsqcup^{\uparrow}_{n\in\mathbb{Z}^+} \sum_{j=1}^{n} \phi_j \cdot \kappa_j \in \overline{\bigcup_{i\in\mathcal{I}} \overline{gconv(A_i)}}$. Thus κ is contained in $\overline{\bigcup_{i\in\mathcal{I}} \overline{gconv(A_i)}}$ and $gconv\left(\bigcup_{i\in\mathcal{I}} A_i\right) \subseteq \overline{\bigcup_{i\in\mathcal{I}} \overline{gconv(A_i)}}$. Hence we conclude that $\overline{gconv\left(\bigcup_{i\in\mathcal{I}} A_i\right)} \subseteq \overline{\bigcup_{i\in\mathcal{I}} \overline{gconv(A_i)}}$.

□

Lemma 3.19. *Let A and B be Scott-compact g-convex subsets of $\underline{\mathcal{K}}(X)$. Then $gconv(A \cup B)$ is also Scott-compact.*

Proof. The unit interval $[0,1]$ equipped with its usual linear order forms a Scott-compact topology. By Tikhonov's theorem,[4] we know that $X \to [0,1] = [0,1]^X$ with the product topology is a Scott-compact space. Hence $\Gamma \stackrel{\text{def}}{=} \{(\phi, \dot{1} - \phi) \mid \phi \in \mathbb{W}(X)\}$ is also a Scott-compact space. The map from $\Gamma \times \underline{\mathcal{K}}(X) \times \underline{\mathcal{K}}(X)$ to $\underline{\mathcal{K}}(X)$ defined by $((\phi, \dot{1} - \phi), \kappa_1, \kappa_2) \mapsto \kappa_1 \,{}_{\phi}\!\diamond\, \kappa_2$ is Scott-continuous. By Corollary 3.16 we know that $gconv(A \cup B)$ is precisely the image of the Scott-compact set $\Gamma \times A \times B$. Because Scott-continuous functions preserve Scott-compactness, we conclude that $gconv(A \cup B)$ is also Scott-compact. □

I now turn to discuss some separation properties for g-convexity.

Lemma 3.20.

1. *If $A \subseteq \underline{\mathcal{K}}(X)$ is g-convex, then for all $x \in X$, the set $\{\kappa(x) \mid \kappa \in A\}$ is convex.*
2. *If $A \subseteq \underline{\mathcal{K}}(X)$ is Scott-compact, then for all $x \in X$, the set $\{\kappa(x) \mid \kappa \in A\}$ is Scott-compact.*
3. *If $A \subseteq \underline{\mathcal{K}}(X)$ is Scott-closed, then for all $x \in X$, the set $\{\kappa(x) \mid \kappa \in A\}$ is Scott-closed.*

Proof.

1. Let $x \in X$, $\kappa_1, \kappa_2 \in A$, and $p \in [0,1]$. We want to show that $p \cdot \kappa_1(x) + (1-p) \cdot \kappa_2(x) \in \{\kappa(x) \mid \kappa \in A\}$. Let $\phi \stackrel{\text{def}}{=} \lambda x.p$. Then $\kappa_1 \,{}_{\phi}\!\diamond\, \kappa_2 \in A$ because of g-convexity. We conclude the proof by $(\kappa_1 \,{}_{\phi}\!\diamond\, \kappa_2)(x) = \phi(x) \cdot \kappa_1(x) + (1 - \phi(x)) \cdot \kappa_2(x) = p \cdot \kappa_1(x) + (1-p) \cdot \kappa_2(x)$.
2. Let $x \in X$. Let $F(\kappa) \stackrel{\text{def}}{=} \kappa(x)$ be a map from $\underline{\mathcal{K}}(X)$ to $\underline{\mathcal{D}}(X)$. Because F is Scott-continuous and Scott-continuous functions preserve Scott-compactness, we conclude that $F(A)$ is Scott-compact because A is Scott-compact.
3. Straightforward by the fact that $\underline{\mathcal{K}}(X) = X \to \underline{\mathcal{D}}(X)$ and $\underline{\mathcal{K}}(X)$ is ordered pointwise.

[4] Let $\{(X_\alpha, \tau_\alpha)\}_{\alpha\in\Lambda}$ be a collection of topological spaces. Then $\prod_{\alpha\in\Lambda} X_\alpha$ is compact iff X_α is compact for all $\alpha \in \Lambda$.

□

LEMMA 3.21. *Let us consider subsets of $\underline{\mathcal{K}}(X)$. Suppose that K is a Scott-compact g-convex set and A is a nonempty Scott-closed g-convex set that is disjoint from K. Then they can be separated by a g-convex Scott-open set, i.e., there is a g-convex Scott-open set V including K and disjoint from A.*

PROOF. We claim that there exists $x \in X$ such that $K(x) \cap A(x) = \emptyset$.

If not, then for all $x \in X$ there is $K(x) \cap A(x) \neq \emptyset$. Hence we can define a kernel κ such that $\kappa(x) \in K(x) \cap A(x)$ for every x. We want to show that $\kappa \in A$ and $\kappa \in K$. This follows from g-convexity of A and K: suppose $\kappa(x) = \kappa_x(x)$ such that $\kappa_x \in K$ for all x, then $\kappa = \sum_{x \in X}(\lambda x'.[x = x']) \cdot \kappa_x$. This contradicts the fact that K and A are disjoint.

Let $x \in X$ such that $K(x) \cap A(x) = \emptyset$. By Lemma 3.20(ii)(iii) we know that $K(x)$ is Scott-compact and $A(x)$ is Scott-closed. By [144, Thm. 3.8] we know that there exist a Scott-continuous linear map F and a number a in $\mathbb{R}^+_\infty$ such that $F(\mu) > a > 1 \geq F(\nu)$ for all μ in $K(x)$ and ν in $A(x)$. Let $V \stackrel{\text{def}}{=} \{\kappa \mid F(\kappa(x)) > a\}$ be a Scott-open subset of $\underline{\mathcal{K}}(X)$. Then we know that $K \subseteq V$ and $A \cap V = \emptyset$. Then it suffices to show that V is g-convex. For any $\{\kappa_i\}_{i \in \mathbb{N}} \subseteq V$ and $\{\phi_i\}_{i \in \mathbb{N}} \subseteq \mathbb{W}(X)$ such that $\sum_{i=1}^\infty \phi_i = \dot{1}$, we have

$$\begin{aligned}
F\left(\left(\sum_{i=1}^\infty \phi_i \cdot \kappa_i\right)(x)\right) &= F\left(\sum_{i=1}^\infty \phi_i(x) \cdot \kappa_i(x)\right) \\
&= F\left(\bigsqcup\nolimits^{\uparrow}_{n \in \mathbb{Z}^+} \sum_{i=1}^n \phi_i(x) \cdot \kappa_i(x)\right) \\
&= \bigsqcup\nolimits^{\uparrow}_{n \in \mathbb{Z}^+} F\left(\sum_{i=1}^n \phi_i(x) \cdot \kappa_i(x)\right) \\
&= \bigsqcup\nolimits^{\uparrow}_{n \in \mathbb{Z}^+} \sum_{i=1}^n \phi_i(x) \cdot F(\kappa_i(x)) \\
&> a,
\end{aligned}$$

hence $\sum_{i=1}^\infty \phi_i \cdot \kappa_i \in V$. □

LEMMA 3.22. *If $K \subseteq \underline{\mathcal{K}}(X)$ is nonempty and Scott-compact, then $gconv(K)$ is Scott-compact.*

PROOF. It suffices to show that any open-cover of K is an open-cover of $gconv(K)$. Let C be an open-cover of K. Let $U = \bigcup C$. If $gconv(K)$ is not contained in U, then by Lemma 3.17, there exist $\{\kappa_i\}_{i \in \mathbb{N}} \subseteq K$ and $\{\phi_i\}_{i \in \mathbb{N}} \subseteq \mathbb{W}(X)$ such that $\sum_{i=1}^\infty \phi_i = \dot{1}$ and $\kappa \stackrel{\text{def}}{=} \sum_{i=1}^\infty \phi_i \cdot \kappa_i \in gconv(K) \setminus U$. Let $A = \downarrow\kappa$ be a Scott-closed set, then A is disjoint from U, and thus disjoint from K. Similar to the proof of Lemma 3.21, we claim that there exist $x \in X$ and a Scott-continuous linear map F and a number $a \in \mathbb{R}^+_\infty$ such that $F(\mu) > a > 1 \geq F(\nu)$ for all μ in $K(x)$ and $\nu \in A(x)$. Then $F(\kappa(x)) = F((\sum_{i=1}^\infty \phi_i \cdot \kappa_i)(x)) = F(\sum_{i=1}^\infty \phi_i(x) \cdot \kappa_i(x)) = \bigsqcup^{\uparrow}_{n \in \mathbb{Z}^+} F(\sum_{i=1}^n \phi_i(x) \cdot \kappa_i(x)) = \bigsqcup^{\uparrow}_{n \in \mathbb{Z}^+} \phi_i(x) \cdot F(\kappa_i(x)) > a > 1$, but because $\kappa \in A$ we also have $F(\kappa(x)) \leq 1$. We then conclude the proof by contradiction. □

3.2.3 A g-convex Powerdomain for Nondeterminism-First

From the literature, a *Plotkin powertheory* [2] is defined by one binary operation $\uplus$, called *formal union*, and the following laws: (i) $A \uplus B = B \uplus A$, (ii) $(A \uplus B) \uplus C = A \uplus (B \uplus C)$, and (iii) $A \uplus A = A$, for all objects A, B, C in the powerdomain. Intuitively, the formal union $\uplus$ represents nondeterministic-choice. Moreover, the formal union induces a semilattice ordering: $A \leq B$ if $A \uplus B = B$. The semilattice ordering is usually not interesting from the perspective of domain theory, however, it is instrumental to describe the relation between conditional-choice and nondeterministic-choice—$A \mathbin{}_{\phi}\!\diamond B \leq A \uplus B$ for all semantic objects A, B—a nondeterministic-choice should *abstract* an arbitrary (possibly probabilistic) conditional-choice.

Let X be a nonempty countable set. As nondeterminism-first interprets programs as collections of input-output transformers, I want to develop a powerdomain on $\underline{\mathcal{K}}(X)$, i.e., kernels on X. To achieve this goal, I need to (i) identify a collection of well-formed semantic objects in $\wp(\underline{\mathcal{K}}(X))$, which admits a formal-union operation described above, (ii) lift conditional-choice $\mathbin{}_{\phi}\!\diamond$ and composition $\otimes$ on kernels to the powerdomain properly, and (iii) prove the powerdomain is a dcpo and the operations are Scott-continuous.

Inspired by studies on convex powerdomains [2, 110, 144], I start with the following collection

$$\mathcal{G}\underline{\mathcal{K}}(X) \stackrel{\text{def}}{=} \{S \subseteq \underline{\mathcal{K}}(X) \mid S \text{ a nonempty g-convex lens}\}$$

to be the set of all g-convex *lenses* of $\underline{\mathcal{K}}(X)$ ordered by *Egli-Miler order* $A \sqsubseteq_G B \stackrel{\text{def}}{=} A \subseteq \downarrow B \wedge \uparrow A \supseteq B$. Recall that a lens of $\underline{\mathcal{K}}(X)$ is a nonempty subset of $\underline{\mathcal{K}}(X)$ that is the intersection of a Scott-closed subset and a Scott-compact saturated subset. I call $\mathcal{G}\underline{\mathcal{K}}(X)$ a *g-convex powerdomain* over kernels on X.

The following theorem establishes a characterization of g-convex powerdomains.

Theorem 3.23. *$(\mathcal{G}\underline{\mathcal{K}}(X), \sqsubseteq_G)$ forms a dcpo, with a least element $\bot_G \stackrel{\text{def}}{=} \{\bot_K\}$.*

Proof. It is straightforward to show that $(\mathcal{G}\underline{\mathcal{K}}(X), \sqsubseteq_G)$ forms a poset and $\bot_G$ is the least element. Then it suffices to show the powerdomain admits directed suprema. For a directed collection $\mathcal{A} = \{A_i\}_{i\in I} \subseteq \mathcal{G}\underline{\mathcal{K}}(X)$, we define $\bigsqcup^{\uparrow}_{i\in I} A_i \stackrel{\text{def}}{=} \overline{\bigcup_{i\in I} \downarrow A_i} \cap \bigcap_{i\in I} \uparrow A_i$. We now show $\bigsqcup^{\uparrow}_{i\in I} A_i$ is indeed the least upper bound of $\mathcal{A}$.

We already know $\underline{\mathcal{K}}(X)$ is coherent by Theorem 3.11. Observe that $\bigsqcup^{\uparrow}_{i\in I} A_i = \overline{\bigcup_{i\in I} \downarrow A_i} \cap \bigcap_{i\in I} \uparrow A_i = \bigcap_{i\in I} (\overline{\bigcup_{i\in I} \uparrow A_i} \cap \uparrow A_i)$, and $\{\overline{\bigcup_{i\in I} \uparrow A_i} \cap \uparrow A_i\}_{i\in I}$ is a filtered family of nonempty lenses, or more generally, nonempty Lawson-closed subsets thus nonempty Lawson-compact subsets because of the coherence of $\underline{\mathcal{K}}(X)$. By Proposition 3.5 we know the filtered family admits a nonempty intersection. Thus $\bigsqcup^{\uparrow}_{i\in I} A_i$ is a nonempty lens that is indeed g-convex by Lemma 3.14 and the g-convexity of A_i's. In this way we show that $\bigsqcup^{\uparrow}_{i\in I} A_i \in \mathcal{G}\underline{\mathcal{K}}(X)$.

Let $B \stackrel{\text{def}}{=} \bigsqcup^{\uparrow}_{i\in I} A_i$. To show that B is the least upper bound of $\mathcal{A}$, we claim that $\downarrow B = \overline{\bigcup_{i\in I} \downarrow A_i}$ and $\uparrow B = \bigcap_{i\in I} \uparrow A_i$. If so, then B is obviously an upper bound of $\mathcal{A}$ and if $A_i \sqsubseteq_G B'$ for all $i \in I$, then $\downarrow A_i \subseteq \downarrow B'$ and $\uparrow A_i \supseteq \uparrow B'$ for all $i \in I$, thus $\downarrow B = \overline{\bigcup_{i\in I} \downarrow A_i} \subseteq \downarrow B'$ and $\uparrow B = \bigcap_{i\in I} \uparrow A_i \supseteq \uparrow B'$, thus $B \sqsubseteq_G B'$. Since B' is arbitrarily chosen, we can conclude that B is the least upper bound of $\mathcal{A}$. We adapt a proof approach from Tix et al. [144]'s work as follows.

- To show $\downarrow B = \overline{\bigcup_{i\in I} \downarrow A_i}$: Inclusion is obvious. For the reversed inclusion, it is sufficient to show $\downarrow B \supseteq \bigcup_{i\in I} \downarrow A_i$ since $\downarrow B$ is Scott-closed. Fix $x \in \downarrow A_i$ for some $i \in I$. Then there exists $y \in A_i$ such that $x \sqsubseteq_K y$. For all $j \in I$ satisfying $A_i \sqsubseteq_G A_j$, there exists $z \in A_j$ such that $y \sqsubseteq_K z$. Therefore $\uparrow x \cap \overline{\bigcup_{i\in I} \downarrow A_i} \cap \uparrow A_j \neq \emptyset$. Again a filtered family of nonempty Lawson-compact sets admits a nonempty intersection by Proposition 3.5, we have $\uparrow x \cap \overline{\bigcup_{i\in I} \downarrow A_i} \cap \bigcap_{j\in I} \uparrow A_j \neq \emptyset$, i.e., $\uparrow x \cap B \neq \emptyset$, thus $x \in \downarrow B$.
- To show $\uparrow B = \bigcap_{i\in I} \uparrow A_i$: Inclusion is obvious. For the reversed inclusion, fix $x \in \bigcap_{i\in I} \uparrow A_i$. Then we have $\downarrow x \cap \overline{\bigcup_{i\in I} \downarrow A_i} \cap \uparrow A_j \neq \emptyset$ for all $j \in I$. By a similar reasoning to the previous case we have $\downarrow x \cap \overline{\bigcup_{i\in I} \downarrow A_i} \cap \bigcap_{j\in I} \uparrow A_j \neq \emptyset$, i.e., $\downarrow x \cap B \neq \emptyset$, thus $x \in \uparrow B$.

□

I now lift conditional-choice ${}_\phi\Diamond$ (where $\phi \in \mathbb{W}(X)$) and composition $\otimes$ for kernels to the powerdomain $\mathcal{GK}(X)$ as follows.

$$A \,{}_\phi\Diamond_G\, B \stackrel{\text{def}}{=} \overline{\{a \,{}_\phi\Diamond\, b \mid a \in A \wedge b \in B\}} \cap \uparrow\{a \,{}_\phi\Diamond\, b \mid a \in A \wedge b \in B\}$$
$$A \otimes_G B \stackrel{\text{def}}{=} \overline{gconv(\{a \otimes b \mid a \in A \wedge b \in B\})} \cap \uparrow gconv(\{a \otimes b \mid a \in A \wedge b \in B\})$$

The operations construct nonempty g-convex lenses by Lemmas 3.14 and 3.22. As conditional-choice and composition operations are Scott-continuous on kernels, the lifted operations are also Scott-continuous in the powerdomain.

LEMMA 3.24. *The operations ${}_\phi\Diamond_G$ and $\otimes_G$ are Scott-continuous for all $\phi \in \mathbb{W}(X)$.*

PROOF. The only nontrivial part of the proof is to show $\otimes_G$ preserves directed suprema. Firstly we claim that $\downarrow(A \otimes_G B) = \overline{gconv(\{a \otimes b \mid a \in \downarrow A \wedge b \in \downarrow B\})}$ and $\uparrow(A \otimes_G B) = \uparrow gconv(\{a \otimes b \mid a \in \uparrow A \wedge b \in \uparrow B\})$. Let's write $A \dot\otimes B$ for $\{a \otimes b \mid a \in A \wedge b \in B\}$.

- To show $\downarrow(A \otimes_G B) = \overline{gconv(\downarrow A \dot\otimes \downarrow B)}$: Inclusion is obvious. For the reversed inclusion, we have $\overline{gconv(\downarrow A \dot\otimes \downarrow B)} \subseteq \overline{gconv(\downarrow(A \dot\otimes B))} = gconv(\overline{\downarrow(A \dot\otimes B)}) = gconv(\overline{A \dot\otimes B}) = \overline{gconv(A \dot\otimes B)} \subseteq \downarrow(A \otimes_G B)$ by Lemma 3.18(i) and Lawson-compactness of $A \otimes_G B$.
- To show $\uparrow(A \otimes_G B) = \uparrow gconv(\uparrow A \dot\otimes \uparrow B)$: Inclusion is obvious. For the reversed inclusion, we have $\uparrow gconv(\uparrow A \dot\otimes \uparrow B) \subseteq \uparrow gconv(\uparrow(A \dot\otimes B)) \subseteq \uparrow gconv(A \dot\otimes B) \subseteq \uparrow(A \otimes_G B)$.

Then it suffices to show that $\otimes_G$ is Scott-continuous in the space of down-closures (i.e., $\{\downarrow A \mid A \in \mathcal{GK}(X)\}$), as well as in the space of up-closures (i.e., $\{\uparrow A \mid A \in \mathcal{GK}(X)\}$).

- Let a directed family $\{A_i\}_{i\in I}$ (ordered by inclusion) and B be nonempty Scott-closed g-convex subsets of $\mathcal{K}(X)$. We want to show that $\overline{gconv(\overline{\bigcup_{i\in I} A_i} \dot\otimes B)} = \bigcup_{i\in I} \overline{gconv(A_i \dot\otimes B)}$, i.e., the left-Scott-continuity. Indeed, we have $\overline{gconv(\overline{\bigcup_{i\in I} A_i} \dot\otimes B)} = \overline{gconv(\overline{\bigcup_{i\in I} A_i \dot\otimes B})} = \overline{gconv(\overline{(\bigcup_{i\in I} A_i) \dot\otimes B})} = \overline{gconv((\bigcup_{i\in I} A_i) \dot\otimes B)} = \overline{gconv(\bigcup_{i\in I}(A_i \dot\otimes B))} = \bigcup_{i\in I} \overline{gconv(A_i \dot\otimes B)}$ by Lemma 3.18 and Scott-continuity of $\otimes$ from Lemma 3.12(ii). The right-Scott-continuity is proved in a similar way.

- Let a directed family $\{A_i\}_{i\in\mathcal{I}}$ (ordered by reversed inclusion) and B be nonempty Scott-compact saturated g-convex subsets of $\underline{\mathcal{K}}(X)$. We want to show that $\uparrow gconv((\bigcap_{i\in\mathcal{I}} A_i) \mathbin{\dot\otimes} B) = \bigcap_{i\in\mathcal{I}} \uparrow gconv(A_i \mathbin{\dot\otimes} B)$. Inclusion is obvious. For the reversed inclusion, choose any g-convex Scott-open set U containing $\uparrow gconv(\bigcap_{i\in\mathcal{I}} A_i \mathbin{\dot\otimes} B)$. As every g-convex Scott-compact saturated subset of a dcpo is the intersection of its g-convex Scott-open neighborhoods (by Lemma 3.21), it suffices to prove that $\bigcap_{i\in\mathcal{I}} \uparrow gconv(A_i \mathbin{\dot\otimes} B)$ is contained in U. Observe that $gconv((\bigcap_{i\in\mathcal{I}} A_i) \mathbin{\dot\otimes} B) \subseteq U$ and also $(\bigcap_{i\in\mathcal{I}} A_i) \mathbin{\dot\otimes} B \subseteq U$, as $\otimes$ is Scott-continuous by Lemma 3.12(ii) and $\bigcap_{i\in\mathcal{I}} A_i$ and B are Scott-compact saturated, we know that $\bigcap_{i\in\mathcal{I}} A_i$ and B have Scott-open neighborhoods V and W respectively such that $V \mathbin{\dot\otimes} W \subseteq U$. Because $\bigcap_{i\in\mathcal{I}} A_i \subseteq V$, by Proposition 3.5 we know there is an $i_o \in \mathcal{I}$ such that $A_{i_o} \subseteq V$. Therefore $A_{i_o} \mathbin{\dot\otimes} B \subseteq V \mathbin{\dot\otimes} W \subseteq U$, and because U is g-convex, we know $gconv(A_{i_o} \mathbin{\dot\otimes} B) \subseteq U$. Recall that U is Scott-open, we conclude that $\bigcap_{i\in\mathcal{I}} \uparrow gconv(A_i \dot\otimes B) \subseteq U$. The right-Scott-continuity is proved in a similar way.

□

Finally, I define a *formal union* operation $\uplus_G$ as in Proposition 3.8 to interpret nondeterministic-choice as $A \uplus_G B \stackrel{\text{def}}{=} \overline{C} \cap \uparrow C$ where C is $gconv(A \cup B)$.

LEMMA 3.25. *The formal union $\uplus_G$ is a Scott-continuous semilattice operation on $\mathcal{GK}(X)$.*

PROOF. It is straightforward to show that $\uplus_G$ is idempotent, commutative, and associative, i.e., $\uplus_G$ is a semilattice operation. Similar to the argument in the proof of Lemma 3.24, it suffices to show the Scott-continuity of $\uplus_G$ with respect to lower closures as well as upper closures.

- Let a directed family $\{A_i\}_{i\in\mathcal{I}}$ (ordered by inclusion) and B be nonempty Scott-closed g-convex subsets of $\underline{\mathcal{K}}(X)$. We want to show $\overline{gconv(\overline{\bigcup_{i\in\mathcal{I}} A_i} \cup B)} = \overline{\bigcup_{i\in\mathcal{I}} \overline{gconv(A_i \cup B)}}$. Indeed, we have $\overline{gconv(\overline{\bigcup_{i\in\mathcal{I}} A_i} \cup B)} = \overline{gconv(\overline{\bigcup_{i\in\mathcal{I}} A_i} \cup B)} = \overline{gconv(\overline{\bigcup_{i\in\mathcal{I}} A_i \cup B})} = \overline{gconv(\bigcup_{i\in\mathcal{I}} A_i \cup B)} = \overline{gconv(\bigcup_{i\in\mathcal{I}} (A_i \cup B))} = \bigcup_{i\in\mathcal{I}} \overline{gconv(A_i \cup B)}$ by Lemma 3.18.
- Let a directed family $\{A_i\}_{i\in\mathcal{I}}$ (ordered by reversed inclusion) and B be nonempty Scott-compact saturated g-convex subsets of $\underline{\mathcal{K}}(X)$. We want to show that $\uparrow gconv((\bigcap_{i\in\mathcal{I}} A_i) \cup B) = \bigcap_{i\in\mathcal{I}} \uparrow gconv(A_i \cup B)$. Inclusion is obvious. For reversed inclusion, it suffices to show that for every open set U that is a neighborhood of $\uparrow gconv((\bigcap_{i\in\mathcal{I}} A_i) \cup B)$, we have that U contains $\bigcap_{i\in\mathcal{I}} \uparrow gconv(A_i \cup B)$ as a subset by Lemma 3.21. Observe that $gconv((\bigcap_{i\in\mathcal{I}} A_i) \cup B) \subseteq U$ thus $(\bigcap_{i\in\mathcal{I}} A_i) \cup B \subseteq U$. Since $\bigcap_{i\in\mathcal{I}} A_i$ and B are Scott-compact saturated sets, there exist Scott-open neighborhoods V and W of $\bigcap_{i\in\mathcal{I}} A_i$ and B, respectively, such that $V \cup W \subseteq U$. Then by Proposition 3.5 we know that there exists $i_o \in \mathcal{I}$ such that $A_{i_o} \subseteq V$ by the fact that $\bigcap_{i\in\mathcal{I}} A_i \subseteq V$. Thus $A_{i_o} \cup B \subseteq V \cup W \subseteq U$. Recall that U is g-convex, we have $gconv(A_{i_o} \cup B) \subseteq U$. Moreover, U is Scott-open, thus saturated, hence we conclude that $\bigcap_{i\in\mathcal{I}} \uparrow gconv(A_i \cup B) \subseteq U$.

□

Example 3.26. Recall the probabilistic program P in Example 3.10:

$$\textbf{if } \star \textbf{ then } t := t + 1 \textbf{ else } t := t - 1 \textbf{ fi}$$

the state space X is $\mathbb{Q}$, and we want to show that for any probabilistic refinement P_r of P (i.e., $\star$ is refined by $\mathbf{prob}(r)$*), for input values t_1, t_2 of t, we have $\mathbb{E}_{t'_1 \sim \Delta_1, t'_2 \sim \Delta_2}[t'_1 - t'_2] = t_1 - t_2$, where the program P_r ends up with a distribution Δ_1 starting with $t = t_1$ and Δ_2 with $t = t_2$.*

With the g-convex powerdomain $\mathcal{GK}(X)$ for nondeterminism-first, $t \coloneqq t + 1$ and $t \coloneqq t - 1$ are assigned semantic objects $\{\lambda t.\, \delta(t+1)\}$ and $\{\lambda t.\, \delta(t-1)\}$, respectively. Thus the nondeterministic-choice is interpreted as a subset of $\{\lambda t.\, \delta(t+1)\} \uplus_G \{\lambda t.\, \delta(t-1)\}$, which is $\{\kappa_r \mid r \in [0,1]\}$, where $\kappa_r = \lambda t.\, r \cdot \delta(t+1) + (1-r) \cdot \delta(t-1)$ is the kernel for the deterministic refinement P_r of P. Therefore for every $r \in [0,1]$, we have $\mathbb{E}_{t'_1 \sim \Delta_1, t'_2 \sim \Delta_2}[t'_1 - t'_2] = \mathbb{E}_{t'_1 \sim \kappa_r(t_1), t'_2 \sim \kappa_r(t_2)}[t'_1] - \mathbb{E}_{t'_1 \sim \kappa_r(t_1), t'_2 \sim \kappa_r(t_2)}[t'_2] = (r(t_1+1) + (1-r)(t_1-1)) - (r(t_2+1) + (1-r)(t_2-1)) = t_1 - t_2$.

In contrast, if one started with the convex powerdomain $\mathcal{P}\underline{\mathcal{D}}(X)$ reviewed in §3.1.3 for nondeterminism-last, we would obtain the semantic object $\lambda t.\, \{r \cdot \delta(t+1) + (1-r) \cdot \delta(t-1) \mid r \in [0,1]\}$ for the program P, as shown in Example 3.10. Now the refinements of P include some κ such that $\kappa(t_1) = 0.5 \cdot \delta(t_1+1) + 0.5 \cdot \delta(t_1-1)$ and $\kappa(t_2) = 0.3 \cdot \delta(t_2+1) + 0.7 \cdot \delta(t_2-1)$, thus we are not able to prove the claim $\mathbb{E}[t'_1 - t'_2] = t_1 - t_2$.

3.3 Algebraic Denotational Semantics

The operational semantics described in §2.3 presents a reasonable model for evaluating single-procedure probabilistic programs without nondeterminism. In this section, I develop a general denotational semantics for CFHGs (introduced in §2.2) of multi-procedure probabilistic programs with nondeterminism. The semantics is *algebraic* in the sense that it could be instantiated with different concrete models of nondeterminism, e.g., nondeterminism-last reviewed in §3.1.3, as well as novel nondeterminism-first developed in §3.2.3. I also show the denotational semantics is equivalent to the operational semantics in §2.3 if we suppress procedure calls and nondeterminism in the programming model.

3.3.1 A Fixpoint Semantics based on Markov Algebras

The algebraic denotational semantics is obtained by composing $Ctrl(e)$ operations along hyperedges. The semantics of programs is determined by an *interpretation*, which consists of two parts: (i) a *semantic algebra*, which defines a set of possible program meanings, and which is equipped with sequencing, conditional-choice, and nondeterministic-choice operators to compose these meanings, and (ii) a *semantic function*, which assigns a meaning to each data action $\mathsf{act} \in \mathsf{Act}$. In my thesis, I propose *Markov algebras* as the semantic algebras:

Definition 3.27. A *Markov algebra* (MA) over a set Cond of deterministic conditions is a 7-tuple $\mathcal{M} = (M, \sqsubseteq_M, \otimes_M, {}_\varphi\Diamond_M, \uplus_M, \bot_M, 1_M)$, where $(M, \sqsubseteq_M)$ forms a dcpo with $\bot_M$ as its least element; $(M, \otimes_M, 1_M)$ forms a monoid (i.e., $\otimes_M$ is an associative binary operator with 1_M as its identity element); ${}_\varphi\Diamond_M$ is a binary operator parametrized by a condition $\varphi \in \mathsf{Cond}$; $\uplus_M$ is idempotent, commutative, associative and for all $a, b \in M$ and $\varphi \in \mathsf{Cond}$ it holds that $a \;{}_\varphi\Diamond_M\; b \leq_M a \uplus_M b$ where $\leq_M$ is the semilattice ordering induced by $\uplus_M$ (i.e., $a \leq_M b$ if $a \uplus_M b = b$); and $\otimes_M$, ${}_\varphi\Diamond_M$, $\uplus_M$ are Scott-continuous.

Example 3.28. Let Ω be a nonempty countable set of program states and Cond *be a set of deterministic conditions, the definition and meaning of which are given in §2.2 and §2.3.*

1. *The convex powerdomain* $\mathcal{P}\underline{\mathcal{D}}(\Omega)$ *admits an MA* $(\Omega \to \mathcal{P}\underline{\mathcal{D}}(\Omega), \dot{\sqsubseteq}_P, \otimes_P, {}_\varphi\diamondsuit_P, \dot{\uplus}_P, \dot{\bot}_P, 1_P)$, *where* $\dot{\sqsubseteq}_P, \dot{\uplus}_P, \dot{\bot}_P$ *are pointwise extensions of* $\sqsubseteq_P, \uplus_P, \bot_P$, *defined in §3.1.3, and* $g \otimes_P h \stackrel{\text{def}}{=} \widehat{\widehat{h}} \circ g$ *where* $\widehat{\widehat{h}}$ *is given by Proposition 3.9,* $g \; {}_\varphi\diamondsuit_P \; h \stackrel{\text{def}}{=} \lambda\omega.g(\omega) \; {}_{[\![\varphi]\!](\omega)}\oplus_P \; h(\omega)$, *as well as* $1_P \stackrel{\text{def}}{=} \lambda\omega.\ \{\delta(\omega)\}$.
2. *The g-convex powerdomain* $\mathcal{GK}(\Omega)$ *admits an MA* $(\mathcal{GK}(\Omega), \sqsubseteq_G, \otimes_G, {}_\varphi\diamondsuit_G, \uplus_G, \bot_G, 1_G)$, *where* $\sqsubseteq_G, \otimes_G, {}_\varphi\diamondsuit_G, \uplus_G, \bot_G$ *come from §3.2.3,*[5] *and* $1_G \stackrel{\text{def}}{=} \{\lambda\omega.\ \delta(\omega)\}$.

Definition 3.29. An *interpretation* is a pair $\mathcal{I} = (\mathcal{M}, [\![\cdot]\!]^{\mathcal{I}})$, where $\mathcal{M}$ is an MA and $[\![\cdot]\!]^{\mathcal{I}} : \mathsf{Act} \to \mathcal{M}$. We call $\mathcal{M}$ the *semantic algebra* of the interpretation and $[\![\cdot]\!]^{\mathcal{I}}$ the *semantic function*.

Example 3.30. We can lift the interpretation of data actions defined in Fig. 2.2 to semantic functions with respect to convex or g-convex powerdomains—$\mathcal{P} = (\mathcal{P}\underline{\mathcal{D}}(\Omega), [\![\cdot]\!]^{\mathcal{P}})$ *with* $[\![\mathsf{act}]\!]^{\mathcal{P}} \stackrel{\text{def}}{=} \lambda\omega.\ \{[\![\mathsf{act}]\!](\omega)\}$ *and* $\mathcal{G} = (\mathcal{GK}(\Omega), [\![\cdot]\!]^{\mathcal{G}})$ *with* $[\![\mathsf{act}]\!]^{\mathcal{G}} \stackrel{\text{def}}{=} \{[\![\mathsf{act}]\!]\}$.

Given a probabilistic program $P = \{H_i\}_{1 \le i \le n}$ where each $H_i = (V_i, E_i, v_i^{\mathsf{entry}}, v_i^{\mathsf{exit}})$ is a CFHG, and an interpretation $\mathcal{I} = (\mathcal{M}, [\![\cdot]\!]^{\mathcal{I}})$, I define $\mathcal{I}[P]$ to be the interpretation of the probabilistic program, as the least fixpoint of the function F_P, which is defined as

$$\lambda\mathbf{S}.\lambda v. \begin{cases} \bigsqcup_M \left\{ \widehat{Ctrl(e)}(\mathbf{S}(u_1), \cdots, \mathbf{S}(u_k)) \mid e = (v, \{u_1, \cdots, u_k\}) \in E \right\} & v \neq v_i^{\mathsf{exit}} \text{ for all } i \\ 1_M & \text{otherwise} \end{cases}$$

where $\widehat{Ctrl(e)}$ for different kinds of control-flow actions is defined as follows:

$$\widehat{seq[\mathsf{act}]}(S_1) \stackrel{\text{def}}{=} [\![\mathsf{act}]\!]^{\mathcal{I}} \otimes_M S_1, \qquad \widehat{cond[\varphi]}(S_1, S_2) \stackrel{\text{def}}{=} S_1 \; {}_\varphi\diamondsuit_M \; S_2,$$
$$\widehat{call[i \to j]}(S_1) \stackrel{\text{def}}{=} \mathbf{S}(v_j^{\mathsf{entry}}) \otimes_M S_1.$$

The least fixpoint of F_P exists by Proposition 3.4 as well as the following lemma. Hence the semantics of the procedure H_i is given by $[\![H_i]\!]_{\mathsf{ds}} \stackrel{\text{def}}{=} (\mathrm{lfp}^{\dot{\sqsubseteq}_M}_{\dot{\bot}_M} F_P)(v_i^{\mathsf{entry}})$.

LEMMA 3.31. *The function* F_P *is Scott-continuous on the dcpo* $(V \to M, \dot{\sqsubseteq}_M)$ *with* $\dot{\bot}_M \stackrel{\text{def}}{=} \lambda v.\bot_M$ *as the least element, where* $\dot{\sqsubseteq}_M$ *is the pointwise extension of* $\sqsubseteq_M$.

PROOF. Appeal to the Scott-continuity of the operations $\otimes_M$, ${}_\varphi\diamondsuit_M$, and $\uplus_M$. □

3.3.2 An Equivalence Result

To justify the denotational semantics proposed in §3.3.1, I go back to the restricted programming language used to define the operational semantics in §2.3. If we suppress the features of multi-procedure and nondeterminism, we should end up with a semantics that is equivalent to the operational semantics $[\![\cdot]\!]_{\mathsf{os}}$ on a countable state space Ω (with the powerset $\wp(\Omega)$ as the σ-algebra).

[5] The conditional-choice is actually interpreted as ${}_{[\![\varphi]\!]}\diamondsuit_G$ in the powerdomain.

LEMMA 3.32. *Let $P = (V, E, v^{\mathsf{entry}}, v^{\mathsf{exit}})$ be a deterministic single-procedure probabilistic program.*

1. *If we interpret P using $\mathscr{P} = (\Omega \to \mathcal{P}\underline{\mathcal{D}}(\Omega), [\![\cdot]\!]^{\mathscr{P}})$, we will have $[\![P]\!]_{\mathsf{ds}} = \lambda\omega.\ \{[\![P]\!]_{\mathsf{os}}(\omega)\}$.*
2. *If we interpret P using $\mathscr{G} = (\mathcal{GK}(\Omega), [\![\cdot]\!]^{\mathscr{G}})$, we will have $[\![P]\!]_{\mathsf{ds}} = \{[\![P]\!]_{\mathsf{os}}\}$.*

PROOF. It is sufficient to show that

$$\lambda\omega.\ \sup_{n\in\mathbb{Z}^+}\{\xrightarrow{\hat{}}_n\}(\langle v^{\mathsf{entry}}, \omega\rangle) = (\mathrm{lfp}^{\dot{\sqsubseteq}_K}_{\lambda v.\bot_K} F_P)(v^{\mathsf{entry}}),$$

and we are instead going to show for all $n \in \mathbb{Z}^+$ and $v \in V$ the following holds

$$\lambda\omega.\xrightarrow{\hat{}}_n(\langle v, \omega\rangle) = F_P^n(\lambda v.\bot_K)(v).$$

By induction on n, the base case is straightforward because both sides equal $\bot_K$. Suppose that for some n, the equality holds for all $v \in V$. Then for all $v \in V$, we want to show that

$$\lambda\omega.\xrightarrow{\hat{}}_{n+1}(\langle v, \omega\rangle) = F_P^{n+1}(\lambda v.\bot_K)(v). \tag{3.4}$$

- If v is not associated with any edges, then $\xrightarrow{\hat{}}_{n+1}(\langle v, \omega\rangle)(\omega') = [\omega = \omega']$ for all ω and ω'. The right-hand-side of (3.4) equals $F_P(F_P^n(\lambda v.\bot_K))(v)$ and by the definition of F_P we know it is equal to $\lambda\omega.\lambda\omega'.[\omega = \omega']$.
- If v is associated with $e = (v, \{u_1, \cdots, u_k\})$, then we know $\lambda\omega.\xrightarrow{\hat{}}_n(\langle u_i, \omega\rangle) = F_P^n(\lambda v.\bot_K)(u_i)$ for all i by induction hypothesis.
  - If $Ctrl(e) = seq[\mathsf{act}]$, then the right-hand-side of (3.4) equals $[\![\mathsf{act}]\!] \otimes F_P^n(\lambda v.\bot_K)(u_1)$. The left-hand-side of (3.4) is

$$\begin{aligned}
&\lambda\omega.\lambda\omega'.\ \sum_\tau \xrightarrow{\hat{}}(\langle v, \omega\rangle)(\tau) \cdot \xrightarrow{\hat{}}_n(\tau)(\omega') \\
&= \lambda\omega.\lambda\omega'.\ \sum_{\omega''} [\![\mathsf{act}]\!](\omega)(\omega'') \cdot \xrightarrow{\hat{}}_n(\langle u_1, \omega''\rangle)(\omega') \\
&= [\![\mathsf{act}]\!] \otimes F_P^n(\lambda v.\bot_K)(u_1).
\end{aligned}$$

  - If $Ctrl(e) = cond[\varphi]$, then the right-hand-side of (3.4) equals $F_P^n(\lambda v.\bot_K)(u_1)\ {}_{[\![\varphi]\!]}\Diamond\ F_P^n(\lambda v.\bot_K)(u_2)$. The left-hand-side of (3.4) is

$$\begin{aligned}
&\lambda\omega.\lambda\omega'.\ \sum_\tau \xrightarrow{\hat{}}(\langle v, \omega\rangle)(\tau) \cdot \xrightarrow{\hat{}}_n(\tau)(\omega') \\
&= \lambda\omega.\lambda\omega'.\Big(\sum_{\omega''} [\![\varphi]\!](\omega) \cdot \delta(\omega)(\omega'') \cdot \xrightarrow{\hat{}}_n(\langle u_1, \omega''\rangle)(\omega') \\
&\qquad + \sum_{\omega''} (1 - [\![\varphi]\!](\omega)) \cdot \delta(\omega)(\omega'') \cdot \xrightarrow{\hat{}}_n(\langle u_2, \omega''\rangle)(\omega')\Big) \\
&= \lambda\omega.\lambda\omega'.\ \big([\![\varphi]\!](\omega) \cdot \xrightarrow{\hat{}}_n(\langle u_1, \omega\rangle)(\omega') + (1 - [\![\varphi]\!](\omega)) \cdot \xrightarrow{\hat{}}_n(\langle u_2, \omega\rangle)(\omega')\big) \\
&= \lambda\omega.\lambda\omega'.\ \big([\![\varphi]\!](\omega) \cdot F_P^n(\lambda v.\bot_K)(u_1)(\omega)(\omega') + (1 - [\![\varphi]\!](\omega)) \cdot F_P^n(\lambda v.\bot_K)(u_2)(\omega)(\omega')\big) \\
&= F_P^n(\lambda v.\bot_K)(u_1)\ {}_{[\![\varphi]\!]}\Diamond\ F_P^n(\lambda v.\bot_K)(u_2).
\end{aligned}$$

  Thus we conclude the proof.

□

3.4 Discussion

3.4.1 Continuous Distributions

One important feature of probabilistic programming that is missing from the development of nondeterminism-first in this chapter is *continuous* probability distributions, such as Normal distributions. Notions from measure theory, such as *measures* and *kernels*, are extensively used to model continuous distributions in probabilistic programming. Kozen [98] studied the relation between deterministic probabilistic programs and continuous distributions via a metric on measures. Many approaches used probability kernels [99, 139], sub-probability kernels [16], and s-finite kernels [14, 140]. A different approach used measurable functions $A \to \mathbb{D}(\mathbb{R}^+ \times B)$ where $\mathbb{D}(S)$ stands for the set of all probability measures on S [141]. Ehrhard et al. [48] provided a category $\mathbf{Cstab}_{\mathsf{m}}$ on stable and measurable maps between cones, and used it to give a denotational semantics for probabilistic PCF. Heunen et al. [69] proposed quasi-Borel spaces that form a new formalization of probability theory replacing measurable spaces, and later Vákár et al. [145] extended quasi-Borel spaces to give a denotational semantics for statistical Fixed-Point Calculus (FPC) [56].

However, those measure-theoretic developments do not work properly when nondeterminism comes into the picture. To overcome this challenge, people have been adapting domain-theoretic results to incorporate nondeterminism-last models. McIver and Morgan built a Plotkin-style powerdomain over probability distributions on a discrete state space [110, 111]. Mislove et al. [115, 116] studied powerdomain constructions for probabilistic CSP. Tix et al. [144] generalized McIver and Morgan's results to continuous state spaces, and construct three powerdomains for the extended probabilistic powerdomains. Although there has been a lot of work on this direction, one has to keep in mind that the domain-theoretic notion of "continuous" distributions is different from the notion in measure theory—instead, the domain-theoretic studies are focused on *computable* distributions. In other words, real numbers are realized by some computable models, such as *partial reals* [49]. These models would become unsatisfactory when one wants to *observe* a random value drawn from a continuous distribution, e.g., the meaning of "$x \sim \textsc{Normal}(0,1)$; **if** $x = 0$ **then** $\cdots$ **fi**" may not be expressible. There has also been some work on domain-theoretic characterizations of measure-theoretic notions. Smolka et al. [139] presented a continuous dcpo on probability kernels for probabilistic networks, with a *parallel-composition* operator that resolves network-related nondeterminism, which is different from both nondeterminism-last and nondeterminism-first.

3.4.2 Higher-Order Functions

In functional programming, higher-order functions are functions that can take functions as arguments, as well as return a function as a result. Some probabilistic programming languages, such as Church [63], are indeed functional programming languages and can express higher-order functions. While operational models for probabilistic functional programming have been proposed (e.g., [16]), developing a denotational semantics for higher-order probabilistic programming has been an open problem for years.

The major challenge is to propose a Cartesian-closed category for semantic objects of probabilistic programming. Intuitively, the Cartesian-closure property ensures that if type A and type B are two objects in the category, then the function space B^A (i.e., an object for the arrow type $A \to B$) is also

```
if h = 1 then
  if prob(0.9) then read_bit(l)
  else l := 1 fi
else
  if prob(0.1) then l := 0
  else read_bit(l) fi
fi
```

(a)

```
if ⋆ then
  if prob(0.9) then read_bit(l)
  else l := 1 fi
else
  if prob(0.1) then l := 0
  else read_bit(l) fi
fi
```

(b)

Fig. 3.4: (a) A concrete program; (b) an abstract program.

contained in the category. The category of measurable spaces is clearly *not* Cartesian-closed. A lot of probabilistic powerdomains also do *not* admit a Cartesian-closed category [84]. Recently, Ehrhard et al. [48] provided a Cartesian-closed category $\mathbf{Cstab}_{\mathsf{m}}$ on stable and measurable maps between cones. Heunen et al. [69] proposed quasi-Borel spaces that form a Cartesian-closed category, and thus support higher-order functions in probabilistic programming. This approach was further extended by Vákár et al. [145] to support recursive types in FPC. Dahlqvist and Kozen [40] presented a denotational semantics for higher-order probabilistic programs with conditioning in terms of linear operators between Banach spaces. However, it is unclear how to model nondeterminism in those frameworks.

3.4.3 Probabilistic Noninterference

A potential application of nondeterminism-first is refinement-based reasoning about security policies, such as *noninterference*, or, more generally, *hyperproperties* [30]. As an example, consider the program in Fig. 3.4(a) with a low-confidentiality one-bit variable l and a high-confidentiality one-bit variable h, where $\mathsf{read\_bit}(l)$ inputs a bit from outside in the sense that l is assigned an unknown bit. We then want to know whether the confidential information could flow from high-confidentiality variables (e.g., h) to low-confidentiality ones (e.g., l). One way [127] to formalize noninterference for probabilistic programs with external unknown inputs is to reason about *transition relations*—pairs of an initial state σ and a final distribution Δ over possible states—such that for any transitions $\langle \sigma_1, \Delta_1 \rangle$, $\langle \sigma_2, \Delta_2 \rangle$, there exists a transition $\langle \sigma_3, \Delta_3 \rangle$ satisfying that

- the initial states σ_1 and σ_3 have the same high-confidentiality information; and
- the transitions $\langle \sigma_2, \Delta_2 \rangle$ and $\langle \sigma_3, \Delta_3 \rangle$ have the same low-confidentiality information.

Back to the example, this means $\sigma_1(h) = \sigma_3(h)$, $\sigma_2(l) = \sigma_3(l)$, and the marginal distributions on the final value of l are identical, i.e., $\sum_{h'} \Delta_2(l', h') = \sum_{h'} \Delta_3(l', h')$ for any $l' \in \{0, 1\}$, where the primed variables stand for the final values of the corresponding variables. The example program does *not* satisfy noninterference because of the following counterexample: suppose $\sigma_1 = [l \mapsto 0, h \mapsto 0], \sigma_2 = [l \mapsto 0, h \mapsto 1], \Delta_1 = \delta([l' \mapsto 0, h' \mapsto 0]), \Delta_2 = \delta([l' \mapsto 1, h' \mapsto 1])$, we know that $\sigma_3 = [l \mapsto 0, h \mapsto 0]$, the program should execute the else-branch of the outside conditional, thus the probability that $l' = 0$ should be at least 0.1, and hence there does not exist a feasible Δ_3. On the other hand, consider the program in Fig. 3.4(b), which is an *abstraction* of the

example program. If we use the nondeterministic-*last* model, the semantics of the abstract program would imply for any input state, *every* marginal distribution on the final value of l is possible. Thus, the abstract program satisfies noninterference. However, the principle of refinement-based reasoning fails in this situation—if a specification satisfies noninterference, its refinements *may* not satisfy noninterference.

In contrast, using the nondeterminism-*first* model developed in this chapter, we can define the semantics of Fig. 3.4(b) as a collection of transition functions:

$$\left\{\lambda(l,h).\ \{\phi(l,h)\cdot\Delta_1 + (1-\phi(l,h))\cdot\Delta_2 \mid \Delta_1 \in A \wedge \Delta_2 \in B\} \mid \phi : \{0,1\}^2 \to [0,1]\right\},$$

where $\phi(l,h)$ represents any refinement of the nondeterministic choice $\star$, and A, B are the semantic objects of the two branches of the outside conditional, respectively, given an input state (l,h):

$$A = \{0.9(1-p)\cdot[l'=0,h'=h] + (0.9p+0.1)\cdot[l'=1,h'=h] \mid p \in [0,1]\},$$
$$B = \{(0.1+0.9q)\cdot[l'=0,h'=h] + 0.9(1-q)\cdot[l'=1,h'=h] \mid q \in [0,1]\},$$

where the probabilities p and q model the unknown inputs from $\mathsf{read\_bit}(l)$. Thus, the abstract program satisfies noninterference if and only if every transition function in the collection satisfies noninterference. By selecting ϕ to be $\lambda(l,h).\ (h=1)$, we obtain exactly the semantics of the concrete program in Fig. 3.4(a) that does *not* satisfies noninterference. Therefore, the abstract program also does not satisfy noninterference.

Chapter 4

PMAF: An Algebraic Framework for Static Analysis of Probabilistic Programs

In this chapter, I present a framework, which I call *PMAF* (for Pre-Markov Algebra Framework), for designing, implementing, and proving the correctness of static analyses of probabilistic programs. I will show how several analyses that may appear to be quite different, can be formulated—and generalized—using PMAF. Examples include Bayesian inference [29, 51, 52], Markov decision problem with rewards [130], and probabilistic-invariant generation [24, 26, 86].

For the purpose of designing a flexible static-analysis framework, I categorize new constructs in probabilistic programs into two kinds, to express *data randomness* (e.g., sampling) and *control-flow randomness* (e.g., probabilistic choice). PMAF is based on the algebraic denotational semantics introduced in §3.3, which is an interpretation of the control-flow graphs for a program's procedures with respect to a semantic Markov algebra. To express both kinds of randomness in the analysis framework, I further introduce a new algebraic structure, called a *pre-Markov algebra*, which is equipped with operations corresponding to control-flow actions in probabilistic programs: *sequencing*, *conditional-choice*, *probabilistic-choice*, and *nondeterministic-choice*. To establish correctness, I introduce *probabilistic abstractions* between a Markov algebra and a pre-Markov algebra that represent the concrete and abstract semantics, respectively.

In this chapter, I will show how, with suitable extensions, a blending of ideas from prior work on (i) static analysis of single-procedure probabilistic programs, and (ii) interprocedural dataflow analysis of standard (non-probabilistic) programs can be used to create a framework for interprocedural analysis of multi-procedure probabilistic programs. In particular,

- The algebraic denotational semantics on which PMAF is based is an interpretation of the control-flow *hyper-graphs* for a program's procedures.

- The abstract semantics is formulated so that the analyzer can obtain *procedure summaries*.

Recall that hyper-graphs contain *hyper-edges*, each of which consists of one source node and possibly several destination nodes. Conditional-branching, probabilistic-branching, and nondeterministic-branching statements can all be represented by hyper-edges. In ordinary control-flow graphs (CFGs), nodes can also have several successors; however, the operator applied at a confluence point q when analyzing a CFG is join ($\sqcup$), and the paths leading up to q are analyzed *independently*. For reasons discussed in §4.1.3, PMAF is based on a *backward* analysis, so the confluence points

represent the program's branch points (i.e., for if-statements and while-loops). If the CFG is treated as a graph, join would be applied at each branch-node, and the subpaths from each successor would be analyzed independently. In contrast, when the CFG is treated as a hyper-graph, i.e., as a control-flow hyper-graph (CFHG), the operator applied at a probabilistic-choice node with probability p is $\lambda a.\lambda b.a \ {}_p\!\oplus\ b$—where ${}_p\!\oplus$ is not join, but an operator that weights the two successor paths by p and $(1-p)$. For instance, in Fig. 4.2(b), the hyper-edge $(v_0, \{v_1, v_5\})$ generates the inequality $\mathscr{A}[v_0] \sqsupseteq \mathscr{A}[v_1] \ {}_{0.75}\!\oplus\ \mathscr{A}[v_5]$, for some analysis $\mathscr{A}$. This approach allows the (hyper-)subpaths from the successors to be analyzed *jointly*.

To perform interprocedural analyses of probabilistic programs, I adopt a common practice from interprocedural analysis of standard non-probabilistic programs: the abstract domain is a *two-vocabulary* domain (each value represents an abstraction of a state transformer) rather than a *one-vocabulary* domain (each value represents an abstraction of a state). In the algebraic approach, an element in the algebra represents a two-vocabulary transformer. Elements can be "multiplied" by the algebra's formal multiplication operator, which is typically interpreted as (an abstraction of) the reversal of transformer composition. The transformer obtained for the set of hyper-paths from the entry of procedure P to the exit of P is the summary for P.

In the case of loops and recursive procedures, PMAF uses widening to ensure convergence. Here my approach is slightly non-standard: I found that for some instantiations of the framework, one could improve precision by using different widening operators for loops controlled by conditional, probabilistic, and nondeterministic branches.

The main advantage of PMAF is that instead of starting from scratch to create a new analysis, one only needs to instantiate PMAF with the implementation of a new pre-Markov algebra. To establish soundness, one just has to establish some well-defined algebraic properties, and can then rely on the soundness of the framework. To implement an analysis, one can rely on an implementation of PMAF to perform sound interprocedural analysis, with respect to the abstraction of the analysis. The PMAF implementation supplies common parts of different static analyses of probabilistic programs, e.g., efficient iteration strategies with widenings and interprocedural summarization. Moreover, any improvements made to the PMAF implementation immediately translate into improvements to *all of its instantiations*.

To evaluate PMAF, I created a prototype implementation, and reformulated two existing intraprocedural probabilistic-program analyses—the Bayesian-inference algorithm proposed by Claret et al. [29], and Markov decision problem with rewards [130]—to fit into PMAF: Reformulation involved changing from the one-vocabulary abstract domains proposed in the original papers to appropriate two-vocabulary abstract domains. I also developed a new program analysis: *linear expectation-invariant analysis* (LEIA). Linear expectation-invariants are (in)equalities involving expected values of linear expressions over program variables.

A related approach to static analysis of probabilistic programs is *probabilistic abstract interpretation* (PAI) [39, 118–120], which lifts standard program analysis to the probabilistic setting. PAI is both general and elegant, but the more concrete approach developed in my work on PMAF has a couple of advantages. First, PMAF is algebraic and provides a simple and well-defined interface for implementing new abstractions. I created an actual implementation of PMAF that can be easily instantiated to specific abstract domains. Second, PMAF is based on a different semantic foundation, which follows the standard interpretation of non-deterministic probabilistic programs in domain theory [45, 82, 83, 115, 116, 144].

```
b1 ~ Bernoulli(0.5);
b2 ~ Bernoulli(0.5);
while (¬b1 ∧ ¬b2) do
  b1 ~ Bernoulli(0.5);
  b2 ~ Bernoulli(0.5)
od
```

(a)

```
while prob(0.75) do
  z ~ Uniform(0, 2);
  if ⋆ then x := x + z
  else y := y + z
  fi
od
```

(b)

Fig. 4.1: (a) A Boolean probabilistic program; (b) An arithmetic probabilistic program.

The concrete semantics of PAI isolates probabilistic choices from the non-probabilistic part of the semantics by interpreting programs as distributions $P : \Omega \to (D \to D)$, where Ω is a probability space and $D \to D$ is the space of non-probabilistic transformers. As a result, the PAI interpretation of the following non-deterministic program is that with probability $1/2$, we have a program that non-deterministically returns 1 or 2; with probability $1/4$, we have a program that returns 1; and with probability $1/4$, a program that returns 2.

$$\begin{array}{lll} \textbf{if} \star & \textbf{then} & \textbf{if prob}(1/2) \textbf{ then return } 1 \textbf{ else return } 2 \\ & \textbf{else} & \textbf{if prob}(1/2) \textbf{ then return } 1 \textbf{ else return } 2 \quad \textbf{fi} \end{array}$$

In contrast, the semantics used in PMAF resolves non-determinism on the outside, and thus the semantics of the program is that it returns 1 with probability $1/2$ and 2 with $1/2$. As a result, one can conclude that the expected return value r is 1.5. However, PAI—and every static analysis based on PAI—can only conclude $r \in \{1.25, 1.5, 1.75\}$.

4.1 Overview

In this section, I briefly introduce two different static analyses of probabilistic programs: Bayesian inference and linear expectation invariant analysis. I then informally explain the main ideas behind the algebraic framework for analyzing probabilistic programs and show how it generalizes the aforementioned analyses.

4.1.1 Example Probabilistic Programs

In PMAF, I categorize the new constructs in probabilistic programs into two kinds of randomness: (i) *data randomness*, i.e., the ability to draw random values from distributions, and (ii) *control-flow randomness*, i.e., the ability to branch probabilistically.

I use the Boolean program in Fig. 4.1(a) to illustrate data randomness. In the program, b_1 and b_2 are two Boolean-valued variables. The *sampling statement* $x \sim \textsc{Dist}(\bar{\theta})$ draws a value from a distribution Dist with a vector of parameters $\bar{\theta}$, and assigns it to the variable x, e.g., $b_1 \sim \textsc{Bernoulli}(0.5)$ assigns to b_1 a random value drawn from a Bernoulli distribution with mean 0.5. Intuitively, the program tosses two fair Boolean-valued coins repeatedly, until one coin shows *true*.

I introduce control-flow randomness through the arithmetic program in Fig. 4.1(b). In the program, x, y, and z are real-valued variables. As in the previous example, we have sampling statements, and $\textsc{Uniform}(l, u)$ represents a uniform distribution on the interval $[l, u]$. The *probabilistic choice* $\textbf{prob}(p)$ returns true with probability p and false with probability $(1 - p)$. Moreover, the program also exhibits *nondeterminism*, as the symbol $\star$ stands for a *nondeterministic choice* that can behave like standard nondeterminism, as well as an arbitrary probabilistic choice [111, §6.6]. Intuitively, the program describes two players x and y playing a round-based game that ends with probability 0.25 after each round. In each round, either player x or player y gains some reward that is uniformly distributed on the interval $[0, 2]$.

4.1.2 Two Static Analyses

Bayesian Inference (BI) Probabilistic programs can be seen as descriptions of probability distributions [23, 63, 112]. For a Boolean probabilistic program, such as the one in Fig. 4.1(a), *Bayesian-inference analysis* [29] calculates the distribution over variable valuations at the end of the program, conditioned on the program terminating. For convenience, I will call the inferred probability distribution the *post-state probability distribution*. The program in Fig. 4.1(a) specifies the post-state distribution over the variables (b_1, b_2) given by: $\mathbb{P}[b_1 = \mathit{false}, b_2 = \mathit{false}] = 0$, and $\mathbb{P}[b_1 = \mathit{false}, b_2 = \mathit{true}] = \mathbb{P}[b_1 = \mathit{true}, b_2 = \mathit{false}] = \mathbb{P}[b_1 = \mathit{true}, b_2 = \mathit{true}] = 1/3$. This distribution also indicates that the program terminates *almost surely*, i.e., the probability that the program terminates is 1.

Linear Expectation Invariant Analysis (LEIA) Loop invariants are crucial to verification of imperative programs [46, 57, 71]. Although loop invariants for traditional programs are usually formulas over program variables, numeric invariants are needed to prove the correctness of probabilistic loops [98, 111]. Such *expectation invariants* are usually defined as random variables—specified as expressions over program variables—with some desirable properties [24, 25, 86]. In this chapter, I work on a more general kind of expectation invariant, defined as follows.

Definition 4.1. For a program P, $\mathbb{E}[\mathcal{E}_2] \bowtie \mathcal{E}_1$ is called an *expectation invariant* if $\mathcal{E}_1$ and $\mathcal{E}_2$ are numeric expressions over P's program variables, $\bowtie$ is one of $\{=, <, >, \leq, \geq\}$, and the following property holds: For any initial valuation of the program variables, the expected value of $\mathcal{E}_2$ in the final valuation (i.e., after the execution of P) is related to the value of $\mathcal{E}_1$ in the initial valuation by $\bowtie$.

I will use variables with primes in $\mathcal{E}_2$ to denote the values in the final valuation. For example, for the program in Fig. 4.1(b), $\mathbb{E}[x' + y'] = x + y + 3$, $\mathbb{E}[z'] = 0.25z + 0.75$, $\mathbb{E}[x'] \leq x + 3$, $\mathbb{E}[x'] \geq x$, $\mathbb{E}[y'] \leq y + 3$, and $\mathbb{E}[y'] \geq y$ are several linear expectation invariants, and LEIA can derive all of these automatically! The expectation invariant $\mathbb{E}[x' + y'] = x + y + 3$ indicates that the expected value of the total reward that the two players would gain is exactly 3.

4.1.3 The Algebraic Framework

This section explains the main ideas behind PMAF, which is general enough to encode the two analyses from §4.1.2.

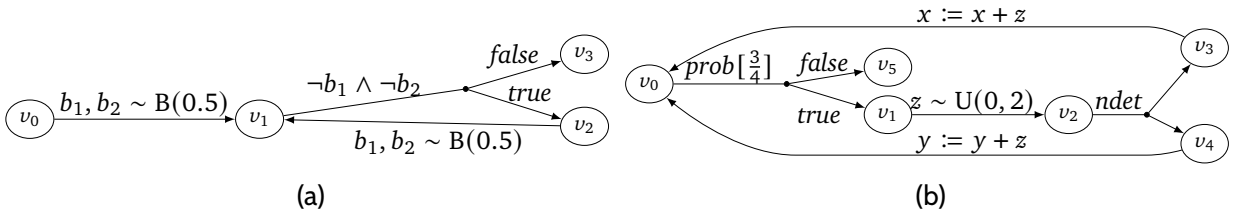


Fig. 4.2: (a) The control-flow hyper-graph of the program in Fig. 4.1(a); (b) The control-flow hyper-graph of the program in Fig. 4.1(b).

Data Randomness vs. Control-Flow Randomness The first principle is to make an *explicit separation between data randomness and control-flow randomness*. This distinction is intended to make the framework more flexible for analysis designers by providing multiple ways to translate the constructs of their specific probabilistic programming language into the constructs of PMAF. Analysis designers may find it useful to use the control-flow-randomness construct directly (e.g., "**if prob**$(0.3)\cdots$"), rather than simulating control-flow randomness by data randomness (e.g., "$p \sim \textsc{Uniform}(0,1)$; **if** $(p < 0.3)\cdots$"). For program analysis, such a simulation can lead to suboptimal results if the constructs used in the simulation require properties to be tracked that are outside the class of properties that a particular analysis's abstract domain is capable of tracking. For example, if an analysis domain only keeps track of expectations, then analysis of "$p \sim \textsc{Uniform}(0,1)$" only indicates that $\mathbb{E}[p] = 0.5$, which does not provide enough information to establish that $\mathbb{P}[p < 0.3] = 0.3$ in the then-branch of "**if** $(p < 0.3)\cdots$". In contrast, when "**prob**$(0.3)\cdots$" is analyzed in the fragment with the explicit control-flow-randomness construct ("**if prob**$(0.3)\cdots$") the analyzer can directly assign the probabilities 0.3 and 0.7 to the outgoing branches, and use those probabilities to compute appropriate expectations in the respective branches.

I achieve the separation between data randomness and control-flow randomness by capturing the different types of randomness in the graphs that I use for representing programs. Recall that in contrast to traditional program analyses, which usually work on control-flow graphs (CFGs), I use *control-flow hyper-graphs* (CFHGs) to model probabilistic programs. Hyper-graphs are directed graphs, each edge of which (i) has one source and possibly multiple destinations, and (ii) has an associated *control-flow action*—either *sequencing*, *conditional-choice*, *probabilistic-choice*, or *nondeterministic-choice*. A traditional CFG represents a collection of execution paths, while in probabilistic programs, paths are no longer independent, and the program specifies a collection of probability distributions over the paths. It is natural to treat a collection of paths as a whole and define distributions over the collections. Intuitively, these kinds of collections might be precisely formalized as *hyper-paths* made up of *hyper-edges* in hyper-graphs.

Fig. 4.2 shows the CFHGs of the two programs in Fig. 4.1. Every edge has an associated action, e.g., the control-flow actions $cond[\neg b_1 \wedge \neg b_2]$, $prob[3/4]$, and *ndet* are conditional-choice, probabilistic-choice, and nondeterministic-choice actions. Note that in Chapter 3, nondeterminism is achieved by allowing multiple outgoing hyper-edges on a single node, but in this chapter, I introduce the nondeterministic choice *ndet* as a control-flow action, for a more uniform treatment of branching edges. Data actions, like $x \coloneqq x + z$ and $b_1 \sim \textsc{Bernoulli}(0.5)$, also perform a trivial control-flow action to transfer control to their only destination node.

Just as the control-flow graph of a procedure typically has a single entry node and a single exit

node, a procedure's control-flow hyper-graph also has a single entry node and a single exit node. In Fig. 4.2(a), the entry and exit nodes are v_0 and v_3, respectively; in Fig. 4.2(b), the entry and exit nodes are v_0 and v_5, respectively.

Backward Analysis Traditional static analyses assign to a CFG node v either backward assertions—about the computations that can lead up to v—or forward assertions—about the computations that can continue from v [35, 37]. Backward assertions are computed via a forward analysis (in the same direction as CFG edges); forward assertions are computed via a backward analysis (counter to the flow of CFG edges).

Because, with PMAF, we work with hyper-graphs rather than CFGs, from the perspective of a node v, there is a difference in how things "look" in the backward and forward direction: hyper-edges fan *out* in the forward direction. Hyper-edges can have two destination nodes, but only one source node.

The second principle of the framework is essentially dictated by this structural asymmetry: the framework *supports backward analyses that compute a particular kind of forward assertion*. In particular, the property to be computed for a node v in the control-flow hyper-graph for procedure P is (an abstraction of) a transformer that summarizes the transformation carried out by the hyper-graph fragment that extends from v to the exit node of P. It is possible to reason in the forward direction—i.e., about computations that lead up to v—but one would have to "break" hyper-paths into paths and "relocate" probabilities, which is more complicated than reasoning in the backward direction. The framework interprets an edge as a property transformer that computes properties of the edge's source node as a function of properties of the edge's destination node(s) and the edge's associated action. These property transformers propagate information in a *hypergraph-leaf-to-hypergraph-root* manner, which is natural in hyper-graph problems. For example, standard formulations of interprocedural dataflow analysis [94, 105, 123, 138] can be viewed as hyper-graph analyses, and propagation is performed in the leaf-to-root direction there as well.

Recall the Boolean program in Fig. 4.1(a). Suppose that we want to perform BI to analyze $\mathbb{P}[b_1 = \mathit{true}, b_2 = \mathit{true}]$ in the post-state distribution. The property to be computed for a node will be a mapping from variable valuations to probabilities, where the probability reflects the chance that a given state will cause the program to terminate in the post-state $(b_1 = \mathit{true}, b_2 = \mathit{true})$. For example, the property that we would hope to compute for node v_1 is the function $\lambda(b_1, b_2).[b_1 \wedge b_2] + [\neg b_1 \wedge \neg b_2] \cdot 1/3$, where $[\varphi]$ is an *Iverson bracket*, which evaluates to 1 if φ is true, and 0 otherwise.

Two-Vocabulary Program Properties In the example of BI above, we can observe that the property transformation discussed above is not suitable for *interprocedural* analysis. Suppose that (i) we want analysis results to tell us something about $\mathbb{P}[b_1 = \mathit{true}, b_2 = \mathit{true}]$ in the post-state distribution of the main procedure, but (ii) to obtain the answer, the analysis must also analyze a call to some other procedure Q. In the main procedure, the analysis is driven by the post-state-probability query $\mathbb{P}[b_1 = \mathit{true}, b_2 = \mathit{true}]$; in general, however, Q will need to be analyzed with respect to some other post-state probability (obtained from the distribution of valuations at the point in main just after the call to Q). One might try to solve this issue by analyzing each procedure multiple times with different post-state-probability queries. However, in an infinite state space, or when the state space is quite large, this approach is no longer feasible.

Following common practice in interprocedural static analysis of traditional programs, the third principle of the framework is to work with *two-vocabulary program properties*. The property sketched in the BI example above is actually *one-vocabulary*, i.e., the property assigned to a control-flow node only involves the state at that node. In contrast, a two-vocabulary property at node v (in the control-flow hyper-graph for procedure P) should describe the state transformation carried out by the hyper-graph fragment that extends from v to the exit node of P.

For instance, LEIA assigns to each control-flow node a conjunction of expectation invariants, which relate the state at the node to the state at the exit node; consequently, LEIA deals with two-vocabulary properties. In §4.3, I reformulate BI to manipulate two-vocabulary properties. As in interprocedural dataflow analysis [36, 138], procedure summaries are used to interpret procedure calls.

Separation of Concerns The fourth principle—which is common to most analysis frameworks—is *separation of concerns*, by which I mean:

> Provide a declarative interface for a client to specify the program properties to be tracked by a desired analysis, but leave it to the framework to furnish the analysis implementation by which the analysis is carried out.

I achieve this goal by adopting (and adapting) ideas from previous work on *algebraic program analysis* [54, 131, 142]. Algebraic program analysis is based on the following idea:

> Any static analysis method performs reasoning in some space of program properties and property transformers; such property transformers should obey algebraic laws.

For instance, the data action **skip**, which does nothing, can be interpreted as the *identity* element in an algebra of program-property transformers.

Concretely, the fourth principle has three aspects:

1. For an intended domain of probabilistic programs, identify an appropriate set of algebraic laws that hold for useful sets of property transformers.

2. Define a specific algebra $\mathcal{A}$ for a program-analysis problem by defining a specific set of property transformers that obey the laws identified in item 1. Give translations from data actions and control-flow actions to such property transformers. (When such a translation is applied to a specific program, it sets up an equation system to be solved over $\mathcal{A}$.)

3. Develop a generic analysis algorithm that solves an equation system over any algebra that satisfies the laws identified in item 1.

Items 1 and 3 are tasks for me, the framework designer; they are the subjects of §4.2. Item 2 is a task for a client of the framework: examples are given in §4.3.

A client of the framework must furnish an *interpretation*—which consists of a *semantic algebra* and a *semantic function*—and a program. The semantic algebra consists of a *universe*, which defines the space of possible program-property transformers, and sequencing, conditional-choice, probabilistic-choice, and nondeterministic-choice operators, corresponding to control-flow actions. The semantic function is a mapping from data actions to the universe. (An interpretation is also called a *domain*.)

$$\mathcal{S}(v_0) \sqsupseteq prob[0.75](\mathcal{S}(v_1), \mathcal{S}(v_5)) \qquad \mathcal{S}(v_3) \sqsupseteq seq[x := x + z](\mathcal{S}(v_0))$$
$$\mathcal{S}(v_1) \sqsupseteq seq[z \sim \textsc{Uniform}(0, 2)](\mathcal{S}(v_2)) \qquad \mathcal{S}(v_4) \sqsupseteq seq[y := y + z](\mathcal{S}(v_0))$$
$$\mathcal{S}(v_2) \sqsupseteq ndet(\mathcal{S}(v_3), \mathcal{S}(v_4)) \qquad \mathcal{S}(v_5) \sqsupseteq \underline{1}$$

Fig. 4.3: The system of inequalities corresponding to Fig. 4.2(b).

To address item 3, my prototype implementation follows the standard *iterative* paradigm of static analysis [35, 88]: I first transform the control-flow hyper-graph into a system of inequalities, and then use a chaotic-iteration algorithm to compute a solution to it (e.g., [18]), which repeatedly applies the interpretation until a fixed point is reached (possibly using widening to ensure convergence). For example, the control-flow hyper-graph in Fig. 4.2(b) can be transformed into the system shown in Fig. 4.3, where $\mathcal{S}(v) \in \mathcal{M}$ are elements in the semantic algebra; $\sqsubseteq$ is the approximation order on $\mathcal{M}$; $[\![\cdot]\!]$ is the semantic function, which maps data actions to $\mathcal{M}$; and $\underline{1}$ is the transformer associated with the exit node.

The soundness of the analysis (with respect to a concrete semantics) is proved by (i) establishing an approximation relation between the concrete semantics and the abstract domain; (ii) showing that the abstract semantic function approximates the concrete one; and (iii) showing that the abstract operators (sequencing, conditional-choice, probabilistic-choice, and nondeterministic-choice) approximate the concrete ones.

For BI, I instantiate the PMAF framework to give lower bounds on post-state distributions, using with an interpretation in which state transformers are probability matrices (see §4.3.1). For LEIA, I design an interpretation using a Cartesian product of polyhedra (see §4.3.3). Once the functions of the interpretations are implemented, and a program is translated into the appropriate hyper-graph, the framework handles the rest of the work, namely, solving the equation system.

4.2 Analysis Framework

To aid in creating abstractions of probabilistic programs, I first identify, in §4.2.1, some algebraic properties that underlie the mechanisms used in the algebraic denotational semantics from §3.3. This algebra will aid my later definitions of abstractions in §4.2.2. I then discuss interprocedural analysis (in §4.2.3) and widening (§4.2.4).

4.2.1 An Algebraic Characterization of Fixpoint Semantics

In the denotational semantics, the concrete semantics is obtained by composing $\widehat{Ctrl(e)}$ operations along hyper-paths. Hence in the algebraic framework, the semantics of probabilistic programs is denoted by an *interpretation*, which consists of two parts: (i) a *semantic algebra*, which defines a set of possible program meanings, and which is equipped with sequencing, conditional-choice, probabilistic-choice, and nondeterministic-choice operators to compose these meanings, and (ii) a *semantic function*, which assigns a meaning to each basic program action.

Recall that in §3.3, I introduce Markov algebras (MAs) as the semantic algebras. The lattices used for abstract interpretation are *pre-Markov algebras* defined below. Note that rather than the possibly-probabilistic deterministic conditions from §2.2, I use and distinguish between purely deterministic conditions (i.e., logical conditions) and purely probabilistic conditions (i.e., $\mathbf{prob}(p)$ for $p \in [0,1]$).

Definition 4.2 (Pre-Markov algebras). A *pre-Markov algebra* (PMA) over a set of logical conditions $\mathcal{L}$ is an 8-tuple $\mathcal{M} = (M, \sqsubseteq, \otimes, {}_{\varphi}\Diamond, {}_{p}\oplus, \uplus, \underline{\bot}, \underline{1})$, where $(M, \sqsubseteq)$ forms a complete lattice with $\underline{\bot}$ as its least element; $(M, \otimes, \underline{1})$ forms a monoid (i.e., $\otimes$ is an associative binary operator with $\underline{1}$ as its identity element); ${}_{\varphi}\Diamond$ is a binary operator parameterized by a condition $\varphi \in \mathcal{L}$; ${}_{p}\oplus$ is a binary operator parameterized by $p \in [0,1]$; $\uplus$ is idempotent, commutative, associative and for all $a, b \in M$ and $\varphi \in \mathcal{L}$, $p \in [0,1]$ it holds that $a \; {}_{\varphi}\Diamond \; b \sqsubseteq a \uplus b$, $a \; {}_{p}\oplus \; b \sqsubseteq a \uplus b$ where $\sqsubseteq$ is the semilattice ordering induced by $\uplus$ (i.e., $a \sqsubseteq b$ if $a \uplus b = b$); and $\otimes$, ${}_{p}\oplus$, ${}_{\varphi}\Diamond$, $\uplus$ are monotone with respect to $\sqsubseteq$. In addition, the following algebraic properties are usually desirable:

$$a = a \; {}_{\varphi}\Diamond \; a, \quad a = a \; {}_{\mathit{true}}\Diamond \; b, \qquad\qquad a \; {}_{\varphi}\Diamond \; b = b \; {}_{\neg\varphi}\Diamond \; a$$
$$a = a \; {}_{p}\oplus \; a, \quad a = a \; {}_{1}\oplus \; b \;, \qquad\qquad a \; {}_{p}\oplus \; b = b \; {}_{1-p}\oplus \; a$$
$$a \; {}_{\varphi}\Diamond \; (b \; {}_{\psi}\Diamond \; c) = (a \; {}_{\varphi'}\Diamond \; b) \; {}_{\psi'}\Diamond \; c \text{ where } \varphi = \varphi' \wedge \psi', \varphi \vee \psi = \psi'$$
$$a \; {}_{p}\oplus \; (b \; {}_{q}\oplus \; c) = (a \; {}_{p'}\oplus \; b) \; {}_{q'}\oplus \; c \text{ where } p = p'q', (1-p)(1-q) = (1-q')$$

The precedence of the operators is that $\otimes$ binds tightest, followed by ${}_{\varphi}\Diamond$, ${}_{p}\oplus$, and $\uplus$.

Remark 4.3. These algebraic properties are not needed to prove soundness of the framework (stated in Theorem 4.7). These laws helped us when designing the abstract domains. Exploiting these algebraic laws to design better algorithms is an interesting direction for future work.

As is standard in abstract interpretation, the order on the algebra should represent an approximation order: $a \sqsubseteq b$ iff a is approximated by b (i.e., if a represents a more precise property than b).

Definition 4.4 (Interpretations). An *interpretation* is a pair $\mathcal{I} = (\mathcal{M}, [\![\cdot]\!])$, where $\mathcal{M}$ is a pre-Markov algebra, and $[\![\cdot]\!] : \mathsf{Act} \to \mathcal{M}$, where Act is the set of data actions for probabilistic programs. We call $\mathcal{M}$ the *semantic algebra* of the interpretation and $[\![\cdot]\!]$ the *semantic function*.

Given a probabilistic program $P = \{H_i\}_{1 \le i \le n}$, where each procedure $H_i = (V_i, E_i, v_i^{\mathsf{entry}}, v_i^{\mathsf{exit}})$ is a CFHG, and an interpretation $\mathcal{I} = (\mathcal{M}, [\![\cdot]\!])$, I define $\mathcal{I}[P]$ to be the interpretation of the probabilistic program. Recall that in this chapter, nondeterministic choices are represented by hyper-edges with the *ndet* control-flow action, thus we can assume each node in a control-flow hyper-graph has at most one outgoing edge. $\mathcal{I}[P]$ is then defined as the *least fixed point* of the function $F_P^\sharp$, which is defined as

$$\lambda \mathcal{S}^\sharp.\lambda v. \begin{cases} \widehat{Ctrl(e)}^\sharp(\mathcal{S}^\sharp(u_1), \ldots, \mathcal{S}^\sharp(u_k)) & e = (v, \{u_1, \ldots, u_k\}) \in E \stackrel{\text{def}}{=} \bigcup_{i=1}^n E_i, \\ \underline{1} & \text{otherwise,} \end{cases}$$

where

$\widehat{seq[\mathsf{act}]}^\sharp(a_1) \stackrel{\text{def}}{=} [\![\mathsf{act}]\!] \otimes a_1$	$\widehat{cond[\varphi]}^\sharp(a_1, a_2) \stackrel{\text{def}}{=} a_1 \; {}_{\varphi}\Diamond \; a_2$
$\widehat{call[i \to j]}^\sharp(a_1) \stackrel{\text{def}}{=} \mathcal{S}^\sharp(v_j^{\mathsf{entry}}) \otimes a_1$	$\widehat{prob[p]}^\sharp(a_1, a_2) \stackrel{\text{def}}{=} a_1 \; {}_{p}\oplus \; a_2$
	$\widehat{ndet}^\sharp(a_1, a_2) \stackrel{\text{def}}{=} a_1 \uplus a_2$

By the Knaster-Tarski theorem (reviewed below), I use the least fixed point of $F_P^\sharp$ to define the interpretation of a probabilistic program P as $\mathscr{I}[P] \stackrel{\text{def}}{=} \text{lfp}^{\dot{\sqsubseteq}}_{\lambda v.\underline{\bot}} F_P^\sharp$. The interpretation of a control-flow node $v \in V \stackrel{\text{def}}{=} \bigcup_{i=1}^n V_i$ is then defined as $\mathscr{I}[v] \stackrel{\text{def}}{=} \mathscr{I}[P](v)$.

Proposition 4.5 (Knaster-Tarski theorem). *Suppose $(L, \sqsubseteq)$ is a complete lattice with a least element $\bot$, and let $f : L \to L$ be a monotone function with respect to $\sqsubseteq$. Then the set of fixed points of f in L also forms a complete lattice under $\sqsubseteq$. In particular, f admits a least fixed point, denoted by $\text{lfp}^{\sqsubseteq}_{\bot} f$.*

4.2.2 Abstractions of Probabilistic Programs

Given an MA C and a PMA $\mathcal{A}$, a *probabilistic abstraction* is defined as follows:

Definition 4.6 (Probabilistic abstractions). A *probabilistic over-abstraction (resp., under-abstraction)* from an MA C to a PMA $\mathcal{A}$ is a concretization mapping, $\gamma : \mathcal{A} \to C$, such that

- $\underline{\bot}_C \sqsubseteq_C \gamma(\underline{\bot}_{\mathcal{A}})$ (resp., $\gamma(\underline{\bot}_{\mathcal{A}}) \sqsubseteq_C \underline{\bot}_C$),
- $\underline{1}_C \sqsubseteq_C \gamma(\underline{1}_{\mathcal{A}})$ (resp., $\gamma(\underline{1}_{\mathcal{A}}) \sqsubseteq_C \underline{1}_C$),
- for all $Q_1, Q_2 \in \mathcal{A}$, $\gamma(Q_1) \otimes_C \gamma(Q_2) \sqsubseteq_C \gamma(Q_1 \otimes_{\mathcal{A}} Q_2)$ (resp., $\gamma(Q_1 \otimes_{\mathcal{A}} Q_2) \sqsubseteq_C \gamma(Q_1) \otimes_C \gamma(Q_2)$),
- for all $Q_1, Q_2 \in \mathcal{A}$, $\gamma(Q_1)\ {}_{\varphi}\Diamond_C\ \gamma(Q_2) \sqsubseteq_C \gamma(Q_1\ {}_{\varphi}\Diamond_{\mathcal{A}}\ Q_2)$ (resp., $\gamma(Q_1\ {}_{\varphi}\Diamond_{\mathcal{A}}\ Q_2) \sqsubseteq_C \gamma(Q_1)\ {}_{\varphi}\Diamond_C\ \gamma(Q_2)$),
- for all $Q_1, Q_2 \in \mathcal{A}$, $\gamma(Q_1)\ {}_{\lambda\omega.p}\Diamond_C\ \gamma(Q_2) \sqsubseteq_C \gamma(Q_1\ {}_p\oplus_{\mathcal{A}}\ Q_2)$ (resp., $\gamma(Q_1\ {}_p\oplus_{\mathcal{A}}\ Q_2) \sqsubseteq_C \gamma(Q_1)\ {}_{\lambda\omega.p}\Diamond_C\ \gamma(Q_2)$), and
- for all $Q_1, Q_2 \in \mathcal{A}$, $\gamma(Q_1) \uplus_C \gamma(Q_2) \sqsubseteq_C \gamma(Q_1 \uplus_{\mathcal{A}} Q_2)$ (resp., $\gamma(Q_1 \uplus_{\mathcal{A}} Q_2) \sqsubseteq_C \gamma(Q_1) \uplus_C \gamma(Q_2)$).

A probabilistic abstraction leads to a sound analyses:

Theorem 4.7. *Let $\mathscr{C}$ and $\mathscr{A}$ be interpretations over the MA C and the PMA $\mathcal{A}$, respectively; let γ be a probabilistic over-abstraction (resp., under-abstraction) from C to $\mathcal{A}$; and let P be an arbitrary probabilistic program. If for all basic actions $\mathsf{act} \in \mathsf{Act}$, $[\![\mathsf{act}]\!]^{\mathscr{C}} \sqsubseteq_C \gamma([\![\mathsf{act}]\!]^{\mathscr{A}})$ (resp., $\gamma([\![\mathsf{act}]\!]^{\mathscr{A}}) \sqsubseteq_C [\![\mathsf{act}]\!]^{\mathscr{C}}$), then it holds that $\mathscr{C}[P] \dot{\sqsubseteq}_C \dot{\gamma}(\mathscr{A}[P])$ (resp., $\dot{\gamma}(\mathscr{A}[P]) \dot{\sqsubseteq}_C \mathscr{C}[P]$).*

Proof. Without loss of generality, I present the proof for over-approximations.

Recall the algebraic denotational semantics from §3.3, $\mathscr{C}[P] = \text{lfp}^{\dot{\sqsubseteq}_C}_{\lambda v.\underline{\bot}_C} F_P^{\mathscr{C}} = \sup_{n\in\mathbb{Z}^+}\{(F_P^{\mathscr{C}})^n(\lambda v.\underline{\bot}_C)\}$ by the Kleene fixed-point theorem, and $\mathscr{A}[P] = \text{lfp}^{\dot{\sqsubseteq}_{\mathcal{A}}}_{\lambda v.\underline{\bot}_{\mathcal{A}}} F_P^{\mathscr{A}}$ obtained by the Knaster-Tarski theorem. We want to show that for all $n \in \mathbb{Z}^+$ it holds that $(F_P^{\mathscr{C}})^n(\lambda v.\underline{\bot}_C) \dot{\sqsubseteq}_C \dot{\gamma}(\mathscr{A}[P])$. We proceed by induction on n. The base case follows directly from the fact that $\underline{\bot}_C$ is the least element in C. For the induction step, suppose we know $(F_P^{\mathscr{C}})^n(\lambda v.\underline{\bot}_C) \dot{\sqsubseteq}_C \dot{\gamma}(\mathscr{A}[P])$ for some $n \in \mathbb{Z}^+$. Let us denote the left hand side (i.e., $(F_P^{\mathscr{C}})^n(\lambda v.\underline{\bot}_C)$) by LHS and $\mathscr{A}[P]$ by SOL. We want to show that $F_P^{\mathscr{C}}(LHS) \dot{\sqsubseteq}_C \dot{\gamma}(SOL)$. This expands to $F_P^{\mathscr{C}}(LHS)(v) \sqsubseteq_C \gamma(SOL(v))$ for all $v \in V$. We proceed by a case analysis on the kind of edges leaving v.

1. If $v = v_i^{\mathsf{exit}}$ for some procedure H_i, then $F_P^{\mathscr{C}}(LHS)(v) = \underline{1}_C$. Then we can conclude this case by showing that $SOL(v) = \underline{1}_{\mathcal{A}}$. Indeed, by definition of SOL, we know that $F_P^{\mathscr{A}}(SOL) = SOL$, thus $F_P^{\mathscr{A}}(SOL)(v) = SOL(v)$. By definition of $F_P^{\mathscr{A}}$, we know that $F_P^{\mathscr{A}}(SOL)(v) = \underline{1}_{\mathcal{A}}$.

2. If $v \neq v_i^{\mathsf{exit}}$ for any procedure H_i, then v is associated with some hyper-edge $e = (v, \{u_1, \cdots, u_k\}) \in E$, and we have

$$\begin{aligned} F_P^{\mathscr{C}}(LHS)(v) &= \widehat{Ctrl(e)}(LHS(u_1), \cdots, LHS(u_k)) \\ &\sqsubseteq_C \widehat{Ctrl(e)}(\gamma(SOL(u_1)), \cdots, \gamma(SOL(u_k))), \end{aligned}$$

by the monotonicity of algebraic operators. If we can prove that for any kind of $Ctrl(e)$ it holds that $\widehat{Ctrl(e)}(\gamma(x_1), \cdots, \gamma(x_k)) \sqsubseteq_C \gamma(\widehat{Ctrl(e)}^\sharp(x_1, \cdots, x_k))$, then we can conclude the case by the following argument:

$$\begin{aligned} F_P^{\mathscr{C}}(LHS)(v) &\sqsubseteq_C \gamma(\widehat{Ctrl(e)}^\sharp(SOL(u_1), \cdots, SOL(u_k))) \\ &= \gamma(F_P^{\mathscr{A}}(SOL)(v)) \\ &= \gamma(SOL(v)). \end{aligned}$$

Now consider the form of $Ctrl(e)$.

- $Ctrl(e) = seq[\mathsf{act}]$: We want to show that $\widehat{seq[\mathsf{act}]}(\gamma(x_1)) \sqsubseteq_C \gamma(\widehat{seq[\mathsf{act}]}^\sharp(x_1))$. It is equivalent to $[\![\mathsf{act}]\!]^{\mathscr{C}} \otimes_C \gamma(x_1) \sqsubseteq_C \gamma([\![\mathsf{act}]\!]^{\mathscr{A}} \otimes_{\mathcal{A}} x_1)$. Indeed, we have

$$[\![\mathsf{act}]\!]^{\mathscr{C}} \otimes_C \gamma(x_1) \sqsubseteq_C \gamma([\![\mathsf{act}]\!]^{\mathscr{A}}) \otimes_C \gamma(x_1) \sqsubseteq_C \gamma([\![\mathsf{act}]\!]^{\mathscr{A}} \otimes_{\mathcal{A}} x_1)$$

  by the monotonicity of $\otimes_C$ and properties of γ.

- $Ctrl(e) = call[i \to j]$: We want to show that $\widehat{call[i \to j]}(\gamma(x_1)) \sqsubseteq_C \gamma(\widehat{call[i \to j]}^\sharp(x_1))$. It is equivalent to $LHS(v_j^{\mathsf{entry}}) \otimes_C \gamma(x_1) \sqsubseteq_C \gamma(SOL(v_j^{\mathsf{entry}}) \otimes_{\mathcal{A}} x_1)$. Indeed, we have

$$LHS(v_j^{\mathsf{entry}}) \otimes_C \gamma(x_1) \sqsubseteq_C \gamma(SOL(v_j^{\mathsf{entry}})) \otimes_C \gamma(x_1) \sqsubseteq_C \gamma(SOL(v_j^{\mathsf{entry}}) \otimes_{\mathcal{A}} x_1)$$

  by induction hypothesis, the monotonicity of $\otimes_C$, and properties of γ.

- $Ctrl(e) = cond[\varphi]$: We want to show that $\widehat{cond[\varphi]}(\gamma(x_1), \gamma(x_2)) \sqsubseteq_C \gamma(\widehat{cond[\varphi]}^\sharp(x_1, x_2))$. It is equivalent to $\gamma(x_1)\ {}_\varphi\Diamond_C\ \gamma(x_2) \sqsubseteq_C \gamma(x_1\ {}_\varphi\Diamond_{\mathcal{A}}\ x_2)$. Appeal to properties of γ.

- $Ctrl(e) = prob[p]$: We want to show that $\widehat{prob[p]}(\gamma(x_1), \gamma(x_2)) \sqsubseteq_C \gamma(\widehat{prob[p]}^\sharp(x_1, x_2))$. It is equivalent to $\gamma(x_1)\ {}_{\lambda\omega.p}\Diamond_C\ \gamma(x_2) \sqsubseteq_C \gamma(x_1\ {}_p\oplus_{\mathcal{A}}\ x_2)$. Appeal to properties of γ.

- $Ctrl(e) = ndet$: We want to show that $\widehat{ndet}(\gamma(x_1), \gamma(x_2)) \sqsubseteq_C \gamma(\widehat{ndet}^\sharp(x_1, x_2))$. It is equivalent to $\gamma(x_1) \uplus_C \gamma(x_2) \sqsubseteq_C \gamma(x_1 \uplus_{\mathcal{A}} x_2)$. Appeal to properties of γ.

□

4.2.3 Interprocedural Analysis Algorithm

We are given a probabilistic program P and an interpretation $\mathscr{A} = (\mathcal{A}, [\![\cdot]\!]^{\mathscr{A}})$, where $\mathcal{A} = (M_{\mathcal{A}}, \sqsubseteq_{\mathcal{A}}, \otimes_{\mathcal{A}}, {}_{\varphi}\diamondsuit_{\mathcal{A}}, {}_{p}\oplus_{\mathcal{A}}, \uplus_{\mathcal{A}}, \underline{\bot}_{\mathcal{A}}, \underline{1}_{\mathcal{A}})$ is a PMA and $[\![\cdot]\!]^{\mathscr{A}}$ is a semantic function. The goal is to compute (an overapproximation of) $\mathscr{A}[P] = \mathrm{lfp}^{\dot{\sqsubseteq}_{\mathcal{A}}}_{\lambda v.\underline{\bot}_{\mathcal{A}}} F^{\sharp}_{P}$. An equivalent way to define $\mathscr{A}[P]$ is to specify it as the least solution to a system of inequalities on $\{\mathscr{A}[v] \mid v \in V\}$ (where $e \in E$ in each case):

	e	$Ctrl(e)$
$\mathscr{A}[v] \sqsupseteq_{\mathcal{A}} [\![\mathsf{act}]\!]^{\mathscr{A}} \otimes_{\mathcal{A}} \mathscr{A}[u_1]$	$(v, \{u_1\})$	$seq[\mathsf{act}]$
$\mathscr{A}[v] \sqsupseteq_{\mathcal{A}} \mathscr{A}[u_1]\ {}_{\varphi}\diamondsuit_{\mathcal{A}}\ \mathscr{A}[u_2]$	$(v, \{u_1, u_2\})$	$cond[\varphi]$
$\mathscr{A}[v] \sqsupseteq_{\mathcal{A}} \mathscr{A}[u_1]\ {}_{p}\oplus_{\mathcal{A}}\ \mathscr{A}[u_2]$	$(v, \{u_1, u_2\})$	$prob[p]$
$\mathscr{A}[v] \sqsupseteq_{\mathcal{A}} \mathscr{A}[u_1] \uplus_{\mathcal{A}} \mathscr{A}[u_2]$	$(v, \{u_1, u_2\})$	$ndet$
$\mathscr{A}[v] \sqsupseteq_{\mathcal{A}} \mathscr{A}[v_j^{\mathsf{entry}}] \otimes_{\mathcal{A}} \mathscr{A}[u_1]$	$(v, \{u_1\})$	$call[i \to j]$
$\mathscr{A}[v] \sqsupseteq_{\mathcal{A}} \underline{1}_{\mathcal{A}}$	if $v = v_i^{\mathsf{exit}}$ for some procedure H_i	

Note that in line 5 a call is treated as a hyper-edge with the action $\lambda(entry, succ).entry \otimes_{\mathcal{A}} succ$. There is no explicit return edge to match a call (as in many multi-procedure program representations, e.g., [132]); instead, each exit node is initialized with the constant $\underline{1}_{\mathcal{A}}$ (line 6).

I mainly adopt known techniques from previous work on interprocedural dataflow analysis, with some adaptations to the PMAF setting, which uses hyper-graphs instead of ordinary graphs (i.e., CFGs).[6] The analysis direction is backward, and the algorithm is similar to methods for computing summary edges in demand interprocedural-dataflow-analysis algorithms ([76, Fig. 4], [135, Fig. 10]). The algorithm uses a standard chaotic-iteration strategy, i.e., Bourdoncle's strategy [18] (except that propagation is performed along hyper-edges instead of edges); it uses a fair iteration strategy for selecting the next edge to consider.

4.2.4 Widening

Widening is a general technique in static analysis to ensure and speed up convergence [34, 36]. To choose the nodes at which widening is to be applied, I treat the hyper-graph as a graph—i.e., each hyper-edge (including calls) contributes one or two ordinary edges. More precisely, I construct a *dependence graph* $G(P) = (N, A)$ from a probabilistic program $P = \{(V_i, E_i, v_i^{\mathsf{entry}}, v_i^{\mathsf{exit}})\}_{1 \le i \le n}$ by defining $N \stackrel{\text{def}}{=} \bigcup_{1 \le i \le n} V_i$, and

$$\begin{aligned} A \stackrel{\text{def}}{=} &\{(u, v) \mid \exists e \in E\colon (v = src(e) \wedge u \in Dst(e))\} \\ &\cup \{(v_j^{\mathsf{entry}}, v) \mid \exists e \in E\colon (v = src(e) \wedge Ctrl(e) = call[i \to j])\}. \end{aligned} \tag{4.1}$$

I then compute a set W of widening points for $G(P)$ via the algorithm of Bourdoncle [18, Fig. 4]. Because of the second set-former in (4.1), W contains widening points that cut each cycle caused by recursion.

[6] As mentioned in §4.1.3, standard formulations of interprocedural dataflow analysis [94, 105, 123, 138] can be viewed as hyper-graph analyses. In that setting, one deals with hyper-graphs with constituent control-flow graphs. With PMAF, because each procedure is represented as a hyper-graph, one has hyper-graphs of constituent hyper-graphs. Fortunately, each procedure's hyper-graph is a *single-entry/single-exit* hyper-graph, so the basic ideas and algorithms from standard interprocedural dataflow analysis carry over to PMAF.

While traditional programs exhibit only one sort of choice operator, probabilistic programs can have three different kinds of choice operators, and hence loops can exhibit three different kinds of behavior. I found that if we used the same widening operator for all widening nodes, there could be a substantial loss in precision. Thus, I equip the framework with three separate widening operators: $\triangledown_c$, $\triangledown_p$, and $\triangledown_n$. Let $v \in W$ be the source of edge $e \in E$. Then the inequalities for widening points become

	e	$Ctrl(e)$
$\mathscr{A}[v] \sqsupseteq_{\mathcal{A}} \mathscr{A}[v] \triangledown_n (\llbracket \mathsf{act} \rrbracket^{\mathscr{A}} \otimes_{\mathcal{A}} \mathscr{A}[u_1])$	$(v, \{u_1\})$	$seq[\mathsf{act}]$
$\mathscr{A}[v] \sqsupseteq_{\mathcal{A}} \mathscr{A}[v] \triangledown_c (\mathscr{A}[u_1] \ {}_{\varphi}\Diamond_{\mathcal{A}} \ \mathscr{A}[u_2])$	$\langle v, \{u_1, u_2\})$	$cond[\varphi]$
$\mathscr{A}[v] \sqsupseteq_{\mathcal{A}} \mathscr{A}[v] \triangledown_p (\mathscr{A}[u_1] \ {}_{p}\oplus_{\mathcal{A}} \ \mathscr{A}[u_2])$	$(v, \{u_1, u_2\})$	$prob[p]$
$\mathscr{A}[v] \sqsupseteq_{\mathcal{A}} \mathscr{A}[v] \triangledown_n (\mathscr{A}[u_1] \uplus_{\mathcal{A}} \mathscr{A}[u_2])$	$(v, \{u_1, u_2\})$	$ndet$
$\mathscr{A}[v] \sqsupseteq_{\mathcal{A}} \mathscr{A}[v] \triangledown_n (\mathscr{A}[v_j^{\mathsf{entry}}] \otimes_{\mathcal{A}} \mathscr{A}[u_1])$	$(v, \{u_1\})$	$call[i \to j]$

Observation 4.8. Recall that in this chapter, I assume that in a probabilistic program, each non-exit node has exactly one outgoing hyper-edge. In each right-hand side above, the second argument to the widening operator re-evaluates the action of the (one outgoing) hyper-edge. Consequently, during an analysis, there is an invariant that whenever a widening operation $a \triangledown b$ is performed, the property $a \sqsubseteq_{\mathcal{A}} b$ holds.

The safety properties for the three widening operators are adaptations of the standard stabilization condition: For every pair of ascending chains $\{a_k\}_{k\in\mathbb{Z}^+}$ and $\{b_k\}_{k\in\mathbb{Z}^+}$,

- the chain $\{c_k\}_{k\in\mathbb{Z}^+}$ defined by $c_0 = a_0 \ {}_{\varphi}\Diamond_{\mathcal{A}} \ b_0$ and $c_{k+1} = c_k \triangledown_c (a_{k+1} \ {}_{\varphi}\Diamond_{\mathcal{A}} \ b_{k+1})$ is eventually stable;
- the chain $\{c_k\}_{k\in\mathbb{Z}^+}$ defined by $c_0 = a_0 \ {}_{p}\oplus_{\mathcal{A}} \ b_0$ and $c_{k+1} = c_k \triangledown_p (a_{k+1} \ {}_{p}\oplus_{\mathcal{A}} \ b_{k+1})$ is eventually stable; and
- the chain $\{c_k\}_{k\in\mathbb{Z}^+}$ defined by $c_0 = a_0 \uplus_{\mathcal{A}} b_0$ and $c_{k+1} = c_k \triangledown_n (a_{k+1} \uplus_{\mathcal{A}} b_{k+1})$ is eventually stable.

4.3 Instantiations

In this section, I instantiate the framework to derive three important analyses: Bayesian inference (BI) (§4.3.1), computing rewards in Markov decision processes (§4.3.2), and linear expectation-invariant analysis (LEIA) (§4.3.3).

4.3.1 Bayesian Inference

Claret et al. [29] proposed a technique to perform Bayesian inference on Boolean programs using dataflow analysis. They use a forward analysis to compute the post-state distribution of a single-procedure, well-structured, probabilistic program. Their analysis is similar to an intraprocedural dataflow analysis: they use discrete joint-probability distributions as dataflow facts, merge these facts at join points, and compute fixpoints in the presence of loops. Let Var be a finite set of program

variables; the set of program states is $\Omega \stackrel{\text{def}}{=} \mathsf{Var} \to \mathbb{2}$, where $\mathbb{2} = \{true, false\}$ is the set of Boolean values. Note that Ω is isomorphic to $\mathbb{2}^{|\mathsf{Var}|}$, and consequently, a distribution can be represented by a vector of length $2^{|\mathsf{Var}|}$ of real numbers in the unit interval $[0, 1]$. (Their implementation uses Algebraic Decision Diagrams [5] to represent distributions compactly.)

The algorithm by Claret et al. [29, Alg. 2] is defined inductively on the structure of programs—for example, the output distribution of $x \sim \textsc{Bernoulli}(r)$ from an input distribution μ, denoted by $Post(\mu, x \sim \textsc{Bernoulli}(r))$, is computed as $\lambda\sigma'.\left(r \cdot \sum_{\{\sigma|\sigma'=\sigma[x\leftarrow true]\}} \mu(\sigma) + (1-r) \cdot \sum_{\{\sigma|\sigma'=\sigma[x\leftarrow false]\}} \mu(\sigma)\right)$.

I have used PMAF to extend their work in two dimensions, creating (i) an *interprocedural* version of Bayesian inference with (ii) *nondeterminism*. Because of nondeterminism, for a given input state the post-state distribution is not unique; consequently, my goal is to compute procedure summaries that gives *lower bounds* on post-state distributions. I consider the following data actions Act and logical conditions $\mathcal{L}$ for Boolean programs, where $p \in [0, 1]$.

$$\mathsf{Act} ::= x := \varphi \mid x \sim \textsc{Bernoulli}(p) \mid \textbf{observe}(\varphi) \mid \textbf{skip}$$
$$\varphi \in \mathcal{L} ::= x \mid true \mid false \mid \textbf{not}\ \varphi \mid \varphi_1\ \textbf{and}\ \varphi_2 \mid \varphi_1\ \textbf{or}\ \varphi_2$$

Similarly, I define interpretations of data actions and logical conditions for Boolean programs as I have done for arithmetic programs in §2.3:

$[\![x := \varphi]\!] \stackrel{\text{def}}{=} \lambda\omega.\ \delta(\omega[x \mapsto [\![\varphi]\!](\omega)])$	$[\![x]\!] \stackrel{\text{def}}{=} \lambda\omega.\ \omega(x)$
$[\![x \sim \textsc{Bernoulli}(p)]\!] \stackrel{\text{def}}{=} \lambda\omega.\ p \cdot \delta(\omega[x \mapsto true])$	$[\![c]\!] \stackrel{\text{def}}{=} \lambda\omega.\ c$ where $c \in \{true, false\}$
$+ (1-p) \cdot \delta(\omega[x \mapsto false])$	$[\![\textbf{not}\ \varphi]\!] \stackrel{\text{def}}{=} \lambda\omega.\ \neg[\![\varphi]\!](\omega)$
$[\![\textbf{observe}(\varphi)]\!] \stackrel{\text{def}}{=} \lambda\omega.\ [\![\varphi]\!](\omega) \cdot \delta(\omega)$	$[\![\varphi_1\ \textbf{and}\ \varphi_2]\!] \stackrel{\text{def}}{=} \lambda\omega.\ [\![\varphi_1]\!](\omega) \wedge [\![\varphi_2]\!](\omega)$
$[\![\textbf{skip}]\!] \stackrel{\text{def}}{=} \lambda\omega.\ \delta(\omega)$	$[\![\varphi_1\ \textbf{or}\ \varphi_2]\!] \stackrel{\text{def}}{=} \lambda\omega.\ [\![\varphi_1]\!](\omega) \vee [\![\varphi_2]\!](\omega)$

To reformulate the domain in the two-vocabulary setting needed for computing procedure summaries, I introduce Var', primed versions of the variables in Var. Var and Var' denote the variables in the pre-state and post-state of a state transformer. A distribution transformer (and therefore a procedure summary) is a matrix of size $2^{|\mathsf{Var}|} \times 2^{|\mathsf{Var}'|}$ of real numbers in the unit interval $[0, 1]$. I define a PMA $\mathcal{B} = (M_{\mathcal{B}}, \sqsubseteq_{\mathcal{B}}, \otimes_{\mathcal{B}}, {}_{\varphi}\diamondsuit_{\mathcal{B}}, {}_{p}\oplus_{\mathcal{B}}, \uplus_{\mathcal{B}}, \underline{\bot}_{\mathcal{B}}, \underline{1}_{\mathcal{B}})$ as follows:

$M_{\mathcal{B}} \stackrel{\text{def}}{=} 2^{\lvert\mathsf{Var}\rvert} \times 2^{\lvert\mathsf{Var}'\rvert} \to [0, 1]$	
$a \sqsubseteq_{\mathcal{B}} b \stackrel{\text{def}}{=} a \dot{\leq} b$	$a \uplus_{\mathcal{B}} b \stackrel{\text{def}}{=} \dot{\min}(a, b)$
$a \otimes_{\mathcal{B}} b \stackrel{\text{def}}{=} a \times b$	$\underline{\bot}_{\mathcal{B}} \stackrel{\text{def}}{=} \lambda(s, t).0$
$a\ {}_{p}\oplus_{\mathcal{B}}\ b \stackrel{\text{def}}{=} p \cdot a + (1-p) \cdot b$	$\underline{1}_{\mathcal{B}} \stackrel{\text{def}}{=} \lambda(s, t).[s = t]$
$a\ {}_{\varphi}\diamondsuit_{\mathcal{B}}\ b \stackrel{\text{def}}{=} \lambda(s, t).\ \textbf{if}\ [\![\varphi]\!](s)\ \textbf{then}\ a(s, t)\ \textbf{else}\ b(s, t)$	

The use of pointwise min in the definition of $a \uplus_{\mathcal{B}} b$ causes the analysis to compute procedure summaries that provide lower bounds on the post-state distributions.

LEMMA 4.9. *$\mathcal{B}$ is a PMA.*

PROOF. $(M_{\mathcal{B}}, \sqsubseteq_{\mathcal{B}})$ forms a complete lattice because all elements in $M_{\mathcal{B}}$ are supported by the bounded interval $[0, 1]$. $(M_{\mathcal{B}}, \otimes_{\mathcal{B}}, \underline{1}_{\mathcal{B}})$ forms a monoid because the set of square matrices (of

the same dimension) with matrix multiplication forms a monoid with the identity matrix as the identity element. The semilattice ordering induced by $\uplus_{\mathcal{B}}$ is the pointwise ordering $\dot{\geq}$, and it is straightforward to check $a \ {}_{\varphi}\diamondsuit_{\mathcal{B}} \ b \dot{\geq} a \uplus_{\mathcal{B}} b$ and $a \ {}_{p}\oplus_{\mathcal{B}} \ b \dot{\geq} a \uplus_{\mathcal{B}} b$ for all $a, b \in M_{\mathcal{B}}$ and $\varphi \in \mathcal{L}$, $p \in [0,1]$. Finally, it is also straightforward to check that the operators $\otimes_{\mathcal{B}}$, ${}_{\varphi}\diamondsuit_{\mathcal{B}}$, ${}_{p}\oplus_{\mathcal{B}}$, $\uplus_{\mathcal{B}}$ are monotone with respect to $\sqsubseteq_{\mathcal{B}}$. □

Let $\mathscr{B} = (\mathcal{B}, [\![\cdot]\!]^{\mathscr{B}})$ be the interpretation for Bayesian inference. I define the semantic function for data actions as follows. Recall that $[\cdot]$ is the *Iverson bracket*, which evaluates to 1 if the argument condition is true, and 0 otherwise.

$$
\begin{aligned}
[\![x \coloneqq \varphi]\!]^{\mathscr{B}} &\stackrel{\text{def}}{=} \lambda(s,t).\ [s[x \mapsto [\![\varphi]\!](s)] = t] \\
[\![x \sim \textsc{Bernoulli}(p)]\!]^{\mathscr{B}} &\stackrel{\text{def}}{=} \lambda(s,t).\ p \cdot [s[x \mapsto \mathit{true}] = t] + (1-p) \cdot [s[x \mapsto \mathit{false}] = t] \\
[\![\textbf{observe}(\varphi)]\!]^{\mathscr{B}} &\stackrel{\text{def}}{=} \lambda(s,t).\ [[\![\varphi]\!](s)] \cdot [s = t] \\
[\![\textbf{skip}]\!]^{\mathscr{B}} &\stackrel{\text{def}}{=} \lambda(s,t).\ [s = t]
\end{aligned}
$$

To prove soundness, I use the denotational semantics based on the g-convex powerdomain $\mathcal{GK}(\Omega)$ (denoted by C in this section) developed in §3.3. I then define the concretization mapping $\gamma_{\mathcal{B}} : M_{\mathcal{B}} \to \mathcal{GK}(\Omega)$ as $\gamma_{\mathcal{B}}(a) \stackrel{\text{def}}{=} \{\kappa \mid \forall s, s' : \kappa(s)(s') \geq a(s,s')\}$, indicating that the abstract domain keeps track of lower bounds.

Lemma 4.10. *$\gamma_{\mathcal{B}}$ is a probabilistic under-abstraction from C to $\mathcal{B}$.*

Proof. By definition, we have $\gamma_{\mathcal{B}}(a) = \uparrow(\lambda s.\lambda s'.a(s,s'))$, i.e., the upper closure of a in the g-convex powerdomain $\mathcal{GK}(\Omega)$.

- We want to show $\gamma_{\mathcal{B}}(\underline{1}_{\mathcal{B}}) \sqsubseteq_C \underline{1}_C$. Appeal to the fact that $\uparrow(\lambda s.\lambda s'.[s = s']) = \uparrow\{\lambda s.\delta(s)\} = \{\lambda s.\delta(s)\} = \underline{1}_C$.
- We want to show for all $Q_1, Q_2 \in \mathcal{B}$, $\gamma_{\mathcal{B}}(Q_1 \otimes_{\mathcal{B}} Q_2) \sqsubseteq_C \gamma_{\mathcal{B}}(Q_1) \otimes_C \gamma_{\mathcal{B}}(Q_2)$. Because $\gamma_{\mathcal{B}}$ always maps to saturated subsets, it is sufficient to show $\gamma_{\mathcal{B}}(Q_1 \times Q_2) \supseteq \uparrow \mathit{gconv}(\gamma_{\mathcal{B}}(Q_1) \otimes_C \gamma_{\mathcal{B}}(Q_2))$. Observe that $\gamma_{\mathcal{B}}(Q_1 \times Q_2)$ is saturated and g-convex, it is sufficient to show $\gamma_{\mathcal{B}}(Q_1) \otimes_C \gamma_{\mathcal{B}}(Q_2) \subseteq \gamma_{\mathcal{B}}(Q_1 \times Q_2)$.
  Fix $\kappa_1 \in \gamma_{\mathcal{B}}(Q_1)$ and $\kappa_2 \in \gamma_{\mathcal{B}}(Q_2)$. Let $q_1 = \lambda s.\lambda s'.Q_1(s,s')$ and $q_2 = \lambda s.\lambda s'.Q_2(s,s')$. Then $\kappa_1 \sqsupseteq_K q_1$ and $\kappa_2 \sqsupseteq_K q_2$. Because the kernel composition operator $\otimes$ is monotone, we know that $\kappa_1 \otimes \kappa_2 \sqsupseteq_K q_1 \otimes q_2$. Observe that

  $$q_1 \otimes q_2 = \lambda s.\lambda s''.\sum_{s' \in \Omega} q_1(s)(s') \cdot q_2(s')(s'') = \lambda s.\lambda s''.(Q_1 \times Q_2)(s,s''),$$

  thus $q_1 \otimes q_2 \in \gamma_{\mathcal{B}}(Q_1 \times Q_2)$. Because $\kappa_1 \otimes \kappa_2 \sqsupseteq_K q_1 \otimes q_2$ and $\gamma_{\mathcal{B}}(Q_1 \times Q_2)$ is saturated, we conclude that $\kappa_1 \otimes \kappa_2 \in \gamma_{\mathcal{B}}(Q_1 \times Q_2)$.
- We want to show that for all $Q_1, Q_2 \in \mathcal{B}$ and $\varphi \in \mathcal{L}$, it holds that $\gamma_{\mathcal{B}}(Q_1 \ {}_{\varphi}\diamondsuit_{\mathcal{B}} \ Q_2) \sqsubseteq_C \gamma_{\mathcal{B}}(Q_1) \ {}_{\varphi}\diamondsuit_C \ \gamma_{\mathcal{B}}(Q_2)$. It is sufficient to show that

  $$\gamma_{\mathcal{B}}(\lambda(s,s').\ \textbf{if}\ [\![\varphi]\!](s)\ \textbf{then}\ Q_1(s,s')\ \textbf{else}\ Q_2(s,s')) \supseteq \uparrow(\gamma_{\mathcal{B}}(Q_1) \ {}_{\varphi}\diamondsuit_C \ \gamma_{\mathcal{B}}(Q_2)).$$

Observe that the left-hand-side is saturated. It is sufficient to show

$$\gamma_{\mathcal{B}}(Q_1)\ {}_{\varphi}\Diamond_{C}\ \gamma_{\mathcal{B}}(Q_2) \subseteq \gamma_{\mathcal{B}}(\lambda(s,s').\ \textbf{if}\ [\![\varphi]\!](s)\ \textbf{then}\ Q_1(s,s')\ \textbf{else}\ Q_2(s,s')).$$

Fix $\kappa_1 \in \gamma_{\mathcal{B}}(Q_1)$ and $\kappa_2 \in \gamma_{\mathcal{B}}(Q_2)$. Let $q_1 = \lambda s.\lambda s'.Q_1(s,s')$ and $q_2 = \lambda s.\lambda s'.Q_2(s,s')$. Then $\kappa_1 \sqsupseteq_K q_1$ and $\kappa_2 \sqsupseteq_K q_2$. Because the kernel conditional-choice operator ${}_{\varphi}\Diamond$ is monotone, we know that $\kappa_1\ {}_{\varphi}\Diamond\ \kappa_2 \sqsupseteq_K q_1\ {}_{\varphi}\Diamond\ q_2$. Observe that

$$\begin{aligned} q_1\ {}_{\varphi}\Diamond\ q_2 &= \lambda s.\lambda s'.[[\![\varphi]\!](s)] \cdot q_1(s)(s') + [1 - [\![\varphi]\!](s)] \cdot q_2(s)(s') \\ &= \lambda s.\lambda s'.\textbf{if}\ [\![\varphi]\!](s)\ \textbf{then}\ Q_1(s,s')\ \textbf{else}\ Q_2(s,s'), \end{aligned}$$

thus $q_1\ {}_{\varphi}\Diamond\ q_2 \in \gamma_{\mathcal{B}}(\lambda(s,s').\textbf{if}\ [\![\varphi]\!](s)\ \textbf{then}\ Q_1(s,s')\ \textbf{else}\ Q_2(s,s'))$. Hence $\kappa_1\ {}_{\varphi}\Diamond\ \kappa_2 \in \gamma_{\mathcal{B}}(\lambda(s,s').\textbf{if}\ [\![\varphi]\!](s)\ \textbf{then}\ Q_1(s,s')\ \textbf{else}\ Q_2(s,s'))$.

- We want to show that for all $Q_1, Q_2 \in \mathcal{B}$ and $p \in [0,1]$, it holds that $\gamma_{\mathcal{B}}(Q_1\ {}_{p}\oplus_{\mathcal{B}}\ Q_2) \sqsubseteq_C \gamma_{\mathcal{B}}(Q_1)\ {}_{\lambda\omega.p}\Diamond_{C}\ \gamma_{\mathcal{B}}(Q_2)$. It is sufficient to show that

$$\gamma_{\mathcal{B}}(p \cdot Q_1 + (1-p) \cdot Q_2) \supseteq \uparrow(\gamma_{\mathcal{B}}(Q_1)\ {}_{\lambda\omega.p}\Diamond_{C}\ \gamma_{\mathcal{B}}(Q_2)).$$

  Observe that the left-hand-side is saturated, it is sufficient to show

$$\gamma_{\mathcal{B}}(Q_1)\ {}_{\lambda\omega.p}\Diamond_{C}\ \gamma_{\mathcal{B}}(Q_2) \subseteq \gamma_{\mathcal{B}}(p \cdot Q_1 + (1-p) \cdot Q_2).$$

  Fix $\kappa_1 \in \gamma_{\mathcal{B}}(Q_1)$ and $\kappa_2 \in \gamma_{\mathcal{B}}(Q_2)$. Let $q_1 = \lambda s.\lambda s'.Q_1(s,s')$ and $q_2 = \lambda s.\lambda s'.Q_2(s,s')$. Then $\kappa_1 \sqsupseteq_K q_1$ and $\kappa_2 \sqsupseteq_K q_2$. Because the kernel condition-choice operator ${}_{\lambda\omega.p}\Diamond$ is monotone, we know that $\kappa_1\ {}_{\lambda\omega.p}\Diamond\ \kappa_2 \sqsupseteq_K q_1\ {}_{\lambda\omega.p}\Diamond\ q_2$. Observe that

$$q_1\ {}_{\lambda\omega.p}\Diamond\ q_2 = \lambda s.\lambda s'.p \cdot q_1(s)(s') + (1-p) \cdot q_2(s)(s') = \lambda s.\lambda s'.p \cdot Q_1(s,s') + (1-p) \cdot Q_2(s,s'),$$

  thus $q_1\ {}_{\lambda\omega.p}\Diamond\ q_2 \in \gamma_{\mathcal{B}}(p \cdot Q_1 + (1-p) \cdot Q_2)$. Hence $\kappa_1\ {}_{\lambda\omega.p}\Diamond\ \kappa_2 \in \gamma_{\mathcal{B}}(p \cdot Q_1 + (1-p) \cdot Q_2)$.

- We want to show that for all $Q_1, Q_2 \in \mathcal{B}$, $\gamma_{\mathcal{B}}(Q_1 \uplus_{\mathcal{B}} Q_2) \sqsubseteq_C \gamma_{\mathcal{B}}(Q_1) \uplus_C \gamma_{\mathcal{B}}(Q_2)$. It is sufficient to show $\gamma_{\mathcal{B}}(\dot{\min}(Q_1, Q_2)) \supseteq \uparrow gconv(\gamma_{\mathcal{B}}(Q_1) \cup \gamma_{\mathcal{B}}(Q_2))$. Observe that the left-hand-side is saturated and g-convex, it is sufficient to show $\gamma_{\mathcal{B}}(Q_1) \cup \gamma_{\mathcal{B}}(Q_2) \subseteq \gamma_{\mathcal{B}}(\dot{\min}(Q_1, Q_2))$. It follows directly from the fact that $\dot{\min}(Q_1, Q_2) \dot{\leq} Q_1$ and $\dot{\min}(Q_1, Q_2) \dot{\leq} Q_2$, as well as the definition of $\gamma_{\mathcal{B}}$, which maps to saturated subsets.

□

I do not define widening operators for BI, because $\gamma_{\mathcal{B}}$ is an under-abstraction and the chaotic-iteration algorithm starts from the bottom element in the abstract domain, the intermediate result at any iteration is a sound answer.

4.3.2 Markov Decision Process with Rewards

Analyses of finite-state Markov decision processes were originally developed in the fields of operational research and finance mathematics [130]. Originally, Markov decision processes were defined as finite-state machines with actions that exhibit probabilistic transitions. In this section, I use a slightly different formalization, using hyper-graphs.

Definition 4.11 (Markov decision processes). A *Markov decision process* (MDP) is a hyper-graph $H = (V, E, v^{\mathsf{entry}}, v^{\mathsf{exit}})$, where every node except v^{exit} has exactly one outgoing hyper-edge; each hyper-edge with just a single destination has an associated *reward*, $seq[\mathbf{reward}(r)]$, where r is a positive rational number; and each hyper-edge with two destinations has either $prob[p]$, where $0 \leq p \leq 1$, or *ndet*. Note that MDPs are a specialization of single-procedure probabilistic programs without conditional-choice.

We can also treat the hyper-graph as a graph: each hyper-edge contributes one or two graph edges. A path through the graph has a *reward*, which is the sum of the rewards that label the edges of the path. (Edges from hyper-edges with the actions $prob[p]$ or *ndet* are considered to have reward 0.) The analysis problem that I wish to solve is to determine, for each node v, the *greatest* expected reward that one can gain by executing the program from v.

It is natural to extend MDPs with procedure calls and multiple procedures, to obtain *recursive Markov decision processes*. The set of program states is defined to be the set of extended nonnegative rational numbers: $\Omega \stackrel{\text{def}}{=} \mathbb{Q}^+_\infty$. To address the maximum-expected-reward problem for a recursive Markov decision process, I define a PMA $\mathcal{R} = (M_\mathcal{R}, \sqsubseteq_\mathcal{R}, \otimes_\mathcal{R}, {}_\varphi\Diamond_\mathcal{R}, {}_p\oplus_\mathcal{R}, \uplus_\mathcal{R}, \underline{\perp}_\mathcal{R}, \underline{1}_\mathcal{R})$ as follows:

$M_\mathcal{R} \stackrel{\text{def}}{=} \mathbb{R}^+_\infty$	${}_\varphi\Diamond_\mathcal{R} \stackrel{\text{def}}{=} \max$	$\underline{\perp}_\mathcal{R} \stackrel{\text{def}}{=} 0$
$\sqsubseteq_\mathcal{R} \stackrel{\text{def}}{=} \leq$	$a\ {}_p\oplus_\mathcal{R}\ b \stackrel{\text{def}}{=} p \cdot a + (1-p) \cdot b$	$\underline{1}_\mathcal{R} \stackrel{\text{def}}{=} 0$
$\otimes_\mathcal{R} \stackrel{\text{def}}{=} +$	$\uplus_\mathcal{R} \stackrel{\text{def}}{=} \max$	

LEMMA 4.12. *$\mathcal{R}$ is a PMA.*

PROOF. $(M_\mathcal{R}, \sqsubseteq_\mathcal{R})$ forms a complete lattice because it is isomorphic to the set of extended nonnegative real numbers. $(M_\mathcal{R}, \otimes_\mathcal{R}, \underline{1}_\mathcal{R})$ forms a monoid because addition + is associative on real numbers and has 0 as its identity element. The semilattice ordering induced by $\uplus_\mathcal{R}$ is the standard real number ordering $\leq$, and it is straightforward to check $a\ {}_\varphi\Diamond_\mathcal{R}\ b \leq a \uplus_\mathcal{R} b$ and $a\ {}_p\oplus_\mathcal{R}\ b \leq a \uplus_\mathcal{R} b$ for all $a, b \in M_\mathcal{R}$ and $\varphi \in \mathcal{L}$, $p \in [0,1]$. Finally, it is also straightforward to check that the operators $\otimes_\mathcal{R}$, ${}_\varphi\Diamond_\mathcal{R}$, ${}_p\oplus_\mathcal{R}$, $\uplus_\mathcal{R}$ are monotone with respect to $\sqsubseteq_\mathcal{R}$. □

Let $\mathscr{R} = (\mathcal{R}, [\![\cdot]\!]^\mathscr{R})$ be the interpretation for a Markov decision process with rewards. Because MDPs do not have logical conditions (i.e., $\mathcal{L} = \emptyset$) and the only data action is $\mathbf{reward}(r)$, I define the concrete interpretation as $[\![\mathbf{reward}(r)]\!] \stackrel{\text{def}}{=} \lambda s.\delta(s + r)$ and the abstract semantic function as $[\![\mathbf{reward}(r)]\!]^\mathscr{R} \stackrel{\text{def}}{=} r$.

To prove soundness, I use the denotational semantics based on the g-convex powerdomain $\mathcal{GK}(\Omega)$ (denoted by C in this section) developed in §3.3. I then define the concretization mapping $\gamma_\mathcal{R} : M_\mathcal{R} \to \mathcal{GK}(\Omega)$ as $\gamma_\mathcal{R}(a) \stackrel{\text{def}}{=} \{\kappa \mid \forall s : \sum_{s' \in \Omega} s' \cdot \kappa(s)(s') \leq s + a\}$, indicating that the abstract domain keeps track of upper bounds.

LEMMA 4.13. *$\gamma_\mathcal{R}$ is a probabilistic over-abstraction from C to $\mathcal{R}$.*

PROOF. By definition, we have $\gamma_\mathcal{R}(a) = \overline{\{\kappa \mid \forall s : \sum_{s' \in \Omega} s' \cdot \kappa(s)(s') = s + a\}}$, where $\overline{U}$ is the Scott closure of U in the g-convex powerdomain $\mathcal{GK}(\Omega)$.

- We want to show $\underline{1}_C \sqsubseteq_C \gamma_\mathcal{R}(\underline{1}_\mathcal{R})$. Appeal to the fact that $\lambda s.\delta(s) \in \gamma_\mathcal{R}(0)$.

- We want to show for all $Q_1, Q_2 \in \mathcal{R}$, $\gamma_{\mathcal{R}}(Q_1) \otimes_C \gamma_{\mathcal{R}}(Q_2) \sqsubseteq_C \gamma_{\mathcal{R}}(Q_1 \otimes_{\mathcal{R}} Q_2)$. Because $\gamma_{\mathcal{R}}$ always maps to Scott-closed subsets, it is sufficient to show that $gconv(\gamma_{\mathcal{R}}(Q_1) \otimes_C \gamma_{\mathcal{R}}(Q_2)) \subseteq \gamma_{\mathcal{R}}(Q_1 + Q_2)$. Observe that $\gamma_{\mathcal{R}}(Q_1 + Q_2)$ is Scott-closed and g-convex, it is sufficient to show that $\gamma_{\mathcal{R}}(Q_1) \otimes_C \gamma_{\mathcal{R}}(Q_2) \subseteq \gamma_{\mathcal{R}}(Q_1 + Q_2)$.
  Fix $\kappa_1 \in \gamma_{\mathcal{R}}(Q_1)$ and $\kappa_2 \in \gamma_{\mathcal{R}}(Q_2)$. Observe that $\sum_{y\in\Omega} y \cdot \kappa_1(s)(y) \leq s + Q_1$ and $\sum_{y\in\Omega} y \cdot \kappa_2(s)(y) \leq s + Q_2$. By the definition of the kernel composition operator $\otimes$, we have

$$\begin{aligned}
\sum_{y\in\Omega} y \cdot (\kappa_1 \otimes \kappa_2)(s)(y) &= \sum_{y\in\Omega} y \cdot (\sum_{z\in\Omega} \kappa_1(s)(z) \cdot \kappa_2(z)(y)) \\
&= \sum_{z\in\Omega} (\sum_{y\in\Omega} y \cdot \kappa_2(z)(y)) \cdot \kappa_1(s)(z) \\
&\leq \sum_{z\in\Omega} (z + Q_2) \cdot \kappa_1(s)(z) \\
&= \sum_{z\in\Omega} z \cdot \kappa_1(s)(z) + Q_2 \cdot \sum_{z\in\Omega} \kappa_1(s)(z) \\
&\leq s + Q_1 + Q_2.
\end{aligned}$$

  Hence $\kappa_1 \otimes \kappa_2 \in \gamma_{\mathcal{R}}(Q_1 + Q_2)$.

- We want to show that for all $Q_1, Q_2 \in \mathcal{R}$ and $p \in [0, 1]$, it holds that $\gamma_{\mathcal{R}}(Q_1) \,{}_{\lambda\omega.p}\diamondsuit_C\, \gamma_{\mathcal{R}}(Q_2) \sqsubseteq_C \gamma_{\mathcal{R}}(Q_1 \,{}_p\oplus_{\mathcal{R}}\, Q_2)$. It is sufficient to show that $\overline{\gamma_{\mathcal{R}}(Q_1) \,{}_{\lambda\omega.p}\diamondsuit\, \gamma_{\mathcal{R}}(Q_2)} \subseteq \gamma_{\mathcal{R}}(p \cdot Q_1 + (1-p) \cdot Q_2)$. Observe that $\gamma_{\mathcal{R}}(p \cdot Q_1 + (1-p) \cdot Q_2)$ is Scott-closed, it is sufficient to show that $\gamma_{\mathcal{R}}(Q_1) \,{}_{\lambda\omega.p}\diamondsuit_C\, \gamma_{\mathcal{R}}(Q_2) \subseteq \gamma_{\mathcal{R}}(p \cdot Q_1 + (1-p) \cdot Q_2)$.
  Fix $\kappa_1 \in \gamma_{\mathcal{R}}(Q_1)$ and $\kappa_2 \in \gamma_{\mathcal{R}}(Q_2)$. Observe that $\sum_{y\in\Omega} y \cdot \kappa_1(s)(y) \leq s + Q_1$ and $\sum_{y\in\Omega} y \cdot \kappa_2(s)(y) \leq s + Q_2$. By the definition of the kernel conditional-choice operator ${}_{\varphi}\diamondsuit$, we have

$$\begin{aligned}
\sum_{y\in\Omega} y \cdot (\kappa_1 \,{}_{\lambda\omega.p}\diamondsuit\, \kappa_2)(s)(y) &= \sum_{y\in\Omega} y \cdot (p \cdot \kappa_1 + (1-p) \cdot \kappa_2)(s)(y) \\
&= \sum_{y\in\Omega} y \cdot p \cdot \kappa_1(s)(y) + \sum_{y\in\Omega} y \cdot (1-p) \cdot \kappa_2(s)(y) \\
&\leq p \cdot Q_1 + (1-p) \cdot Q_2.
\end{aligned}$$

  Hence $\kappa_1 \,{}_{\lambda\omega.p}\diamondsuit\, \kappa_2 \in \gamma_{\mathcal{R}}(p \cdot Q_1 + (1-p) \cdot Q_2)$.

- We want to show for all $Q_1, Q_2 \in \mathcal{R}$, $\gamma_{\mathcal{R}}(Q_1) \uplus_C \gamma_{\mathcal{R}}(Q_2) \sqsubseteq_C \gamma_{\mathcal{R}}(Q_1 \uplus_{\mathcal{R}} Q_2)$. It is sufficient to show that $\overline{gconv(\gamma_{\mathcal{R}}(Q_1) \cup \gamma_{\mathcal{R}}(Q_2))} \subseteq \gamma_{\mathcal{R}}(\max(Q_1, Q_2))$. Observe that $\gamma_{\mathcal{R}}(\max(Q_1, Q_2))$ is Scott-closed and g-convex, it is sufficient to show that $\gamma_{\mathcal{R}}(Q_1) \cup \gamma_{\mathcal{R}}(Q_2) \subseteq \gamma_{\mathcal{R}}(\max(Q_1, Q_2))$. It follows directly from the fact that $Q_1 \leq \max(Q_1, Q_2)$ and $Q_2 \leq \max(Q_1, Q_2)$, as well as the definition of $\gamma_{\mathcal{R}}$, which maps to Scott-closed subsets.

□

I then use a trivial widening in this analysis: if after some fixed number of iterations the analysis does not converge, it returns ∞ as the result.

4.3.3 Linear Expectation-Invariant Analysis

Several examples of expectation invariants obtained via linear expectation-invariant analysis (LEIA) were given in §4.1.2. This section gives details of the abstract domain for LEIA.

I make use of an existing abstract domain, namely, the domain of *convex polyhedra* [38]. Elements of the polyhedral domain are defined by linear-inequality and linear-equality constraints among program variables. For LEIA, I use two-vocabulary polyhedra over *nonnegative* program variables. Let $x = (x_1, \cdots, x_n)^T$ be a column vector of nonnegative program variables and $x' = (x'_1, \cdots, x'_n)^T$ be a column vector of the "primed" versions of corresponding program variables. A polyhedron $P \subseteq (\mathbb{R}^+)^{2n}$ captures linear-inequality constraints among x and x', which can be interpreted as a relation between pre-state and post-state variable valuations.

A polyhedron $P = \{(x'^T\ x^T)^T \in (\mathbb{R}^+)^{2n} \mid A'x' + Ax \leq b \wedge D'x' + Dx = e\}$, can be encoded as the intersection of a finite number of closed half spaces and a finite number of subspaces, where A', A, D', D are matrices and b, e are vectors. The associated *constraint set* is defined as $C_P = \{A'x' + Ax \leq b, D'x' + Dx = e\}$. Let $\mathcal{P}$ be the set of polyhedra; $\mathcal{P}$ is equipped with meet, join, renaming, forgetting, and comparison operations.

LEIA uses *expectation polyhedra*. They are actually the same as polyhedra, except that the two vocabularies are $x = (x_1, \cdots, x_n)^T$ and $\mathbb{E}[x'] = (\mathbb{E}[x'_1], \cdots, \mathbb{E}[x'_n])^T$. An expectation polyhedron represents a constraint set of the form

$$\{A'\mathbb{E}[x'] + Ax \leq b, D'\mathbb{E}[x'] + Dx = e\}. \tag{4.2}$$

Because of the linearity of the expectation operator $\mathbb{E}$, an equivalent way to express (4.2) is as follows:

$$\{\mathbb{E}[A'x'] + Ax \leq b, \mathbb{E}[D'x'] + Dx = e\}.$$

Let $\mathcal{EP}$ be the set of expectation polyhedra. $\mathcal{EP}$ is equipped with the same set of operations as $\mathcal{P}$.

I define the state space to be $\Omega = (\mathbb{R}^+)^n$. I then define a PMA $\mathcal{I}$ with a universe $M_{\mathcal{I}} \stackrel{\text{def}}{=} \mathcal{P} \times \mathcal{EP}$. An element $(P, EP) \in \mathcal{I}$ consists of

(i) a set of standard constraints $P \in \mathcal{P}$, and

(ii) a set of expectation constraints $EP \in \mathcal{EP}$, such that $\mathbf{0} \sqcup P[\mathbb{E}[x']/x'] \sqsupseteq EP$ holds, where $\mathbf{0} \stackrel{\text{def}}{=} \bigwedge_{i=1}^{n}(\mathbb{E}[x'_i] = 0)$.

The latter property means that, if necessary, one can always "rebuild" a pessimistic $\mathcal{EP}$ component from the $\mathcal{P}$ component as $\mathbf{0} \sqcup P[\mathbb{E}[x']/x']$.[7]

Because the state space Ω is *not* countable, I use the denotational semantics based on the convex powerdomain $\Omega \to \mathcal{P}\underline{\mathcal{D}}(\Omega)$ (denoted by C in this section) reviewed in §3.3. Note that to support distributions on real numbers, the state space Ω is equipped with a coherent dcpo [110, 144]. I define the concretization mapping $\gamma_{\mathcal{I}}$ as follows:

$$\gamma_{\mathcal{I}}(P, EP) = \lambda s.\ \{\mu \mid \mu(\{s' \mid [s'^T\ s^T]^T \models P\}) = \mu(\Omega) \wedge [\textstyle\int s'^T \cdot \mu(ds')\ s^T]^T \models \mathbf{0} \sqcup EP\}.$$

[7] The intuition is that P represents a convex over-approximation to some desired set of points; the expected value has to lie somewhere inside $\vec{0} \sqcup P$, where "$\vec{0} \sqcup \ldots$" is needed to account for sub-probability distributions. For instance, for a nonnegative interval $[lo, hi]$, it must hold that $expected \in ([0, 0] \sqcup [lo, hi])$; i.e., $0 \leq expected \leq hi$.

Comparison The comparison operation on ordinary polyhedra can be defined as standard set inclusion. For expectation polyhedra, taking into account sub-probability distributions, I define $EP_1 \sqsubseteq EP_2$ to be $\mathbf{0} \sqcup EP_1 \subseteq \mathbf{0} \sqcup EP_2$, so that any element inside or below EP_1 should also be inside or below EP_2. Consequently, I define $(P_1, EP_1) \sqsubseteq_{\mathcal{I}} (P_2, EP_2) \stackrel{\text{def}}{=} P_1 \subseteq P_2 \wedge \mathbf{0} \sqcup EP_1 \subseteq \mathbf{0} \sqcup EP_2$.

Composition For ordinary polyhedra, the composition of P_1 and P_2 can be defined as

$$(\exists x'' : C_{P_1}[x''/x'] \wedge C_{P_2}[x''/x]) \implies C_{P_1 \otimes P_2},$$

where I introduce an intermediate vocabulary $x'' = (x''_1, \cdots, x''_n)^T$, and use it to connect P_1 and P_2. Consequently, I define $P_1 \otimes P_2$ to be $\exists x'' : C_{P_1}[x''/x'] \wedge C_{P_2}[x''/x]$. Operationally, composition involves first introducing a new vocabulary; renaming the variables properly; performing a meet, and finally forgetting the intermediate vocabulary.

Somewhat surprisingly, because of the *tower property* in probability theory, exactly the same steps can be used to compose expectation polyhedra. Informally, the tower property means that $\mathbb{E}[X] = \mathbb{E}[\mathbb{E}[X \mid Y]]$, where X and Y are two random variables, and $\mathbb{E}[X \mid Y]$ is a conditional expectation. For instance, suppose that EP_1 and EP_2 are defined by the constraint sets $\{\mathbb{E}(x') = x + 2\}$ and $\{\mathbb{E}(x') = 7x\}$, respectively. Following the renaming recipe above, we have $\mathbb{E}(x'') = x + 2$ and $\mathbb{E}(x' \mid x'') = 7x''$. By the tower property, we have $\mathbb{E}(x') = \mathbb{E}(\mathbb{E}(x' \mid x''))$ $= \mathbb{E}(7x'') = 7\mathbb{E}(x'') = 7x + 14$. Operationally, the tower property allows one to compose linear expectation invariants, and eliminate the intermediate vocabulary x''. Consequently, I define

$$(P_1, EP_1) \otimes_{\mathcal{I}} (P_2, EP_2) \stackrel{\text{def}}{=} (P_1 \otimes P_2, EP_1 \otimes EP_2).$$

Conditional-choice For the ordinary-polyhedron component, a conditional-choice ${}_{\varphi}\diamondsuit$ is performed by first meeting each operand with the logical constraint φ, and then joining the results. However, for the expectation-polyhedron component, conditioning can split the probability space in almost arbitrary ways. Consequently, the constraints on post-state expectations as a function of pre-state valuations are not necessarily true after conditioning. Thus, I define

$$\begin{aligned}(P_1, EP_1)\ {}_{\varphi}\diamondsuit_{\mathcal{I}}\ (P_2, EP_2) \stackrel{\text{def}}{=}\ & \textbf{let } P = (\{\varphi\} \sqcap P_1) \sqcup (\{\neg\varphi\} \sqcap P_2) \\ & \textbf{in } (P, (EP_1 \sqcup EP_2) \sqcap (\mathbf{0} \sqcup P[\mathbb{E}[x']/x'])).\end{aligned}$$

The $\sqcap$ in the second component is performed to maintain the invariant that $\mathbf{0} \sqcup P[\mathbb{E}[x']/x'] \sqsupseteq$ the second component.

Probabilistic-choice For the ordinary-polyhedron component, I merely join the components of the two operands. For the expectation-polyhedron component, I introduce two more vocabularies and have

$$(\exists x'', x''' : C_{EP_1}[x''/\mathbb{E}[x']] \wedge C_{EP_2}[x'''/\mathbb{E}[x']] \wedge \bigwedge_{i=1}^{n} \mathbb{E}[x'_i] = p \cdot x''_i + (1-p) \cdot x'''_i) \implies C_{EP_1\ {}_p\oplus EP_2}.$$

Consequently, I define $EP_1\ {}_p\oplus\ EP_2$ to be

$$\exists x'', x''' : \left(C_{EP_1}[x''/\mathbb{E}[x']] \wedge C_{EP_2}[x'''/\mathbb{E}[x']] \wedge \bigwedge_{i=1}^{n} \mathbb{E}[x'_i] = p \cdot x''_i + (1-p) \cdot x'''_i \right),$$

and $(P_1, EP_1)\ {}_p\oplus_{\mathcal{I}}\ (P_2, EP_2) \stackrel{\text{def}}{=} (P_1 \sqcup P_2, EP_1\ {}_p\oplus\ EP_2)$.

Nondeterministic-choice The nondeterministic-choice operations on both ordinary polyhedra and expectation polyhedra can be defined as join. Hence, I define $(P_1, EP_1) \uplus_{\mathcal{I}} (P_2, EP_2) \stackrel{\text{def}}{=} (P_1 \sqcup P_2, EP_1 \sqcup EP_2)$.

Bottom and Unit Element I define $\underline{\bot}_{\mathcal{I}} \stackrel{\text{def}}{=} (\mathit{false}, \mathbf{0})$, and $\underline{1}_{\mathcal{I}} \stackrel{\text{def}}{=} (\{x_i' = x_i \mid 1 \le i \le n\}, \{\mathbb{E}[x_i'] = x_i \mid 1 \le i \le n\})$.

Semantic Function Some examples of the semantic mapping $[\![\cdot]\!]^{\mathcal{F}}$ are as follows, where $\min(\mathscr{D})$ and $\max(\mathscr{D})$ represents the interval of the support of a distribution $\mathscr{D}$, while $\mathrm{mean}(\mathscr{D})$ stands for its average. Note that LEIA does not support observation statements, which might change the post-state probability distribution in almost arbitrary ways.

$$
\begin{aligned}
[\![x_i := \mathcal{E}]\!]^{\mathcal{F}} &\stackrel{\text{def}}{=} \Big(\{x_i' = \mathcal{E}(x)\} \cup \{x_j' = x_j \mid j \neq i\}, \{\mathbb{E}[x_i'] = \mathcal{E}(x)\} \cup \{\mathbb{E}[x_j'] = x_j \mid j \neq i\}\Big)\\
[\![x_i \sim \mathscr{D}]\!]^{\mathcal{F}} &\stackrel{\text{def}}{=} \Big(\{\min(\mathscr{D}) \le x_i' \le \max(\mathscr{D})\} \cup \{x_j' = x_j \mid j \neq i\},\\
&\qquad\qquad \{\mathbb{E}[x_i'] = \mathrm{mean}(\mathscr{D})\} \cup \{\mathbb{E}[x_j'] = x_j \mid j \neq i\}\Big)\\
[\![\mathbf{skip}]\!]^{\mathcal{F}} &\stackrel{\text{def}}{=} \underline{1}_{\mathcal{I}}
\end{aligned}
$$

Note I assume all expressions in the program are linear. For nonlinear arithmetic programs, one can adopt some linearization techniques [54, 113].

LEMMA 4.14. *$\mathcal{I}$ is a PMA.*

PROOF. Most of the properties appeal to the properties of the polyhedron domain [38]. The only nontrivial property is that $a\ {}_p\oplus_{\mathcal{I}}\ b \le_{\mathcal{I}} a \uplus_{\mathcal{I}} b$ for abstract elements a, b and $p \in [0,1]$, where $\le_{\mathcal{I}}$ is the semilattice ordering induced by $\uplus_{\mathcal{I}}$. It suffices to show that for any polyhedra EP_1 and EP_2, it holds that $EP_1\ {}_p\oplus\ EP_2 \subseteq EP_1 \sqcup EP_2$. By the properties of the polyhedron join, we know that

$$
\begin{aligned}
C_{EP_1 \sqcup EP_2} \iff \exists x'', x''' \colon (&C_{EP_1}[x''/\mathbb{E}[x']] \wedge C_{EP_2}[x'''/\mathbb{E}[x']] \wedge\\
&\bigwedge_{i=1}^{n} (\mathbb{E}[x_i'] \ge \min(x_i'', x_i''') \wedge \mathbb{E}[x_i'] \le \max(x_i'', x_i'''))),
\end{aligned}
$$

thus by the definition of polyhedron probabilistic-choice operator ${}_p\oplus$, $\mathbb{E}[x_i']$ is a convex combination of x_i'' and x_i''' thus must be included in the interval $[\min(x_i'', x_i'''), \max(x_i'', x_i''')]$. Therefore, we have $C_{EP_1 \sqcup EP_2} \iff C_{EP_1\ {}_p\oplus\ EP_2}$ and $EP_1\ {}_p\oplus\ EP_2 \subseteq EP_1 \sqcup EP_2$. □

LEMMA 4.15. *$\gamma_{\mathcal{I}}$ is a probabilistic over-abstraction from C to $\mathcal{I}$.*

PROOF. By definition, we have

$$
\gamma_{\mathcal{I}}(P, EP) = \lambda s.\ \overline{\{\mu \mid \mu(\{s' \mid [s'^T\ s^T]^T \in P) = \mu(\Omega) \wedge [\textstyle\int y^T \cdot \mu(dy)\ s^T]^T \in EP\}},
$$

where $\overline{U}$ is the Scott-closure of U in the convex powerdomain $\mathcal{P}\underline{\mathcal{D}}(\Omega)$.

- We want to show $\underline{1}_C \sqsubseteq_C \gamma_{\mathcal{I}}(\underline{1}_{\mathcal{I}})$. Appeal to the fact that $\lambda s.\{\delta(s)\} \in \gamma_{\mathcal{I}}(\{x_i' = x_i \mid 1 \le i \le n\}, \{\mathbb{E}[x_i'] = x_i \mid 1 \le i \le n\})$.
- We want to show for all $(P_1, EP_1), (P_2, EP_2) \in \mathcal{I}$, it holds that $\gamma_{\mathcal{I}}(P_1, EP_1) \otimes_C \gamma_{\mathcal{I}}(P_1, EP_1) \sqsubseteq_C \gamma_{\mathcal{I}}((P_1, EP_1) \otimes_{\mathcal{I}} (P_2, EP_2))$. Let $g = \gamma_{\mathcal{I}}(P_1, EP_1)$ and $h = \gamma_{\mathcal{I}}(P_2, EP_2)$. Fix $s \in \Omega$. Then it suffices to show $\widehat{\widehat{h}}(g(s)) \sqsubseteq_P \gamma_{\mathcal{I}}((P_1, EP_1) \otimes_{\mathcal{I}} (P_2, EP_2))(s)$ (recall Proposition 3.9). Because $\gamma_{\mathcal{I}}$ always maps to Scott-closed convex subsets, the ordering $\sqsubseteq_P$ can be reduced to set inclusion $\subseteq$. Since $\widehat{\widehat{h}}$ is linear with respect to lifted probabilistic choices, it suffices to show that for any $\mu \in g(s)$, the set $\widehat{h}(\mu)$ (the linear function $\widehat{h}$ is obtained by [144, Thm. 2.11], which is similar to Proposition 3.7) is contained as a subset in

$$\gamma_{\mathcal{I}}((P_1, EP_1) \otimes_{\mathcal{I}} (P_2, EP_2))(s) = \gamma_{\mathcal{I}}(P_1 \otimes P_2, EP_1 \otimes EP_2)(s).$$

Fix some $\mu \in g(s)$.
First, we claim that for any $\nu \in \widehat{h}(\mu)$, it holds that $\nu(\{s'' \mid [s''^T\ s^T]^T \in P_1 \otimes P_2\}) = \nu(\Omega)$. Because $\widehat{h}$ is linear with respect to probabilistic choices, it suffices to show that for any $s' \in \mathrm{supp}(\mu)$ and $\nu \in h(s')$, it holds that

$$\nu(\{s'' \mid [s''^T\ s^T]^T \in P_1 \otimes P_2\}) = \nu(\Omega).$$

By the definition of h, we have $\nu(\{s'' \mid [s''^T\ s'^T]^T \in P_2\}) = \nu(\Omega)$. Because $s' \in \mathrm{supp}(\mu)$, $\mu \in g(s)$, and by the definition of g, we have $[s'^T\ s^T]^T \in P_1$. Thus, for any s'' satisfying $[s''^T\ s'^T]^T \in P_2$, it holds that $[s''^T\ s^T]^T \in P_1 \otimes P_2$. Therefore, we can conclude this claim by

$$\nu(\Omega) = \nu(\{s'' \mid [s''^T\ s'^T]^T \in P_2\}) \le \nu(\{s' \mid [s''^T\ s^T]^T \in P_1 \otimes P_2\}) \le \nu(\Omega).$$

Second, we claim that for any $\nu \in \widehat{h}(\mu)$, it holds that $[\int y^T \cdot \nu(dy)\ s^T]^T \in \mathbf{0} \sqcup (EP_1 \otimes EP_2)$. Because $\widehat{h}$ is linear with respect to probabilistic choices, and by assuming the Axiom of Choice, we can choose $\pi_{s'} \in h(s')$ for each state s' such that $\nu = \int \pi_{s'} \cdot \mu(ds')$. By the definition of h, we know that for any state s', it holds that $[\int y^T \cdot \pi_{s'}(dy)\ s'^T]^T \in \mathbf{0} \sqcup EP_2$. Because EP_2 is convex, we have

$$\begin{aligned} & [\textstyle\int (\int y^T \cdot \pi_{s'}(dy)) \cdot \mu(ds')\ \int s'^T \cdot \mu(ds')]^T \in \mathbf{0} \sqcup EP_2 \\ \Longrightarrow\ & [\textstyle\int y^T \cdot \nu(dy)\ \int s'^T \cdot \mu(ds')]^T \in \mathbf{0} \sqcup EP_2. \end{aligned}$$

By the definition of g, we have $[\int s'^T \cdot \mu(ds')\ s^T]^T \in \mathbf{0} \sqcup EP_1$. Thus, by the definition of polyhedron composition $\otimes$, we know that

$$[\textstyle\int y^T \cdot \nu(dy)\ s^T]^T \in (\mathbf{0} \sqcup EP_1) \otimes (\mathbf{0} \sqcup EP_2) \subseteq \mathbf{0} \sqcup (EP_1 \otimes EP_2).$$

- We want to show for all $(P_1, EP_1), (P_2, EP_2) \in \mathcal{I}$ and $\varphi \in \mathcal{L}$, it holds that $\gamma_{\mathcal{I}}(P_1, EP_1)\ {}_{\varphi}\Diamond_C\ \gamma_{\mathcal{I}}(P_2, EP_2) \sqsubseteq_C \gamma_{\mathcal{I}}((P_1, EP_1)\ {}_{\varphi}\Diamond_{\mathcal{I}}\ (P_2, EP_2))$. Let $g = \gamma_{\mathcal{I}}(P_1, EP_1)$ and $h = \gamma_{\mathcal{I}}(P_2, EP_2)$. Fix $s \in \Omega$. Then it suffices to show $g(s)\ {}_{[\![\varphi]\!](s)]}\oplus_P\ h(s) \sqsubseteq_P \gamma_{\mathcal{I}}((P_1, EP_1)\ {}_{\varphi}\Diamond_{\mathcal{I}}\ (P_2, EP_2))(s)$. Because $\gamma_{\mathcal{I}}$ maps to Scott-closed convex subsets, the ordering $\sqsubseteq_P$ can be reduced to set inclusion $\subseteq$. Fix $\mu_1 \in g(s)$ and $\mu_2 \in h(s)$. It then suffices to show that

$$\mu \overset{\text{def}}{=} [\![\varphi]\!](s)] \cdot \mu_1 + (1 - [\![\varphi]\!](s)]) \cdot \mu_2 \in \gamma_{\mathcal{I}}(P, (EP_1 \sqcup EP_2) \sqcap (\mathbf{0} \sqcup P[\mathbb{E}[x']/x']))(s),$$

where $P \stackrel{\text{def}}{=} (\{\varphi\} \sqcap P_1) \sqcup (\{\neg\varphi\} \sqcap P_2)$.
First, we claim that $\mu(\{s' \mid [s'^T\ s^T]^T \in P\}) = \mu(\Omega)$. By the definition of g and h, we know that $\mu_1(\{s' \mid [s'^T\ s^T]^T \in P_1\}) = \mu_1(\Omega)$ and $\mu_2(\{s' \mid [s'^T\ s^T]^T \in P_2\}) = \mu_2(\Omega)$. If $[\![\varphi]\!](s) = \mathit{true}$, we have

$$\begin{aligned}\mu(\Omega) = \mu_1(\Omega) &= \mu_1(\{s' \mid [s'^T\ s^T]^T \in P_1\})\\ &= \mu_1(\{s' \mid [s'^T\ s^T]^T \in P_1 \wedge [\![\varphi]\!](s)\})\\ &\le \mu_1(\{s' \mid [s'^T\ s^T]^T \in \{\varphi\} \sqcap P_1\})\\ &\le \mu_1(\{s' \mid [s'^T\ s^T]^T \in P\})\\ &= \mu(\{s' \mid [s'^T\ s^T]^T \in P\}) \le \mu(\Omega).\end{aligned}$$

Similarly, if $[\![\varphi]\!](s) = \mathit{false}$, we also have $\mu(\Omega) = \mu(\{s' \mid [s'^T\ s^T]^T \in P\})$.
Second, we claim that

$$\begin{aligned}[\textstyle\int y^T \cdot \mu(dy)\ s^T]^T &\in \mathbf{0} \sqcup ((EP_1 \sqcup EP_2) \sqcap (\mathbf{0} \sqcup P[\mathbb{E}[x']/x']))\\ &= (\mathbf{0} \sqcup EP_1 \sqcup EP_2) \sqcap (\mathbf{0} \sqcup P[\mathbb{E}[x']/x']).\end{aligned}$$

The $(\mathbf{0} \sqcup P[\mathbb{E}[x']/x'])$ part appeals to the fact that $\mu(\Omega) = \mu(\{y \mid [y^T\ s^T]^T \in P\})$ and P is convex. For the $(\mathbf{0} \sqcup EP_1 \sqcup EP_2)$ part, if $[\![\varphi]\!](s) = \mathit{true}$, then $\mu = \mu_1$, thus $[\int y^T \cdot \mu(dy)\ s^T]^T \in (\mathbf{0} \sqcup EP_1)$. Similarly, if $[\![\varphi]\!](s) = \mathit{false}$, we have $\mu = \mu_2$ and thus $[\int y^T \cdot \mu(dy)\ s^T]^T \in (\mathbf{0} \sqcup EP_2)$. Therefore, we conclude that $[\int y^T \cdot \mu(dy)\ s^T]^T \in \mathbf{0} \sqcup EP_1 \sqcup EP_2$.

- We want to show for all $(P_1, EP_1), (P_2, EP_2) \in \mathcal{I}$ and $p \in [0,1]$, it holds that $\gamma_{\mathcal{I}}(P_1, EP_1)\ {}_p\oplus_C\ \gamma_{\mathcal{I}}(P_2, EP_2) \sqsubseteq_C \gamma_{\mathcal{I}}((P_1, EP_1)\ {}_p\oplus_{\mathcal{I}}\ (P_2, EP_2))$. Let $g = \gamma_{\mathcal{I}}(P_1, EP_1)$ and $h = \gamma_{\mathcal{I}}(P_2, EP_2)$. Fix $s \in \Omega$. Then it is sufficient to show that $g(s)\ {}_p\oplus_P\ h(s) \sqsubseteq_P \gamma_{\mathcal{I}}((P_1, EP_1)\ {}_p\oplus_{\mathcal{I}}\ (P_2, EP_2))(s)$. Because $\gamma_{\mathcal{I}}$ maps to Scott-closed convex subsets, the ordering $\sqsubseteq_P$ can be reduced to set inclusion $\subseteq$. Fix $\mu_1 \in g(s)$ and $\mu_2 \in h(s)$. It then suffices to show that

$$\mu \stackrel{\text{def}}{=} p \cdot \mu_1 + (1-p) \cdot \mu_2 \in \gamma_{\mathcal{I}}(P_1 \sqcup P_2, EP_1\ {}_p\oplus\ EP_2)(s).$$

First, we claim that $\mu(\{s' \mid [s'^T\ s^T]^T \in P_1 \sqcup P_2) = \mu(\Omega)$. By the definition of g and h, we know that $\mu_1(\{s' \mid [s'^T\ s^T]^T \in P_1\}) = \mu_1(\Omega)$ and $\mu_2(\{s' \mid [s'^T\ s^T]^T \in P_2\}) = \mu_2(\Omega)$. Thus, we have

$$\begin{aligned}\mu(\Omega) &= p \cdot \mu_1(\Omega) + (1-p) \cdot \mu_2(\Omega)\\ &= p \cdot \mu_1(\{s' \mid [s'^T\ s^T]^T \in P_1\}) + (1-p) \cdot \mu_2(\{s' \mid [s'^T\ s^T]^T \in P_2\})\\ &\le p \cdot \mu_1(\{s' \mid [s'^T\ s^T]^T \in P_1 \sqcup P_2\}) + (1-p) \cdot \mu_2(\{s' \mid [s'^T\ s^T]^T \in P_1 \sqcup P_2\})\\ &= \mu(\{s' \mid [s'^T\ s^T]^T \in P_1 \sqcup P_2\}) \le \mu(\Omega).\end{aligned}$$

Second, we claim that $[\int y^T \cdot \mu(dy)\ s^T]^T \in \mathbf{0} \sqcup (EP_1\ {}_p\oplus\ EP_2)$. By the definition of g and h, we know that $[\int y^T \cdot \mu_1(dy)\ s^T]^T \in \mathbf{0} \sqcup EP_1$ and $[\int y^T \cdot \mu_2(dy)\ s^T]^T \in \mathbf{0} \sqcup EP_2$. By the definition of the polyhedron probabilistic-choice operator ${}_p\oplus$, we have $[(p \cdot \int y^T \cdot \mu_1(dy) + (1-p) \cdot \int y^T \cdot \mu_2(dy))\ s^T]^T \in (\mathbf{0} \sqcup EP_1)\ {}_p\oplus\ (\mathbf{0} \sqcup EP_2)$, thus conclude that $[\int y^T \cdot \mu(dy)\ s^T]^T \in \mathbf{0} \sqcup (EP_1\ {}_p\oplus\ EP_2)$ by the fact $\mu = p \cdot \mu_1 + (1-p) \cdot \mu_2$ and $(\mathbf{0} \sqcup EP_1)\ {}_p\oplus\ (\mathbf{0} \sqcup EP_2) \subseteq \mathbf{0} \sqcup (EP_1\ {}_p\oplus\ EP_2)$.

- We want to show that for all $(P_1, EP_1), (P_2, EP_2) \in \mathcal{I}$, it holds that $\gamma_{\mathcal{I}}(P_1, EP_1) \uplus_C \gamma_{\mathcal{I}}(P_2, EP_2) \sqsubseteq_C \gamma_{\mathcal{I}}((P_1, EP_1) \uplus_{\mathcal{I}} (P_2, EP_2))$. Note that $\gamma_{\mathcal{I}}$ maps to Scott-closed convex subsets. Fix $s \in \Omega$. It then suffices to show that $\gamma_{\mathcal{I}}(P_1, EP_1)(s) \cup \gamma_{\mathcal{I}}(P_2, EP_2)(s) \subseteq \gamma_{\mathcal{I}}(P_1 \sqcup P_2, EP_1 \sqcup EP_2)(s)$. Without loss of generality, we show the proof for $\gamma_{\mathcal{I}}(P_1, EP_1)(s) \subseteq \gamma_{\mathcal{I}}(P_1 \sqcup P_2, EP_1 \sqcup EP_2)(s)$. Fix $\mu_1 \in \gamma_{\mathcal{I}}(P_1, EP_1)(s)$.
  First, we claim that $\mu_1(\{s' \mid [s'^T\ s^T]^T \in P_1 \sqcup P_2\}) = \mu_1(\Omega)$. Appeal to the fact that

$$\mu_1(\Omega) = \mu_1(\{s' \mid [s'^T\ s^T]^T \in P_1\}) \leq \mu_1(\{s' \mid [s'^T\ s^T]^T \in P_1 \sqcup P_2\}) \leq \mu_1(\Omega).$$

  Second, we claim that $[\int y^T \cdot \mu_1(dy)\ s^T]^T \in \mathbf{0} \sqcup EP_1 \sqcup EP_2$. By the definition of μ_1, we can conclude this claim by the fact that $[\int y^T \cdot \mu_1(dy)\ s^T]^T \in \mathbf{0} \sqcup EP_1$.

□

Widening Let $\triangledown$ be the standard widening operator on ordinary polyhedra [67]. Recall from Observation 4.8 that whenever a widening operation $a \triangledown b$ is performed, the property $a \sqsubseteq_{\mathcal{A}} b$ holds for an analysis $\mathcal{A}$. There is a subtle issue with expectation invariants when dealing with conditional or nondeterministic loops.

Observation 4.16. In a conventional program, if we have a loop "**while** B **do** S **od**," and I is a loop-invariant, then $I \wedge \neg B$ (which implies I) holds on exiting the loop. In contrast, for a conditional or nondeterministic loop in a probabilistic program, an expectation-invariant that holds at the beginning and end of the loop body does not necessarily hold on exiting the loop.

Example 4.17. Consider the following program:

while $\neg(x = y)$ **do**
  if prob$(1/2)$ **then** $x := x + 1$ **else** $y := y + 1$ **fi**
od

For the loop body, we can derive an expectation invariant $\mathbb{E}[x' - y'] = x - y$*; however, for the entire loop this property does not hold: at the end of the loop* $x = y$ *must hold, and hence* $\mathbb{E}[x' - y']$ *should be equal to* 0*.*

Because of this issue, I use a pessimistic widening operator for conditional-choice and nondeterministic-choice: the widening operator forgets the expectation invariants and rebuilds them from standard invariants.

$$(P_1, EP_1) \triangledown_c (P_2, EP_2) \stackrel{\text{def}}{=} (P_1 \triangledown P_2, \mathbf{0} \sqcup P_2[\mathbb{E}[x']/x'])$$
$$(P_1, EP_1) \triangledown_n (P_2, EP_2) \stackrel{\text{def}}{=} (P_1 \triangledown P_2, \mathbf{0} \sqcup P_2[\mathbb{E}[x']/x'])$$

I do not have a good method for $(P_1, EP_1) \triangledown_p (P_2, EP_2)$. I found that the following approach loses precision:

$$\textbf{let } P = (P_1 \triangledown P_2) \textbf{ in } (P, (EP_1 \triangledown EP_2) \sqcap (\mathbf{0} \sqcup P[\mathbb{E}[x']/x']))$$

In my experiments, I use $(P_1, EP_1) \triangledown_p (P_2, EP_2) \stackrel{\text{def}}{=} (P_1 \triangledown P_2, EP_2)$, which does no extrapolation in the $\mathcal{EP}$ component.

4.4 Evaluation

In this section, I first describe the implementation of PMAF, and the three instantiations introduced in §4.3. Then, I evaluate the effectiveness and performance of the three analyses.

4.4.1 Implementation

PMAF is implemented in OCaml; the core framework consists of about 400 lines of code. The framework is implemented as a functor parametrized by a module representing a PMA, with some extra functions, such as widening and printing. This organization allows any analysis that can be formulated in PMAF to be implemented as a plugin. Also, the core framework relies on control-flow hyper-graphs, and provides users the flexibility to employ it with any front end. I use OCamlGraph [32] as the implementation of fixed-point computation and Bourdoncle's algorithm [18].

The plugin for Bayesian inference is about 400 lines of code, including a lexer and a parser for the imperative language that I use in the examples of this paper. I use Lacaml [122] to manipulate matrices. The plugins for the Markov decision problem with rewards and linear expectation-invariant analysis are about 200 lines and 500 lines, respectively. I use APRON [80] for polyhedron operations. Most of the code in the plugins is to implement the PMA structure of the analysis domain.

Because of the numerical reasoning required when analyzing probabilistic programs, I need to be concerned about finite numerical precision in my implementations of the instantiations (although they are sound on a theoretical machine operating on reals). In my implementation, I use the fact that ascending chains of floating numbers always converge in a finite number of steps. The user could use the technique proposed by Darulova and Kuncak [42] to obtain a sound guarantee on numerical precision.

4.4.2 Experiments

Evaluation Platform My experiments were performed on a machine with an Intel Core i5 2.4 GHz processor and 8GB of RAM under Mac OS X 10.13.4. A replication package for the evaluation results in this section is publicly available [147].

Bayesian Inference and Markov Decision Problem with Rewards I tested my framework on Bayesian inference and Markov decision problem with rewards on handcrafted examples. The results of the evaluation of the two analyses are described in Table 4.1. The tables contains the number of lines; whether the program is non-recursive, tail-recursive, or recursive; the number of procedure calls; and the time taken by the implementation (measured by running each program 5 times and computing the 20% trimmed mean).

Table 4.1: Top: Bayesian inference. Bottom: Markov decision problem with rewards. (Time is in seconds.)

Program	#loc	rec?	#call	time
compare	17	n	0	2.22
dice	12	n	0	0.02
eg1	10	n	0	0.02
eg1-tail	16	t	2	0.02
eg2	10	n	0	0.02
eg2-tail	16	t	2	0.01
recursive	14	r	1	0.01
binary10	184	n	90	0.03
loop	10	n	0	0.03
quicksort7	109	n	42	0.03
recursive	13	t	1	0.03
student	43	t	8	0.03

My framework computed the same answer (modulo floating-point round-off errors) as PReMo

Table 4.2: Linear expectation-invariant analysis.

Program	Expectation invariants	#loc	rec?	#call	time
2d-walk	$\mathbb{E}[x'] = x,\ \mathbb{E}[y'] = y,\ \mathbb{E}[dist'] = dist,$ $\mathbb{E}[count'] \leq count + 1,\ \mathbb{E}[count'] \geq count$	47	n	0	0.24
aggregate-rv	$\mathbb{E}[2x' - i'] = 2x - i,\ \mathbb{E}[x'] \leq x + 1/2,\ \mathbb{E}[x'] \geq x$	11	n	0	0.06
biased-coin	$\mathbb{E}[x'] \leq x + 1/2,\ \mathbb{E}[x'] \geq x - 1/2$	25	n	0	0.06
binom-update ($p = 1/4$)	$\mathbb{E}[4x' - n'] = 4x - n,\ \mathbb{E}[x'] \leq x + 1/4,\ \mathbb{E}[x'] \geq x$	14	n	0	0.06
coupon5	$\mathbb{E}[count' - i'] = count - i$ (1st), $\mathbb{E}[4count' - 5i'] = 4count - 5i$ (2nd), $\mathbb{E}[3count' - 5i'] = 3count - 5i$ (3rd), $\mathbb{E}[2count' - 5i'] = 2count - 5i$ (4th), $\mathbb{E}[count' - 5i'] = count - 5i$ (5th)	58	n	0	0.07
dist	$\mathbb{E}[x'] = x,\ \mathbb{E}[y'] = y,\ \mathbb{E}[z'] = 1/2 \cdot x + 1/2 \cdot y$	5	n	0	0.05
eg	$\mathbb{E}[x' + y'] = x + y + 3,\ \mathbb{E}[z'] = 1/4 \cdot z + 3/4,$ $\mathbb{E}[x'] \leq x + 3,\ \mathbb{E}[x'] \geq x$	8	n	0	0.89
eg-tail	$\mathbb{E}[z'] \geq 1/4 \cdot z,\ \mathbb{E}[x'] \geq x,\ \mathbb{E}[y'] \geq y,$ $\mathbb{E}[x' + y'] \geq x + y + 3/4$	11	t	1	0.13
hare-turtle	$\mathbb{E}[2h' - 5t'] = 2h - 5t,\ \mathbb{E}[h'] \leq h + 5/2,\ \mathbb{E}[h'] \geq h$	15	n	0	0.06
hawk-dove	$\mathbb{E}[p1b' - count'] = p1b - count,$ $\mathbb{E}[p2b' - count'] = p2b - count,$ $\mathbb{E}[p1b'] \leq p1b + 1,\ \mathbb{E}[p1b'] \geq p1b$	29	n	0	0.08
mot-ex	$\mathbb{E}[2x' - y'] = 2x - y,\ \mathbb{E}[4x' - 3count'] = 4x - 3count,$ $\mathbb{E}[x'] \leq x + 3/4,\ \mathbb{E}[x'] \geq x$	16	n	0	0.06
recursive	$\mathbb{E}[x'] = x + 9$	13	r	2	0.37
uniform-dist	$\mathbb{E}[n'] \leq 2n,\ \mathbb{E}[n'] \geq n,\ \mathbb{E}[g'] \leq 2g + 1/2,\ \mathbb{E}[g'] \geq g$	14	n	0	0.06

[156], a tool for probabilistic recursive models. I did not compare with probabilistic abstract interpretation [39] because its semantic foundation is substantially different from that of my framework—as I mentioned in the beginning of this chapter, the order for resolving probabilistic behavior and nondeterministic behavior is different.

The analysis time of Bayesian inference grows exponentially with respect to the number of program variables.[8] The time cost comes from the explicit matrix representation of domain elements. One could use Algebraic Decision Diagrams [5] as a compact representation to improve the efficiency.

The analyzer for the Markov decision problem with rewards works quickly and obtains some interesting results. quicksort7 is a model of a randomized Quicksort algorithm on an array of size 7 (obtained from [156]), and my analysis results are consistent with the worst-case expected number of comparisons being $\Theta(n \log n)$.[9] binary10 is a model of randomized binary search algorithm on an array of size 10, and my analysis results are consistent with the worst-case expected number of comparisons being $\Theta(\log n)$.

[8] One should not assume that exponential growth makes the analysis useless; after all, predicate-abstraction domains [65] also grow exponentially: the universe of assignments to a set of Boolean variables grows exponentially in the number of variables. Finding useful coarser abstractions for Bayesian inference—by analogy with the techniques of Ball et al. [6] for predicate abstraction—might be an interesting direction for future work.

[9] The analysis computes *worst-case expected number* because the underlying semantics resolves nondeterminism first and probabilistic-choice second, and thus the analysis computes $\max_{\text{nondet. resolution}} \mathbb{E}[\#\text{comparisons under resolution}]$.

Linear Expectation-Invariant Analysis I performed a more thorough evaluation of linear expectation-invariant analysis. I collected several examples from the literature on probabilistic invariant generation [25, 86], and handcrafted some new examples to demonstrate particular capabilities of my domain, e.g., analysis of recursive programs. For the examples obtained from the loop-invariant-generation benchmark, I extracted the loop body as my test programs. Also, I performed a positive-negative decomposition to make sure all program variables are nonnegative. That is, I represented each variable x as $x^+ - x^-$ where $x^+, x^- \geq 0$, and replaced every operation on variables with appropriate operations on the decomposed variables.

The results of the evaluation are shown in Table 4.2, which lists the expectation invariants obtained, and the time taken by the implementation. In general, the analysis runs quickly—all the examples are processed in less than one second. The analysis time mainly depends on the number of program variables and the size of the control-flow hyper-graph.

As shown in Table 4.2, my analysis can derive nontrivial expectation invariants, e.g., relations among different program variables such as $\mathbb{E}[x'+y'] = x+y+3$, $\mathbb{E}[2x'-y'] = 2x-y$. In most cases, my results are at least as precise as those in [25, 86]. Exceptions are biased-coin and uniform-dist, collected from [86], where their invariant-generation algorithm uses a template-based approach and the form of expectations can be more complicated, e.g., $[P_1] \cdot \mathcal{E}_1 + [P_2] \cdot \mathcal{E}_2$ where P_1, P_2 are linear assertions and $\mathcal{E}_1, \mathcal{E}_2$ are linear expressions. Nevertheless, my analysis is fully automated and applicable to general programs, while [86] requires interactive proofs for nested loops, and [25] works only for single loops.

4.5 Discussion

In this section, I discuss some related work and limitations of PMAF.

Static Analysis for Standard Programs PMAF is an extension of interprocedural dataflow analysis [94, 105, 123, 138] to probabilistic programs, but it does not support some language features that standard dataflow analysis has been used to address, e.g., calls through function pointers.

Compared to the Galois connections that are ordinarily used in abstract interpretation [35, 37], my definition of probabilistic abstractions is based on just a concretization function, so PMAF does not have the full power of standard abstract-interpretation machinery.

Static Analysis for Probabilistic Programs Most closely related to my work on PMAF is probabilistic abstract interpretation [39, 118–120], which is discussed in the beginning of this chapter. There is a long line of research on manual reasoning techniques for probabilistic programs [55, 85, 99, 110, 126]. The main difference to this work is that I focus on the design and implementation of automatic techniques that that rely on computing (and approximating) fixed points.

Other work focuses on specialized automatic analyses for specific properties. Claret et al. [29] proposed a dataflow analysis for Bayesian inference on Boolean programs that I have reformulated in PMAF to lift it to the interprocedural level. There are different techniques for automatically

proving probabilistic termination, such as probabilistic pushdown automata [19, 20] and martingales and stochastic invariants [27, 28]. Martingales for automatic analysis of probabilistic programs have been pioneered by Chakarov and Sankaranarayanan [24]. Compared with existing techniques for probabilistic invariant generation [7, 24, 25, 28], the expectation-invariant analysis proposed in §4.3.3 is designed as a two-vocabulary domain utilizing the well-studied polyhedral abstract domain.

Other Analyses Based on Hyper-Graphs Hyper-graph-based analyses go back to the join-over-all-hyper-path-valuations of Knuth [95]. Other analyses based on hyper-graphs includes Möncke and Wilhelm [117] framework for finding join-over-all-hyper-path-valuations for *partially ordered* abstract domains. In the hyper-paths in this chapter, I use simple edges to model calls, as well as use binary hyper-edges to model conditional, probabilistic, and nondeterministic choice. For *acyclic* hyper-graphs, Eisner has considered semirings for computing expectations and variances of random variables [107]. He works with a discrete sample space: all hyper-paths in a given hyper-graph, and the value of a random variable for a given hyper-path is built up as the sum of the values contributed by each hyper-edge. In my work, I consider *cyclic* hyper-graphs, and the nature of the computation that a hyper-path represents is more complex than that considered by Eisner.

Chapter 5

Central Moment Analysis of Cost Accumulators in Probabilistic Programs

In this chapter, I propose a novel static analysis for deriving symbolic interval bounds on higher *central moments* for *cost accumulators* in probabilistic programs. Cost accumulators are quantities that can only be incremented or decremented through computation and do not influence the control flow, such as termination time [11, 26, 27, 85, 126], rewards in Markov decision processes (MDPs) [130], position information in control systems [10, 17, 136], and cash flow during bitcoin mining [154]. In general, it is not tractable to compute the result distributions of probabilistic programs automatically and precisely: Composing simple distributions can quickly complicate the result distribution, and randomness in the control flow can easily lead to state-space explosion. Monte-Carlo simulation [134] is a common approach to study the result distributions, but the technique does not provide formal guarantees, and can sometimes be inefficient [11].

Existing work [17, 104, 124, 154] has proposed successful static-analysis approaches that leverage *aggregate* information of a cost accumulator X, such as X's *expected* value $\mathbb{E}[X]$ (i.e., X's "first moment"). The intuition why it is beneficial to compute aggregate information—in lieu of distributions—is that aggregate measures like expectations *abstract* distributions to a single number, while still indicating non-trivial properties. Moreover, expectations are transformed by statements in a probabilistic program in a manner similar to the weakest-precondition transformation of formulas in a non-probabilistic program [111]. One important kind of aggregate information is *moments*. In this chapter, I focus on *central* moments (i.e., $\mathbb{E}[(X-\mathbb{E}[X])^k]$ for any $k \geq 2$), whereas most previous work focused on *raw* moments (i.e., $\mathbb{E}[X^k]$ for any $k \geq 1$). Central moments can provide more information about distributions. For example, the *variance* $\mathbb{V}[X]$ (i.e., $\mathbb{E}[(X-\mathbb{E}[X])^2]$, X's "second central moment") indicates how X can deviate from its mean, the *skewness* (i.e., $\frac{\mathbb{E}[(X-\mathbb{E}[X])^3]}{(\mathbb{V}[X])^{3/2}}$, X's "third standardized moment") indicates how lopsided the distribution of X is, and the *kurtosis* (i.e., $\frac{\mathbb{E}[(X-\mathbb{E}[X])^4]}{(\mathbb{V}[X])^2}$, X's "fourth standardized moment") measures the heaviness of the tails of the distribution of X. One application of moments is to answer queries about *tail bounds*, e.g., the assertions about probabilities of the form $\mathbb{P}[X \geq d]$, via *concentration-of-measure* inequalities from probability theory [47]. With central moments, one has an opportunity to obtain more precise tail bounds of the form $\mathbb{P}[X \geq d]$, and becomes able to derive bounds on tail probabilities of the form $\mathbb{P}[|X - \mathbb{E}[X]| \geq d]$.

Central moments $\mathbb{E}[(X-\mathbb{E}[X])^k]$ can be seen as polynomials of raw moments $\mathbb{E}[X], \cdots, \mathbb{E}[X^k]$,

e.g., the variance $\mathbb{V}[X] = \mathbb{E}[(X - \mathbb{E}[X])^2]$ can be rewritten as $\mathbb{E}[X^2] - \mathbb{E}^2[X]$, where $\mathbb{E}^k[X]$ denotes $(\mathbb{E}[X])^k$. Central moments can usually provide more information about the distribution of X than raw moments $\mathbb{E}[X^k]$. To derive bounds on central moments, we need both *upper* and *lower* bounds on the raw moments, because of the presence of *subtraction*. For example, to upper-bound $\mathbb{V}[X]$, a static analyzer needs to have an *upper* bound on $\mathbb{E}[X^2]$ and a *lower* bound on $\mathbb{E}^2[X]$.

In this chapter, I present the first fully automatic analysis for deriving symbolic *interval* bounds on higher central moments for cost accumulators in probabilistic programs with general recursion and continuous distributions. One challenge is to support *inter*procedural reasoning to reuse analysis results for functions. My solution makes use of a "lifting" technique from the natural-language-processing community. That technique derives an algebra for second moments from an algebra for first moments [107]. I generalize the technique to develop *moment semirings*, and use them to derive a novel *frame* rule to handle function calls with *moment-polymorphic recursion* (see §5.1.2).

Previous work has successfully automated inference of upper [124] or lower bounds [154] on the expected cost of probabilistic programs. Kura et al. [104] developed a system to derive upper bounds on higher *raw* moments of program runtimes. However, even in combination, existing approaches can*not* solve tasks such as deriving a lower bound on the second raw moment of runtimes, or deriving an upper bound on the variance of accumulators that count live heap cells. Fig. 5.1(a) summarizes the features of related work on moment inference for probabilistic programs. To the best of my knowledge, my work is the first moment-analysis tool that supports all of the listed programming and analysis features. Fig. 5.1(b) and (c) compare my work with related work in terms of tail-bound analysis on a concrete program (see §5.4). The bounds are derived for the cost accumulator *tick* in a random-walk program that I will present in §5.1. It can be observed that for $d \geq 20$, the most precise tail bound for *tick* is the one obtained via an upper bound on the variance $\mathbb{V}[tick]$ (*tick*'s second central moment).

My work incorporates ideas known from the literature:

- Using the expected-potential method (or ranking super-martingales) to derive upper bounds on the expected program runtimes or monotone costs [24, 26, 27, 55, 104, 124].

- Using the *Optional Stopping Theorem* from probability theory to ensure the soundness of lower-bound inference for probabilistic programs [7, 68, 137, 154].

- Using *linear programming* (LP) to efficiently automate the (expected) potential method for (expected) cost analysis [73, 75, 152].

The contributions of my work in this chapter are as follows:

- I develop moment semirings to compose the moments for a cost accumulator from two computations, and to enable interprocedural reasoning about higher moments.

- I instantiate moment semirings with the symbolic interval domain, use that to develop a derivation system for interval bounds on higher central moments for cost accumulators, and automate the derivation via LP solving.

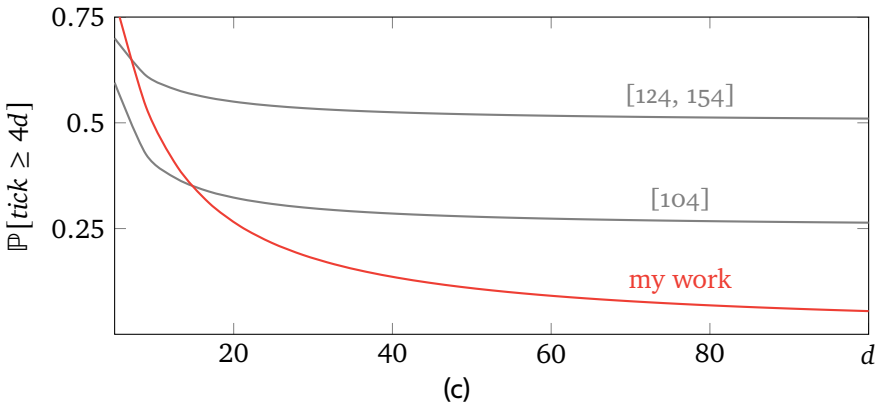
- I prove the soundness of my derivation system for programs that satisfy the criterion of my extension to the Optional Stopping Theorem, and develop an algorithm for checking this criterion automatically.

feature	[17]	[124]	[104]	[154]	my work
loop		✓	✓	✓	✓
recursion		✓			✓
continuous distributions	✓		✓	✓	✓
non-monotone costs	✓			✓	✓
higher moments	✓		✓		✓
interval bounds	✓			✓	✓

(a)

	[124, 154]	[104]	my work
Derived bound	$\mathbb{E}[tick] \leq 2d + 4$	$\mathbb{E}[tick^2] \leq 4d^2 + 22d + 28$	$\mathbb{V}[tick] \leq 22d + 28$
Moment type	raw	raw	central
Concentration inequality	Markov (degree = 1)	Markov (degree = 2)	Cantelli
Tail bound $\mathbb{P}[tick \geq 4d]$	$\approx \frac{1}{2}$	$\approx \frac{1}{4}$	$\xrightarrow{d\to\infty} 0$

(b)



(c)

Fig. 5.1: (a) Comparison in terms of supporting features. (b) Comparison in terms of moment bounds for the running example. (c) Comparison in terms of derived tail bounds.

- I implemented the analysis and evaluated it on a broad suite of benchmarks from the literature. The experimental results show that on a variety of examples, my analyzer is able to use higher central moments to obtain tighter tail bounds on program runtimes than the system of Kura et al. [104], which uses only upper bounds on raw moments.

5.1 Overview

In this section, I demonstrate the expected-potential method for both first-moment analysis (previous work) and higher central-moment analysis (my work) (§5.1.1), and discuss the challenges to supporting interprocedural reasoning and to ensuring the soundness of my approach (§5.1.2).

*Example 5.1. The program in Fig. 5.2 implements a bounded, biased random walk. The main function consists of a single statement "***call** rdwalk*" that invokes a recursive function. The variables*

```
1  func rdwalk() begin
2    { 2(d − x) + 4 }
3    if x < d then
4      { 2(d − x) + 4 }
5      t ~ Uniform(−1, 2);
6      { 2(d − x − t) + 5 }
7      x := x + t;
8      { 2(d − x) + 5 }
9      call rdwalk;
10     { 1 }
11     tick(1)
12     { 0 }
13   fi
14 end
```

```
1  # VID ≝ {x, d, t}
2  # FID ≝ {rdwalk}
3  # pre-condition: {d > 0}
4  func main() begin
5    x := 0;
6    call rdwalk
7  end
```

Fig. 5.2: A bounded, biased random walk, implemented using recursion. The annotations show the derivation of an *upper* bound on the expected accumulated cost.

x and d represent the current position and the ending position of the random walk, respectively. We assume that $d > 0$ holds initially. In each step, the program samples the length of the current move from a uniform distribution on the interval $[-1, 2]$. The statement **tick**(1) *adds one to a cost accumulator that counts the number of steps before the random walk ends. We denote this accumulator by tick in the rest of this section. The program terminates with probability one and its expected accumulated cost is bounded by $2d + 4$.*

5.1.1 The Expected-Potential Method for Higher-Moment Analysis

My approach to higher-moment analysis is inspired by the *expected-potential method* [124], which is also known as *ranking super-martingales* [24, 26, 104, 154], for expected-cost bound analysis of probabilistic programs.

The classic *potential method* of amortized analysis [143] can be automated to derive symbolic cost bounds for non-probabilistic programs [73, 75]. The basic idea is to define a *potential function* $\phi : \Sigma \to \mathbb{R}^+$ that maps program states $\sigma \in \Sigma$ to nonnegative numbers, where we assume each state σ contains a cost-accumulator component $\sigma.\alpha$. If a program executes with initial state σ to final state σ', then it holds that $\phi(\sigma) \geq (\sigma'.\alpha - \sigma.\alpha) + \phi(\sigma')$, where $(\sigma'.\alpha - \sigma.\alpha)$ describes the accumulated cost from σ to σ'. The potential method also enables *compositional* reasoning: if a statement S_1 executes from σ to σ' and a statement S_2 executes from σ' to σ'', then we have $\phi(\sigma) \geq (\sigma'.\alpha - \sigma.\alpha) + \phi(\sigma')$ and $\phi(\sigma') \geq (\sigma''.\alpha - \sigma'.\alpha) + \phi(\sigma'')$; therefore, we derive $\phi(\sigma) \geq (\sigma''.\alpha - \sigma.\alpha) + \phi(\sigma'')$ for the sequential composition $S_1; S_2$. For non-probabilistic programs, the initial potential provides an *upper* bound on the accumulated cost.

This approach has been adapted to reason about expected costs of probabilistic programs [124, 154]. To derive upper bounds on the *expected* accumulated cost of a program S with initial state σ, one needs to take into consideration the *distribution* of all possible executions. More precisely, the

potential function should satisfy the following property:

$$\phi(\sigma) \geq \mathbb{E}_{\sigma' \sim [\![S]\!](\sigma)}[C(\sigma, \sigma') + \phi(\sigma')], \tag{5.1}$$

where the notation $\mathbb{E}_{x\sim\mu}[f(x)]$ represents the expected value of $f(x)$, where x is drawn from the distribution μ, $[\![S]\!](\sigma)$ is the distribution over final states of executing S from σ, and $C(\sigma, \sigma') \stackrel{\text{def}}{=} \sigma'.\alpha - \sigma.\alpha$ is the execution cost from σ to σ'.

Example 5.2. Fig. 5.2 annotates the rdwalk *function from Example 5.1 with the derivation of an upper bound on the expected accumulated cost. The annotations, taken together, define an expected-potential function $\phi : \Sigma \to \mathbb{R}^+$ where a program state $\sigma \in \Sigma$ consists of a program point and a valuation for program variables. To justify the upper bound $2(d - x) + 4$ for the function* rdwalk*, one has to show that the potential right before the* **tick**(1) *statement should be at least* 1*. This property is established by* backward *reasoning on the function body:*

- *For* **call** rdwalk*, we apply the "induction hypothesis" that the expected cost of the function* rdwalk *can be upper-bounded by $2(d-x)+4$. Adding the* 1 *unit of potential needed by the tick statement, we obtain $2(d - x) + 5$ as the pre-annotation of the function call.*
- *For $x \coloneqq x + t$, we substitute x with $x + t$ in the post-annotation of this statement to obtain the pre-annotation.*
- *For $t \sim \textsc{Uniform}(-1, 2)$, because its post-annotation is $2(d - x - t) + 5$, we compute its pre-annotation as*

$$\begin{aligned}\mathbb{E}_{t\sim\textsc{Uniform}(-1,2)}[2(d - x - t) + 5] &= 2(d - x) + 5 - 2 \cdot \mathbb{E}_{t\sim\textsc{Uniform}(-1,2)}[t] \\ &= 2(d - x) + 5 - 2 \cdot \frac{1}{2} \\ &= 2(d - x) + 4,\end{aligned}$$

  which is exactly the upper bound we want to justify.

My Approach In this chapter, I focus on the derivation of higher central moments. Observing that a central moment $\mathbb{E}[(X-\mathbb{E}[X])^k]$ can be rewritten as a polynomial of raw moments $\mathbb{E}[X], \cdots, \mathbb{E}[X^k]$, I reduce the problem of bounding central moments to reasoning about upper and lower bounds on raw moments. For example, the variance can be written as $\mathbb{V}[X] = \mathbb{E}[X^2] - \mathbb{E}^2[X]$, so it suffices to analyze the *upper* bound of the second moment $\mathbb{E}[X^2]$ and the *lower* bound on the square of the first moment $\mathbb{E}^2[X]$. For higher central moments, this approach requires both upper and lower bounds on higher raw moments. For example, consider the fourth central moment of a *nonnegative* random variable X: $\mathbb{E}[(X - \mathbb{E}[X])^4] = \mathbb{E}[X^4] - 4\mathbb{E}[X^3]\mathbb{E}[X] + 6\mathbb{E}[X^2]\mathbb{E}^2[X] - 3\mathbb{E}^4[X]$. Deriving an upper bound on the fourth central moment requires lower bounds on the first (i.e., $\mathbb{E}[X]$) and third (i.e., $\mathbb{E}[X^3]$) raw moments.

I now sketch the development of *moment semirings*. I first consider only the upper bounds on higher moments of *nonnegative* costs. To do so, I extend the range of the expected-potential function ϕ to real-valued vectors $(\mathbb{R}^+)^{m+1}$, where $m \in \mathbb{N}$ is the degree of the target moment. I update the potential inequality (5.1) as follows:

$$\phi(\sigma) \geq \mathbb{E}_{\sigma' \sim [\![S]\!](\sigma)}[\overrightarrow{\langle C(\sigma, \sigma')^k \rangle_{0\leq k\leq m}} \otimes \phi(\sigma')], \tag{5.2}$$

```
1  func rdwalk() begin
2    { ⟨1, 2(d − x) + 4, 4(d − x)² + 22(d − x) + 28⟩ }
3    if x < d then
4      { ⟨1, 2(d − x) + 4, 4(d − x)² + 22(d − x) + 28⟩ }
5      t ~ Uniform(−1, 2);
6      { ⟨1, 2(d − x − t) + 5, 4(d − x − t)² + 26(d − x − t) + 37⟩ }
7      x := x + t;
8      { ⟨1, 2(d − x) + 5, 4(d − x)² + 26(d − x) + 37⟩ }
9      call rdwalk;
10     { ⟨1, 1, 1⟩ }
11     tick(1)
12     { ⟨1, 0, 0⟩ }
13   fi
14 end
```

Fig. 5.3: Derivation of an *upper* bound on the first and second moment of the accumulated cost.

where $\overrightarrow{\langle v_k \rangle_{0 \le k \le m}}$ denotes an $(m+1)$-dimensional vector, the order $\le$ on vectors is defined pointwise, and $\otimes$ is some *composition* operator. Recall that $[\![S]\!](\sigma)$ denotes the distribution over final states of executing S from σ, and $C(\sigma, \sigma')$ describes the cost for the execution from σ to σ'. Intuitively, for $\phi(\sigma) = \overrightarrow{\langle \phi(\sigma)_k \rangle_{0 \le k \le m}}$ and each k, the component $\phi(\sigma)_k$ is an upper bound on the k-th moment of the cost for the computation starting from σ. The 0-th moment is the *termination probability* of the computation, and I assume it is always one for now. We *cannot* simply define $\otimes$ as pointwise addition because, for example, $(a+b)^2 \neq a^2 + b^2$ in general. If we think of b as the cost for some probabilistic computation, and we prepend a constant cost a to the computation, then by linearity of expectations, we have $\mathbb{E}[(a+b)^2] = \mathbb{E}[a^2 + 2ab + b^2] = a^2 + 2 \cdot a \cdot \mathbb{E}[b] + \mathbb{E}[b^2]$, i.e., reasoning about the second moment requires us to keep track of the first moment. Similarly, we should have

$$\phi(\sigma)_2 \ge \mathbb{E}_{\sigma' \sim [\![S]\!](\sigma)}[C(\sigma, \sigma')^2 + 2 \cdot C(\sigma, \sigma') \cdot \phi(\sigma')_1 + \phi(\sigma')_2],$$

for the second-moment component, where $\phi(\sigma')_1$ and $\phi(\sigma')_2$ denote $\mathbb{E}[b]$ and $\mathbb{E}[b^2]$, respectively. Therefore, the composition operator $\otimes$ for second-moment analysis (i.e., $m = 2$) should be defined as

$$\langle 1, r_1, s_1 \rangle \otimes \langle 1, r_2, s_2 \rangle \stackrel{\text{def}}{=} \langle 1, r_1 + r_2, s_1 + 2r_1 r_2 + s_2 \rangle. \tag{5.3}$$

Example 5.3. Fig. 5.3 annotates the rdwalk *function from Example 5.1 with the derivation of an upper bound on both the first and second moment of the accumulated cost. To justify the first and second moment of the accumulated cost for the function* rdwalk*, We again perform backward reasoning:*

- *For* **tick**(1)*, it transforms a post-annotation a by $\lambda a.(\langle 1,1,1 \rangle \otimes a)$; thus, the pre-annotation is $\langle 1,1,1 \rangle \otimes \langle 1,0,0 \rangle = \langle 1,1,1 \rangle$.*
- *For* **call** rdwalk*, we apply the "induction hypothesis", i.e., the upper bound shown on line 2. We use the $\otimes$ operator to compose the induction hypothesis with the post-annotation of this function call:*

$$\begin{aligned}
&\langle 1, 2(d-x)+4, 4(d-x)^2+22(d-x)+28\rangle \otimes \langle 1,1,1\rangle \\
&= \langle 1, 2(d-x)+5, (4(d-x)^2+22(d-x)+28)+2\cdot(2(d-x)+4)+1\rangle \\
&= \langle 1, 2(d-x)+5, 4(d-x)^2+26(d-x)+37\rangle.
\end{aligned}$$

- *For $x \coloneqq x+t$, we substitute x with $x+t$ in the post-annotation of this statement to obtain the pre-annotation.*
- *For $t \sim \textsc{Uniform}(-1,2)$, because the post-annotation involves both t and t^2, we compute from the definition of uniform distributions that*

$$\mathbb{E}_{t\sim\textsc{Uniform}(-1,2)}[t] = \frac{1}{2}, \quad \mathbb{E}_{t\sim\textsc{Uniform}(-1,2)}[t^2] = 1.$$

Then the upper bound on the second moment is derived as follows:

$$\begin{aligned}
&\mathbb{E}_{t\sim\textsc{Uniform}(-1,2)}[4(d-x-t)^2+26(d-x-t)+37] \\
&= (4(d-x)^2+26(d-x)+37) - (8(d-x)+26)\cdot\mathbb{E}_{t\sim\textsc{Uniform}(-1,2)}[t] \\
&\quad + 4\cdot\mathbb{E}_{t\sim\textsc{Uniform}(-1,2)}[t^2] \\
&= 4(d-x)^2+22(d-x)+28,
\end{aligned}$$

which is the same as the desired upper bound on the second moment of the accumulated cost for the function rdwalk. *(See Fig. 5.3, line 2.)*

I generalize the composition operator $\otimes$ to moments with arbitrarily high degrees, via a family of algebraic structures, which I name *moment semirings* (see §5.2.2). These semirings are *algebraic* in the sense that they can be instantiated with any partially ordered semiring, not just $\mathbb{R}^+$.

Interval Bounds Moment semirings not only provide a general method to analyze higher moments, but also enable reasoning about upper and lower bounds on moments *simultaneously*. The simultaneous treatment is also essential for analyzing programs with *non-monotone* costs (see §5.2.3).

I instantiate moment semirings with the standard interval semiring $\mathcal{I} = \{[a,b] \mid a \le b\}$. The algebraic approach allows me to systematically incorporate the interval-valued bounds, by *reinterpreting* operations in eq. (5.3) under $\mathcal{I}$:

$$\begin{aligned}
&\langle [1,1], [r_1^{\mathsf{L}}, r_1^{\mathsf{U}}], [s_1^{\mathsf{L}}, s_1^{\mathsf{U}}]\rangle \otimes \langle [1,1], [r_2^{\mathsf{L}}, r_2^{\mathsf{U}}], [s_2^{\mathsf{L}}, s_2^{\mathsf{U}}]\rangle \\
&\overset{\text{def}}{=} \langle [1,1], [r_1^{\mathsf{L}}, r_1^{\mathsf{U}}] +_{\mathcal{I}} [r_2^{\mathsf{L}}, r_2^{\mathsf{U}}], [s_1^{\mathsf{L}}, s_2^{\mathsf{U}}] +_{\mathcal{I}} 2\cdot([r_1^{\mathsf{L}}, r_1^{\mathsf{U}}] \cdot_{\mathcal{I}} [r_2^{\mathsf{L}}, r_2^{\mathsf{U}}]) +_{\mathcal{I}} [s_2^{\mathsf{L}}, s_2^{\mathsf{U}}]\rangle \\
&= \langle [1,1], [r_1^{\mathsf{L}}+r_2^{\mathsf{L}}, r_1^{\mathsf{U}}+r_2^{\mathsf{U}}], [s_1^{\mathsf{L}}+2\cdot\min S + s_2^{\mathsf{L}}, s_1^{\mathsf{U}}+2\cdot\max S + s_2^{\mathsf{U}}]\rangle,
\end{aligned}$$

where $S \overset{\text{def}}{=} \{r_1^{\mathsf{L}} r_2^{\mathsf{L}}, r_1^{\mathsf{L}} r_2^{\mathsf{U}}, r_1^{\mathsf{U}} r_2^{\mathsf{L}}, r_1^{\mathsf{U}} r_2^{\mathsf{U}}\}$. I then update the potential inequality eq. (5.2) as follows:

$$\phi(\sigma) \sqsupseteq \mathbb{E}_{\sigma'\sim[\![S]\!](\sigma)}[\overrightarrow{\langle [C(\sigma,\sigma')^k, C(\sigma,\sigma')^k]\rangle_{0\le k\le m}} \otimes \phi(\sigma')],$$

where the order $\sqsubseteq$ is defined as pointwise interval inclusion.

Example 5.4. Suppose that the interval bound on the first moment of the accumulated cost of the rdwalk *function from Example 5.1 is $[2(d-x), 2(d-x)+4]$. We can now derive the upper bound on the variance $\mathbb{V}[tick] \le 22d+28$ shown in Fig. 5.1(b) (where we substitute x with 0 because the main function initializes x to 0 on line 5 in Fig. 5.2):*

$$\begin{aligned}\mathbb{V}[tick] &= \mathbb{E}[tick^2] - \mathbb{E}^2[tick]\\ &\le (\textit{upper bound on } \mathbb{E}[tick^2]) - (\textit{lower bound on } \mathbb{E}[tick])^2\\ &= (4d^2 + 22d + 28) - (2d)^2\\ &= 22d + 28.\end{aligned}$$

In §5.4, I describe how to use moment bounds to derive the tail bounds shown in Fig. 5.1(c).

5.1.2 Two Major Challenges

Interprocedural Reasoning Recall that in the derivation of Fig. 5.3, I use the $\otimes$ operator to compose the upper bounds on moments for **call** rdwalk and its post-annotation $\langle 1, 1, 1\rangle$. However, this approach does *not* work in general, because the post-annotation might be symbolic (e.g., $\langle 1, x, x^2\rangle$) and the callee might mutate referenced program variables (e.g., x). One workaround is to derive a *pre*-annotation for each possible *post*-annotation of a recursive function, i.e., the moment annotations for a recursive function is *polymorphic*. This workaround would *not* be effective for non-tail-recursive functions: for example, we need to reason about the rdwalk function in Fig. 5.3 with *infinitely* many post-annotations $\langle 1, 0, 0\rangle$, $\langle 1, 1, 1\rangle$, $\langle 1, 2, 4\rangle$, ..., i.e., $\langle 1, i, i^2\rangle$ for all $i \in \mathbb{Z}^+$.

My solution to *moment-polymorphic recursion* is to introduce a *combination* operator $\oplus$ in a way that if ϕ_1 and ϕ_2 are two expected-potential functions, then

$$\phi_1(\sigma) \oplus \phi_2(\sigma) \ge \mathbb{E}_{\sigma' \sim [\![S]\!](\sigma)}[\overrightarrow{\langle C(\sigma,\sigma')^k\rangle_{0\le k\le m}} \otimes (\phi_1(\sigma') \oplus \phi_2(\sigma'))].$$

I then use the $\oplus$ operator to derive a *frame* rule:

$$\frac{\{\ Q_1\ \}\ S\ \{\ Q_1'\ \} \qquad \{\ Q_2\ \}\ S\ \{\ Q_2'\ \}}{\{\ Q_1 \oplus Q_2\ \}\ S\ \{\ Q_1' \oplus Q_2'\ \}}$$

I define $\oplus$ as pointwise addition, i.e., for second moments,

$$\langle p_1, r_1, s_1\rangle \oplus \langle p_2, r_2, s_2\rangle \stackrel{\text{def}}{=} \langle p_1 + p_2, r_1 + r_2, s_1 + s_2\rangle, \tag{5.4}$$

and because the 0-th-moment (i.e., termination-probability) component is no longer guaranteed to be one, I redefine $\otimes$ to consider the termination probabilities:

$$\langle p_1, r_1, s_1\rangle \otimes \langle p_2, r_2, s_2\rangle \stackrel{\text{def}}{=} \langle p_1p_2, p_2r_1 + p_1r_2, p_2s_1 + 2r_1r_2 + p_1s_2\rangle. \tag{5.5}$$

Remark 5.5. As I will show in §5.2.2, the composition operator $\otimes$ and combination operator $\oplus$ form a moment semiring*; consequently, we can use* algebraic *properties of semirings (e.g., distributivity) to aid higher-moment analysis. For example, a vector $\langle 0, r_1, s_1\rangle$ whose termination-probability component is zero does not seem to make sense, because moments with respect to a zero distribution should also be zero. However, by distributivity, we have*

$$\begin{aligned}&\langle 1, r_3, s_3\rangle \otimes \langle 1, r_1 + r_2, s_1 + s_2\rangle\\ =\ &\langle 1, r_3, s_3\rangle \otimes (\langle 0, r_1, s_1\rangle \oplus \langle 1, r_2, s_2\rangle)\\ =\ &(\langle 1, r_3, s_3\rangle \otimes \langle 0, r_1, s_1\rangle) \oplus (\langle 1, r_3, s_3\rangle \oplus \langle 1, r_2, s_2\rangle).\end{aligned}$$

If we think of $\langle 1, r_1 + r_2, s_1 + s_2 \rangle$ *as a post-annotation of a computation whose moments are bounded by* $\langle 1, r_3, s_3 \rangle$*, the equation above indicates that we can use* $\oplus$ *to* decompose *the post-annotation into subparts, and then reason about each subpart separately. This fact inspires me to develop a decomposition technique for moment-polymorphic recursion.*

Example 5.6. With the $\oplus$ *operator and the frame rule, we only need to analyze the* rdwalk *function from Example 5.1 with* three *post-annotations:* $\langle 1, 0, 0 \rangle$*,* $\langle 0, 1, 1 \rangle$*, and* $\langle 0, 0, 2 \rangle$*, which form a kind of "elimination sequence." We construct this sequence in an* on-demand *manner; the first post-annotation is the identity element* $\langle 1, 0, 0 \rangle$ *of the moment semiring.*

For post-annotation $\langle 1, 0, 0 \rangle$*, as shown in Fig. 5.3, we need to know the moment bound for* rdwalk *with the post-annotation* $\langle 1, 1, 1 \rangle$*. Instead of reanalyzing* rdwalk *with the post-annotation* $\langle 1, 1, 1 \rangle$*, We use the* $\oplus$ *operator to compute the "difference" between it and the previous post-annotation* $\langle 1, 0, 0 \rangle$*. Observing that* $\langle 1, 1, 1 \rangle = \langle 1, 0, 0 \rangle \oplus \langle 0, 1, 1 \rangle$*, we now analyze* rdwalk *with* $\langle 0, 1, 1 \rangle$ *as the post-annotation:*

call rdwalk;
$\{\ \langle 0,\ 1,\ 3 \rangle\ \}\ \ \# = \langle 1,\ 1,\ 1 \rangle \otimes \langle 0,\ 1,\ 1 \rangle$
tick(1)
$\{\ \langle 0,\ 1,\ 1 \rangle\ \}$

Again, because $\langle 0, 1, 3 \rangle = \langle 0, 1, 1 \rangle \oplus \langle 0, 0, 2 \rangle$*, we need to further analyze* rdwalk *with* $\langle 0, 0, 2 \rangle$ *as the post-annotation:*

call rdwalk;
$\{\ \langle 0,\ 0,\ 2 \rangle\ \}\ \ \# = \langle 1,\ 1,\ 1 \rangle \otimes \langle 0,\ 0,\ 2 \rangle$
tick(1)
$\{\ \langle 0,\ 0,\ 2 \rangle\ \}$

With the post-annotation $\langle 0, 0, 2 \rangle$*, we can now reason* monomorphically *without analyzing any new post-annotation! We can perform a succession of reasoning steps similar to what we have done in Example 5.2 to justify the following bounds ("unwinding" the elimination sequence):*

- $\{\langle 0, 0, 2 \rangle\}$ rdwalk $\{\langle 0, 0, 2 \rangle\}$*: Directly by backward reasoning with the post-annotation* $\langle 0, 0, 2 \rangle$*.*
- $\{\langle 0, 1, 4(d-x)+9 \rangle\}$ rdwalk $\{\langle 0, 1, 1 \rangle\}$*: To analyze the recursive call with post-annotation* $\langle 0, 1, 3 \rangle$*, we use the frame rule with the post-call-site annotation* $\langle 0, 0, 2 \rangle$ *to derive* $\langle 0, 1, 4(d - x) + 11 \rangle$ *as the pre-annotation:*

  $\{\ \langle 0,\ 1,\ 4(d-x)+11 \rangle\ \}\ \ \# = \langle 0,\ 1,\ 4(d-x)+9 \rangle \oplus \langle 0,\ 0,\ 2 \rangle$
  call rdwalk;
  $\{\ \langle 0,\ 1,\ 3 \rangle\ \}\ \ \# = \langle 0,\ 1,\ 1 \rangle \oplus \langle 0,\ 0,\ 2 \rangle$

- $\{\langle 1, 2(d-x)+4, 4(d-x)^2+22(d-x)+28 \rangle\}$ rdwalk $\{\langle 1, 0, 0 \rangle\}$*: To analyze the recursive call with post-annotation* $\langle 1, 1, 1 \rangle$*, we use the frame rule with the post-call-site annotation* $\langle 0, 1, 1 \rangle$ *to derive* $\langle 1, 2(d - x) + 5, 4(d - x)^2 + 26(d - x) + 37 \rangle$ *as the pre-annotation:*

  $\{\ \langle 1, 2(d-x)+5, 4(d-x)^2+26(d-x)+37 \rangle\ \}$
  $\# = \langle 1, 2(d-x)+4, 4(d-x)^2+22(d-x)+28 \rangle \oplus \langle 0, 1, 4(d-x)+9 \rangle$
  call rdwalk;
  $\{\ \langle 1,\ 1,\ 1 \rangle\ \}\ \ \# = \langle 1,\ 0,\ 0 \rangle \oplus \langle 0,\ 1,\ 1 \rangle$

```
func geo() begin { ⟨1, 2^x⟩ }
  x := x + 1; { ⟨1, 2^(x−1)⟩ }
  # expected-potential method for lower bounds:
  # 2^(x−1) < 1/2 · (2^x + 1) + 1/2 · 0
  if prob(1/2) then { ⟨1, 2^x + 1⟩ }
    tick(1); { ⟨1, 2^x⟩ }
    call geo { ⟨1, 0⟩}
  fi
end
```

Fig. 5.4: A purely probabilistic loop with annotations for a *lower* bound on the first moment of the accumulated cost.

In §5.2.3, I present an automatic inference system for the expected-potential method that is extended with interval-valued bounds on higher moments, with support for moment-polymorphic recursion.

Soundness of the Analysis Unlike the classic potential method, the expected-potential method is *not* always sound when reasoning about the moments for cost accumulators in probabilistic programs.

Counterexample 5.7. Consider the program in Fig. 5.4 that describes a purely probabilistic loop that exits the loop with probability $1/2$ *in each iteration. The expected accumulated cost of the program should be* one *[68]. However, the annotations in Fig. 5.4 justify a potential function* 2^x *as a* lower *bound on the expected accumulated cost, no matter what value* x *has at the beginning, which is apparently* unsound.

Why does the expected-potential method fail in this case? The short answer is that dualization only works for some problems: upper-bounding the sum of nonnegative ticks is equivalent to lower-bounding the sum of nonpositive ticks; lower-bounding the sum of nonnegative ticks—the issue in Fig. 5.4—is equivalent to upper-bounding the sum of nonpositive ticks; however, the two kinds of problems are *inherently different* [68]. Intuitively, the classic potential method for bounding the costs of non-probabilistic programs is a *partial*-correctness method, i.e., derived upper/lower bounds are sound if the analyzed program terminates [125]. With probabilistic programs, many programs do not terminate *definitely*, but only *almost surely*, i.e., they terminate with probability one, but have some execution traces that are non-terminating. The programs in Figures 5.2 and 5.4 are both almost-surely terminating. For the expected-potential method, the potential at a program state can be seen as an *average* of potentials needed for all possible computations that continue from the state. If the program state can lead to a non-terminating execution trace, the potential associated with that trace might be problematic, and as a consequence, the expected-potential method might fail.

Previous research [7, 68, 137, 154] has employed the *Optional Stopping Theorem* (OST) from probability theory to address this soundness issue. The classic OST provides a collection of *sufficient* conditions for reasoning about expected gain *upon termination* of stochastic processes, where the expected gain at any time is *invariant*. By constructing a stochastic process for executions

$$
\begin{aligned}
S &::= \textbf{skip} \mid \textbf{tick}(c) \mid x \coloneqq E \mid x \sim D \mid \textbf{call}\ f \mid \textbf{while}\ L\ \textbf{do}\ S\ \textbf{od} \\
&\quad \mid \textbf{if}\ \textbf{prob}(p)\ \textbf{then}\ S_1\ \textbf{else}\ S_2\ \textbf{fi} \mid \textbf{if}\ L\ \textbf{then}\ S_1\ \textbf{else}\ S_2\ \textbf{fi} \mid S_1; S_2 \\
L &::= \textbf{true} \mid \textbf{not}\ L \mid L_1\ \textbf{and}\ L_2 \mid E_1 \leq E_2 \\
E &::= x \mid c \mid E_1 + E_2 \mid E_1 \times E_2 \\
D &::= \textsc{Uniform}(a, b) \mid \cdots
\end{aligned}
$$

Fig. 5.5: Syntax of the probabilistic programming language, where $p \in [0, 1]$, $a, b, c \in \mathbb{R}$, $a < b$, $x \in$ VID is a variable, and $f \in$ FID is a function identifier.

of probabilistic programs and setting the expected-potential function as the invariant, one can apply the OST to justify the soundness of the expected-potential function. In other article, I have studied and proposed an extension to the classic OST with a *new* sufficient condition that is suitable for reasoning about higher moments [150]. I then prove the soundness of my central-moment inference for programs that satisfy this condition, and develop an algorithm to check this condition automatically (see §5.3).

5.2 Derivation System for Higher Moments

In this section, I describe the inference system used by my analysis. I first present a probabilistic programming language (§5.2.1). I then introduce *moment semirings* to compose higher moments for a cost accumulator from two computations (§5.2.2). I use moment semirings to develop my derivation system, which is presented as a declarative program logic (§5.2.3). Finally, I sketch how I reduce the inference of a derivation to LP solving (§5.2.4).

5.2.1 A Probabilistic Programming Language

In this chapter, I use a syntactic representation of Appl—instead of using control-flow hypergraphs—to simplify the presentation of the derivation system. Recall that Appl supports general recursion and continuous distributions. I also assume that all the program variables are real-valued for brevity.

Fig. 5.5 presents the syntax as a grammar, where the metavariables S, L, E, and D stand for statements, conditions, expressions, and distributions, respectively. Each distribution D is associated with a probability measure $\mu_D \in \mathbb{D}(\mathbb{R})$. The statement "$x \sim D$" is a *random-sampling* assignment, which draws from the distribution μ_D to obtain a sample value and then assigns it to x. The statement "**if prob**(p) **then** S_1 **else** S_2 **fi**" is a *probabilistic-branching* statement, which executes S_1 with probability p, or S_2 with probability $(1 - p)$.

The statement "**call** f" makes a (possibly recursive) call to the function with identifier $f \in$ FID. In this chapter, I assume that the functions only manipulate states that consist of global program variables. The statement **tick**(c), where $c \in \mathbb{R}$ is a constant, is used to define the *cost model*. It adds c to an anonymous global cost accumulator. Note that my implementation supports

local variables, function parameters, return statements, as well as accumulation of non-constant costs; the restrictions imposed here are not essential, and are introduced solely to simplify the presentation.

I use a pair $\langle \mathscr{D}, S_{\mathsf{main}} \rangle$ to represent a program, where $\mathscr{D}$ is a finite map from function identifiers to their bodies and S_{main} is the body of the main function. In §5.3.2, I present an operational semantics for Appl, which is similar to the operational semantics presented in §2.3. The reason *not* to use a denotational semantics is to enable a direct adaptation of Optional Stopping Theorems (see §5.3.3).

5.2.2 Moment Semirings

As discussed in §5.1.1, I want to design a *composition* operation $\otimes$ and a *combination* operation $\oplus$ to compose and combine higher moments of accumulated costs such that

$$\phi(\sigma) \sqsupseteq \mathbb{E}_{\sigma' \sim [\![S]\!](\sigma)}[\overrightarrow{\langle C(\sigma,\sigma')^k \rangle_{0 \le k \le m}} \otimes \phi(\sigma')],$$
$$\phi_1(\sigma) \oplus \phi_2(\sigma) \sqsupseteq \mathbb{E}_{\sigma' \sim [\![S]\!](\sigma)}[\overrightarrow{\langle C(\sigma,\sigma')^k \rangle_{0 \le k \le m}} \otimes (\phi_1(\sigma') \oplus \phi_2(\sigma'))],$$

where the expected-potential functions ϕ, ϕ_1, ϕ_2 map program states to interval-valued vectors, $C(\sigma,\sigma')$ is the cost for the computation from σ to σ', and m is the degree of the target moment. In eqs. (5.4) and (5.5), I gave a definition of $\otimes$ and $\oplus$ suitable for first and second moments, respectively. In this section, I generalize them to reason about upper and lower bounds of higher moments. My approach is inspired by the work of Li and Eisner [107], which develops a method to "lift" techniques for first moments to those for second moments. Instead of restricting the elements of semirings to be vectors of numbers, I propose *algebraic* moment semirings that can also be instantiated with vectors of intervals, which we need for the interval-bound analysis that was demonstrated in §5.1.1.

Definition 5.8. The m-th order *moment semiring* $\mathcal{M}_{\mathcal{R}}^{(m)} = (|\mathcal{R}|^{m+1}, \oplus, \otimes, \underline{0}, \underline{1})$ is parametrized by a partially ordered semiring $\mathcal{R} = (|\mathcal{R}|, \le, +, \cdot, 0, 1)$, where

$$\overrightarrow{\langle u_k \rangle_{0 \le k \le m}} \oplus \overrightarrow{\langle v_k \rangle_{0 \le k \le m}} \stackrel{\text{def}}{=} \overrightarrow{\langle u_k + v_k \rangle_{0 \le k \le m}}, \tag{5.6}$$
$$\overrightarrow{\langle u_k \rangle_{0 \le k \le m}} \otimes \overrightarrow{\langle v_k \rangle_{0 \le k \le m}} \stackrel{\text{def}}{=} \overrightarrow{\langle \textstyle\sum_{i=0}^{k} \binom{k}{i} \times (u_i \cdot v_{k-i}) \rangle_{0 \le k \le m}}, \tag{5.7}$$

$\binom{k}{i}$ is the binomial coefficient; the scalar product $n \times u$ is an abbreviation for $\sum_{i=1}^{n} u$, for $n \in \mathbb{Z}^+, u \in \mathcal{R}$; $\underline{0} \stackrel{\text{def}}{=} \langle 0, 0, \cdots, 0 \rangle$; and $\underline{1} \stackrel{\text{def}}{=} \langle 1, 0, \cdots, 0 \rangle$. We define the partial order $\sqsubseteq$ as the pointwise extension of the partial order $\le$ on $\mathcal{R}$.

Intuitively, the definition of $\otimes$ in eq. (5.7) can be seen as the multiplication of two moment-generating functions for distributions with moments $\overrightarrow{\langle u_k \rangle_{0 \le k \le m}}$ and $\overrightarrow{\langle v_k \rangle_{0 \le k \le m}}$, respectively. I then prove a composition property for moment semirings.

Lemma 5.9. *For all $u, v \in \mathcal{R}$, it holds that*

$$\overrightarrow{\langle (u+v)^k \rangle_{0 \le k \le m}} = \overrightarrow{\langle u^k \rangle_{0 \le k \le m}} \otimes \overrightarrow{\langle v^k \rangle_{0 \le k \le m}},$$

where u^n is an abbreviation for $\prod_{i=1}^{n} u$, for $n \in \mathbb{Z}^+, u \in \mathcal{R}$.

Proof. Let RHS denote the right-hand-side of the target equation. Observe that

$$RHS_k = \sum_{i=0}^{k} \binom{k}{i} \times (u^i \cdot v^{k-i}).$$

We prove by induction on k that $(u+v)^k = RHS_k$.

- Base case (i.e., $k = 0$): We have $(u+v)^0 = 1$. On the other hand, we have

$$RHS_0 = \binom{0}{0} \times (u^0 \cdot v^0) = 1 \times (1 \cdot 1) = 1.$$

- Suppose that $(u+v)^k = RHS_k$ for some k. Then

$$\begin{aligned}
(u+v)^{k+1} &= (u+v) \cdot (u+v)^k \\
&= (u+v) \cdot \sum_{i=0}^{k} \binom{k}{i} \times (u^i \cdot v^{k-i}) \\
&= \sum_{i=0}^{k} \binom{k}{i} \times (u^{i+1} \cdot v^{k-i}) + \sum_{i=0}^{k} \binom{k}{i} \times (u^i \cdot v^{k-i+1}) \\
&= \sum_{i=1}^{k+1} \binom{k}{i-1} \times (u^i \cdot v^{k-i+1}) + \sum_{i=0}^{k} \binom{k}{i} \times (u^i \cdot v^{k-i+1}) \\
&= \sum_{i=0}^{k+1} (\binom{k}{i-1} + \binom{k}{i}) \times (u^i \cdot v^{k-i+1}) \\
&= \sum_{i=0}^{k+1} \binom{k+1}{i} \times (u^k \cdot v^{k-i+1}) \\
&= RHS_{k+1}.
\end{aligned}$$

□

5.2.3 Inference Rules

I present the derivation system as a declarative program logic that uses moment semirings to enable compositional reasoning and moment-polymorphic recursion.

Interval-Valued Moment Semirings My derivation system infers upper and lower bounds simultaneously, rather than separately, which is essential for *non-monotone* costs. Consider a program "**tick**$(-1); S$" and suppose that we have $\langle 1, 2, 5\rangle$ and $\langle 1, -2, 5\rangle$ as the upper and lower bounds on the first two moments of the cost for S, respectively. If we only use the upper bound, we derive $\langle 1, -1, 1\rangle \otimes \langle 1, 2, 5\rangle = \langle 1, 1, 2\rangle$, which is *not* an upper bound on the moments of the cost for the program; if the *actual* moments of the cost for S are $\langle 1, 0, 5\rangle$, then the *actual* moments of the cost for "**tick**$(-1); S$" are $\langle 1, -1, 1\rangle \otimes \langle 1, 0, 5\rangle = \langle 1, -1, 4\rangle \not\leq \langle 1, 1, 2\rangle$. Thus, in the analysis, I instantiate moment semirings with the interval domain $\mathcal{I}$. For the program "**tick**$(-1); S$", its interval-valued bound on the first two moments is $\langle [1,1], [-1,-1], [1,1]\rangle \otimes \langle [1,1], [-2,2], [5,5]\rangle = \langle [1,1], [-3,1], [2,10]\rangle$.

Template-Based Expected-Potential Functions The basic approach to automated inference using potential functions is to introduce a *template* for the expected-potential functions. Let me fix $m \in \mathbb{N}$ as the degree of the target moment. Because I use $\mathcal{M}_{\mathcal{I}}^{(m)}$-valued expected-potential functions whose range is vectors of intervals, the templates are vectors of intervals whose ends are represented *symbolically*. In this chapter, I represent the ends of intervals by *polynomials* in $\mathbb{R}[\mathsf{VID}]$ over program variables.

More formally, I lift the interval semiring $\mathcal{I}$ to a *symbolic* interval semiring $\mathcal{PI}$ by representing the ends of the k-th interval by polynomials in $\mathbb{R}_{kd}[\mathsf{VID}]$ up to degree kd for some fixed $d \in \mathbb{N}$. Let $\mathcal{M}_{\mathcal{PI}}^{(m)}$ be the m-th order moment semiring instantiated with the symbolic interval semiring. Then the potential annotation is represented as $Q = \overrightarrow{\langle [L_k, U_k] \rangle_{0 \le k \le m}} \in \mathcal{M}_{\mathcal{PI}}^{(m)}$, where L_k's and U_k's are polynomials in $\mathbb{R}_{kd}[\mathsf{VID}]$. Q defines an $\mathcal{M}_{\mathcal{I}}^{(m)}$-valued expected-potential function $\phi_Q(\sigma) \stackrel{\text{def}}{=} \overrightarrow{\langle [\sigma(L_k), \sigma(U_k)] \rangle_{0 \le k \le m}}$, where σ is a program state, and $\sigma(L_k)$ and $\sigma(U_k)$ are L_k and U_k evaluated over σ, respectively.

Inference Rules I formalize my derivation system for moment analysis in a Hoare-logic style. The judgment has the form $\Delta \vdash_h \{\Gamma; Q\}\ S\ \{\Gamma'; Q'\}$, where S is a statement, $\{\Gamma; Q\}$ is a precondition, $\{\Gamma'; Q'\}$ is a postcondition, $\Delta = \langle \Delta_k \rangle_{0 \le k \le m}$ is a context of function specifications, and $h \in \mathbb{Z}^+$ specifies some restrictions put on Q, Q' that I will explain later. The *logical context* $\Gamma : (\mathsf{VID} \to \mathbb{R}) \to \{\top, \bot\}$ is a predicate that describes reachable states at a program point. The *potential annotation* $Q \in \mathcal{M}_{\mathcal{PI}}^{(m)}$ specifies a map from program states to the moment semiring that is used to define interval-valued expected-potential functions. The semantics of the triple $\{\cdot; Q\}\ S\ \{\cdot; Q'\}$ is that if the rest of the computation after executing S has its moments of the accumulated cost bounded by $\phi_{Q'}$, then the whole computation has its moments of the accumulated cost bounded by ϕ_Q. The parameter h restricts all i-th-moment components in Q, Q', such that $i < h$, to be $[0, 0]$. I call such potential annotations *h-restricted*; this construction is motivated by an observation from Example 5.6, where I illustrated the benefits of carrying out interprocedural analysis using an "elimination sequence" of annotations for recursive function calls, where the successive annotations have a greater number of zeros, filling from the left. *Function specifications* are valid pairs of pre- and post-conditions for all declared functions in a program. For each k, such that $0 \le k \le m$, and each function f, a valid specification $(\Gamma; Q, \Gamma'; Q') \in \Delta_k(f)$ is justified by the judgment $\Delta \vdash_k \{\Gamma; Q\}\ \mathscr{D}(f)\ \{\Gamma'; Q'\}$, where $\mathscr{D}(f)$ is the function body of f, and Q, Q' are k-restricted. The validity of a context Δ for function specifications is then established by the validity of all specifications in Δ, denoted by $\vdash \Delta$. To perform context-sensitive interprocedural analysis, a function can have multiple specifications.

Fig. 5.6 presents the inference rules. The rule (Q-Tick) is the only rule that deals with costs in a program. To accumulate the moments of the cost, I use the $\otimes$ operation in the moment semiring $\mathcal{M}_{\mathcal{PI}}^{(m)}$. The rule (Q-Sample) accounts for sampling statements. Because "$x \sim D$" randomly assigns a value to x in the support of distribution D, I quantify x out universally from the logical context. To compute $Q = \mathbb{E}_{x \sim \mu_D}[Q']$, where x is drawn from distribution D, I assume the moments for D are well-defined and computable, and substitute x^i, $i \in \mathbb{N}$ with the corresponding moments in Q'. I make this assumption because every component of Q' is a polynomial over program variables. For example, if $D = \textsc{Uniform}(-1, 2)$, we know the following facts

$$\mathbb{E}_{x \sim \mu_D}[x^0] = 1, \mathbb{E}_{x \sim \mu_D}[x^1] = \frac{1}{2}, \mathbb{E}_{x \sim \mu_D}[x^2] = 1, \mathbb{E}_{x \sim \mu_D}[x^3] = \frac{5}{4}.$$

(Valid-Ctx)
$$\frac{\forall (h, f) \in \mathrm{dom}(\Delta) : \forall (\Gamma; Q, \Gamma'; Q') \in \Delta(f) : \Delta \vdash_h \{\Gamma; Q\}\ \mathscr{D}(f)\ \{\Gamma'; Q'\}}{\vdash \Delta}$$

(Q-Skip)
$$\frac{}{\Delta \vdash_h \{\Gamma; Q\}\ \mathbf{skip}\ \{\Gamma; Q\}}$$

(Q-Tick)
$$\frac{Q = \overrightarrow{\langle [c^k, c^k] \rangle_{0 \le k \le m}} \otimes Q'}{\Delta \vdash_h \{\Gamma; Q\}\ \mathbf{tick}(c)\ \{\Gamma; Q'\}}$$

(Q-Assign)
$$\frac{\Gamma = [E/x]\Gamma' \qquad Q = [E/x]Q'}{\Delta \vdash_h \{\Gamma; Q\}\ x \coloneqq E\ \{\Gamma'; Q'\}}$$

(Q-Sample)
$$\frac{\Gamma = \forall x \in \mathrm{supp}(\mu_D) : \Gamma' \qquad Q = \mathbb{E}_{x \sim \mu_D}[Q']}{\Delta \vdash_h \{\Gamma; Q\}\ x \sim D\ \{\Gamma'; Q'\}}$$

(Q-Loop)
$$\frac{\Delta \vdash_h \{\Gamma \wedge L; Q\}\ S\ \{\Gamma; Q\}}{\Delta \vdash_h \{\Gamma; Q\}\ \mathbf{while}\ L\ \mathbf{do}\ S\ \mathbf{od}\ \{\Gamma \wedge \neg L; Q\}}$$

(Q-Seq)
$$\frac{\Delta \vdash_h \{\Gamma; Q\}\ S_1\ \{\Gamma'; Q'\} \qquad \Delta \vdash_h \{\Gamma'; Q'\}\ S_2\ \{\Gamma''; Q''\}}{\Delta \vdash_h \{\Gamma; Q\}\ S_1; S_2\ \{\Gamma''; Q''\}}$$

(Q-Call-Mono)
$$\frac{(\Gamma; Q, \Gamma'; Q') \in \Delta_m(f)}{\Delta \vdash_m \{\Gamma; Q\}\ \mathbf{call}\ f\ \{\Gamma'; Q'\}}$$

(Q-Call-Poly)
$$\frac{h < m \qquad \Delta_h(f) = (\Gamma; Q_1, \Gamma'; Q_1') \qquad \Delta \vdash_{h+1} \{\Gamma; Q_2\}\ \mathscr{D}(f)\ \{\Gamma'; Q_2'\}}{\Delta \vdash_h \{\Gamma; Q_1 \oplus Q_2\}\ \mathbf{call}\ f\ \{\Gamma'; Q_1' \oplus Q_2'\}}$$

(Q-Prob)
$$\frac{\Delta \vdash_h \{\Gamma; Q_1\}\ S_1\ \{\Gamma'; Q'\} \qquad \Delta \vdash_h \{\Gamma; Q_2\}\ S_2\ \{\Gamma'; Q'\} \qquad Q = P \oplus R \qquad P = \langle [p, p], [0, 0], \cdots, [0, 0] \rangle \otimes Q_1 \qquad R = \langle [1-p, 1-p], [0, 0], \cdots, [0, 0] \rangle \otimes Q_2}{\Delta \vdash_h \{\Gamma; Q\}\ \mathbf{if}\ \mathbf{prob}(p)\ \mathbf{then}\ S_1\ \mathbf{else}\ S_2\ \mathbf{fi}\ \{\Gamma'; Q'\}}$$

(Q-Cond)
$$\frac{\Delta \vdash_h \{\Gamma \wedge L; Q\}\ S_1\ \{\Gamma'; Q'\} \qquad \Delta \vdash \{\Gamma \wedge \neg L; Q\}\ S_2\ \{\Gamma'; Q'\}}{\Delta \vdash \{\Gamma; Q\}\ \mathbf{if}\ L\ \mathbf{then}\ S_1\ \mathbf{else}\ S_2\ \mathbf{fi}\ \{\Gamma'; Q'\}}$$

(Q-Weaken)
$$\frac{\Delta \vdash_h \{\Gamma_0; Q_0\}\ S\ \{\Gamma_0'; Q_0'\} \qquad \Gamma \models \Gamma_0 \qquad \Gamma_0' \models \Gamma' \qquad \Gamma \models Q \sqsupseteq Q_0 \qquad \Gamma_0' \models Q_0' \sqsupseteq Q'}{\Delta \vdash_h \{\Gamma; Q\}\ S\ \{\Gamma'; Q'\}}$$

Fig. 5.6: Inference rules of the derivation system.

Then for $Q' = \langle [1,1], [1+x^2, xy^2+x^3y] \rangle$, by the linearity of expectations, we compute $Q = \mathbb{E}_{x\sim\mu_D}[Q']$ as follows:

$$\begin{aligned}\mathbb{E}_{x\sim\mu_D}[Q'] &= \langle [1,1], [\mathbb{E}_{x\sim\mu_D}[1+x^2], \mathbb{E}_{x\sim\mu_D}[xy^2+x^3y]\rangle \\ &= \langle [1,1], [1+\mathbb{E}_{x\sim\mu_D}[x^2], y^2\mathbb{E}_{x\sim\mu_D}[x] + y\mathbb{E}_{x\sim\mu_D}[x^3]]\rangle \\ &= \langle [1,1], [2, \frac{1}{2}\cdot y^2 + \frac{5}{4}\cdot y]\rangle.\end{aligned}$$

The other probabilistic rule (Q-Prob) deals with probabilistic branching. Intuitively, if the moments of the execution of S_1 and S_2 are q_1 and q_2, respectively, and those of the accumulated cost of the computation after the branch statement is bounded by $\phi_{Q'}$, then the moments for the whole computation should be bounded by a "weighted average" of $(q_1 \otimes \phi_{Q'})$ and $(q_2 \otimes \phi_{Q'})$, with respect to the branching probability p. I implement the weighted average by the combination operator $\oplus$ applied to $\langle [p,p], [0,0], \cdots, [0,0]\rangle \otimes q_1 \otimes \phi_{Q'}$ and $\langle [1-p, 1-p], [0,0], \cdots, [0,0]\rangle \otimes q_2 \otimes \phi_{Q'}$, because the 0-th moments denote probabilities.

The rules (Q-Call-Poly) and (Q-Call-Mono) handle function calls. Recall that in Example 5.6, I use the $\oplus$ operator to combine multiple potential functions for a function to reason about recursive function calls. The restriction parameter h is used to ensure that the derivation system only needs to reason about *finitely* many post-annotations for each call site. In rule (Q-Call-Poly), where h is smaller than the target moment m, I fetch the pre- and post-condition Q_1, Q_1' for the function f from the specification context Δ_h. I then combine it with a *frame* of $(h+1)$-restricted potential annotations Q_2, Q_2' for the function f. The frame is used to account for the interval bounds on the moments for the computation after the function call for most non-tail-recursive programs. When h reaches the target moment m, I use the rule (Q-Call-Mono) to reason *moment-monomorphically*, because setting h to $m+1$ implies that the frame can only be $\langle [0,0], [0,0], \cdots, [0,0]\rangle$.

The structural rule (Q-Weaken) is used to strengthen the pre-condition and relax the post-condition. The entailment relation $\Gamma \models \Gamma'$ states that the logical implication $\Gamma \implies \Gamma'$ is valid. In terms of the bounds on higher moments for cost accumulators, if the triple $\{\cdot; Q\}\ S\ \{\cdot; Q'\}$ is valid, then I can safely widen the intervals in the pre-condition Q and narrow the intervals in the post-condition Q'.

Example 5.10. Fig. 5.7 presents the logical context and the complete potential annotation for the first and second moments for the cost accumulator tick of the rdwalk *function from Example 5.1. Similar to the reasoning in Example 5.6, we can justify the derivation using moment-polymorphic recursion and the moment bounds for* rdwalk *with post-annotations* $\langle [0,0], [1,1], [1,1]\rangle$ *and* $\langle [0,0], [0,0], [2,2]\rangle$.

5.2.4 Automatic Linear-Constraint Generation

I adapt existing techniques [21, 124] to automate my inference system by (i) using an abstract interpreter to infer logical contexts, (ii) generating templates and linear constraints by inductively applying the derivation rules to the analyzed program, and (iii) employing an off-the-shelf LP solver to discharge the linear constraints. During the generation phase, the coefficients of monomials in the polynomials from the ends of the intervals in every qualitative context $Q \in \mathcal{M}^{(m)}_{\mathcal{PI}}$ are recorded as symbolic names, and the inequalities among those coefficients—derived from the inference rules in Fig. 5.6—are emitted to the LP solver.

```
1  func rdwalk() begin
2    { x < d + 2; ⟨[1,1], [2(d−x), 2(d−x)+4],
3      [4(d−x)^2 + 6(d−x) − 4, 4(d−x)^2 + 22(d−x) + 28]⟩ }
4    if x < d then
5      { x < d; ⟨[1,1], [2(d−x), 2(d−x)+4],
6        [4(d−x)^2 + 6(d−x) − 4, 4(d−x)^2 + 22(d−x) + 28]⟩ }
7      t ~ Uniform(−1, 2);
8      { x < d ∧ t ≤ 2; ⟨[1,1], [2(d−x−t)+1, 2(d−x−t)+5],
9        [4(d−x−t)^2 + 10(d−x−t) − 3, 4(d−x−t)^2 + 26(d−x−t) + 37)]⟩ }
10     x := x + t;
11     { x < d + 2; ⟨[1,1], [2(d−x)+1, 2(d−x)+5],
12       [4(d−x)^2 + 10(d−x) − 3, 4(d−x)^2 + 26(d−x) + 37]⟩ }
13     call rdwalk;
14     { ⊤; ⟨[1,1], [1,1], [1,1]⟩ }
15     tick(1)
16     { ⊤; ⟨[1,1], [0,0], [0,0]⟩ }
17   fi
18 end
```

Fig. 5.7: The rdwalk function with annotations for the interval-bounds on the first and second moments.

Generating Linear Constraints Fig. 5.8 demonstrates the generation process for some of the bounds in Fig. 5.3. Let B_k be a vector of *monomials* over program variables VID of degree up to k. Then a polynomial $\sum_{b \in B_k} q_b \cdot b$, where $q_b \in \mathbb{R}$ for all $b \in B_k$, can be represented as a vector of its coefficients $(q_b)_{b \in B_k}$. I denote coefficient vectors by uppercase letters, while I use lowercase letters as names of the coefficients. I also assume that the degree of the polynomials for the k-th moments is up to k.

For (Q-Tick), I generate constraints that correspond to the composition operation $\otimes$ of the

$$\frac{\begin{array}{c} p_1^{tk} = u_1^{tk} \quad q_1^{tk} = u_1^{tk} + v_1^{tk} \quad q_x^{tk} = v_x^{tk} \quad q_N^{tk} = v_N^{tk} \quad q_r^{tk} = v_r^{tk} \\ t_1^{tk} = w_1^{tk} + 2v_1^{tk} + u_1^{tk} \quad t_x^{tk} = w_x^{tk} + 2v_x^{tk} \quad t_{x^2}^{tk} = w_{x^2}^{tk} \quad \cdots \end{array}}{\Delta \vdash \{\top; (P^{tk}, Q^{tk}, T^{tk})\}\ \mathbf{tick}(1)\ \{\top; (U^{tk}, V^{tk}, W^{tk})\}} \text{ (Q-Tick)}$$

$$\frac{\begin{array}{c} p_1^{sa} = u_1^{sa} \quad q_1^{sa} = v_1^{sa} + \frac{1}{2} \cdot v_r^{sa} \quad q_x^{sa} = v_x^{sa} \quad q_N^{sa} = v_N^{sa} \quad q_r^{sa} = 0 \\ t_1^{sa} = w_1^{sa} + \frac{1}{2} \cdot w_r^{sa} + 1 \cdot w_{r^2}^{sa} \quad t_x^{sa} = w_x^{sa} + \frac{1}{2} \cdot w_{r \cdot x}^{sa} \quad t_{x^2}^{sa} = w_{x^2}^{sa} \quad \cdots \end{array}}{\Delta \vdash \{x < N; (P^{sa}, Q^{sa}, T^{sa})\}\ r \sim \text{Uniform}(-1, 2)\ \{x < N \wedge r \leq 2; (U^{sa}, V^{sa}, W^{sa})\}} \text{ (Q-Sample)}$$

Fig. 5.8: Generate linear constraints, guided by inference rules.

moment semiring. For example, the second-moment component should satisfy

$$\begin{aligned}
&\sum_{b\in B_2} t_b^{tk}\cdot b\\
&= \text{the second-moment component of } \big((1,1,1)\otimes(\sum_{b\in B_0} u_b^{tk}\cdot b, \sum_{b\in B_1} v_b^{tk}\cdot b, \sum_{b\in B_2} w_b^{tk}\cdot b)\big)\\
&= \sum_{b\in B_2} w_b^{tk}\cdot b + 2\cdot\sum_{b\in B_1} v_b^{tk}\cdot b + \sum_{b\in B_0} u_b^{tk}\cdot b.
\end{aligned}$$

Then we extract $t_1^{tk} = w_1^{tk} + 2v_1^{tk} + u_1^{tk}$ for $b = 1$, and $t_x^{tk} = w_x^{tk} + 2v_x^{tk}$ for $b = x$, etc. For (Q-Sample), I generate constraints to perform "partial evaluation" on the polynomials by substituting r with the moments of $\textsc{Uniform}(-1,2)$. As I discussed in §5.2.3, let D denote $\textsc{Uniform}(-1,2)$, then $\mathbb{E}_{r\sim D}[w_r^{sa}\cdot r] = w_r^{sa}\cdot\mathbb{E}_{r\sim D}[r] = \frac{1}{2}\cdot w_r^{sa}$, $\mathbb{E}_{r\sim D}[w_{r^2}^{sa}\cdot r^2] = w_{r^2}^{sa}\cdot\mathbb{E}_{r\sim D}[r^2] = 1\cdot w_{r^2}^{sa}$. Then we generate a constraint $t_1^{sa} = w_1^{sa} + \frac{1}{2}\cdot w_r^{sa} + 1\cdot w_{r^2}^{sa}$ for t_1^{sa}.

The loop rule (Q-Loop) involves constructing loop *invariants* Q, which is in general a nontrivial problem for automated static analysis. Instead of computing the loop invariant Q explicitly, my system represents Q directly as a template with unknown coefficients, then uses Q as the post-annotation to analyze the loop body and obtain a pre-annotation, and finally generates linear constraints that indicate the pre-annotation equals to Q.

The structural rule (Q-Weaken) can be applied at any point during the derivation. In my implementation, I apply it where the control flow has a branch, because different branches might have different costs. To handle the judgment $\Gamma \models Q \sqsupseteq Q'$, i.e., to generate constraints that ensure one interval is always contained in another interval, where the ends of the intervals are polynomials, I adapt the idea of *rewrite functions* [21, 124]. Intuitively, to ensure that $[L_1, U_1] \sqsupseteq [L_2, U_2]$, i.e., $L_1 \le L_2$ and $U_2 \le U_1$, under the logical context Γ, I generate constraints indicating that there exist two polynomials T_1, T_2 that are always nonnegative under Γ, such that $L_1 = L_2 + T_1$ and $U_1 = U_2 - T_2$. Here, T_1 and T_2 are like slack variables, except that because all quantities are polynomials, they are too (i.e., slack polynomials). In my implementation, Γ is a set of linear constraints over program variables of the form $\mathcal{E} \ge 0$, then I can represent T_1, T_2 by *conical* combinations (i.e., linear combinations with nonnegative scalars) of expressions $\mathcal{E}$ in Γ.

Solving Linear Constraints The LP solver not only finds assignments to the coefficients that satisfy the constraints, it can also optimize a linear objective function. In the central-moment analysis, I construct an objective function that tries to minimize imprecision. For example, let us consider upper bounds on the variance. I randomly pick a concrete valuation of program variables that satisfies the pre-condition (e.g., $d > 0$ in Fig. 5.2), and then substitute program variables with the concrete valuation in the polynomial for the upper bound on the variance (obtained from bounds on the raw moments). The resulting linear combination of coefficients, which I set as the objective function, stands for the variance under the concrete valuation. Thus, minimizing the objective function produces the most precise upper bound on the variance under the specific concrete valuation. Also, I can extract a *symbolic* upper bound on the variance using the assignments to the coefficients. Because the derivation of the bounds only uses the given pre-condition, the symbolic bounds apply to all valuations of program variables that satisfy the pre-condition.

5.3 Soundness of Higher-Moment Analysis

In this section, I study the soundness of the derivation system for higher-moment analysis. I first present a small-step operational cost semantics for the probabilistic programming language (§5.3.1). I then develop a Markov-chain semantics to reason about how *stepwise* costs contribute to the *global* accumulated cost (§5.3.2). With the Markov-chain semantics, I formulate higher-moment analysis with respect to the semantics and prove the soundness of my derivation system for higher-moment analysis based on a recent extension to the *Optional Stopping Theorem* (§5.3.3). Finally, I sketch the algorithmic approach for ensuring the soundness of my analysis (§5.3.4).

5.3.1 A Small-Step Operational Semantics

I start with a small-step operational semantics with continuations, which I will use later to construct the Markov-chain semantics. Similarly to §2.3, I follow a distribution-based approach [16, 98] to define an operational cost semantics. A probabilistic semantics steps a program configuration to a probability distribution on configurations. A *program configuration* $\sigma \in \Sigma$ is a quadruple $\langle \gamma, S, K, \alpha \rangle$ where $\gamma : \mathsf{VID} \to \mathbb{R}$ is a program state that maps variables to values, S is the statement being executed, K is a continuation that describes what remains to be done after the execution of S, and $\alpha \in \mathbb{R}$ is the global cost accumulator. To describe these distributions formally, I need to construct a measurable space of program configurations. My approach is to construct a measurable space for each of the four components of configurations, and then use their product measurable space as the semantic domain.

- Valuations $\gamma : \mathsf{VID} \to \mathbb{R}$ are finite real-valued maps, so I define $(V, \mathcal{V}) \stackrel{\text{def}}{=} (\mathbb{R}^{\mathsf{VID}}, \mathcal{B}(\mathbb{R}^{\mathsf{VID}}))$ as the canonical structure on a finite-dimensional space.

- The executing statement S can contain real numbers, so I need to "lift" the Borel σ-algebra on $\mathbb{R}$ to program statements. Intuitively, statements with exactly the same structure can be treated as vectors of parameters that correspond to their real-valued components. Formally, I achieve this by constructing a metric space on statements and then extracting a Borel σ-algebra from the metric space. Fig. 5.9 presents an inductively defined metric d_S on statements, as well as metrics d_E, d_L, and d_D on expressions, conditions, and distributions, respectively, as they are required by d_S. I denote the result measurable space by $(S, \mathcal{S})$.

- A *continuation* K is either an empty continuation **Kstop**, a loop continuation **Kloop** $L\ S\ K$, or a sequence continuation **Kseq** $S\ K$. Similarly, I construct a measurable space $(K, \mathcal{K})$ on continuations by extracting from a metric space. Fig. 5.9 shows the definition of a metric d_K on continuations.

- The cost accumulator $\alpha \in \mathbb{R}$ is a real number, so I define $(W, \mathcal{W}) \stackrel{\text{def}}{=} (\mathbb{R}, \mathcal{B}(\mathbb{R}))$ as the canonical measurable space on $\mathbb{R}$.

Then the semantic domain is defined as the product measurable space of the four components: $(\Sigma, \mathcal{O}) \stackrel{\text{def}}{=} (V, \mathcal{V}) \otimes (S, \mathcal{S}) \otimes (K, \mathcal{K}) \otimes (W, \mathcal{W})$.

An execution of an Appl program $\langle \mathscr{D}, S_{\mathsf{main}} \rangle$ is initialized with $\langle \lambda\_.0, S_{\mathsf{main}}, \mathbf{Kstop}, 0 \rangle$, and the termination configurations have the form $\langle \_, \mathbf{skip}, \mathbf{Kstop}, \_ \rangle$. Different from a standard semantics

$$d_E(x, x) \stackrel{\text{def}}{=} 0$$

$$d_E(c_1, c_2) \stackrel{\text{def}}{=} |c_1 - c_2|$$

$$d_E(E_{11} + E_{12}, E_{21} + E_{22}) \stackrel{\text{def}}{=} d_E(E_{11}, E_{21}) + d_E(E_{12}, E_{22})$$

$$d_E(E_{11} \times E_{12}, E_{21} \times E_{22}) \stackrel{\text{def}}{=} d_E(E_{11}, E_{21}) + d_E(E_{12}, E_{22})$$

$$d_E(E_1, E_2) \stackrel{\text{def}}{=} \infty \text{ otherwise}$$

$$d_L(\textbf{true}, \textbf{true}) \stackrel{\text{def}}{=} 0$$

$$d_L(\textbf{not } L_1, \textbf{not } L_2) \stackrel{\text{def}}{=} d_L(L_1, L_2)$$

$$d_L(L_{11} \textbf{ and } L_{12}, L_{21} \textbf{ and } L_{22}) \stackrel{\text{def}}{=} d_L(L_{11}, L_{21}) + d_L(L_{12}, L_{22})$$

$$d_L(E_{11} \leq E_{12}, E_{21} \leq E_{22}) \stackrel{\text{def}}{=} d_E(E_{11}, E_{21}) + d_E(E_{12}, E_{22})$$

$$d_L(L_1, L_2) \stackrel{\text{def}}{=} \infty \text{ otherwise}$$

$$d_D(\textsc{Uniform}(a_1, b_1), \textsc{Uniform}(a_2, b_2)) \stackrel{\text{def}}{=} |a_1 - a_2| + |b_1 - b_2|$$

$$d_D(D_1, D_2) \stackrel{\text{def}}{=} \infty \text{ otherwise}$$

$$d_S(\textbf{skip}, \textbf{skip}) \stackrel{\text{def}}{=} 0$$

$$d_S(\textbf{tick}(c_1), \textbf{tick}(c_2)) \stackrel{\text{def}}{=} |c_1 - c_2|$$

$$d_S(x \coloneqq E_1, x \coloneqq E_2) \stackrel{\text{def}}{=} d_E(E_1, E_2)$$

$$d_S(x \sim D_1, x \sim D_2) \stackrel{\text{def}}{=} d_D(D_1, D_2)$$

$$d_S(\textbf{call } f, \textbf{call } f) \stackrel{\text{def}}{=} 0$$

$$d_S(\textbf{if prob}(p_1) \textbf{ then } S_{11} \textbf{ else } S_{12} \textbf{ fi}, \textbf{if prob}(p_2) \textbf{ then } S_{21} \textbf{ else } S_{22} \textbf{ fi}) \stackrel{\text{def}}{=} |p_1 - p_2| + d_S(S_{11}, S_{21}) + d_S(S_{12}, S_{22})$$

$$d_S(\textbf{if } L_1 \textbf{ then } S_{11} \textbf{ else } S_{12} \textbf{ fi}, \textbf{if } L_2 \textbf{ then } S_{21} \textbf{ else } S_{22} \textbf{ fi}) \stackrel{\text{def}}{=} d_L(L_1, L_2) + d_S(S_{11}, S_{21}) + d_S(S_{12}, S_{22})$$

$$d_S(\textbf{while } L_1 \textbf{ do } S_1 \textbf{ od}, \textbf{while } L_2 \textbf{ do } S_2 \textbf{ od}) \stackrel{\text{def}}{=} d_L(L_1, L_2) + d_S(S_1, S_2)$$

$$d_S(S_{11}; S_{12}, S_{21}; S_{22}) \stackrel{\text{def}}{=} d_S(S_{11}, S_{21}) + d_S(S_{12}, S_{22})$$

$$d_S(S_1, S_2) \stackrel{\text{def}}{=} \infty \text{ otherwise}$$

$$d_K(\textbf{Kstop}, \textbf{Kstop}) \stackrel{\text{def}}{=} 0$$

$$d_K(\textbf{Kloop } L_1\ S_1\ K_1, \textbf{Kloop } L_2\ S_2\ K_2) \stackrel{\text{def}}{=} d_L(L_1, L_2) + d_S(S_1, S_2) + d_K(K_1, K_2)$$

$$d_K(\textbf{Kseq } S_1\ K_1, \textbf{Kseq } S_2\ K_2) \stackrel{\text{def}}{=} d_S(S_1, S_2) + d_K(K_1, K_2)$$

$$d_K(K_1, K_2) \stackrel{\text{def}}{=} \infty \text{ otherwise}$$

Fig. 5.9: Metrics for expressions, conditions, distributions, statements, and continuations.

where each program configuration steps to at most one new configuration, a probabilistic semantics may pick several different new configurations. The evaluation relation has the form $\sigma \mapsto \mu$ where $\mu \in \mathbb{D}(\Sigma)$ is a probability measure over configurations. Fig. 5.10 presents the rules of the evaluation relation. Note that expressions E and conditions L are deterministic, so I define a standard big-step evaluation relation for them, written $\gamma \vdash E \Downarrow r$ and $\gamma \vdash L \Downarrow b$, where γ is a valuation, $r \in \mathbb{R}$, and $b \in \{\top, \bot\}$. Most of the rules in Fig. 5.10, except (E-Sample) and (E-Prob), are also deterministic as they step to a Dirac measure. The rule (E-Prob) constructs a distribution whose support has exactly two elements, which stand for the two branches of the probabilistic choice. The rule (E-Sample) "pushes" the probability distribution of D to a distribution over post-sampling program configurations.

Example 5.11. Suppose that a random sampling statement is being executed, i.e., the current configuration is

$$\langle \{t \mapsto t_0\}, (t \sim \textsc{Uniform}(-1, 2)), K_0, \alpha_0 \rangle.$$

The probability measure for the uniform distribution is $\lambda O. \int_O \frac{[-1 \le x \le 2]}{3} dx$. *Thus, by the rule (E-Sample), we derive the post-sampling probability measure over configurations as* $\lambda A. \int_{\mathbb{R}} [\langle \{t \mapsto r\}, \textbf{skip}, K_0, \alpha_0 \rangle \in A] \cdot \frac{[-1 \le r \le 2]}{3} dr$.

5.3.2 A Markov-Chain Semantics

In this section, I harness Markov-chain-based reasoning [85, 126] to develop a Markov-chain cost semantics, based on the evaluation relation $\sigma \mapsto \mu$. An advantage of this approach is that it allows me to study how the cost of every single evaluation step contributes to the accumulated cost at the exit of the program and later adapt Optional Stopping Theorems to reason about soundness in §5.3.3.

First, I prove that the evaluation relation $\mapsto$ can be interpreted as a probability kernel.

Lemma 5.12. *Let* $\gamma : \mathsf{VID} \to \mathbb{R}$ *be a valuation.*

- *Let E be an expression. Then there exists a unique $r \in \mathbb{R}$ such that $\gamma \vdash E \Downarrow r$.*
- *Let L be a condition. Then there exists a unique $b \in \{\top, \bot\}$ such that $\gamma \vdash L \Downarrow b$.*

Proof. By induction on the structure of E and L. □

Lemma 5.13. *For every configuration $\sigma \in \Sigma$, there exists a unique $\mu \in \mathbb{D}(\Sigma, O)$ such that $\sigma \mapsto \mu$.*

Proof. Let $\sigma = \langle \gamma, S, K, \alpha \rangle$. Then by case analysis on the structure of S, followed by a case analysis on the structure of K when $S = \textbf{skip}$. The rest of the proof appeals to Lemma 5.12. □

Theorem 5.14. *The evaluation relation $\mapsto$ defines a probability kernel on program configurations.*

Proof. Lemma 5.13 tells me that $\mapsto$ can be seen as a function $\hat{\mapsto}$ defined as follows:

$$\hat{\mapsto}(\sigma, A) \stackrel{\text{def}}{=} \mu(A) \quad \text{where} \quad \sigma \mapsto \mu.$$

$\boxed{\gamma \vdash E \Downarrow r}$ "the expression E evaluates to a real value r under the valuation γ"

$$\text{(E-Var)}\ \frac{\gamma(x) = r}{\gamma \vdash x \Downarrow r} \qquad \text{(E-Const)}\ \frac{}{\gamma \vdash c \Downarrow c} \qquad \text{(E-Add)}\ \frac{\gamma \vdash E_1 \Downarrow r_1 \qquad \gamma \vdash E_2 \Downarrow r_2 \qquad r = r_1 + r_2}{\gamma \vdash E_1 + E_2 \Downarrow r}$$

$$\text{(E-Mul)}\ \frac{\gamma \vdash E_1 \Downarrow r_1 \qquad \gamma \vdash E_2 \Downarrow r_2 \qquad r = r_1 \cdot r_2}{\gamma \vdash E_1 \times E_2 \Downarrow r}$$

$\boxed{\gamma \vdash L \Downarrow b}$ "the condition L evaluates to a Boolean value b under the valuation γ"

$$\text{(E-Top)}\ \frac{}{\gamma \vdash \textbf{true} \Downarrow \top} \qquad \text{(E-Neg)}\ \frac{\gamma \vdash L \Downarrow b}{\gamma \vdash \textbf{not}\ L \Downarrow \neg b} \qquad \text{(E-Conj)}\ \frac{\gamma \vdash L_1 \Downarrow b_1 \qquad \gamma \vdash L_2 \Downarrow b_2}{\gamma \vdash L_1\ \textbf{and}\ L_2 \Downarrow b_1 \wedge b_2} \qquad \text{(E-Le)}\ \frac{\gamma \vdash E_1 \Downarrow r_1 \qquad \gamma \vdash E_2 \Downarrow r_2}{\gamma \vdash E_1 \leq E_2 \Downarrow [r_1 \leq r_2]}$$

$\boxed{\langle \gamma, S, K, \alpha \rangle \mapsto \mu}$ "the configuration $\langle \gamma, S, K, \alpha \rangle$ steps to a probability distribution μ on $\langle \gamma', S', K', \alpha' \rangle$'s"

$$\text{(E-Skip-Stop)}\ \frac{}{\langle \gamma, \textbf{skip}, \textbf{Kstop}, \alpha \rangle \mapsto \delta(\langle \gamma, \textbf{skip}, \textbf{Kstop}, \alpha \rangle)}$$

$$\text{(E-Skip-Loop)}\ \frac{\gamma \vdash L \Downarrow b}{\langle \gamma, \textbf{skip}, \textbf{Kloop}\ S\ L\ K, \alpha \rangle \mapsto [b] \cdot \delta(\langle \gamma, S, \textbf{Kloop}\ S\ L\ K, \alpha \rangle) + [\neg b] \cdot \delta(\langle \gamma, \textbf{skip}, K, \alpha \rangle)}$$

$$\text{(E-Skip-Seq)}\ \frac{}{\langle \gamma, \textbf{skip}, \textbf{Kseq}\ S\ K, \alpha \rangle \mapsto \delta(\langle \gamma, S, K, \alpha \rangle)} \qquad \text{(E-Tick)}\ \frac{}{\langle \gamma, \textbf{tick}(c), K, \alpha \rangle \mapsto \delta(\langle \gamma, \textbf{skip}, K, \alpha + c \rangle)}$$

$$\text{(E-Assign)}\ \frac{\gamma \vdash E \Downarrow r}{\langle \gamma, x \coloneqq E, K, \alpha \rangle \mapsto \delta(\langle \gamma[x \mapsto r], \textbf{skip}, K, \alpha \rangle)} \qquad \text{(E-Sample)}\ \frac{}{\langle \gamma, x \sim D, K, \alpha \rangle \mapsto \mu_D \gg\!= \lambda r.\delta(\langle \gamma[x \mapsto r], \textbf{skip}, K, \alpha \rangle)}$$

$$\text{(E-Call)}\ \frac{}{\langle \gamma, \textbf{call}\ f, K, \alpha \rangle \mapsto \delta(\langle \gamma, \mathscr{D}(f), K, \alpha \rangle)}$$

$$\text{(E-Prob)}\ \frac{}{\langle \gamma, \textbf{if}\ \textbf{prob}(p)\ \textbf{then}\ S_1\ \textbf{else}\ S_2\ \textbf{fi}, K, \alpha \rangle \mapsto p \cdot \delta(\langle \gamma, S_1, K, \alpha \rangle) + (1-p) \cdot \delta(\langle \gamma, S_2, K, \alpha \rangle)}$$

$$\text{(E-Cond)}\ \frac{\gamma \vdash L \Downarrow b}{\langle \gamma, \textbf{if}\ L\ \textbf{then}\ S_1\ \textbf{else}\ S_2\ \textbf{fi}, K, \alpha \rangle \mapsto [b] \cdot \delta(\langle \gamma, S_1, K, \alpha \rangle) + [\neg b] \cdot \delta(\langle \gamma, S_2, K, \alpha \rangle)}$$

$$\text{(E-Loop)}\ \frac{}{\langle \gamma, \textbf{while}\ L\ \textbf{do}\ S\ \textbf{od}, K, \alpha \rangle \mapsto \delta(\langle \gamma, \textbf{skip}, \textbf{Kloop}\ L\ S\ K, \alpha \rangle)} \qquad \text{(E-Seq)}\ \frac{}{\langle \gamma, S_1; S_2, K, \alpha \rangle \mapsto \delta(\langle \gamma, S_1, \textbf{Kseq}\ S_2\ K, \alpha \rangle)}$$

Fig. 5.10: Rules of the operational semantics of Appl.

It is clear that $\lambda A.\hat{\mapsto}(\sigma, A)$ is a probability measure. On the other hand, to show that $\lambda\sigma.\hat{\mapsto}(\sigma, A)$ is measurable for any $A \in \mathcal{O}$, we need to prove that for $B \in \mathcal{B}(\mathbb{R})$, it holds that $\mathcal{O}(A, B) \overset{\text{def}}{=} (\lambda\sigma.\hat{\mapsto}(\sigma, A))^{-1}(B) \in \mathcal{O}$.

We introduce *skeletons* of programs to separate real numbers from discrete structures.

$$
\begin{aligned}
\hat{S} &::= \textbf{skip} \mid \textbf{tick}(\square_\ell) \mid x \coloneqq \hat{E} \mid x \sim \hat{D} \mid \textbf{call}\ f \mid \textbf{while}\ \hat{L}\ \textbf{do}\ \hat{S}\ \textbf{od} \\
&\quad \mid \textbf{if}\ \textbf{prob}(\square_\ell)\ \textbf{then}\ \hat{S}_1\ \textbf{else}\ \hat{S}_2\ \textbf{fi} \mid \textbf{if}\ \hat{L}\ \textbf{then}\ \hat{S}_1\ \textbf{else}\ \hat{S}_2\ \textbf{fi} \mid \hat{S}_1; \hat{S}_2 \\
\hat{L} &::= \textbf{true} \mid \textbf{not}\ \hat{L} \mid \hat{L}_1\ \textbf{and}\ \hat{L}_2 \mid \hat{E}_1 \le \hat{E}_2 \\
\hat{E} &::= x \mid \square_\ell \mid \hat{E}_1 + \hat{E}_2 \mid \hat{E}_1 \times \hat{E}_2 \\
\hat{D} &::= \textsc{Uniform}(\square_{\ell_a}, \square_{\ell_b}) \mid \cdots \\
\hat{K} &::= \textbf{Kstop} \mid \textbf{Kloop}\ \hat{L}\ \hat{S}\ \hat{K} \mid \textbf{Kseq}\ \hat{S}\ \hat{K}
\end{aligned}
$$

The *holes* $\square_\ell$ are placeholders for real numbers parameterized by *locations* $\ell \in \mathsf{LOC}$. We assume that the holes in a program structure are always pairwise distinct. Let $\eta : \mathsf{LOC} \to \mathbb{R}$ be a map from holes to real numbers and $\eta(\hat{S})$ (resp., $\eta(\hat{L})$, $\eta(\hat{E})$, $\eta(\hat{D})$, $\eta(\hat{K})$) be the instantiation of a statement (resp., condition, expression, distribution, continuation) skeleton by substituting $\eta(\ell)$ for $\square_\ell$. One important property of skeletons is that the "distance" between any concretizations of two different skeletons is always infinity with respect to the metrics in Fig. 5.9.

Observe that

$$
\mathcal{O}(A, B) = \bigcup_{\hat{S}, \hat{K}} \mathcal{O}(A, B) \cap \{\langle \gamma, \eta(\hat{S}), \eta(\hat{K}), \alpha\rangle \mid \text{any } \gamma, \alpha, \eta\}
$$

and that $\hat{S}, \hat{K}$ are countable families of statement and continuation skeletons. Thus it suffices to prove that every set in the union, which we denote by $\mathcal{O}(A, B) \cap \mathscr{C}(\hat{S}, \hat{K})$ later in the proof, is measurable. Note that $\mathscr{C}(\hat{S}, \hat{K})$ itself is indeed measurable. Further, the skeletons $\hat{S}$ and $\hat{K}$ are able to determine the evaluation rule for all concretized configurations. Thus we can proceed by a case analysis on the evaluation rules.

To aid the case analysis, we define a deterministic evaluation relation $\overset{\text{det}}{\longmapsto}$ by getting rid of the $\delta(\cdot)$ notations in the rules in Fig. 5.10 except probabilistic ones (E-Sample) and (E-Prob). Obviously, $\overset{\text{det}}{\longmapsto}$ can be interpreted as a measurable function on configurations.

- If the evaluation rule is deterministic, then we have

$$
\begin{aligned}
\mathcal{O}(A, B) \cap \mathscr{C}(\hat{S}, \hat{K}) &= \{\sigma \mid \sigma \mapsto \mu, \mu(A) \in B\} \cap \mathscr{C}(\hat{S}, \hat{K}) \\
&= \{\sigma \mid \sigma \overset{\text{det}}{\longmapsto} \sigma', [\sigma' \in A] \in B\} \cap \mathscr{C}(\hat{S}, \hat{K}) \\
&= \begin{cases}
\mathscr{C}(\hat{S}, \hat{K}) & \text{if } \{0, 1\} \subseteq B, \\
\overset{\text{det}}{\longmapsto}^{-1}(A) \cap \mathscr{C}(\hat{S}, \hat{K}) & \text{if } 1 \in B \text{ and } 0 \notin B, \\
\overset{\text{det}}{\longmapsto}^{-1}(A^c) \cap \mathscr{C}(\hat{S}, \hat{K}) & \text{if } 0 \in B \text{ and } 1 \notin B, \\
\emptyset & \text{if } \{0, 1\} \cap B = \emptyset.
\end{cases}
\end{aligned}
$$

The sets in all the cases are measurable, so is the set $\mathcal{O}(A, B) \cap \mathscr{C}(\hat{S}, \hat{K})$.

- Rule (E-Prob): Consider B with the form $(-\infty, t]$ with $t \in \mathbb{R}$. If $t \geq 1$, then $\mathcal{O}(A, B) = \Sigma$. Otherwise, let us assume $t < 1$. Let $\hat{S} =$ **if prob**$(\square)$ **then** $\hat{S}_1$ **else** $\hat{S}_2$ **fi**. Then we have

$$\begin{aligned}
\mathcal{O}(A,B) \cap \mathscr{C}(\hat{S},\hat{K}) &= \{\sigma \mid \sigma \mapsto \mu, \mu(A) \in B\} \cap \mathscr{C}(\hat{S},\hat{K}) \\
&= \{\sigma \mid \sigma \mapsto p \cdot \delta(\sigma_1) + (1-p) \cdot \delta(\sigma_2), \\
&\qquad p \cdot [\sigma_1 \in A] + (1-p) \cdot [\sigma_2 \in A] \in B\} \cap \mathscr{C}(\hat{S},\hat{K}) \\
&= \mathscr{C}(\hat{S},\hat{K}) \cap \{\langle \gamma, \textbf{if prob}(p) \textbf{ then } S_1 \textbf{ else } S_2 \textbf{ fi}, K, \alpha\rangle \mid \\
&\qquad p \cdot [\langle \gamma, S_1, K, \alpha\rangle \in A] + (1-p) \cdot [\langle \gamma, S_2, K, \alpha\rangle \in A] \leq t\} \\
&= \mathscr{C}(\hat{S},\hat{K}) \cap \\
&\quad \{\langle \gamma, \textbf{if prob}(p) \textbf{ then } S_1 \textbf{ else } S_2 \textbf{ fi}, K, \alpha\rangle \mid \\
&\qquad (\langle \gamma, S_1, K, \alpha\rangle \in A, \langle \gamma, S_2, K, \alpha\rangle \notin A, p \leq t) \vee \\
&\qquad (\langle \gamma, S_2, K, \alpha\rangle \in A, \langle \gamma, S_1, K, \alpha\rangle \notin A, 1-p \leq t)\}.
\end{aligned}$$

  The set above is measurable because A and A^c (i.e., the complement of A) are measurable, as well as $\{p \mid p \leq t\}$ and $\{p \mid p \geq 1-t\}$ are measurable in $\mathbb{R}$.

- Rule (E-Sample): Consider B with the form $(-\infty, t]$ with $t \in \mathbb{R}$. Similar to the previous case, we assume that $t < 1$. Let $\hat{S} = x \sim \textsc{Uniform}(\square_{\ell_a}, \square_{\ell_b})$, without loss of generality. Then we have

$$\begin{aligned}
\mathcal{O}(A,B) \cap \mathscr{C}(\hat{S},\hat{K}) &= \{\sigma \mid \sigma \mapsto \mu, \mu(A) \in B\} \cap \mathscr{C}(\hat{S},\hat{K}) \\
&= \{\sigma \mid \sigma \mapsto \mu_D \gg\!= \kappa_\sigma, \int \kappa_\sigma(r)(A)\mu_D(dr) \leq t\} \cap \mathscr{C}(\hat{S},\hat{K}) \\
&= \mathscr{C}(\hat{S},\hat{K}) \cap \{\sigma \mid \sigma \mapsto \mu_D \gg\!= \kappa_\sigma, \\
&\qquad \mu_D(\{r \mid \langle \gamma[x \mapsto r], \textbf{skip}, K, \alpha\rangle \in A\}) \leq t\} \\
&= \mathscr{C}(\hat{S},\hat{K}) \cap \{\langle \gamma, x \sim \textbf{uniform}(a,b), K, \alpha\rangle \mid a < b, \\
&\qquad \mu_{\textsc{Uniform}(a,b)}(\{r \mid \langle \gamma[x \mapsto r], \textbf{skip}, K, \alpha\rangle \in A\}) \leq t\},
\end{aligned}$$

  where $\kappa_{\langle \gamma, S, K, \alpha\rangle} \stackrel{\text{def}}{=} \lambda r.\delta(\langle \gamma[x \mapsto r], \textbf{skip}, K, \alpha\rangle)$. For fixed γ, K, α, the set $\{r \mid \langle \gamma[x \mapsto r], \textbf{skip}, K, \alpha\rangle \in A\}$ is measurable in $\mathbb{R}$. For the distributions considered in this chapter, there is a sub-probability kernel $\kappa_D : \mathbb{R}^{\text{ar}(D)} \rightsquigarrow \mathbb{R}$, where $\text{ar}(D)$ is the number of parameters of D. For example, $\kappa_{\textsc{Uniform}}(a,b)$ is defined to be $\mu_{\textsc{Uniform}(a,b)}$ if $a < b$, or $\mathbf{0}$ otherwise. Therefore, $\lambda(a,b).\kappa_{\textsc{Uniform}}(a,b)(\{r \mid \langle \gamma[x \mapsto r], \textbf{skip}, K, \alpha\rangle \in A\})$ is measurable, and its inversion on $(-\infty, t]$ is a measurable set on distribution parameters (a,b). Hence the set above is measurable.

□

I now review a standard mechanism in measure theory that constructs a probability measure by composing probability kernels. If μ is a probability measure on $(S, \mathcal{S})$ and $\kappa : (S, \mathcal{S}) \rightsquigarrow (T, \mathcal{T})$ is a probability kernel, then we can construct the a probability measure on $(S, \mathcal{S}) \otimes (T, \mathcal{T})$ that captures all transitions from μ through κ: $\mu \otimes \kappa \stackrel{\text{def}}{=} \lambda(A,B).\int_A \kappa(x,B)\mu(dx)$. If μ is a probability measure on $(S_0, \mathcal{S}_0)$ and $\kappa_i : (S_{i-1}, \mathcal{S}_{i-1}) \rightsquigarrow (S_i, \mathcal{S}_i)$ is a probability kernel for $i = 1, \cdots, n$,where

$n \in \mathbb{Z}^+$, then we can construct a probability measure on $\bigotimes_{i=0}^{n}(S_i, \mathcal{S}_i)$, i.e., the space of sequences of n transitions by iteratively applying the kernels to μ:

$$\mu \otimes \bigotimes_{i=1}^{0} \kappa_i \stackrel{\text{def}}{=} \mu,$$
$$\mu \otimes \bigotimes_{i=1}^{k+1} \kappa_i \stackrel{\text{def}}{=} (\mu \otimes \bigotimes_{i=1}^{k} \kappa_i) \otimes \kappa_{k+1}, \qquad 0 \le k < n.$$

Let $(S_i, \mathcal{S}_i)$, $i \in \mathcal{I}$ be a family of measurable spaces. Their product, denoted by $\bigotimes_{i\in\mathcal{I}}(S_i, \mathcal{S}_i) = (\prod_{i\in\mathcal{I}} S_i, \bigotimes_{i\in\mathcal{I}} \mathcal{S}_i)$, is the product space with the smallest σ-algebra such that for each $i \in \mathcal{I}$, the coordinate map π_i is measurable. The theorem below is widely used to construct a probability measures on an infinite product via probability kernels.

Proposition 5.15 (Ionescu-Tulcea). *Let $(S_i, \mathcal{S}_i)$, $i \in \mathbb{Z}^+$ be a sequence of measurable spaces. Let μ_0 be a probability measure on $(S_0, \mathcal{S}_0)$. For each $i \in \mathbb{N}$, let $\kappa_i : \bigotimes_{k=0}^{i-1}(S_k, \mathcal{S}_k) \rightsquigarrow (S_i, \mathcal{S}_i)$ be a probability kernel. Then there exists a sequence of probability measures $\mu_i \stackrel{\text{def}}{=} \mu_0 \otimes \bigotimes_{k=1}^{i} \kappa_k$, $i \in \mathbb{Z}^+$, and there exists a uniquely defined probability measure μ on $\bigotimes_{k=0}^{\infty}(S_k, \mathcal{S}_k)$ such that $\mu_i(A) = \mu(A \times \prod_{k=i+1}^{\infty} S_k)$ for all $i \in \mathbb{Z}^+$ and $A \in \bigotimes_{k=0}^{i} \mathcal{S}_i$.*

Let $(\Omega, \mathcal{F}) \stackrel{\text{def}}{=} \bigotimes_{n=0}^{\infty}(\Sigma, O)$ be a measurable space of infinite traces on program configurations. Let $\{\mathcal{F}_n\}_{n\in\mathbb{Z}^+}$ be a filtration, i.e., an increasing sequence $\mathcal{F}_0 \subseteq \mathcal{F}_1 \subseteq \cdots \subseteq \mathcal{F}$ of sub-σ-algebras in $\mathcal{F}$, generated by coordinate maps $X_n(\omega) \stackrel{\text{def}}{=} \omega_n$ for $n \in \mathbb{Z}^+$. Let $\langle \mathscr{D}, S_{\mathsf{main}} \rangle$ be an Appl program. Let $\mu_0 \stackrel{\text{def}}{=} \delta(\langle \lambda\_.0, S_{\mathsf{main}}, \mathbf{Kstop}, 0 \rangle)$ be the initial distribution. Let $\mathbb{P}$ be the probability measure on infinite traces induced by Proposition 5.15 and Theorem 5.14. Then $(\Omega, \mathcal{F}, \mathbb{P})$ forms a probability space on *infinite* traces of the program. Intuitively, $\mathbb{P}$ specifies the probability distribution over all possible executions of a probabilistic program. The probability of an assertion θ with respect to $\mathbb{P}$, written $\mathbb{P}[\theta]$, is defined as $\mathbb{P}(\{\omega \mid \theta(\omega) \text{ is true}\})$.

To formulate the accumulated cost at the exit of the program, I define the *stopping time* $T : \Omega \to \mathbb{Z}^+ \cup \{\infty\}$ of a probabilistic program as a random variable on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ of program traces:

$$T(\omega) \stackrel{\text{def}}{=} \inf\{n \in \mathbb{Z}^+ \mid \omega_n = \langle \_, \mathbf{skip}, \mathbf{Kstop}, \_ \rangle\},$$

i.e., $T(\omega)$ is the number of evaluation steps before the trace ω reaches some termination configuration $\langle \_, \mathbf{skip}, \mathbf{Kstop}, \_ \rangle$. I define the accumulated cost $A_T : \Omega \to \mathbb{R}$ with respect to the stopping time T as

$$A_T(\omega) \stackrel{\text{def}}{=} A_{T(\omega)}(\omega),$$

where $A_n : \Omega \to \mathbb{R}$ captures the accumulated cost at the n-th evaluation step for $n \in \mathbb{Z}^+$, which is defined as

$$A_n(\omega) \stackrel{\text{def}}{=} \alpha_n \text{ where } \omega_n = \langle \_, \_, \_, \alpha_n \rangle.$$

The m-th moment of the accumulated cost is given by the expectation $\mathbb{E}[A_T^m]$ with respect to $\mathbb{P}$.

5.3.3 Soundness of the Derivation System

The Expected-Potential Method for Moment Analysis I fix a degree $m \in \mathbb{N}$ and let $\mathcal{M}_{\mathcal{I}}^{(m)}$ be the m-th order moment semiring instantiated with the interval semiring $\mathcal{I}$. I now formally define $\mathcal{M}_{\mathcal{I}}^{(m)}$-valued expected-potential functions.

Definition 5.16. A measurable map $\phi : \Sigma \to \mathcal{M}_{\mathcal{I}}^{(m)}$ is said to be an *expected-potential function* if

(i) $\phi(\sigma) = \underline{1}$ if $\sigma = \langle \_, \mathbf{skip}, \mathbf{Kstop}, \_ \rangle$, and

(ii) $\phi(\sigma) \sqsupseteq \mathbb{E}_{\sigma' \sim \mapsto(\sigma)}[\overrightarrow{\left([(\alpha' - \alpha)^k, (\alpha' - \alpha)^k]\right)_{0 \le k \le m}} \otimes \phi(\sigma')]$ where $\sigma = \langle \_, \_, \_, \alpha \rangle, \sigma' = \langle \_, \_, \_, \alpha' \rangle$ for all $\sigma \in \Sigma$.

Intuitively, $\phi(\sigma)$ is an interval bound on the moments for the accumulated cost of the computation that *continues from* the configuration σ. I define $\mathbf{\Phi}_n$ and $\mathbf{Y}_n$, where $n \in \mathbb{Z}^+$, to be $\mathcal{M}_{\mathcal{I}}^{(m)}$-valued random variables on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ of the Markov-chain semantics as

$$\mathbf{\Phi}_n(\omega) \stackrel{\text{def}}{=} \phi(\omega_n), \mathbf{Y}_n(\omega) \stackrel{\text{def}}{=} \overrightarrow{\langle [A_n(\omega)^k, A_n(\omega)^k] \rangle_{0 \le k \le m}} \otimes \mathbf{\Phi}_n(\omega).$$

In the definition of $\mathbf{Y}_n$, I use $\otimes$ to compose the powers of the accumulated cost at step n and the expected potential function that stands for the moments of the accumulated cost for the rest of the computation.

Lemma 5.17. *By the properties of potential functions, we can prove that* $\mathbb{E}[\mathbf{Y}_{n+1} \mid \mathbf{Y}_n] \sqsubseteq \mathbf{Y}_n$ *almost surely, for all* $n \in \mathbb{Z}^+$.

To prove Lemma 5.17, I first investigate several properties of the interval-valued moment semiring. I show that $\otimes$ and $\oplus$ are monotone if the operations of the underlying semiring are monotone.

Lemma 5.18. *Let* $\mathcal{R} = (|\mathcal{R}|, \le, +, \cdot, 0, 1)$ *be a partially ordered semiring. If* $+$ *and* $\cdot$ *are monotone with respect to* $\le$*, then* $\otimes$ *and* $\oplus$ *in the moment semiring* $\mathcal{M}_{\mathcal{R}}^{(m)}$ *are also monotone with respect to* $\sqsubseteq$.

Proof. It is straightforward to show $\oplus$ is monotone. For the rest of the proof, without loss of generality, we show that $\overrightarrow{\langle u_k \rangle_{0 \le k \le m}} \otimes \overrightarrow{\langle v_k \rangle_{0 \le k \le m}} \sqsubseteq \overrightarrow{\langle u_k \rangle_{0 \le k \le m}} \otimes \overrightarrow{\langle w_k \rangle_{0 \le k \le m}}$ if $\overrightarrow{\langle v_k \rangle_{0 \le k \le m}} \sqsubseteq \overrightarrow{\langle w_k \rangle_{0 \le k \le m}}$. By the definition of $\sqsubseteq$, we know that $v_k \le w_k$ for all $k = 0, 1, \cdots, m$. Then for each k, we have

$$\begin{aligned}
(\overrightarrow{\langle u_k \rangle_{0 \le k \le m}} \otimes \overrightarrow{\langle v_k \rangle_{0 \le k \le m}})_k &= \sum_{i=0}^{k} \binom{k}{i} \times (u_i \cdot v_{k-i}) \\
&\le \sum_{i=0}^{k} \binom{k}{i} \times (u_i \cdot w_{k-i}) \\
&= (\overrightarrow{\langle u_k \rangle_{0 \le k \le m}} \otimes \overrightarrow{\langle w_k \rangle_{0 \le k \le m}})_k.
\end{aligned}$$

Then we conclude by the definition of $\sqsubseteq$. □

As I allow potential functions to be *interval*-valued, I show that the interval semiring $\mathcal{I}$ satisfies the monotonicity required in Lemma 5.18.

Lemma 5.19. *The operations* $+_{\mathcal{I}}$ *and* $\cdot_{\mathcal{I}}$ *are monotone with respect to* $\le_{\mathcal{I}}$.

Proof. It is straightforward to show $+_{\mathcal{I}}$ is monotone. For the rest of the proof, it suffices to show that $[a, b] \cdot_{\mathcal{I}} [c, d] \le_{\mathcal{I}} [a', b'] \cdot_{\mathcal{I}} [c, d]$ if $[a, b] \le_{\mathcal{I}} [a', b']$, i.e., $[a, b] \subseteq [a', b']$ or $a \ge a', b \le b'$.

We claim that $\min S_{a,b,c,d} \ge \min S_{a',b',c,d}$, i.e., $\min\{ac, ad, bc, bd\} \ge \min\{a'c, a'd, b'c, b'd\}$.

- If $0 \le c \le d$: Then $ac \le bc$, $ad \le bd$, $a'c \le b'c$, $a'd \le b'd$. It then suffices to show that $\min\{ac, ad\} \ge \min\{a'c, a'd\}$. Because $d \ge c \ge 0$ and $a \ge a'$, we conclude that $ac \ge a'c$ and $ad \ge a'd$.
- If $c < 0 \le d$: Then $ac \ge bc$, $ad \le bd$, $a'c \ge b'c$, $a'd \ge b'd$. It then suffices to show that $\min\{bc, ad\} \ge \min\{b'c, a'd\}$. Because $d \ge 0 > c$ and $a \ge a', b \le b'$, we conclude that $bc \ge b'c$ and $ad \le a'd$.
- If $c \le d < 0$: Then $ac \ge bc$, $ad \ge bd$, $a'c \ge b'c$, $a'd \ge b'd$. It then suffices to show that $\min\{bc, bd\} \ge \min\{b'c, b'd\}$. Because $0 > d \ge c$ and $b \le b'$, we conclude that $bc \ge b'c$ and $bd \ge b'd$.

In a similar way, we can also prove that $\max S_{a,b,c,d} \le \max S_{a',b',c,d}$. Therefore, we conclude that $\cdot_{\mathcal{I}}$ is monotone. □

LEMMA 5.20. *If $\{[a_n, b_n]\}_{n\in\mathbb{Z}^+}$ is a montone sequence in $\mathcal{I}$, i.e., $[a_0, b_0] \le_{\mathcal{I}} [a_1, b_1] \le_{\mathcal{I}} \cdots \le_{\mathcal{I}} [a_n, b_n] \le_{\mathcal{I}} \cdots$, and $[a_n, b_n] \le_{\mathcal{I}} [c, d]$ for all $n \in \mathbb{Z}^+$. Let $[a, b] = \lim_{n\to\infty}[a_n, b_n]$ (the limit is well-defined by the monotone convergence theorem for series). Then $[a, b] \le_{\mathcal{I}} [c, d]$.*

PROOF. By the definition of $\le_{\mathcal{I}}$, we know that $\{a_n\}_{n\in\mathbb{Z}^+}$ is non-increasing and $\{b_n\}_{n\in\mathbb{Z}^+}$ is non-decreasing. Because $a_n \ge c$ for all $n \in \mathbb{Z}^+$, we conclude that $\lim_{n\to\infty} a_n \ge c$. Because $b_n \le d$ for all $n \in \mathbb{Z}^+$, we conclude that $\lim_{n\to\infty} b_n \le d$. Thus we conclude that $[a, b] \le_{\mathcal{I}} [c, d]$. □

LEMMA 5.21. *Let $X, Y : \Omega \to \mathcal{M}_{\mathcal{I}}^{(m)}$ be integrable. Then $\mathbb{E}[X \oplus Y] = \mathbb{E}[X] \oplus \mathbb{E}[Y]$.*

PROOF. Appeal to linearity of expectations and the fact that $\oplus$ is the pointwise extension of $+_{\mathcal{I}}$, as well as $+_{\mathcal{I}}$ is the pointwise extension of numeric addition. □

LEMMA 5.22. *If $X : \Omega \to \mathcal{M}_{\mathcal{I}}^{(m)}$ is $\mathcal{G}$-measurable and bounded, a.s., as well as $X(\omega) = \overrightarrow{\langle [a_k(\omega), a_k(\omega)]\rangle_{0\le k\le m}}$ for all $\omega \in \Omega$, then $\mathbb{E}[X \otimes Y \mid \mathcal{G}] = X \otimes \mathbb{E}[Y \mid \mathcal{G}]$ almost surely.*

PROOF. Fix $\omega \in \Omega$. Let $Y(\omega) = \overrightarrow{\langle [b_k(\omega), c_k(\omega)]\rangle_{0\le k\le m}}$. Then we have

$$\begin{aligned}
\mathbb{E}[X \otimes Y \mid \mathcal{G}](\omega) &= \mathbb{E}[\overrightarrow{\langle [a_k, a_k]\rangle_{0\le k\le m}} \otimes \overrightarrow{\langle [b_k, c_k]\rangle_{0\le k\le m}} \mid \mathcal{G}](\omega) \\
&= \mathbb{E}[\overrightarrow{\langle \textstyle\sum_{\mathcal{I}}{}_{i=0}^{k} \binom{k}{i} \times_{\mathcal{I}} ([a_i, a_i] \cdot_{\mathcal{I}} [b_{k-i}, c_{k-i}])\rangle_{0\le k\le m}} \mid \mathcal{G}](\omega) \\
&= \overrightarrow{\langle \mathbb{E}[\textstyle\sum_{\mathcal{I}}{}_{i=0}^{k} \binom{k}{i} \times_{\mathcal{I}} ([a_i, a_i] \cdot_{\mathcal{I}} [b_{k-i}, c_{k-i}]) \mid \mathcal{G}](\omega)\rangle_{0\le k\le m}} \\
&= \overrightarrow{\langle \textstyle\sum_{\mathcal{I}}{}_{i=0}^{k} \binom{k}{i} \times_{\mathcal{I}} \mathbb{E}[[a_i, a_i] \cdot_{\mathcal{I}} [b_{k-i}, c_{k-i}] \mid \mathcal{G}](\omega)\rangle_{0\le k\le m}}.
\end{aligned}$$

On the other hand, we have

$$\begin{aligned}
X(\omega) \otimes \mathbb{E}[Y \mid \mathcal{G}](\omega) &= \langle X_0(\omega), \cdots, X_m(\omega)\rangle \otimes \mathbb{E}[\langle Y_0, \cdots, Y_m\rangle \mid \mathcal{G}](\omega) \\
&= \langle X_0(\omega), \cdots, X_m(\omega)\rangle \otimes \langle \mathbb{E}[Y_0 \mid \mathcal{G}](\omega), \cdots, \mathbb{E}[Y_m \mid \mathcal{G}](\omega)\rangle \\
&= \overrightarrow{\langle \textstyle\sum_{\mathcal{I}}{}_{i=0}^{k} \binom{k}{i} \times_{\mathcal{I}} (X_i(\omega) \cdot_{\mathcal{I}} \mathbb{E}[Y_{k-i} \mid \mathcal{G}](\omega))\rangle_{0\le k\le m}} \\
&= \overrightarrow{\langle \textstyle\sum_{\mathcal{I}}{}_{i=0}^{k} \binom{k}{i} \times_{\mathcal{I}} ([a_i(\omega), a_i(\omega)] \cdot_{\mathcal{I}} \mathbb{E}[[b_{k-i}, c_{k-i}] \mid \mathcal{G}](\omega))\rangle_{0\le k\le m}}.
\end{aligned}$$

Thus, it suffices to show that for each i, $\mathbb{E}[[a_i, a_i] \cdot_{\mathcal{I}} [b_{k-i}, c_{k-i}] \mid \mathcal{G}] = [a_i, a_i] \cdot_{\mathcal{I}} \mathbb{E}[[b_{k-i}, c_{k-i}] \mid \mathcal{G}]$ almost surely.

For ω such that $a_i(\omega) \geq 0$:

$$\begin{aligned}
\mathbb{E}[[a_i, a_i] \cdot_{\mathcal{I}} [b_{k-i}, c_{k-i}] \mid \mathcal{G}](\omega) &= \mathbb{E}[[a_i b_{k-i}, a_i c_{k-i}] \mid \mathcal{G}](\omega) \\
&= [\mathbb{E}[a_i b_{k-i} \mid \mathcal{G}](\omega), \mathbb{E}[a_i c_{k-i} \mid \mathcal{G}](\omega)] \\
&= [a_i(\omega) \cdot \mathbb{E}[b_{k-i} \mid \mathcal{G}](\omega), a_i(\omega) \cdot \mathbb{E}[c_{k-i} \mid \mathcal{G}](\omega)], a.s., \\
&= [a_i(\omega), a_i(\omega)] \cdot_{\mathcal{I}} \mathbb{E}[[b_{k-i}, c_{k-i}] \mid \mathcal{G}](\omega).
\end{aligned}$$

For ω such that $a_i(\omega) < 0$:

$$\begin{aligned}
\mathbb{E}[[a_i, a_i] \cdot_{\mathcal{I}} [b_{k-i}, c_{k-i}] \mid \mathcal{G}](\omega) &= \mathbb{E}[[a_i c_{k-i}, a_i b_{k-i}] \mid \mathcal{G}](\omega) \\
&= [\mathbb{E}[a_i c_{k-i} \mid \mathcal{G}](\omega), \mathbb{E}[a_i b_{k-i} \mid \mathcal{G}](\omega)] \\
&= [a_i(\omega) \cdot \mathbb{E}[c_{k-i} \mid \mathcal{G}](\omega), a_i(\omega) \cdot \mathbb{E}[b_{k-i} \mid \mathcal{G}](\omega)], a.s., \\
&= [a_i(\omega), a_i(\omega)] \cdot_{\mathcal{I}} \mathbb{E}[[b_{k-i}, c_{k-i}] \mid \mathcal{G}](\omega).
\end{aligned}$$

□

Proof of Lemma 5.17. A sequence of random variables $\{X_n\}_{n \in \mathbb{Z}^+}$ is said to be *adapted* to a filtration $\{\mathcal{F}_n\}_{n \in \mathbb{Z}^+}$ if for each $n \in \mathbb{Z}^+$, X_n is $\mathcal{F}_n$-measurable. Then $\{\Phi_n\}_{n \in \mathbb{Z}^+}$ and $\{A_n\}_{n \in \mathbb{Z}^+}$ are adapted to the coordinate-generated filtration $\{\mathcal{F}_n\}_{n \in \mathbb{Z}^+}$ as $\Phi_n(\omega)$ and $A_n(\omega)$ depend on ω_n. By the property of the operational semantics, we know that $\alpha_n(\omega) \leq C \cdot n$ almost surely for some $C \geq 0$. Then using Lemma 5.22, we have

$$\begin{aligned}
\mathbb{E}[Y_{n+1} \mid \mathcal{F}_n](\omega) &= \mathbb{E}[A_{n+1} \otimes \Phi_{n+1} \mid \mathcal{F}_n](\omega) \\
&= \mathbb{E}[A_n \otimes \overrightarrow{\langle [(\alpha_{n+1} - \alpha_n)^k, (\alpha_{n+1} - \alpha_n)^k] \rangle_{0 \leq k \leq m}} \otimes \Phi_{n+1} \mid \mathcal{F}_n](\omega) \\
&= A_n(\omega) \otimes \mathbb{E}[\overrightarrow{\langle [(\alpha_{n+1} - \alpha_n)^k, (\alpha_{n+1} - \alpha_n)^k] \rangle_{0 \leq k \leq m}} \otimes \Phi_{n+1} \mid \mathcal{F}_n](\omega), a.s., \\
&= A_n(\omega) \otimes \mathbb{E}[\overrightarrow{\langle [(\alpha_{n+1} - \alpha_n)^k, (\alpha_{n+1} - \alpha_n)^k] \rangle_{0 \leq k \leq m}} \otimes \phi(\omega_{n+1}) \mid \mathcal{F}_n].
\end{aligned}$$

Recall the property of the expected-potential function ϕ in Defintion 5.16. Then by Lemma 5.18 with Lemma 5.19, we have

$$\begin{aligned}
\mathbb{E}[Y_{n+1} \mid \mathcal{F}_n](\omega) &\sqsubseteq A_n(\omega) \otimes \phi(\omega_n), a.s., \\
&= A_n(\omega) \otimes \Phi_n(\omega) \\
&= Y_n.
\end{aligned}$$

As a corollary, we have $\mathbb{E}[Y_n] \sqsubseteq \mathbb{E}[Y_0]$ for all $n \in \mathbb{Z}^+$. □

I call $\{\mathbf{Y}_n\}_{n \in \mathbb{Z}^+}$ a *moment invariant*. My goal is to establish that $\mathbb{E}[\mathbf{Y}_T] \sqsubseteq \mathbb{E}[\mathbf{Y}_0]$, i.e., the initial interval-valued potential $\overrightarrow{\mathbb{E}[\mathbf{Y}_0] = \mathbb{E}[\underline{1} \otimes \mathbf{\Phi}_0]} = \overrightarrow{\mathbb{E}[\mathbf{\Phi}_0]}$ brackets the higher moments of the accumulated cost $\overrightarrow{\mathbb{E}[\mathbf{Y}_T] = \mathbb{E}[\langle [A_T^k, A_T^k] \rangle_{0 \leq k \leq m} \otimes \underline{1}]} = \overrightarrow{\langle [\mathbb{E}[A_T^k], \mathbb{E}[A_T^k]] \rangle_{0 \leq k \leq m}}$.

Soundness The soundness of the derivation system is proved with respect to the Markov-chain semantics. Let $\|\overrightarrow{\langle [a_k, b_k]\rangle_{0\le k\le m}}\|_\infty \stackrel{\text{def}}{=} \max_{0\le k\le m}\{\max\{|a_k|, |b_k|\}\}$.

THEOREM 5.23. *Let $\langle \mathscr{D}, S_{\mathsf{main}}\rangle$ be a probabilistic program. Suppose $\Delta \vdash \{\Gamma; Q\}\ S_{\mathsf{main}}\ \{\Gamma'; \underline{1}\}$, where $Q \in \mathcal{M}^{(m)}_{\mathcal{PI}}$ and the ends of the k-th interval in Q are polynomials in $\mathbb{R}_{kd}[\mathsf{VID}]$. Let $\{\mathbf{Y}_n\}_{n\in\mathbb{Z}^+}$ be the moment invariant extracted from the Markov-chain semantics with respect to the derivation of $\Delta \vdash \{\Gamma; Q\}\ S_{\mathsf{main}}\ \{\Gamma'; \underline{1}\}$. If the following conditions hold:*

(i) $\mathbb{E}[T^{md}] < \infty$, and

(ii) there exists $C \ge 0$ such that for all $n \in \mathbb{Z}^+$, $\|\mathbf{Y}_n\|_\infty \le C \cdot (n+1)^{md}$ almost surely,

Then $\overrightarrow{\langle [\mathbb{E}[A_T^k], \mathbb{E}[A_T^k]]\rangle_{0\le k\le m}} \sqsubseteq \phi_Q(\lambda\_.0)$.

The intuitive meaning of $\overrightarrow{\langle [\mathbb{E}[A_T^k], \mathbb{E}[A_T^k]]\rangle_{0\le k\le m}} \sqsubseteq \phi_Q(\lambda\_.0)$ is that the moment $\mathbb{E}[A_T^k]$ of the accumulated cost upon program termination is bounded by the interval in the k^{th}-moment component of $\phi_Q(\lambda\_.0)$, where Q is the quantitative context and $\lambda\_.0$ is the initial state.

As I discussed in §5.1.2 and Counterexample 5.7, the expected-potential method is *not* always sound for deriving bounds on higher moments for cost accumulators in probabilistic programs. The extra conditions Theorem 5.23(i) and (ii) impose constraints on the analyzed program and the expected-potential function, which allow me to reduce the soundness to the *optional stopping problem* from probability theory.

Optional Stopping Let me represent the moment invariant $\{\mathbf{Y}_n\}_{n\in\mathbb{Z}^+}$ as

$$\{\langle [L_n^{(0)}, U_n^{(0)}], [L_n^{(1)}, U_n^{(1)}], \cdots, [L_n^{(m)}, U_n^{(m)}]\rangle\}_{n\in\mathbb{Z}^+},$$

where $L_n^{(k)}, U_n^{(k)} : \Omega \to \mathbb{R}$ are real-valued random variables on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ of the Markov-chain semantics, for $n \in \mathbb{Z}^+$, $0 \le k \le m$. I then have the observations below as direct corollaries of Lemma 5.17:

- For any k, the sequence $\{U_n^{(k)}\}_{n\in\mathbb{Z}^+}$ satisfies $\mathbb{E}[U_{n+1}^{(k)} \mid U_n^{(k)}] \le U_n^{(k)}$ almost surely, for all $n \in \mathbb{Z}^+$, and we want to find sufficient conditions for $\mathbb{E}[U_T^{(k)}] \le \mathbb{E}[U_0^{(k)}]$.
- For any k, the sequence $\{L_n^{(k)}\}_{n\in\mathbb{Z}^+}$ satisfies $\mathbb{E}[L_{n+1}^{(k)} \mid L_n^{(k)}] \ge L_n^{(k)}$ almost surely, for all $n \in \mathbb{Z}^+$, and we want to find sufficient conditions for $\mathbb{E}[L_T^{(k)}] \ge \mathbb{E}[L_0^{(k)}]$.

These kinds of questions can be reduced to *optional stopping problem* from probability theory. Recent research [7, 68, 137, 154] has used and extended the *Optional Stopping Theorem* (OST) from probability theory to establish *sufficient* conditions for the soundness for analysis of probabilistic programs. However, the classic OST turns out to be *not* suitable for higher-moment analysis. I extend OST with a *new* sufficient condition that allows me to prove Theorem 5.23. In another article [150], I presented details of such OST extensions; in this section, I only sketch the development that is sufficient for my thesis. I first review an important convergence theorem for series of random variables.

PROPOSITION 5.24 (DOMINATED CONVERGENCE THEOREM). *If $\{f_n\}_{n\in\mathbb{Z}^+}$ is a sequence of measurable functions on a measure space $(S, \mathcal{S}, \mu)$, $\{f_n\}_{n\in\mathbb{Z}^+}$ converges to f pointwise, and $\{f_n\}_{n\in\mathbb{Z}^+}$ is dominated*

by a nonnegative integrable function g (i.e., $|f_n(x)| \le g(x)$ for all $n \in \mathbb{Z}^+$, $x \in S$), then f is integrable and $\lim_{n\to\infty} \mu(f_n) = \mu(f)$.

Further, the theorem still holds if f is chosen as a measurable function and "$\{f_n\}_{n\in\mathbb{Z}^+}$ converges to f pointwise and is dominated by g" holds almost everywhere.

Now I prove the following extension of OST to deal with interval-valued potential functions.

THEOREM 5.25. *If $\mathbb{E}[\|Y_n\|_\infty] < \infty$ for all $n \in \mathbb{Z}^+$, then $\mathbb{E}[Y_T]$ exists and $\mathbb{E}[Y_T] \sqsubseteq \mathbb{E}[Y_0]$ in the following situation:*

There exist $\ell \in \mathbb{N}$ and $C \ge 0$ such that $\mathbb{E}[T^\ell] < \infty$ and for all $n \in \mathbb{Z}^+$, $\|Y_n\|_\infty \le C \cdot (n+1)^\ell$ almost surely.

PROOF. By $\mathbb{E}[T^\ell] < \infty$ where $\ell \ge 1$, we know that $\mathbb{P}[T < \infty] = 1$. By the property of the operational semantics, for $\omega \in \Omega$ such that $T(\omega) < \infty$, we have $Y_n(\omega) = Y_T(\omega)$ for all $n \ge T(\omega)$. Then we have

$$\begin{aligned}
\mathbb{P}[\lim_{n\to\infty} Y_n = Y_T] &= \mathbb{P}(\{\omega \mid \lim_{n\to\infty} Y_n(\omega) = Y_T(\omega)\}) \\
&\ge \mathbb{P}(\{\omega \mid \lim_{n\to\infty} Y_n(\omega) = Y_T(\omega) \wedge T(\omega) < \infty\}) \\
&= \mathbb{P}(\{\omega \mid Y_{T(\omega)}(\omega) = Y_T(\omega) \wedge T(\omega) < \infty\}) \\
&= \mathbb{P}(\{\omega \mid T(\omega) < \infty\}) \\
&= 1.
\end{aligned}$$

On the other hand, $Y_n(\omega)$ can be treated as a vector of real numbers. Let $a_n : \Omega \to \mathbb{R}$ be a real-valued component in Y_n. Because $\mathbb{E}[\|Y_n\|_\infty] < \infty$ and $\|Y_n\|_\infty \le C \cdot (n+1)^\ell$ almost surely, we know that $\mathbb{E}[|a_n|] \le \mathbb{E}[\|Y_n\|_\infty] < \infty$ and $|a_n| \le \|Y_n\|_\infty \le C \cdot (n+1)^\ell$ almost surely. Therefore,

$$|a_n| = |a_{\min(T,n)}| \le C \cdot (\min(T,n)+1)^\ell \le C \cdot (T+1)^\ell, \text{a.s.}$$

Recall that $\mathbb{E}[T^\ell] < \infty$. Then $\mathbb{E}[(T+1)^\ell] = \mathbb{E}[T^\ell + O(T^{\ell-1})] < \infty$. By Proposition 5.24, with the function g set to $\lambda\omega.C \cdot (T(\omega)+1)^\ell$, we know that $\lim_{n\to\infty} \mathbb{E}[a_n] = \mathbb{E}[a_T]$. Because a_n is an arbitrary real-valued component in Y_n, we know that $\lim_{n\to\infty} \mathbb{E}[Y_n] = \mathbb{E}[Y_T]$. By Lemma 5.17, we know that $\mathbb{E}[Y_n] \sqsubseteq \mathbb{E}[Y_0]$ for all $n \in \mathbb{Z}^+$. By Lemma 5.20, we conclude that $\lim_{n\to\infty} \mathbb{E}[Y_n] \sqsubseteq \mathbb{E}[Y_0]$, i.e., $\mathbb{E}[Y_T] \sqsubseteq \mathbb{E}[Y_0]$. □

Proof of Theorem 5.23 To reduce the soundness proof to the extended OST for interval-valued bounds, I construct an *annotated transition kernel* from validity judgements $\vdash \Delta$ and $\Delta \vdash \{\Gamma; Q\}\ S_{\mathsf{main}}\ \{\Gamma'; Q'\}$. Before proceeding to the proof, I extend the derivation system with rules for program configurations and include them in Fig. 5.11. Moreover, I use a more declarative rule shown below for function calls that merges the two rules for function calls in Fig. 5.6 into one:

$$\frac{\forall i \in I : (\Gamma; Q_i, \Gamma'; Q_i') \in \Delta(f)}{\Delta \vdash \{\Gamma; \bigoplus_{i\in I} Q_i\}\ \mathbf{call}\ f\ \{\Gamma'; \bigoplus_{i\in I} Q_i'\}} \text{(Q-CALL)}$$

$$\frac{\gamma \models \Gamma \qquad \Delta \vdash \{\Gamma; Q\}\ S\ \{\Gamma'; Q'\} \qquad \Delta \vdash \{\Gamma'; Q'\}\ K}{\Delta \vdash \{\Gamma; Q\}\ \langle \gamma, S, K, \alpha\rangle}\ (\textsc{Valid-Cfg}) \qquad \frac{}{\Delta \vdash \{\Gamma; Q\}\ \mathbf{Kstop}}\ (\text{QK-}\textsc{Stop})$$

$$\frac{\Delta \vdash \{\Gamma \wedge L; Q\}\ S\ \{\Gamma; Q\} \qquad \Delta \vdash \{\Gamma \wedge \neg L; Q\}\ K}{\Delta \vdash \{\Gamma; Q\}\ \mathbf{Kloop}\ L\ S\ K}\ (\text{QK-}\textsc{Loop}) \qquad \frac{\Delta \vdash \{\Gamma; Q\}\ S\ \{\Gamma'; Q'\} \qquad \Delta \vdash \{\Gamma'; Q'\}\ K}{\Delta \vdash \{\Gamma; Q\}\ \mathbf{Kseq}\ S\ K}\ (\text{QK-}\textsc{Seq})$$

$$\frac{\Delta \vdash \{\Gamma'; Q'\}\ K \qquad \Gamma \models \Gamma' \qquad \Gamma \models Q \sqsupseteq Q'}{\Delta \vdash \{\Gamma; Q\}\ K}\ (\text{QK-}\textsc{Weaken})$$

Fig. 5.11: Extra inference rules of the derivation system.

Lemma 5.26. *Suppose* $\vdash \Delta$ *and* $\Delta \vdash \{\Gamma; Q\}\ S_{\mathsf{main}}\ \{\Gamma'; Q'\}$. *An* annotated program configuration *has the form* $\langle \Gamma, Q, \gamma, S, K, \alpha\rangle$ *such that* $\Delta \vdash \{\Gamma; Q\}\ \langle \gamma, S, K, \alpha\rangle$. *Then there exists a probability kernel* κ *over annotated program configurations such that:*

For all $\sigma = \langle \Gamma, Q, \gamma, S, K, \alpha\rangle \in \mathrm{dom}(\kappa)$*, it holds that*

(i) κ *is the same as the evaluation relation* $\mapsto$ *if the annotations are omitted, i.e.,*

$$\kappa(\sigma) \gg\!= \lambda\langle \_, \_, \gamma', S', K', \alpha'\rangle.\delta(\langle \gamma', S', K', \alpha'\rangle) = \mapsto(\langle \gamma, S, K, \alpha\rangle),$$

and

(ii) $\phi_Q(\gamma) \sqsupseteq \mathbb{E}_{\sigma' \sim \kappa(\sigma)}[\overrightarrow{\langle [(\alpha' - \alpha)^k, (\alpha' - \alpha)^k]\rangle_{0 \le k \le m}} \otimes \phi_{Q'}(\gamma')]$ *where* $\sigma' = \langle \_, Q', \gamma', \_, \_, \alpha'\rangle$.

Before proving the soundness lemma, I show that the derivation system for bound inference admits a *relaxation* rule.

Lemma 5.27. *Suppose that* $\vdash \Delta$. *If* $\Delta \vdash \{\Gamma; Q_1\}\ S\ \{\Gamma'; Q_1'\}$ *and* $\Delta \vdash \{\Gamma; Q_2\}\ S\ \{\Gamma'; Q_2'\}$*, then the judgment* $\Delta \vdash \{\Gamma; Q_1 \oplus Q_2\}\ S\ \{\Gamma'; Q_1' \oplus Q_2'\}$ *is derivable.*

Proof. By nested induction on the derivation of the judgment $\Delta \vdash \{\Gamma; Q_1\}\ S\ \{\Gamma'; Q_1'\}$, followed by inversion on $\Delta \vdash \{\Gamma; Q_2\}\ S\ \{\Gamma'; Q_2'\}$. We assume the derivations have the same shape and the same logical contexts; in practice, we can ensure this by explicitly inserting weakening positions, e.g., all the branching points, and by doing a first pass to obtain logical contexts.

- $\dfrac{}{\Delta \vdash \{\Gamma; Q_1\}\ \mathbf{skip}\ \{\Gamma; Q_1\}}$ (Q-Skip)

  By inversion, we have $Q_2 = Q_2'$.

  Then by (Q-Skip), we immediately have $\Delta \vdash \{\Gamma; Q_1 \oplus Q_2\}\ \mathbf{skip}\ \{\Gamma; Q_1 \oplus Q_2\}$.

- $\dfrac{Q_1 = \overrightarrow{\langle [c^k, c^k]\rangle_{0 \le k \le m}} \otimes Q_1'}{\Delta \vdash \{\Gamma; Q_1\}\ \mathbf{tick}(c)\ \{\Gamma; Q_1'\}}$ (Q-Tick)

By inversion, we have $Q_2 = \overrightarrow{\langle [c^k, c^k] \rangle_{0 \le k \le m}} \otimes Q_2'$.
By distributivity, we have $\overrightarrow{\langle [c^k, c^k] \rangle_{0 \le k \le m}} \otimes (Q_1' \oplus Q_2') = (\overrightarrow{\langle [c^k, c^k] \rangle_{0 \le k \le m}} \otimes Q_1') \oplus (\overrightarrow{\langle [c^k, c^k] \rangle_{0 \le k \le m}} \oplus Q_2') = Q_1 \oplus Q_2$.
Then we conclude by (Q-Tick).

- (Q-Assign)
$$\frac{\Gamma = [E/x]\Gamma' \qquad Q_1 = [E/x]Q_1'}{\Delta \vdash \{\Gamma; Q_1\}\ x \coloneqq E\ \{\Gamma'; Q_1'\}}$$
By inversion, we have $Q_2 = [E/x]Q_2'$.
Then we know that $[E/x](Q_1' \oplus Q_2') = [E/x]Q_1' \oplus [E/x]Q_2' = Q_1 \oplus Q_2$.
Then we conclude by (Q-Assign).

- (Q-Sample)
$$\frac{\Gamma = \forall x \in \mathrm{supp}(\mu_D) : \Gamma' \qquad Q_1 = \mathbb{E}_{x \sim \mu_D}[Q_1']}{\Delta \vdash \{\Gamma; Q_1\}\ x \sim D\ \{\Gamma'; Q_1'\}}$$
By inversion, we have $Q_2 = \mathbb{E}_{x \sim \mu_D}[Q_2']$.
By Lemma 5.21, we know that $\mathbb{E}_{x \sim \mu_D}[Q_1' \oplus Q_2'] = \mathbb{E}_{x \sim \mu_D}[Q_1'] \oplus \mathbb{E}_{x \sim \mu_D}[Q_2'] = Q_1 \oplus Q_2$.
Then we conclude by (Q-Sample).

- (Q-Call)
$$\frac{\forall i \in I : (\Gamma; Q_{1i}, \Gamma'; Q_{1i}') \in \Delta(f)}{\Delta \vdash \{\Gamma; \bigoplus_{i \in I} Q_{1i}\}\ \mathbf{call}\ f\ \{\Gamma'; \bigoplus_{i \in I} Q_{1i}'\}}$$
By inversion, there exists J such that $Q_2 = \bigoplus_{j \in J} Q_{2j}$ and $Q_2' = \bigoplus_{j \in J} Q_{2j}'$ where $(\Gamma; Q_{2j}, \Gamma'; Q_{2j}') \in \Delta(f)$ for each $j \in J$.
Then by (Q-Call), we have $\Delta \vdash \{\Gamma; \bigoplus_{i \in I} Q_{1i} \oplus \bigoplus_{j \in J} Q_{2j}\}\ \mathbf{call}\ f\ \{\Gamma'; \bigoplus_{i \in I} Q_{1i}' \oplus \bigoplus_{j \in J} Q_{2j}'\}$.

- (Q-Prob)
$$\frac{\Delta \vdash \{\Gamma; Q_{11}\}\ S_1\ \{\Gamma'; Q_1'\} \qquad \Delta \vdash \{\Gamma; Q_{12}\}\ S_2\ \{\Gamma'; Q_1'\} \qquad Q_1 = P_1 \oplus R_1 \qquad P_1 = \langle [p, p], [0,0], \cdots, [0,0] \rangle \otimes Q_{11} \qquad R_1 = \langle [1-p, 1-p], [0,0], \cdots, [0,0] \rangle \otimes Q_{12}}{\Delta \vdash \{\Gamma; Q_1\}\ \mathbf{if}\ \mathbf{prob}(p)\ \mathbf{then}\ S_1\ \mathbf{else}\ S_2\ \mathbf{fi}\ \{\Gamma'; Q_1'\}}$$
By inversion, we know that $Q_2 = P_2 \oplus R_2$ for some Q_{21}, Q_{22} such that $\Delta \vdash \{\Gamma; Q_{21}\}\ S_1\ \{\Gamma'; Q_2'\}$, $\Delta \vdash \{\Gamma; Q_{22}\}\ S_2\ \{\Gamma'; Q_2'\}$, $P_2 = \langle [p, p], [0,0], \cdots, [0,0] \rangle \otimes Q_{21}$, and $R_2 = \langle [1-p, 1-p], [0,0], \cdots, [0,0] \rangle \otimes Q_{22}$.
By induction hypothesis, we have $\Delta \vdash \{\Gamma; Q_{11} \oplus Q_{21}\}\ S_1\ \{\Gamma'; Q_1' \oplus Q_2'\}$ and $\Delta \vdash \{\Gamma; Q_{12} \oplus Q_{22}\}\ S_2\ \{\Gamma'; Q_1' \oplus Q_2'\}$.

Then we have

$$\begin{aligned}
&\langle [p,p], \cdots, [0,0] \rangle \otimes (Q_{11} \oplus Q_{21}) \\
&= (\langle [p,p], \cdots, [0,0] \rangle \otimes Q_{11}) \oplus (\langle [p,p], \cdots, [0,0] \rangle \oplus Q_{21}) \\
&= P_1 \oplus P_2, \\
&\langle [1-p,1-p], \cdots, [0,0] \rangle \otimes (Q_{12} \oplus Q_{22}) \\
&= (\langle [1-p,1-p], \cdots, [0,0] \rangle \otimes Q_{12}) \oplus (\langle [1-p,1-p], \cdots, [0,0] \rangle \otimes Q_{22}) \\
&= R_1 \oplus R_2, \\
&(P_1 \oplus P_2) \oplus (R_1 \oplus R_2) \\
&= (P_1 \oplus R_1) \oplus (P_2 \oplus R_2) = Q_1 \oplus Q_2.
\end{aligned}$$

Thus we conclude by (Q-Prob).

- (Q-Cond)
$$\frac{\Delta \vdash \{\Gamma \wedge L; Q_1\}\ S_1\ \{\Gamma'; Q_1'\} \qquad \Delta \vdash \{\Gamma \wedge \neg L; Q_1\}\ S_2\ \{\Gamma'; Q_1'\}}{\Delta \vdash \{\Gamma; Q_1\}\ \textbf{if}\ L\ \textbf{then}\ S_1\ \textbf{else}\ S_2\ \textbf{fi}\ \{\Gamma'; Q_1'\}}$$
By inversion, we have $\Delta \vdash \{\Gamma \wedge L; Q_2\}\ S_1\ \{\Gamma'; Q_2'\}$, and $\Delta \vdash \{\Gamma \wedge \neg L; Q_2\}\ S_2\ \{\Gamma'; Q_2'\}$.
By induction hypothesis, we have $\Delta \vdash \{\Gamma \wedge L; Q_1 \oplus Q_2\}\ S_1\ \{\Gamma'; Q_1' \oplus Q_2'\}$ and $\Delta \vdash \{\Gamma \wedge \neg L; Q_1 \oplus Q_2\}\ S_2\ \{\Gamma'; Q_1' \oplus Q_2'\}$.
Then we conclude by (Q-Cond).

- (Q-Loop)
$$\frac{\Delta \vdash \{\Gamma \wedge L; Q_1\}\ S\ \{\Gamma; Q_1\}}{\Delta \vdash \{\Gamma; Q_1\}\ \textbf{while}\ L\ \textbf{do}\ S\ \textbf{od}\ \{\Gamma \wedge \neg L; Q_1\}}$$
By inversion, we have $\Delta \vdash \{\Gamma \wedge L; Q_2\}\ S\ \{\Gamma; Q_2\}$.
By induction hypothesis, we have $\Delta \vdash \{\Gamma \wedge L; Q_1 \oplus Q_2\}\ S\ \{\Gamma; Q_1 \oplus Q_2\}$.
Then we conclude by (Q-Loop).

- (Q-Seq)
$$\frac{\Delta \vdash \{\Gamma; Q_1\}\ S_1\ \{\Gamma''; Q_1''\} \qquad \Delta \vdash \{\Gamma''; Q_1''\}\ S_2\ \{\Gamma'; Q_1'\}}{\Delta \vdash \{\Gamma; Q_1\}\ S_1; S_2\ \{\Gamma'; Q_1'\}}$$
By inversion, there exists Q_2'' such that $\Delta \vdash \{\Gamma; Q_2\}\ S_1\ \{\Gamma''; Q_2''\}$, and $\Delta \vdash \{\Gamma''; Q_2''\}\ S_2\ \{\Gamma'; Q_2'\}$.
By induction hypothesis, we have $\Delta \vdash \{\Gamma; Q_1 \oplus Q_2\}\ S_1\ \{\Gamma''; Q_1'' \oplus Q_2''\}$ and $\Delta \vdash \{\Gamma''; Q_1'' \oplus Q_2''\}\ S_2\ \{\Gamma'; Q_1' \oplus Q_2'\}$.
Then we conclude by (Q-Seq).

- (Q-Weaken)
$$\frac{\Delta \vdash \{\Gamma_0; Q_0\}\ S\ \{\Gamma_0'; Q_0'\} \qquad \Gamma \models \Gamma_0 \qquad \Gamma_0' \models \Gamma' \qquad \Gamma \models Q_1 \sqsupseteq Q_0 \qquad \Gamma_0' \models Q_0' \sqsupseteq Q_1'}{\Delta \vdash \{\Gamma; Q_1\}\ S\ \{\Gamma'; Q_1'\}}$$
By inversion, there exist Q_3, Q_3' such that $\Gamma \models Q_2 \sqsupseteq Q_3$, $\Gamma_0' \models Q_3' \sqsupseteq Q_2'$, and $\Delta \vdash \{\Gamma_0; Q_3\}\ S\ \{\Gamma_0'; Q_3'\}$.
By induction hypothesis, we have $\Delta \vdash \{\Gamma_0; Q_0 \oplus Q_3\}\ S\ \{\Gamma_0'; Q_0' \oplus Q_3'\}$.
To apply (Q-Weaken), we need to show that $\Gamma \models Q_1 \oplus Q_2 \sqsupseteq Q_0 \oplus Q_3$ and $\Gamma_0' \models Q_0' \oplus Q_3' \sqsupseteq Q_1' \oplus Q_2'$.
Then appeal to Lemmas 5.18 and 5.19.

□

Now I can construct the annotated transition kernel to reduce the proof of the soundness lemma to OST.

Proof of Lemma 5.26. Let $\nu \overset{\text{def}}{=} \mapsto(\langle \gamma, S, K, \alpha\rangle)$. By inversion on $\Delta \vdash \{\Gamma; Q\}\ \langle \gamma, S, K, \alpha\rangle$, we know that $\gamma \models \Gamma$, $\Delta \vdash \{\Gamma; Q\}\ S\ \{\Gamma'; Q'\}$, and $\Delta \vdash \{\Gamma'; Q'\}\ K$ for some Γ', Q'. We now construct a probability measure μ as $\kappa(\langle \Gamma, Q, \gamma, S, K, \alpha\rangle)$ by induction on the derivation of $\Delta \vdash \{\Gamma; Q\}\ S\ \{\Gamma'; Q'\}$.

(Q-Skip)

$$\frac{}{\Delta \vdash \{\Gamma; Q\}\ \textbf{skip}\ \{\Gamma; Q\}}$$

- By induction on the derivation of $\Delta \vdash \{\Gamma; Q\}\ K$.

  (QK-Stop)

  $$\frac{}{\Delta \vdash \{\Gamma; Q\}\ \textbf{Kstop}}$$

  – We have $\nu = \delta(\langle \gamma, \textbf{skip}, \textbf{Kstop}, \alpha\rangle)$.
  Then we set $\mu = \delta(\langle \Gamma, Q, \gamma, \textbf{skip}, \textbf{Kstop}, \alpha\rangle)$.
  It is clear that $\phi_Q(\gamma) = \underline{1} \otimes \phi_Q(\gamma)$.

  (QK-Loop)

  $$\frac{\Delta \vdash \{\Gamma \wedge L; Q\}\ S\ \{\Gamma; Q\} \qquad \Delta \vdash \{\Gamma \wedge \neg L; Q\}\ K}{\Delta \vdash \{\Gamma; Q\}\ \textbf{Kloop}\ L\ S\ K}$$

  – Let $b \in \{\bot, \top\}$ be such that $\gamma \vdash L \Downarrow b$.
  If $b = \top$, then $\nu = \delta(\langle \gamma, S, \textbf{Kloop}\ L\ S\ K, \alpha\rangle)$.
  We set $\mu = \delta(\langle \Gamma \wedge L, Q, \gamma, S, \textbf{Kloop}\ L\ S\ K, \alpha\rangle)$.
  In this case, we know that $\gamma \models \Gamma \wedge L$.
  By the premise, we know that $\Delta \vdash \{\Gamma \wedge L; Q\}\ S\ \{\Gamma; Q\}$.
  It then remains to show that $\Delta \vdash \{\Gamma; Q\}\ \textbf{Kloop}\ L\ S\ K$.
  By (QK-Loop), it suffices to show that $\Delta \vdash \{\Gamma \wedge L; Q\}\ S\ \{\Gamma; Q\}$ and $\Delta \vdash \{\Gamma \wedge \neg L; Q\}\ K$.
  Then appeal to the premise.
  If $b = \bot$, then $\mu = \delta(\langle \gamma, \textbf{skip}, K, \alpha\rangle)$.
  We set $\mu = \delta(\langle \Gamma \wedge \neg L, Q, \gamma, \textbf{skip}, K, \alpha\rangle)$.
  In this case, we know that $\gamma \models \Gamma \wedge \neg L$.
  By (Q-Skip), we have $\Delta \vdash \{\Gamma \wedge \neg L; Q\}\ \textbf{skip}\ \{\Gamma \wedge \neg L; Q\}$.
  It then remains to show that $\Delta \vdash \{\Gamma \wedge \neg L; Q\}\ K$.
  Then appeal to the premise.
  In both cases, γ and Q do not change, thus we conclude that $\phi_Q(\gamma) = \underline{1} \otimes \phi_Q(\gamma)$.

  (QK-Seq)

  $$\frac{\Delta \vdash \{\Gamma; Q\}\ S\ \{\Gamma'; Q'\} \qquad \Delta \vdash \{\Gamma'; Q'\}\ K}{\Delta \vdash \{\Gamma; Q\}\ \textbf{Kseq}\ S\ K}$$

  – We have $\nu = \delta(\langle \gamma, S, K, \alpha\rangle)$.
  Then we set $\mu = \delta(\langle \Gamma, Q, \gamma, S, K, \alpha\rangle)$.
  By the premise, we know that $\Delta \vdash \{\Gamma; Q\}\ S\ \{\Gamma'; Q'\}$ and $\Delta \vdash \{\Gamma'; Q'\}\ K$.

Because γ and Q do not change, we conclude that $\phi_Q(\gamma) = \underline{1} \otimes \phi_Q(\gamma)$.

(QK-Weaken)
$$\frac{\Delta \vdash \{\Gamma'; Q'\}\ K \qquad \Gamma \models \Gamma' \qquad \Gamma \models Q \sqsupseteq Q'}{\Delta \vdash \{\Gamma; Q\}\ K}$$

– Because $\gamma \models \Gamma$ and $\Gamma \models \Gamma'$, we know that $\gamma \models \Gamma'$.
Let μ' be obtained from the induction hypothesis on $\Delta \vdash \{\Gamma'; Q'\}\ K$.
Then $\phi_{Q'}(\gamma) \sqsupseteq \mathbb{E}_{\sigma' \sim \mu'}[\overrightarrow{\langle [(\alpha' - \alpha)^k, (\alpha' - \alpha)^k] \rangle_{0 \le k \le m}} \otimes \phi_{Q''}(\gamma')]$, where $\sigma' = \langle \_, Q'', \gamma', \_, \_, \alpha' \rangle$.
We set $\mu = \mu'$.
Because $\Gamma \models Q \sqsupseteq Q'$ and $\gamma \models \Gamma$, we conclude that $\phi_Q(\gamma) \sqsupseteq \phi_{Q'}(\gamma)$.

(Q-Tick)
$$\frac{Q = \overrightarrow{\langle [c^k, c^k] \rangle_{0 \le k \le m}} \otimes Q'}{\Delta \vdash \{\Gamma; Q\}\ \mathbf{tick}(c)\ \{\Gamma; Q'\}}$$

• We have $\nu = \delta(\langle \gamma, \mathbf{skip}, K, \alpha + c \rangle)$.
Then we set $\mu = \delta(\langle \Gamma, Q', \gamma, \mathbf{skip}, K, \alpha + c \rangle)$.
By (Q-Skip), we have $\Delta \vdash \{\Gamma; Q'\}\ \mathbf{skip}\ \{\Gamma; Q'\}$.
Then by the assumption, we have $\Delta \vdash \{\Gamma; Q'\}\ K$.
It remains to show that $\phi_Q(\gamma) \sqsupseteq \overrightarrow{\langle [c^k, c^k] \rangle_{0 \le k \le m}} \otimes \phi_{Q'}(\gamma)$.
Indeed, we have $\phi_Q(\gamma) = \overrightarrow{\langle [c^k, c^k] \rangle_{0 \le k \le m}} \otimes \phi_{Q'}(\gamma)$ by the premise.

(Q-Assign)
$$\frac{\Gamma = [E/x]\Gamma' \qquad Q = [E/x]Q'}{\Delta \vdash \{\Gamma; Q\}\ x \coloneqq E\ \{\Gamma'; Q'\}}$$

• Let $r \in \mathbb{R}$ be such that $\gamma \vdash E \Downarrow r$.
We have $\nu = \delta(\langle \gamma[x \mapsto r], \mathbf{skip}, K, \alpha \rangle)$.
Then we set $\mu = \delta(\langle \Gamma', Q', \gamma[x \mapsto r], \mathbf{skip}, K, \alpha \rangle)$.
Because $\gamma \vdash \Gamma$, i.e., $\gamma \vdash [E/x]\Gamma'$, we know that $\gamma[x \mapsto r] \vdash \Gamma'$.
By (Q-Skip), we have $\Delta \vdash \{\Gamma'; Q'\}\ \mathbf{skip}\ \{\Gamma'; Q'\}$.
Then by the assumption, we have $\Delta \vdash \{\Gamma'; Q'\}\ K$.
It remains to show that $\phi_Q(\gamma) = \underline{1} \otimes \phi_{Q'}(\gamma[x \mapsto r])$.
By the premise, we have $Q = [E/x]Q'$, thus $\phi_Q(\gamma) = \phi_{[E/x]Q'}(\gamma) = \phi_{Q'}(\gamma[x \mapsto r])$.

(Q-Sample)
$$\frac{\Gamma = \forall x \in \mathrm{supp}(\mu_D) : \Gamma' \qquad Q = \mathbb{E}_{x \sim \mu_D}[Q']}{\Delta \vdash \{\Gamma; Q\}\ x \sim D\ \{\Gamma'; Q'\}}$$

• We have $\nu = \mu_D \gg\!= \lambda r. \delta(\langle \gamma[x \mapsto r], \mathbf{skip}, K, \alpha \rangle)$.
Then we set $\mu = \mu_D \gg\!= \lambda r. \delta(\langle \Gamma', Q', \gamma[x \mapsto r], \mathbf{skip}, K, \alpha \rangle)$.
For all $r \in \mathrm{supp}(\mu_D)$, because $\gamma \models \forall x \in \mathrm{supp}(\mu_D) : \Gamma'$, we know that $\gamma[x \mapsto r] \models \Gamma'$.
By (Q-Skip), we have $\Delta \vdash \{\Gamma'; Q'\}\ \mathbf{skip}\ \{\Gamma'; Q'\}$.
Then by the assumption, we have $\Delta \vdash \{\Gamma'; Q'\}\ K$.

It remains to show that $\phi_Q(\gamma) \sqsupseteq \mathbb{E}_{r\sim\mu_D}[\underline{1} \otimes \phi_{Q'}(\gamma[x \mapsto r])]$.
Indeed, because $Q = \mathbb{E}_{x\sim\mu_D}[Q']$, we know that $\phi_Q(\gamma) = \phi_{\mathbb{E}_{x\sim\mu_D}[Q']}(\gamma) = \mathbb{E}_{r\sim\mu_D}[\phi_{Q'}(\gamma[x \mapsto r])]$.

(Q-Call)
$$\frac{\forall i \in I\colon (\Gamma; Q_i, \Gamma'; Q_i') \in \Delta(f)}{\Delta \vdash \{\Gamma; \bigoplus_{i\in I} Q_i\}\ \mathbf{call}\ f\ \{\Gamma'; \bigoplus_{i\in I} Q_i'\}}$$

- We have $\nu = \delta(\langle \gamma, \mathscr{D}(f), K, \alpha\rangle)$.
Then we set $\mu = \delta(\langle \Gamma, \bigoplus_{i\in I} Q_i, \gamma, \mathscr{D}(f), K, \alpha\rangle)$.
By the premise, we know that $\Delta \vdash \{\Gamma; Q_i\}\ \mathscr{D}(f)\ \{\Gamma'; Q_i'\}$ for each $i \in I$.
By Lemma 5.27 and simple induction, we know that $\Delta \vdash \{\Gamma; \bigoplus_{i\in I} Q_i\}\ \mathscr{D}(f)\ \{\Gamma'; \bigoplus_{i\in I} Q_i'\}$.
Because γ and $\bigoplus_i Q_i$ do not change, we conclude that $\phi_{\bigoplus_i Q_i}(\gamma) = \underline{1} \otimes \phi_{\bigoplus_i Q_i}(\gamma)$.

(Q-Prob)
$$\frac{Q = P \oplus R \qquad P = \langle [p,p], [0,0], \cdots, [0,0]\rangle \otimes Q_1 \qquad \Delta \vdash \{\Gamma; Q_1\}\ S_1\ \{\Gamma'; Q'\} \qquad R = \langle [1-p, 1-p], [0,0], \cdots, [0,0]\rangle \otimes Q_2 \qquad \Delta \vdash \{\Gamma; Q_2\}\ S_2\ \{\Gamma'; Q'\}}{\Delta \vdash \{\Gamma; Q\}\ \mathbf{if}\ \mathbf{prob}(p)\ \mathbf{then}\ S_1\ \mathbf{else}\ S_2\ \mathbf{fi}\ \{\Gamma'; Q'\}}$$

- We have $\nu = p \cdot \delta(\langle \gamma, S_1, K, \alpha\rangle) + (1-p) \cdot \delta(\langle \gamma, S_2, K, \alpha\rangle)$.
Then we set $\mu = p \cdot \delta(\langle \Gamma, Q_1, \gamma, S_1, K, \alpha\rangle + (1-p) \cdot \delta(\langle \Gamma, Q_2, \gamma, S_2, K, \alpha\rangle)$.
From the assumption and the premise, we know that $\gamma \models \Gamma$, $\Delta \vdash \{\Gamma'; Q'\}\ K$, and $\Delta \vdash \{\Gamma; Q_1\}\ S_1\ \{\Gamma'; Q'\}$, $\Delta \vdash \{\Gamma; Q_2\}\ S_2\ \{\Gamma'; Q'\}$.
It remains to show that $\phi_Q(\gamma)_k \geq_{\mathcal{I}} (p \cdot \phi_{Q_1}(\gamma)_k) +_{\mathcal{I}} ((1-p) \cdot \phi_{Q_2}(\gamma)_k)$, where the scalar product $p \cdot [a,b] \stackrel{\text{def}}{=} [pa, pb]$ for $p \geq 0$.
On the other hand, from the premise, we have $Q_k = P_k +_{\mathcal{PI}} R_k$ and $P_k = (([p,p], \cdots, [0,0]) \otimes Q_1)_k = \binom{k}{0} \times_{\mathcal{PI}} ([p,p] \cdot_{\mathcal{PI}} (Q_1)_k) = p \cdot (Q_1)_k$, as well as $R_k = (1-p) \cdot (Q_2)_k$.
Therefore, we have $\phi_Q(\gamma)_k = \phi_{\overrightarrow{\langle P_k +_{\mathcal{PI}} R_k\rangle_{0\leq k\leq m}}}(\gamma)_k = p \cdot \phi_{Q_1}(\gamma)_k +_{\mathcal{I}} (1-p) \cdot \phi_{Q_2}(\gamma)_k$.

(Q-Cond)
$$\frac{\Delta \vdash \{\Gamma \wedge L; Q\}\ S_1\ \{\Gamma'; Q'\} \qquad \Delta \vdash \{\Gamma \wedge \neg L; Q\}\ S_2\ \{\Gamma'; Q'\}}{\Delta \vdash \{\Gamma; Q\}\ \mathbf{if}\ L\ \mathbf{then}\ S_1\ \mathbf{else}\ S_2\ \mathbf{fi}\ \{\Gamma'; Q'\}}$$

- Let $b \in \{\top, \bot\}$ be such that $\gamma \vdash L \Downarrow b$.
If $b = \top$, then $\nu = \delta(\langle \gamma, S_1, K, \alpha\rangle)$.
We set $\mu = \delta(\langle \Gamma \wedge L, Q, \gamma, S_1, K, \alpha\rangle)$.
In this case, we know that $\gamma \models \Gamma \wedge L$.
By the premise and the assumption, we know that $\Delta \vdash \{\Gamma \wedge L; Q\}\ S_1\ \{\Gamma'; Q'\}$ and $\Delta \vdash \{\Gamma'; Q'\}\ K$.
If $b = \bot$, then $\nu = \delta(\langle \gamma, S_2, K, \alpha\rangle)$.
We set $\mu = \delta(\langle \Gamma \wedge \neg L, Q, \gamma, S_2, K, \alpha\rangle)$.
In this case, we know that $\gamma \models \Gamma \wedge \neg L$.
By the premise and the assumption, we know that $\Delta \vdash \{\Gamma \wedge \neg L; Q\}\ S_2\ \{\Gamma'; Q'\}$ and $\Delta \vdash \{\Gamma'; Q'\}\ K$.
In both cases, γ and Q do not change, thus we conclude that $\phi_Q(\gamma) = \underline{1} \otimes \phi_Q(\gamma)$.

(Q-Loop)
$$\frac{\Delta \vdash \{\Gamma \wedge L; Q\}\ S\ \{\Gamma; Q\}}{\Delta \vdash \{\Gamma; Q\}\ \textbf{while}\ L\ \textbf{do}\ S_1\ \textbf{od}\ \{\Gamma \wedge \neg L; Q\}}$$

- We have $\nu = \delta(\langle \gamma, \textbf{skip}, \textbf{Kloop}\ L\ S\ K, \alpha\rangle)$.
  Then we set $\mu = \delta(\langle \Gamma, Q, \gamma, \textbf{skip}, \textbf{Kloop}\ L\ S\ K, \alpha\rangle)$.
  By (Q-Skip), we have $\Delta \vdash \{\Gamma; Q\}\ \textbf{skip}\ \{\Gamma; Q\}$.
  Then by the assumption $\Delta \vdash \{\Gamma \wedge \neg L; Q\}\ K$ and the premise, we know that $\Delta \vdash \{\Gamma; Q\}\ \textbf{Kloop}\ L\ S\ K$ by (QK-Loop).
  Because γ and Q do not change, we conclude that $\phi_Q(\gamma) = \underline{1} \otimes \phi_Q(\gamma)$.

(Q-Seq)
$$\frac{\Delta \vdash \{\Gamma; Q\}\ S_1\ \{\Gamma'; Q'\} \qquad \Delta \vdash \{\Gamma'; Q'\}\ S_2\ \{\Gamma''; Q''\}}{\Delta \vdash \{\Gamma; Q\}\ S_1; S_2\ \{\Gamma''; Q''\}}$$

- We have $\nu = \delta(\langle \gamma, S_1, \textbf{Kseq}\ S_2\ K, \alpha\rangle)$.
  Then we set $\mu = \delta(\langle \Gamma, Q, \gamma, S_1, \textbf{Kseq}\ S_2\ K, \alpha\rangle)$.
  By the first premise, we have $\Delta \vdash \{\Gamma; Q\}\ S_1\ \{\Gamma'; Q'\}$.
  By the assumption $\Delta \vdash \{\Gamma''; Q''\}\ K$ and the second premise, we know that $\Delta \vdash \{\Gamma'; Q'\}\ \textbf{Kseq}\ S_2\ K$ by (QK-Seq).
  Because γ and Q do not change, we conclude that $\phi_Q(\gamma) = \underline{1} \otimes \phi_Q(\gamma)$.

(Q-Weaken)
$$\frac{\Delta \vdash \{\Gamma_0; Q_0\}\ S\ \{\Gamma_0'; Q_0'\} \qquad \Gamma \models \Gamma_0 \qquad \Gamma_0' \models \Gamma' \qquad \Gamma \models Q \sqsupseteq Q_0 \qquad \Gamma_0' \models Q_0' \sqsupseteq Q'}{\Delta \vdash \{\Gamma; Q\}\ S\ \{\Gamma'; Q'\}}$$

- By $\gamma \models \Gamma$ and $\Gamma \models \Gamma_0$, we know that $\gamma \models \Gamma_0$.
  By the assumption $\Delta \vdash \{\Gamma'; Q'\}\ K$ and the premise $\Gamma_0' \models \Gamma'$, $\Gamma_0' \models Q_0' \sqsupseteq Q'$, we derive $\Delta \vdash \{\Gamma_0'; Q_0'\}\ K$ by (QK-Weaken).
  Thus let μ_0 be obtained by the induction hypothesis on $\Delta \vdash \{\Gamma_0; Q_0\}\ S\ \{\Gamma_0'; Q_0'\}$.
  Then $\phi_{Q_0}(\gamma) \sqsupseteq \mathbb{E}_{\sigma' \sim \mu_0}[\overrightarrow{\langle [(\alpha' - \alpha)^k, (\alpha' - \alpha)^k]\rangle_{0 \le k \le m}} \otimes \phi_{Q''}(\gamma')]$, where $\sigma' = \langle \_, Q'', \gamma', \_, \_, \alpha'\rangle$.
  We set $\mu = \mu_0$.
  By the premise $\Gamma \models Q \sqsupseteq Q_0$ and $\gamma \models \Gamma$, we conclude that $\phi_Q(\gamma) \sqsupseteq \phi_{Q_0}(\gamma)$.

□

Therefore, I can use the annotated kernel κ above to re-construct the trace-based moment semantics in §5.3.2. Then I can define the potential function on annotated program configurations as $\phi(\sigma) \stackrel{\text{def}}{=} \phi_Q(\gamma)$ where $\sigma = \langle \_, Q, \gamma, \_, \_, \_\rangle$.

The next step is to apply the extended OST for interval bounds (Theorem 5.25). Recall that the theorem requires that for some $\ell \in \mathbb{N}$ and $C \ge 0$, $\|Y_n\|_\infty \le C \cdot (n+1)^\ell$ almost surely for all $n \in \mathbb{Z}^+$. One sufficient condition for the requirement is to assume the *bounded-update* property, i.e., every (deterministic or probabilistic) assignment to a program variable updates the variable with a bounded change. As observed by Wang et al. [154], bounded updates are common in practice. I formulate the idea as follows.

LEMMA 5.28. *If there exists $C_0 \geq 0$ such that for all $n \in \mathbb{Z}^+$ and $x \in \mathsf{VID}$, it holds that $\mathbb{P}[|\gamma_{n+1}(x) - \gamma_n(x)| \leq C_0] = 1$ where ω is an infinite trace, $\omega_n = \langle \gamma_n, \_, \_, \_ \rangle$, and $\omega_{n+1} = \langle \gamma_{n+1}, \_, \_, \_ \rangle$, then there exists $C \geq 0$ such that for all $n \in \mathbb{Z}^+$, $\|Y_n\|_\infty \leq C \cdot (n+1)^{md}$ almost surely.*

PROOF. Let $C_1 \geq 0$ be such that for all $\mathbf{tick}(c)$ statements in the program, $|c| \leq C_1$. Then for all ω, if $\omega_n = \langle \_, \_, \_, \alpha_n \rangle$, then $|\alpha_n| \leq n \cdot C_1$. On the other hand, we know that $\mathbb{P}[|\gamma_n(x) - \gamma_0(x)| \leq C_0 \cdot n] = 1$ for any variable x. As we assume all the program variables are initialized to zero, we know that $\mathbb{P}[|\gamma_n(x)| \leq C_0 \cdot n] = 1$. From the construction in the proof of Lemma 5.26, we know that all the templates used to define the interval-valued potential function should have almost surely bounded coefficients. Let $C_2 \geq 0$ be such a bound. Also, the k-th component in a template is a polynomial in $\mathbb{R}_{kd}[\mathsf{VID}]$. Therefore, $\Phi_n(\omega) = \phi(\omega_n) = \phi_{Q_n}(\gamma_n)$, and

$$|\phi_{Q_n}(\gamma_n)_k| \leq \sum_{i=0}^{kd} C_2 \cdot |\mathsf{VID}|^i \cdot |C_0 \cdot n|^i \leq C_3 \cdot (n+1)^{kd}, \text{ a.s.},$$

for some sufficiently large constant C_3. Thus

$$\begin{aligned} |(Y_n)_k| = |(A_n \otimes \Phi_n)_k| &= |\sum_{i=0}^{k}{}_{\mathcal{I}} \binom{k}{i} \times_{\mathcal{I}} ((A_n)_i \cdot_{\mathcal{I}} (\Phi_n)_{k-i})| \\ &\leq \sum_{i=0}^{k} \binom{k}{i} \cdot (n \cdot C_1)^i \cdot (C_3 \cdot (n+1))^{(k-i)d} \\ &\leq C_4 \cdot (n+1)^{kd}, \text{ a.s.}, \end{aligned}$$

for some sufficiently large constant C_4. Therefore $\|Y_n\|_\infty \leq C_5 \cdot (n+1)^{md}$, a.s., for some sufficiently large constant C_5. □

Now I prove the soundness of the bound inference for central moment analysis.

PROOF OF THEOREM 5.23. By Lemma 5.28, there exists $C \geq 0$ such that $\|Y_n\|_\infty \leq C \cdot (n+1)^{md}$ almost surely for all $n \in \mathbb{Z}^+$. By the assumption, we also know that $\mathbb{E}[T^{md}] < \infty$. Thus by Theorem 5.25, we conclude that $\mathbb{E}[Y_T] \sqsubseteq \mathbb{E}[Y_0]$, i.e., $\mathbb{E}[A_T] \sqsubseteq \mathbb{E}[\Phi_0] = \phi_Q(\lambda\_.0)$. □

5.3.4 An Algorithm for Checking Soundness Criteria

Termination Analysis I reuse my system for automatically deriving higher moments, which I developed in §5.2.3 and §5.2.4, for checking if $\mathbb{E}[T^{md}] < \infty$ (Theorem 5.23(i)). To reason about termination time, I assume that every program statement increments the cost accumulator by one. For example, the inference rule (Q-SAMPLE) becomes

$$\frac{\Gamma = \forall x \in \mathrm{supp}(\mu_D) : \Gamma' \qquad Q = \langle 1, 1, \cdots, 1 \rangle \otimes \mathbb{E}_{x \sim \mu_D}[Q']}{\Delta \vdash \{\Gamma; Q\}\ x \sim D\ \{\Gamma'; Q'\}}$$

However, I cannot apply Theorem 5.23 for the soundness of the termination-time analysis, because that would introduce a circular dependence. Instead, I use a different proof technique to reason about $\mathbb{E}[T^{md}]$, taking into account the *monotonicity* of the runtimes. My upper-bound analysis of higher moments of runtimes is similar to the approach of Kura et al. [104]. In this section, I assume $\mathcal{R} = (\mathbb{R}^+_\infty, \leq, +, \cdot, 0, 1)$ to be a partially ordered semiring on extended nonnegative real numbers.

Definition 5.29. A map $\psi : \Sigma \to \mathcal{M}_{\mathcal{R}}^{(m)}$ is said to be an *expected-potential function* for upper bounds on stopping time if

(i) $\psi(\sigma)_0 = 1$ for all $\sigma \in \Sigma$,

(ii) $\psi(\sigma) = \underline{1}$ if $\sigma = \langle \_, \mathbf{skip}, \mathbf{Kstop}, \_ \rangle$, and

(iii) $\psi(\sigma) \sqsupseteq \mathbb{E}_{\sigma' \sim \mapsto (\sigma)}[\langle 1, 1, \cdots, 1 \rangle \otimes \psi(\sigma')]$ for all non-terminating configuration $\sigma \in \Sigma$.

Intuitively, $\psi(\sigma)$ is an upper bound on the moments of the evaluation steps upon termination for the computation that *continues from* the configuration σ. I define A_n and Ψ_n where $n \in \mathbb{Z}^+$ to be random variables on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ of the trace semantics as $A_n(\omega) \stackrel{\text{def}}{=} \overrightarrow{\langle n^k \rangle}_{0 \le k \le m}$ and $\Psi_n(\omega) \stackrel{\text{def}}{=} \psi(\omega_n)$. Then I define $A_T(\omega) \stackrel{\text{def}}{=} A_{T(\omega)}(\omega)$. Note that $A_T = \overrightarrow{\langle T^k \rangle}_{0 \le k \le m}$.

I now show that a valid potential function for stopping time *always* gives a sound upper bound by applying the Monotone Convergence Theorem reviewed below.

Proposition 5.30 (Monotone convergence theorem). *If $\{f_n\}_{n \in \mathbb{Z}^+}$ is a non-decreasing sequence of nonnegative measurable functions on a measure space $(S, \mathcal{S}, \mu)$, and $\{f_n\}_{n \in \mathbb{Z}^+}$ converges to f pointwise, then f is measurable and* $\lim_{n \to \infty} \mu(f_n) = \mu(f) \le \infty$.

Further, the theorem still holds if f is chosen as a measurable function and "$\{f_n\}_{n \in \mathbb{Z}^+}$ converges to f pointwise" holds almost everywhere*, rather than* everywhere.

Theorem 5.31. $\mathbb{E}[A_T] \sqsubseteq \mathbb{E}[\Psi_0]$.

Proof. Let $C_n(\omega) \stackrel{\text{def}}{=} \langle 1, 1, \cdots, 1 \rangle$ if $n < T(\omega)$, otherwise $C_n(\omega) \stackrel{\text{def}}{=} \langle 1, 0, \cdots, 0 \rangle$. Then $A_T = \bigotimes_{i=0}^{\infty} C_i$. By Proposition 5.30, we know that $\mathbb{E}[A_T] = \lim_{n \to \infty} \mathbb{E}[\bigotimes_{i=0}^{n} C_i]$. Thus it suffices to show that for all $n \in \mathbb{Z}^+$, $\mathbb{E}[\bigotimes_{i=0}^{n} C_i] \sqsubseteq \mathbb{E}[\Psi_0]$.

Observe that $\{C_n\}_{n \in \mathbb{Z}^+}$ is adapted to $\{\mathcal{F}_n\}_{n \in \mathbb{Z}^+}$, because the event $\{T \le n\}$ is $\mathcal{F}_n$-measurable. Then we have

$$\begin{aligned} \mathbb{E}[\bigotimes_{i=0}^{n} C_i \otimes \Psi_{n+1} \mid \mathcal{F}_n] &= \bigotimes_{i=0}^{n-1} C_i \otimes \mathbb{E}[C_n \otimes \Psi_{n+1} \mid \mathcal{F}_n], \text{a.s.}, \\ &\sqsubseteq \bigotimes_{i=0}^{n-1} C_i \otimes \Psi_n. \end{aligned}$$

Therefore, $\mathbb{E}[\bigotimes_{i=0}^{n} C_i \otimes \Psi_{n+1}] \sqsubseteq \mathbb{E}[\Psi_0]$ for all $n \in \mathbb{Z}^+$ by a simple induction. Because $\Psi_{n+1} \sqsupseteq \underline{1}$, we conclude that

$$\mathbb{E}[\bigotimes_{i=0}^{n} C_i] \sqsubseteq \mathbb{E}[\bigotimes_{i=0}^{n} C_i \otimes \Psi_{n+1}] \sqsubseteq \mathbb{E}[\Psi_0].$$

□

Boundedness of $\|Y_n\|_\infty$, $n \in \mathbb{Z}^+$ To ensure that the condition in Theorem 5.23(ii) holds, I check if the analyzed program satisfies the *bounded-update* property: every (deterministic or probabilistic) assignment to a program variable updates the variable with a change bounded by a constant C almost surely. Then the absolute value of every program variable at evaluation step n can be bounded by $C \cdot n = O(n)$. Thus, a polynomial up to degree $\ell \in \mathbb{N}$ over program variables can be bounded by $O(n^\ell)$ at evaluation step n. As observed by Wang et al. [154], bounded updates are common in practice.

5.4 Tail-Bound Analysis

One application of the central-moment analysis is to bound the probability that the accumulated cost deviates from some given quantity. In this section, I sketch how I produce the tail bounds shown in Fig. 5.1(c).

There are a lot of *concentration-of-measure* inequalities in probability theory [47]. Among those, one of the most important is *Markov's inequality*:

Proposition 5.32. *If X is a nonnegative random variable and $a > 0$, then $\mathbb{P}[X \geq a] \leq \frac{\mathbb{E}[X^k]}{a^k}$ for any $k \in \mathbb{N}$.*

Recall that Fig. 5.1(b) presents upper bounds on the raw moments $\mathbb{E}[tick] \leq 2d + 4$ and $\mathbb{E}[tick^2] \leq 4d^2 + 22d + 28$ for the cost accumulator *tick*. With Markov's inequality, I derive the following tail bounds:

$$\mathbb{P}[tick \geq 4d] \leq \frac{\mathbb{E}[tick]}{4d} \leq \frac{2d+4}{4d} \xrightarrow{d\to\infty} \frac{1}{2}, \tag{5.8}$$

$$\mathbb{P}[tick \geq 4d] \leq \frac{\mathbb{E}[tick^2]}{(4d)^2} \leq \frac{4d^2+22d+28}{16d^2} \xrightarrow{d\to\infty} \frac{1}{4}. \tag{5.9}$$

Note that (5.9) provides an asymptotically more precise bound on $\mathbb{P}[tick \geq 4d]$ than (5.8) does, when d approaches infinity.

Central-moment analysis can obtain an even more precise tail bound. As presented in Fig. 5.1(b), my analysis derives $\mathbb{V}[tick] \leq 22d + 28$ for the variance of *tick*. We can now employ concentration inequalities that involve variances of random variables. Recall *Cantelli's inequality*:

Proposition 5.33. *If X is a random variable and $a > 0$, then $\mathbb{P}[X - \mathbb{E}[X] \geq a] \leq \frac{\mathbb{V}[X]}{\mathbb{V}[X]+a^2}$ and $\mathbb{P}[X - \mathbb{E}[X] \leq -a] \leq \frac{\mathbb{V}[X]}{\mathbb{V}[X]+a^2}$.*

With Cantelli's inequality, I obtain the following tail bound, where I assume $d \geq 2$:

$$\begin{aligned} &\mathbb{P}[tick \geq 4d] = \mathbb{P}[tick - (2d+4) \geq 2d-4] \\ &\leq \mathbb{P}[tick - \mathbb{E}[tick] \geq 2d-4] \leq \frac{\mathbb{V}[tick]}{\mathbb{V}[tick] + (2d-4)^2} \\ &= 1 - \frac{(2d-4)^2}{\mathbb{V}[tick] + (2d-4)^2} \leq \frac{22d+28}{4d^2+6d+44} \xrightarrow{d\to\infty} 0. \end{aligned} \tag{5.10}$$

For all $d \geq 15$, (5.10) gives a more precise bound than both (5.8) and (5.9). It is also clear from Fig. 5.1(c), where I plot the three tail bounds (5.8), (5.9), and (5.10), that the asymptotically most precise bound is the one obtained via variances.

In general, for higher central moments, I employ *Chebyshev's inequality* to derive tail bounds:

Proposition 5.34. *If X is a random variable and $a > 0$, then $\mathbb{P}[|X - \mathbb{E}[X]| \geq a] \leq \frac{\mathbb{E}[(X-\mathbb{E}[X])^{2k}]}{a^{2k}}$ for any $k \in \mathbb{N}$.*

In my experiments, I use Chebyshev's inequality to derive tail bounds from the fourth central moments. I will show in Fig. 5.14 that these tail bounds can be more precise than those obtained from both raw moments and variances.

5.5 Evaluation

In this section, I first describe the implementation of the automatic moment-analysis tool in §5.5.1. I then evaluate the performance of the tool in §5.5.2, compared with state-of-the-art analysis tools for higher moments.

5.5.1 Implementation

The prototype implementation of my moment-analysis tool is open-source and publicly available.[10] The tool is still under active development; thus, in this section, I first describe the implementation that produced the evaluation results in my paper [149] on which this chapter is based, and then discuss some enhancements I have implemented to improve the usability and efficiency of the tool.

The `pldi21` branch of my open-source tool retains the version used by my paper [149]. I implemented the central moment analysis in OCaml, and the implementation consists of about 5,300 LOC. The tool works on imperative arithmetic probabilistic programs. The language supports recursive functions, continuous distributions, unstructured control-flow, and local variables. To infer the bounds on the central moments for a cost accumulator in a program, the user needs to specify the order of the analyzed moment, and a maximal degree for the polynomials to be used in potential-function templates. Using APRON [80], I implemented an interprocedural numeric analysis to infer the logical contexts used in the derivation. My tool relies on the inferred logical contexts to implement the weakening rule (Q-Weaken) in Fig. 5.6. Recall that if we want to relax a symbolic interval, we need to find two *nonnegative* polynomials: one is subtracted from the lower bound; the other is added to the upper bound. For example, if $n \geq x$ and $m \geq y$ hold at a program point, then we can use $(n-x)$, $(m-y)$, $(n-x)(m-y)$, etc. as the candidate nonnegative polynomials. The bound-inference rules are implemented in a syntax-directed manner, *except* that I apply weakening rules only at branch statements. Intuitively, the two branches of a conditional statement have different logical contexts, so we might need different nonnegative polynomials to relax the bounds of two branches. I use the off-the-shelf solver Gurobi [66] for LP solving, and the SMT solver Z3 [43] to generate a concrete input that satisfies a given pre-condition. (Recall that in §5.2.4, I described how to use the concrete input to construct an objective function for LP solving.)

In the `master` branch of the tool repo, I have implemented some enhancements towards better usability and efficiency. The *usability* of the `pldi21` version is not satisfactory because it can only handle arithmetic probabilistic programs with real-valued program variables. For example, to analyze programs that involve array manipulation, the user had to reimplement a purely arithmetic program that over-approximates the behavior of the original program. Besides, a usable programming language should usually support multiple data types, such as real numbers, integers, Booleans, etc. It is already nontrivial to support those features in a static analyzer for non-probabilistic programs, and probabilities may pose new challenges; for example, as discussed in §5.3.3, probabilistic termination is very different from and much trickier than non-probabilistic termination. Another concern is *efficiency*: despite the fact that my prototype implementation in the `pldi21` version achieved reasonable efficiency and scalability in the experimental evaluation (see §5.5.2), the worst-case time complexity can become exponential in terms of the number of program variables and the depth of the call graph. In the rest of this section, I describe my implementation

[10] https://bitbucket.org/probabilistic/ginfer/

```
1  func compare(guess, secret)
2  //@auxiliary k s.t. 1 ≤ k ≤ N ∧ ∧_{j=k+1}^{N} (secret[j] = guess[j]) ∧ (secret[k] < guess[k]);
3  begin
4    i := N; cmp := 0;
5    while i > 0 do
6      tick(2);
7      while i > 0 do
8        if prob(0.5) then break fi;
9        tick(5);
10       if cmp > 0 ∨ (cmp = 0 ∧ guess[i] > secret[i]) then
11         //@assert(i ≤ k);
12         cmp := 1
13       else
14         //@assert(i > k);
15         tick(5);
16         if cmp < 0 ∨ (cmp = 0 ∧ guess[i] < secret[i]) then
17           //@assert(false);
18           cmp := −1
19         fi
20       fi;
21       tick(1); i := i − 1
22     od
23   od;
24   return cmp
25 end
```

Fig. 5.12: Assisted moment-bound derivation using a logical state. The derived upper bound on the variance of the accumulated cost is $26N^2 + 42N - 10k^2 - 10k$.

strategies for supporting array manipulation, more basic data types, probability encapsulation, an analysis for neededness of variables, and tunable context sensitivity.

Array Manipulation Soundly and precisely handling the program heap in static analysis is a hard problem and researchers have proposed many techniques to analyze heap manipulation (e.g., [64, 79]). In my implementation, I use a relatively lightweight semi-automatic approach that is first used by Carbonneaux et al. [22]; the idea is to introduce a *logical state* using *auxiliary variables* that are used in bound derivation but do *not* influence program behavior. The auxiliary variables provide a mechanism for users to specify logical or quantitative invariants, which can reflect properties of the heap contents and thus aid the moment-bound derivation. I introduce special syntactic forms for annotations of the declaration, manipulation, and assertion of auxiliary variables, and then implemented in the type checker a pass to make sure that the normal part of a program cannot refer to any auxiliary variables. In this way, the user does not need to reimplement a program; instead, they just need to add annotations, which can be treated as comments by a compiler.

Fig. 5.12 illustrates the idea on the compare function that compares two N-bit vectors *guess*

and *secret*. Note that I will later use this function in §5.6 to demonstrate an application of using central-moment analysis to reason about timing attacks. The function iterates over the bits from high-index to low-index, and it introduces some *random delays* (by the probabilistic branching on line 8) to add noise to its accumulated cost. Intuitively, the cost accumulator models the running time of the function. Suppose that for some fixed k, we want to analyze the compare function under the condition that the highest $(N-k)$ bits of *guess* and *secret* are identical, and $secret[k] < guess[k]$. The analysis result on moments of the running time can then indicate how the length of the common prefix of the two input vectors would influence the running time. In Fig. 5.12, the parts of the code marked in blue are user-provided annotations. The auxiliary variable k is introduced to specify a complicated array-related pre-condition. Because the program never mutates *secret* or *guess*, the assertions on lines 11, 14, and 17 can be directly justified using the logical-state invariant specified on line 2. With the extra information, the central-moment analysis tool is able to derive a fine-grained upper bound (which involves k) on the variance of the accumulated cost. Note that although the user just needs to add annotations about the logical state, they must verify the annotations are consistent on themselves. Integrating the moment-analysis tool with verification tools that can justify program variants is interesting future work.

More Basic Data Types It is often more desirable to support multiple data types in a programming language than just allowing real-valued program variables. Once one has multiple types in the system, the moment-bound analysis tool must find a proper way to reference program variables of different types in symbolic bounds. For example, consider the function f below with a Boolean-valued variable b:

```
func f(b) begin
  if b then
    if prob(0.4) then tick(1) else tick(2) fi
  else
    if prob(0.6) then tick(1) else tick(2) fi
  fi
end
```

Instead of using 1.6 as an upper bound on the expected accumulated cost of the function, my tool is able to derive a more precise bound that involves b as $[b] \cdot 1.6 + [\neg b] \cdot 1.4$, where $[\varphi]$ is the Iverson bracket which evaluates to 1 if φ is true, and to 0 otherwise. To support such reasoning, I adapt a systematic approach proposed by Hoffmann et al. [72] to express resource bounds in terms of values of different types for functional programs. The basic idea is to introduce for each type τ a set of *base monomials* that map inhabitants of type τ to real numbers, and then use those base monomials to construct polynomials that express moment bounds. I implemented the following simple type system:

$$\tau ::= \mathsf{real} \mid \mathsf{int} \mid \mathsf{bool} \mid \tau[],$$

where inhabitants of the type $\tau[]$ are arrays whose elements are of type τ. I now define base monomials $\mathcal{B}(\tau)$ for each type τ:

$$\mathcal{B}(\mathsf{real}) \stackrel{\text{def}}{=} \{\lambda v.\ v\}, \qquad \mathcal{B}(\mathsf{int}) \stackrel{\text{def}}{=} \{\lambda v.\ v\},$$

$$\mathcal{B}(\mathsf{bool}) \stackrel{\text{def}}{=} \{\lambda v.\ [v], \lambda v.\ [\neg v]\}, \qquad \mathcal{B}(\tau[]) \stackrel{\text{def}}{=} \{\lambda v.\ 1\}.$$

Note that the only base monomial for an array is the constant-one function; as a consequence, the moment analysis would not investigate the values in an array. Then, for a context $\Gamma = x_1 : \tau_1, \cdots, x_n : \tau_n$ of variable-type bindings, I define the set of monomials over program variables $x_1, \cdots, x_n$ as follows, where V is a map from variables to values:

$$\mathcal{M}(\Gamma) \stackrel{\text{def}}{=} \{\lambda V.\ \prod_{i=1}^{n} b_i(V(x_i))^{d_i} \mid b_i \in \mathcal{B}(\tau_i), d_i \in \mathbb{Z}^+\},$$

and thus the polynomial moment bounds over Γ can be expressed as linear combinations of finitely many monomials from $\mathcal{M}(\Gamma)$. Because my tool requires the user to provide a maximal degree for the polynomials to be used in the potential-function templates, I simply use monomials whose degree does not exceed the maximal degree.

Probability Encapsulation Another interesting direction for extending the type system is to add a type that *encapsulates* probabilities [152]; that is, the programming language has a type for *non-constant* probabilities and programs can manipulate those probabilities and flip a coin with respect to them in probabilistic branching. The motivation for supporting a probability-encapsulation type is that although most of the static analyzers for probabilistic programs assume that probabilistic branches are of constant probabilities, *non-constant* probabilities can become useful in verification tasks. For example, let us consider the following function that simulates a fair coin using a coin that shows heads with probability p and we want to verify the function is correct for any $p \in [0, 1]$:

```
func fair(p) begin
  if prob(p) then
    if prob(p) then call fair(p)
    else tick(1) fi # In this case, the outcome should be heads.
  else
    if prob(p) then tick(0) # In this case, the outcome should be tails.
    else call fair(p) fi
  fi
end
```

Because there is exactly one unit of cost when the simulation function decides to return heads as the coin-flip outcome, the expected accumulated cost is exactly the probability that the function returns heads. Indeed, my moment-bound analysis tool is able to derive $1/2$ as both the lower and the upper bounds on the expected accumulated cost for any possible coin-flip probability p.

To achieve this, I adapt the approach by Wang et al. [152] that adds a probability-encapsulation type to a functional programming language. I extend the simple type system mentioned earlier in this section with a primitive probability type as follows:

$$\tau ::= \mathsf{real} \mid \mathsf{int} \mid \mathsf{bool} \mid \tau[] \mid \mathsf{prob},$$

where the introduction form $\mathsf{P}(c)$ for values of type prob simply takes a real number $c \in [0, 1]$, and the elimination form "**if prob**(p) **then** $\cdots$ **else** $\cdots$ **fi**" is a probabilistic branch on a value p of type prob. I then define the set of base monomials for prob by

$$\mathcal{B}(\mathsf{prob}) \stackrel{\text{def}}{=} \{\lambda \mathsf{P}(c).\ c, \lambda \mathsf{P}(c).\ (1 - c)\}.$$

Furthermore, it is convenient to incorporate the ability to multiply and invert encapsulated probabilities in the programming language. The major challenge was to add inference rules for those new program constructs, as well as effectively automate newly added rules in the moment analysis tool. I implemented the following two rules for probability multiplication and probability inversion, where for a program variable x of type prob, I write x for the base monomial $\lambda \mathsf{P}(c).\ c$ and $\overline{x}$ for the base monomial $\lambda \mathsf{P}(c).\ (1-c)$. Meanwhile, because the set of base monomials is not necessarily linearly independent, (e.g., $\{1, x, \overline{x}\}$ is not linearly independent as $\overline{x} = 1 + (-1) \cdot x$), I also took care of canonical representations of polynomial templates in my implementation.

$$\frac{Q = [(y \cdot z,\ 1 - (1-\overline{y}) \cdot (1-\overline{z}))/(x, \overline{x})]Q'}{\Delta \vdash_h \{\Gamma; Q\}\ x \coloneqq \mathsf{prob\_mul}(y, z)\ \{\Gamma; Q'\}}\ (\textsc{Prob-Mult}) \qquad \frac{Q = [(\overline{y}, y)/(x, \overline{x})]Q'}{\Delta \vdash_h \{\Gamma; Q\}\ x \coloneqq \mathsf{prob\_inv}(y)\ \{\Gamma; Q'\}}\ (\textsc{Prob-Inv})$$

Analysis of Neededness Besides the analysis capability, the analysis efficiency is also an important aspect to evaluate a static analyzer. Recall that my central-moment analysis framework uses polynomials over program variables as the templates for moment bounds; therefore, even with a fixed maximal degree on the polynomials, the number of possible monomials grows *exponentially* in terms of the number of program variables. It is obviously redundant to use all program variables to express the moment bound at every program point. For example, consider the program below:

```
1 while x < d do
2     t ~ Uniform(−1, 2);
3     x := x + t;
4     tick(1)
5 od
```

There are three program variables x, d, and t, but not all variables are *needed* to encode the moment bound at every program location; for example, the variable t is just used to save a temporary value drawn from a distribution, so it is only needed between the time it is created and the time it is used, i.e., between line 2 and line 3 of the code.

Inspired by the liveness analysis, I implemented a intra-procedural data-flow analysis to evaluate the *neededness* of every program variable at every program point for expressing moment bounds. Fig. 5.13 presents the neededness analysis as an inference system. The judgement $\vdash \{U\}\ S\ \{U'\}$ should be read in a *backward* manner: if the continuation after a statement S needs a set U' of program variables in the moment bounds, then a set U of program variables is needed before the statement S. Thus, the rules formulate a backward data-flow analysis. I denote by $\mathrm{FV}(E)$ and $\mathrm{FV}(L)$ the set of free variables that appear in the expression E and the condition L, respectively. The interesting cases are the rule (N-Loop) and (N-Cond). As I described earlier in this section, my tool would apply the weakening rule (Q-Weaken) at the branching statements. For a conditional branch whose predicate is L, the set of nonnegative polynomials that can be used for weakening might be different in different branches, and such a difference depends on L. Thus, I enforce that the free variables of the branch predicate L are needed at the beginning of succeeding branches.

Tunable Context Sensitivity Another source of the exponential time complexity of the moment analysis is the treatment of *context sensitivity*, i.e., function calls to the same function at different

$$\text{(N-Skip)}\ \frac{}{\vdash \{U\}\ \textbf{skip}\ \{U\}} \qquad \text{(N-Tick)}\ \frac{}{\vdash \{U\}\ \textbf{tick}(c)\ \{U\}} \qquad \text{(N-Assign)}\ \frac{U = \textbf{if}\ x \in U'\ \textbf{then}\ (U' \setminus \{x\}) \cup \mathrm{FV}(E)\ \textbf{else}\ U'}{\vdash \{U\}\ x \coloneqq E\ \{U'\}}$$

$$\text{(N-Sample)}\ \frac{U = \textbf{if}\ x \in U'\ \textbf{then}\ U' \setminus \{x\}\ \textbf{else}\ U'}{\vdash \{U\}\ x \sim D\ \{U'\}} \qquad \text{(N-Loop)}\ \frac{\vdash \{U\}\ S\ \{U\} \qquad \mathrm{FV}(L) \subseteq U}{\vdash \{U\}\ \textbf{while}\ L\ \textbf{do}\ S\ \textbf{od}\ \{U\}} \qquad \text{(N-Call)}\ \frac{}{\vdash \{U\}\ \textbf{call}\ f\ \{U\}}$$

$$\text{(N-Seq)}\ \frac{\vdash \{U\}\ S_1\ \{U'\} \qquad \vdash \{U'\}\ S_2\ \{U''\}}{\vdash \{U\}\ S_1; S_2\ \{U''\}} \qquad \text{(N-Prob)}\ \frac{\vdash \{U_1\}\ S_1\ \{U'\} \qquad \vdash \{U_2\}\ S_2\ \{U'\} \qquad U = U_1 \cup U_2}{\vdash \{U\}\ \textbf{if}\ \textbf{prob}(p)\ \textbf{then}\ S_1\ \textbf{else}\ S_2\ \textbf{fi}\ \{U'\}}$$

$$\text{(N-Cond)}\ \frac{\vdash \{U_1\}\ S_1\ \{U'\} \qquad \vdash \{U_2\}\ S_2\ \{U'\} \qquad U = U_1 \cup U_2 \qquad \mathrm{FV}(L) \subseteq U_1 \qquad \mathrm{FV}(L) \subseteq U_2}{\vdash \{U\}\ \textbf{if}\ L\ \textbf{then}\ S_1\ \textbf{else}\ S_2\ \textbf{fi}\ \{U'\}} \qquad \text{(N-Weaken)}\ \frac{\vdash \{U_0\}\ S\ \{U_0'\} \qquad U_0 \subseteq U \qquad U' \subseteq U_0'}{\vdash \{U\}\ S\ \{U'\}}$$

Fig. 5.13: Inference rules of the neededness analysis.

call sites can use different function specifications in the bound derivation. More specifically, in my prototype implementation of the `pldi21` version, I collapse the cycles in the call graph and analyze each function at least once for every path in the resulting graph. This implementation strategy can make the moment analysis extremely slow when the call graph has a complex structure.

To tackle this problem, I adapt different treatments for context sensitivity of static analysis, and in the moment-analysis tool, I allow the user to specify the granularity of the context sensitivity. I implemented *k-limiting* context sensitivity [138], i.e., the static analysis does not distinguish two function calls if both have the same k immediate call sites. I also reimplemented the built-in context sensitivity of the `pldi21` version as the *acyclic* context sensitivity, i.e., the static analysis only remembers the longest prefix of the call stack such that no call sites can appear twice in the prefix. My preliminary experiments have shown that 0-limiting context sensitivity is sufficient for many recursive probabilistic programs, but a thorough evaluation on a broader suite of recursive benchmarks is left for future work. Before ending this section, I demonstrate an example that indeed requires k-limiting context sensitivity for $k > 0$.

Example 5.35. Consider the following probabilistic variant of the McCarthy 91 function:

```
func f91(x) begin
  if x > 100 then
    x := x − 10; return x
  else
    x := x + 11;
    x := call f91(x); tick(1);
    if prob(1/3) then
      x := call f91(x); tick(1)
    fi;
    return x
  fi
end
```

I assume the pre-condition $x \leq 100$ *in the analysis. Using* 0*-limiting context sensitivity, my tool cannot derive an upper bound on the expected accumulated cost. With* 1*- and* 2*-limiting context sensitivity, my tool is able to derive* $55.5 - 0.5x$ *and* $54.5 - 0.5x$ *as the upper bounds, respectively. With the acyclic context sensitivity, my tool derives the bound* $55 - 0.5x$*. The results meet my expectation: k-limiting sensitivity with larger k should yield (not strictly) more precise bounds. Also, for the* ***f91*** *function above, there are two recursive call sites, so with the acyclic context sensitivity, the analyzer handles call stacks whose length is at most two, thus the result cannot be more precise than the analysis result under* 2*-limiting sensitivity.*

5.5.2 Experiments

Evaluation Setup I evaluated my tool to answer the following three research questions:

1. How does the raw-moment inference part of my tool compare to existing techniques for expected-cost bound analysis [124, 154]?

2. How does my tool compare to the state of the art in tail-probability analysis (which is based only on higher *raw* moments [104])?

3. How scalable is my tool? Can it analyze programs with many recursive functions?

A replication package for the evaluation results in this section is publicly available [151].

For the first question, I collected a broad suite of challenging examples from related work [104, 124, 154] with different loop and recursion patterns, as well as probabilistic branching, discrete sampling, and continuous sampling. My tool achieved comparable precision and efficiency with the prior work on expected-cost bound analysis [124, 154]. The details are included in Tables 5.4 and 5.5.

For the second question, I evaluated my tool on the complete benchmarks from Kura et al. [104]. I also conducted a case study of a timing-attack analysis for a program provided by DARPA during engagements of the STAC program [41], where central moments are more useful than raw moments to bound the success probability of an attacker. I include the case study in §5.6.

For the third question, I conducted case studies on two sets of synthetic benchmark programs:

- coupon-collector programs with N coupons ($N \in [1, 10^3]$), where each program is implemented as a set of tail-recursive functions, each of which represents a state of coupon

collection, i.e., the number of coupons collected so far; and

- random-walk programs with N consecutive one-dimensional random walks ($N \in [1, 10^3]$), each of which starts at a position that equals the number of steps taken by the previous random walk to reach the ending position (the origin). Each program is implemented as a set of non-tail-recursive functions, each of which represents a random walk. The random walks in the same program can have different transition probabilities.

The largest synthetic program has nearly 16,000 LOC. I then ran my tool to derive an upper bound on the fourth (resp., second) central moment of the runtime for each coupon-collector (resp., random-walk) program.

The experiments were performed on a machine with an Intel Core i7 3.6GHz processor and 16GB of RAM under macOS Catalina 10.15.7.

Results Some of the evaluation results to answer the second research question are presented in Table 5.1. The programs (1-1) and (1-2) are coupon-collector problems with a total of two and four coupons, respectively. The other five are variants of random walks. The first three are one-dimensional random walks: (2-1) is integer-valued, (2-2) is real-valued with continuous sampling, and (2-3) exhibits adversarial nondeterminism. The programs (2-4) and (2-5) are two-dimensional random walks. The table contains the inferred upper bounds on the moments for runtimes of these programs, and the running times of the analyses. I compared my results with Kura et al. [104]'s inference tool for raw moments. My tool is as precise as, and sometimes more precise than the prior work on all the benchmark programs. Meanwhile, my tool is able to infer an upper bound on the raw moments of degree up to four on all the benchmarks, while the prior work reports failure on some higher moments for the random-walk programs. In terms of efficiency, my tool completed each example in less than 10 seconds, while the prior work took more than a few minutes on some programs. One reason why my tool is more efficient is that I always reduce higher-moment inference with non-linear polynomial templates to efficient LP solving, but the prior work requires semidefinite programming (SDP) for polynomial templates.

Besides raw moments, my tool is also capable of inferring upper bounds on the central moments of runtimes for the benchmarks. To evaluate the quality of the inferred central moments, Fig. 5.14 plots the upper bounds of tail probabilities on runtimes T obtained by Kura et al. [104], and those by my central-moment analysis. Specifically, the prior work uses Markov's inequality (Proposition 5.32), while I am also able to apply Cantelli's and Chebyshev's inequality (Propositions 5.33 and 5.34) with central moments. My tool outperforms the prior work on programs (1-1), (1-2), (2-3), and (2-5), and derives better tail bounds when d is large on programs (2-2) and (2-4), while it obtains similar curves on program (2-1).

Scalability In Fig. 5.15, I demonstrate the running times of my tool on the two sets of synthetic benchmark programs; Fig. 5.15a plots the analysis times for coupon-collector programs as a function of the independent variable N (the total number of coupons), and Fig. 5.15b plots the analysis times for random-walk programs as a function of N (the total number of random walks). The evaluation statistics show that my tool achieves good scalability in both case studies: the runtime is almost a linear function of the program size, which is the number of recursive functions for both case studies. Two reasons why my tool is scalable on the two sets of programs are (i) my analysis

Table 5.1: Inferred upper bounds on the raw/central moments of runtimes, with comparison to Kura et al. [104]. "T/O" stands for timeout after 30 minutes. "N/A" means that the tool is not applicable. "-" indicates that the tool fails to infer a bound. Entries with more precise results or less analysis time are marked in bold.

program	moment	my work		Kura et al. [104]	
		upper bnd.	time (sec)	upper bnd.	time (sec)
(1-1)	2^{nd} raw	**201**	0.019	**201**	**0.015**
	3^{rd} raw	**3,829**	**0.019**	**3,829**	0.020
	4^{th} raw	**90,705**	**0.023**	**90,705**	0.027
	2^{nd} central	**32**	**0.029**	N/A	N/A
	4^{th} central	**9,728**	**0.058**	N/A	N/A
(1-2)	2^{nd} raw	**2,357**	1.068	3,124	**0.037**
	3^{rd} raw	**148,847**	1.512	171,932	**0.062**
	4^{th} raw	**11,285,725**	1.914	12,049,876	**0.096**
	2^{nd} central	**362**	**3.346**	N/A	N/A
	4^{th} central	**955,973**	**9.801**	N/A	N/A
(2-1)	2^{nd} raw	**2,320**	**0.016**	**2,320**	11.380
	3^{rd} raw	**691,520**	**0.018**	-	16.056
	4^{th} raw	**340,107,520**	**0.021**	-	23.414
	2^{nd} central	**1,920**	**0.026**	N/A	N/A
	4^{th} central	**289,873,920**	**0.049**	N/A	N/A
(2-2)	2^{nd} raw	**8,375**	**0.022**	**8,375**	38.463
	3^{rd} raw	**1,362,813**	**0.028**	-	73.408
	4^{th} raw	**306,105,209**	**0.035**	-	141.072
	2^{nd} central	**5,875**	**0.029**	N/A	N/A
	4^{th} central	**447,053,126**	**0.086**	N/A	N/A
(2-3)	2^{nd} raw	**3,675**	**0.039**	6,710	48.662
	3^{rd} raw	**618,584**	0.049	19,567,045	**0.039**
	4^{th} raw	**164,423,336**	**0.055**	-	T/O
	2^{nd} central	**3,048**	**0.053**	N/A	N/A
	4^{th} central	**196,748,763**	**0.123**	N/A	N/A
(2-4)	2^{nd} raw	**6,625**	**0.035**	10,944	216.352
	3^{rd} raw	**742,825**	**0.048**	-	453.435
	4^{th} raw	**101,441,320**	**0.072**	-	964.579
	2^{nd} central	**6,624**	**0.051**	N/A	N/A
	4^{th} central	**313,269,063**	**0.215**	N/A	N/A
(2-5)	2^{nd} raw	**21,060**	**0.045**	-	216.605
	3^{rd} raw	**9,860,940**	**0.063**	-	467.577
	4^{th} raw	**7,298,339,760**	**0.101**	-	1133.947
	2^{nd} central	**20,160**	**0.068**	N/A	N/A
	4^{th} central	**8,044,220,161**	**0.271**	N/A	N/A

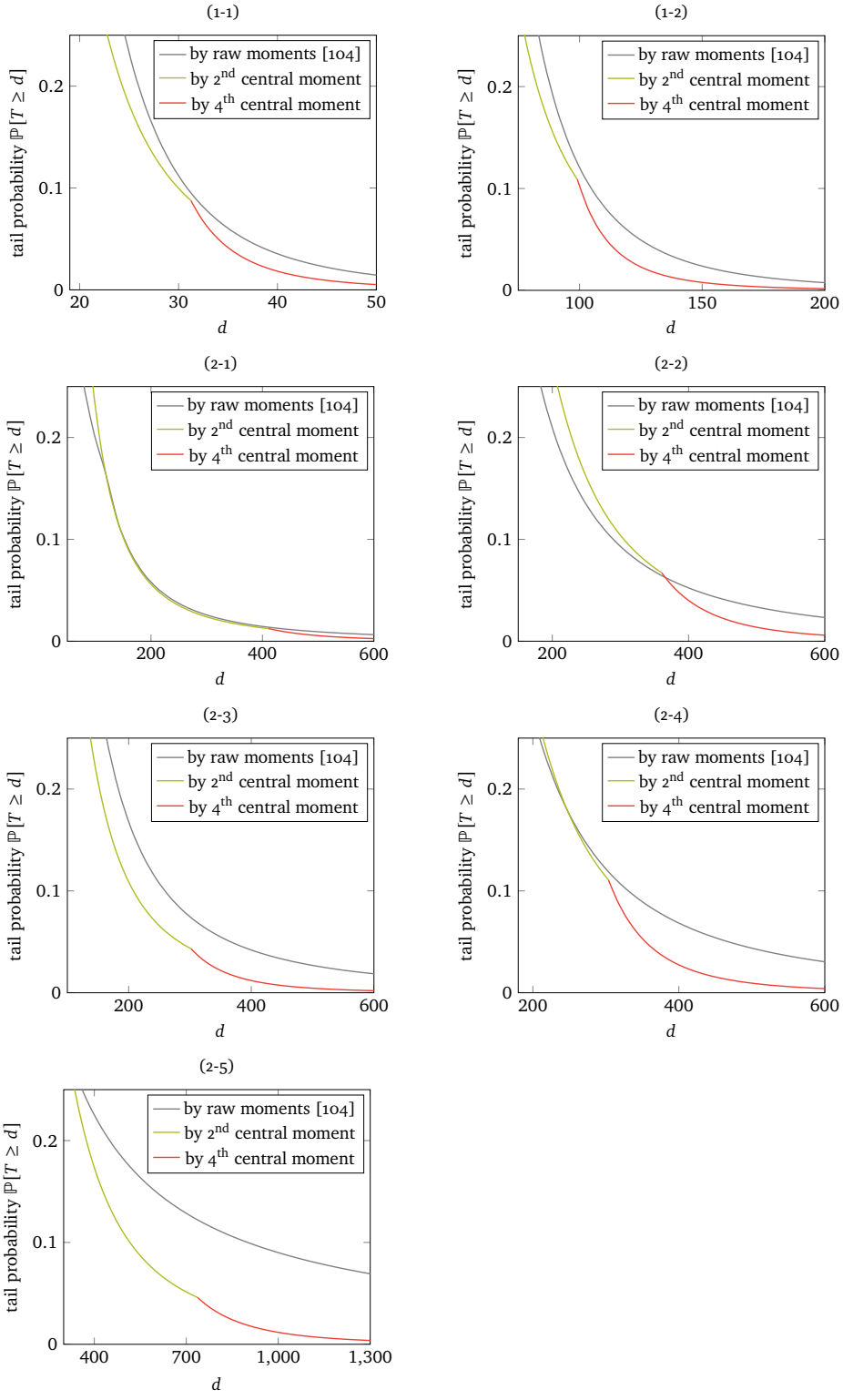
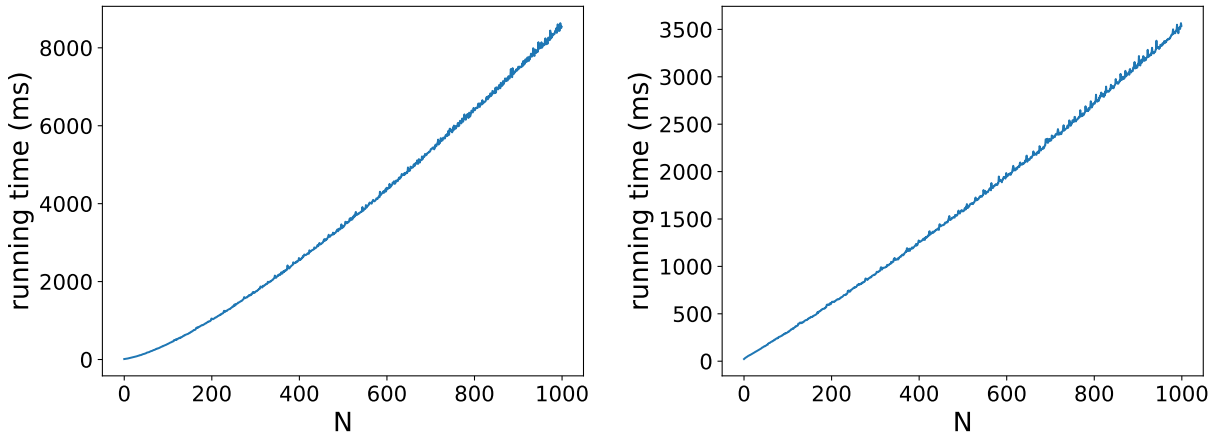


Fig. 5.14: Upper bound of the tail probability $\mathbb{P}[T \geq d]$ as a function of d, with comparison to Kura et al. [104]. Each gray line is the minimum of tail bounds obtained from the raw moments of degree up to four inferred by Kura et al. [104]. Green lines and red lines are the tail bounds given by 2nd and 4th central moments inferred by my tool, respectively.



(a) Coupon Collector (b) Random Walk

Fig. 5.15: Running times of my tool on two sets of synthetic benchmark programs. Each figure plots the runtimes as a function of the size of the analyzed program.

is compositional and uses function summaries to analyze function calls, and (ii) for a fixed set of templates and a fixed diameter of the call graph, the number of linear constraints generated by my tool grows linearly with the size of the program, and the LP solvers available nowadays can handle large problem instances efficiently.

Discussion Higher central moments can also provide more information about the *shape* of a distribution, e.g., the *skewness* (i.e., $\frac{\mathbb{E}[(T-\mathbb{E}[T])^3]}{(\mathbb{V}[T])^{3/2}}$) indicates how lopsided the distribution of T is, and the *kurtosis* (i.e., $\frac{\mathbb{E}[(T-\mathbb{E}[T])^4]}{(\mathbb{V}[T])^2}$) measures the heaviness of the tails of the distribution of T. I used my tool to analyze two variants of the random-walk program (2-1). The two random walks have different transition probabilities and step lengths, but they have the same expected runtime $\mathbb{E}[T]$. Table 5.2 presents the skewness and kurtosis derived from the moment bounds inferred by my tool. A positive skew indicates that the mass of the distribution is concentrated on the *left*, and larger skew means the concentration is more *left*. A larger kurtosis, on the other hand, indicates that the distribution has *fatter* tails. Therefore, as the derived skewness and kurtosis indicate, the distribution of the runtime T for rdwalk-2 should be more left-leaning and have fatter tails than the distribution for rdwalk-1. Density estimates for the runtime T, obtained by simulation, are shown in Fig. 5.16.

Table 5.2: Skewness & kurtosis.

program	skewness	kurtosis
rdwalk-1	2.1362	10.5633
rdwalk-2	2.9635	17.5823

My tool can also derive *symbolic* bounds on higher moments. Table 5.3 presents the inferred upper bounds on the variances for the random-walk benchmarks, where I replace the concrete inputs with symbolic pre-conditions.

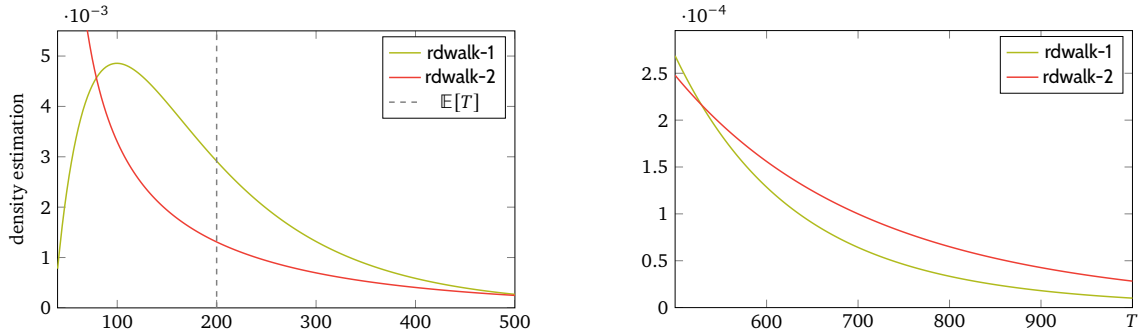


Fig. 5.16: Density estimation for the runtime T of two variants rdwalk-1 and rdwalk-2 of (2-1).

Table 5.3: Inferred symbolic upper bounds on the variances.

program	pre-condition	upper bound on the variance
(2-1)	$x \geq 0$	$1920x$
(2-2)	$x \geq 0$	$2166.6667x + 1541.6667$
(2-3)	$x \geq 0$	$284.2060x^2 + 955.25x$
(2-4)	$x \geq 0 \wedge y > 0$	$144(x+y)^2 + 816(x+y) + 1056$
(2-5)	$x \geq y$	$7920(x-y) + 12240$

5.6 Case Study: Timing Attack

In the case study, I motivate the use of central-moment analysis on a probabilistic program with a *timing-leak* vulnerability, and demonstrate how the results from an analysis can be used to bound the success rate of an attack program that attempts to exploit the vulnerability. The program is extracted and modified from a web application provided by DARPA during engagements as part of the STAC program [41]. In essence, the program models a password checker that compares an input *guess* with an internally stored password *secret*, represented as two N-bit vectors. The program in Fig. 5.17(a) is the interface of the checker, and Fig. 5.17(b) is the comparison function compare, which carries out most of the computation. The statements of the form "**tick**$(\cdot)$" represent a cost model for the running time of compare, which is assumed to be observable by the attacker. compare iterates over the bits from high-index to low-index, and the running time expended during the processing of bit i depends on the current comparison result (stored in *cmp*), as well as on the values of the i-th bits of *guess* and *secret*. Because the running time of compare might *leak* information about the relationship between *guess* and *secret*, compare introduces some *random delays* to add noise to its running time. However, we will see shortly that such a countermeasure does *not* protect the program from a timing attack.

I now show how the moments of the running time of compare—the kind of information provided by my central-moment analysis (§5.2)—are useful for analyzing the success probability of the attack program given in Fig. 5.17(c). Let T be the random variable for the running time of compare. A standard timing attack for such programs is to guess the bits of *secret* successively. The idea is the following: Suppose that we have successfully obtained the bits $secret[i+1]$ through $secret[N]$; we now guess that the next bit, $secret[i]$, is 1 and set $guess[i] := 1$. Theoretically, if the following

```
1  func check(guess) begin
2    cmp := compare(guess, secret);
3    if cmp = 0 then
4      login()
5    fi
6  end
```

(a)

```
1  func compare(guess, secret) begin
2    i := N; cmp := 0;
3    while i > 0 do
4      tick(2);
5      while i > 0 do
6        if prob(0.5) then break fi;
7        tick(5);
8        if cmp > 0 ∨ (cmp = 0 ∧ guess[i] > secret[i])
9        then cmp := 1
10       else
11         tick(5);
12         if cmp < 0 ∨ (cmp = 0 ∧ guess[i] < secret[i])
13         then cmp := −1
14         fi
15       fi;
16       tick(1);
17       i := i − 1
18     od
19   od;
20   return cmp
21 end
```

(b)

```
1  guess := 0⃗;
2  i := N;
3  while i > 0 do
4    next := guess;
5    next[i] := 1;
6    est := estimateTime(K, check(next));
7    if est ≤ 14N − 2.5i then
8      guess[i] := 0
9    else
10     guess[i] := 1
11   fi;
12   i := i − 1
13 od
```

(c)

Fig. 5.17: (a) The interface of the password checker. (b) A function that compares two bit vectors, adding some random noise. (c) An attack program that attempts to exploit the timing properties of compare to find the value of the password stored in *secret*.

two conditional expectations

$$\mathbb{E}[T_1] \stackrel{\text{def}}{=} \mathbb{E}[T \mid \textstyle\bigwedge_{j=i+1}^{N}(secret[j] = guess[j]) \wedge (secret[i] = 1 \wedge guess[i] = 1)] \tag{5.11}$$

$$\mathbb{E}[T_0] \stackrel{\text{def}}{=} \mathbb{E}[T \mid \textstyle\bigwedge_{j=i+1}^{N}(secret[j] = guess[j]) \wedge (secret[i] = 0 \wedge guess[i] = 1)] \tag{5.12}$$

have a significant difference, then there is an opportunity to check our guess by running the program multiple times, using the *average* running time as an estimate of $\mathbb{E}[T]$, and choosing the value of $guess[i]$ according to whichever of (5.11) and (5.12) is closest to our estimate. However, if the difference between $\mathbb{E}[T_1]$ and $\mathbb{E}[T_0]$ is not significant enough, or the program produces a large amount of noise in its running time, the attack might not be realizable in practice. To determine whether the timing difference represents an exploitable vulnerability, we need to reason about the attack program's success rate.

Toward this end, we can analyze the failure probability for setting $guess[i]$ incorrectly, which happens when, due to an unfortunate fluctuation, the running-time estimate *est* is closer to one of $\mathbb{E}[T_1]$ and $\mathbb{E}[T_0]$, but the truth is actually the other. For instance, suppose that $\mathbb{E}[T_0] < \mathbb{E}[T_1]$ and $est < \frac{1}{2}(\mathbb{E}[T_0] + \mathbb{E}[T_1])$; the attack program would pick T_0 as the truth, and set $guess[i]$ to 0. If such a choice is *incorrect*, then the actual distribution of *est* on the i-th round of the attack program

satisfies $\mathbb{E}[est] = \mathbb{E}[T_1]$, and the probability of this failure event is

$$\begin{aligned}\mathbb{P}\left[est < \frac{\mathbb{E}[T_0] + \mathbb{E}[T_1]}{2}\right] &= \mathbb{P}\left[est - \mathbb{E}[T_1] < \frac{\mathbb{E}[T_0] - \mathbb{E}[T_1]}{2}\right] \\ &= \mathbb{P}\left[est - \mathbb{E}[est] < \frac{\mathbb{E}[T_0] - \mathbb{E}[T_1]}{2}\right]\end{aligned}$$

under the condition given by the conjunction in (5.11). This formula has exactly the same shape as a *tail probability*, which makes it possible to utilize moments and *concentration-of-measure* inequalities [47] to bound the probability.

The attack program is parameterized by $K > 0$, which represents the number of trials it performs for each bit position to obtain an estimate of the running time. I have applied the central-moment-analysis technique developed in this chapter, and obtained the following inequalities on the mean (i.e., the first moment), the second moment, and the variance (i.e., the second central moment) of the quantities (5.11) and (5.12).

$$\mathbb{E}[T_1] \geq 13N, \qquad \mathbb{E}[T_1] \leq 15N, \qquad \mathbb{V}[T_1] \leq 26N^2 + 42N, \tag{5.13}$$

$$\mathbb{E}[T_0] \geq 13N - 5i, \qquad \mathbb{E}[T_0] \leq 15N - 5i, \qquad \mathbb{V}[T_0] \leq 26N^2 + 42N - 10i^2 - 10i. \tag{5.14}$$

To bound the probability that the attack program makes an incorrect guess for the i-th bit, I continue with a case analysis:

- Suppose that $secret[i] = 1$, but the attack program assigns $guess[i] := 0$. The truth—with respect to the actual distribution of the running time T of compare for the i-th bit—is that $\mathbb{E}[est] = \mathbb{E}[T_1]$, but the attack program in Fig. 5.17(c) executes the then-branch of the conditional statement. Thus, our task reduces to that of bounding $\mathbb{P}[est < 14N - 2.5i]$. The estimate *est* is the average of K i.i.d. random variables drawn from a distribution with mean $\mathbb{E}[T_1]$ and variance $\mathbb{V}[T_1]$. I derive the following, using the inequalities from (5.13):

$$\mathbb{E}[est] = \mathbb{E}[T_1] \geq 13N, \qquad \mathbb{V}[est] = \frac{\mathbb{V}[T_1]}{K} \leq \frac{26N^2 + 42N}{K}. \tag{5.15}$$

  I am now able to derive an upper bound on $\mathbb{P}[est < 14N - 2.5i]$ using Cantelli's inequality, where I assume $N < 2.5i$:

$$\begin{aligned}&\mathbb{P}[est \leq 14N - 2.5i] \\ &= \mathbb{P}[est - 13N \leq N - 2.5i] \\ &\leq \mathbb{P}[est - \mathbb{E}[est] \leq N - 2.5i] && \dagger\ \mathbb{E}[est] \geq 13N \text{ by (5.15)}\ \dagger \\ &\leq \frac{\mathbb{V}[est]}{\mathbb{V}[est] + (N - 2.5i)^2} && \dagger\ \text{Proposition 5.33}\ \dagger \\ &= \frac{26N^2 + 42N}{26N^2 + 42N + K(N - 2.5i)^2}.\end{aligned}$$

- The other case, in which $secret[i] = 0$ but the attack program chooses to set $guess[i] := 1$, can be analyzed in a similar way to the previous case, and the bound obtained is the following,

where I assume $N < 2.5i$:

$$\begin{aligned}\mathbb{P}[est > 14N - 2.5i] &\leq \mathbb{P}[est \geq 14N - 2.5i] \\ &\leq \frac{26N^2 + 42N - 10i^2 - 10i}{26N^2 + 42N - 10i^2 - 10i + K(N - 2.5i)^2}.\end{aligned}$$

Let F_1^i and F_0^i, respectively, denote the two upper bounds on the failure probabilities for the i-th bit. Note that both cases require $N < 2.5i$.

For the attack program to succeed, it has to succeed for all bits. Let us consider fix the number of bits $N = 32$. Solving $N < 2.5i$ yields $i \geq 13$; thus, for $i = 1, \cdots, 12$, we cannot rely on the tail bounds above. Luckily, the attack program can enumerate all the possibilities to resolve the last 12 bits (i.e., $2^{12} = 4{,}096$ trials). If in each iteration the number of trials that the attack program uses to estimate the running time is $K = 10^4$, I derive a *lower* bound on the success rate of the attack program from the upper bounds on the failure probabilities derived above:

$$\mathbb{P}[\textsc{Success for all but the last 12 bits}] \geq \prod_{i=13}^{32}(1 - \max(F_1^i, F_0^i)) \geq 0.049833,$$

which is low, but not insignificant. However, the somewhat low probability is caused by a property of compare: if *guess* and *secret* share a very long prefix, then the running-time behavior on different values of *guess* becomes indistinguishable. However, if I increase the number of bits for the brute-force enumeration, for example, the attack program enumerates all the possibilities to resolve the last 14 bits (i.e., $2^{14} = 16{,}384$ trials), and I obtain:

$$\mathbb{P}[\textsc{Success for all but the last 14 bits}] \geq 0.796052,$$

which is a much higher probability! In this way, the attack program needs to perform a total of $10{,}000 \times 18 + 16{,}384 = 196{,}384$ calls to check.

Overall, the analysis above concludes that the check and compare procedures in Fig. 5.17 are vulnerable to a timing attack.

Table 5.4: Inferred upper bounds of the expectations of monotone costs, with comparison to Ngo et al. [124]. ABSYNTH uses a finer-grained set of base functions, and it supports bounds of the form $|[x, y]|$, which is defined as $\max(0, y - x)$.

program	pre-condition	upper bound by my tool	upper bound by ABSYNTH [124]
2drdwalk	$d < n$	$2(n - d + 1)$ (deg 1, 0.269s)	$2\|[d, n + 1]\|$ (deg 1, 0.170s)
C4B_t09	$x > 0$	$17x$ (deg 1, 0.061s)	$17\|[0, x]\|$ (deg 1, 0.014s)
C4B_t13	$x > 0 \wedge y > 0$	$1.25x + y$ (deg 1, 0.060s)	$1.25\|[0, x]\| + \|[0, y]\|$ (deg 1, 0.008s)
C4B_t15	$x > y \wedge y > 0$	$1.1667x$ (deg 1, 0.072s)	$1.3333\|[0, x]\|$ (deg 1, 0.014s)
C4B_t19	$i > 100 \wedge k > 0$	$k + 2i - 49$ (deg 1, 0.059s)	$\|[0, 51 + i + k]\| + 2\|[0, i]\|$ (deg 1, 0.010s)
C4B_t30	$x > 0 \wedge y > 0$	$0.5x + 0.5y + 2$ (deg 1, 0.044s)	$0.5\|[0, x + 2]\| + 0.5\|[0, y + 2]\|$ (deg 1, 0.007s)
C4B_t61	$l \geq 8$	$1.4286l$ (deg 1, 0.046s)	$\|[0, l]\| + 0.5\|[1, l]\|$ (deg 1, 0.007s)
bayes_net	$n > 0$	$4n$ (deg 1, 0.264s)	$4\|[0, n]\|$ (deg 1, 0.057s)
ber	$x < n$	$2(n - x)$ (deg 1, 0.035s)	$2\|[x, n]\|$ (deg 1, 0.004s)
bin	$n > 0$	$0.2(n + 9)$ (deg 1, 0.036s)	$0.2\|[0, n + 9]\|$ (deg 1, 0.030s)
condand	$n > 0 \wedge m > 0$	$2m$ (deg 1, 0.042s)	$2\|[0, m]\|$ (deg 1, 0.004s)
cooling	$mt > st \wedge t > 0$	$mt - st + 0.42t + 2.1$ (deg 1, 0.071s)	$0.42\|[0, t + 5]\| + \|[st, mt]\|$ (deg 1, 0.017s)
coupon	$\top$	11.6667 (deg 4, 0.066s)	15 (deg 1, 0.016s)
cowboy_duel	$\top$	1.2 (deg 1, 0.030s)	1.2 (deg 1, 0.004s)
cowboy_duel_3	$\top$	2.0833 (deg 1, 0.110s)	2.0833 (deg 1, 0.142s)
fcall	$x < n$	$2(n - x)$ (deg 1, 0.053s)	$2\|[x, n]\|$ (deg 1, 0.004s)
filling_vol	$volTF > 0$	$0.6667volTF + 7$ (deg 1, 0.082s)	$0.3333(\|[0, volTF + 10]\| + \|[0, volTF + 11]\|)$ (deg 1, 0.079s)
geo	$\top$	5 (deg 1, 0.061s)	5 (deg 1, 0.003s)
hyper	$x < n$	$5(n - x)$ (deg 1, 0.035s)	$5\|[x, n]\|$ (deg 1, 0.005s)
linear01	$x > 2$	$0.6x$ (deg 1, 0.034s)	$0.6\|[0, x]\|$ (deg 1, 0.008s)
prdwalk	$x < n$	$1.1429(n - x + 4)$ (deg 1, 0.037s)	$1.1429\|[x, n + 4]\|$ (deg 1, 0.011s)
prnes	$y > 0 \wedge n < 0$	$-68.4795n + 0.0526(y - 1)$ (deg 1, 0.071s)	$68.4795\|[n, 0]\| + 0.0526\|[0, y]\|$ (deg 1, 0.016s)
prseq	$y > 9 \wedge x - y > 2$	$1.65x - 1.5y$ (deg 1, 0.061s)	$1.65\|[y, x]\| + 0.15\|[0, y]\|$ (deg 1, 0.011s)
prspeed	$x+1 < n \wedge y < m$	$2(m - y) + 0.6667(n - x)$ (deg 1, 0.065s)	$2\|[y, m]\| + 0.6667\|[x, n]\|$ (deg 1, 0.010s)
race	$h < t$	$0.6667(t - h + 9)$ (deg 1, 0.039s)	$0.6667\|[h, t + 9]\|$ (deg 1, 0.027s)
rdseql	$x > 0 \wedge y > 0$	$2.25x + y$ (deg 1, 0.059s)	$2.25\|[0, x]\| + \|[0, y]\|$ (deg 1, 0.008s)
rdspeed	$x+1 < n \wedge y < m$	$2(m - y) + 0.6667(n - x)$ (deg 1, 0.062s)	$2\|[y, m]\| + 0.6667\|[x, n]\|$ (deg 1, 0.010s)
rdwalk	$x < n$	$2(n - x + 1)$ (deg 1, 0.035s)	$2\|[x, n + 1]\|$ (deg 1, 0.004s)
reject_sampl	$n > 0$	$2n$ (deg 2, 0.071s)	$2\|[0, n]\|$ (deg 1, 0.350s)
rfind_lv	$\top$	2 (deg 1, 0.033s)	2 (deg 1, 0.004s)
rfind_mc	$k > 0$	2 (deg 1, 0.047s)	$\|[0, k]\|$ (deg 1, 0.007s)
robot	$n > 0$	$0.2778(n + 7)$ (deg 1, 0.047s)	$0.3846\|[0, n + 6]\|$ (deg 1, 0.017s)
roulette	$n < 10$	$-4.9333n + 98.6667$ (deg 1, 0.057s)	$4.9333\|[n, 20]\|$ (deg 1, 0.073s)
sprdwalk	$x < n$	$2(n - x)$ (deg 1, 0.036s)	$2\|[x, n]\|$ (deg 1, 0.004s)
trapped_miner	$n > 0$	$7.5n$ (deg 1, 0.081s)	$7.5\|[0, n]\|$ (deg 1, 0.015s)
complex	$y, w, n, m > 0$	$4mn + 2n + w + 0.6667(y + 1)$ (deg 2, 0.142s)	$(\|[0, w]\| + 0.3333\|[0, y]\|)\|[0, y + 1]\| + 0.6667 + (4\|[0, m]\| + 2)\|[0, n]\|$ (deg 2, 0.451s)
multirace	$n > 0 \wedge m > 0$	$2mn + 4n$ (deg 2, 0.080s)	$2\|[0, m]\|\|[0, n]\| + 4\|[0, n]\|$ (deg 2, 0.692s)
pol04	$x > 0$	$4.5x^2 + 10.5x$ (deg 2, 0.052s)	$1.5\|[0, x]\|^2 + 3\|[1, x]\|\|[0, x]\| + 10.5\|[0, x]\|$ (deg 2, 0.101s)
pol05	$x > 0$	$0.6667(x^2 + 3x)$ (deg 2, 0.059s)	$2\|[0, x + 1]\|\|[0, x]\|$ (deg 2, 0.133s)
pol07	$n > 1$	$1.5n^2 - 4.5n + 3$ (deg 2, 0.057s)	$1.5\|[1, n]\|\|[2, n]\|$ (deg 2, 0.203s)
rdbub	$n > 0$	$3n^2$ (deg 2, 0.055s)	$3\|[0, n]\|^2$ (deg 2, 0.030s)
recursive	$l < h$	$0.25(h - l)^2 + 1.75(h - l)$ (deg 2, 0.313s)	$0.25\|[l, h]\|^2 + 1.75\|[l, h]\|$ (deg 2, 0.398s)
trader	$mP > 0 \wedge sP > mP$	$1.5(sP^2 - mP^2 + sP - mP)$ (deg 2, 0.073s)	$1.5\|[mP, sP]\|^2 + 3\|[mP, sP]\|\|[0, mP]\| + 1.5\|[mP, sP]\|$ (deg 2, 0.192s)

Table 5.5: Inferred upper and lower bounds of the expectation of (possibly) non-monotone costs, with comparison to Wang et al. [154]. To ensure soundness, my tool has to perform an extra termination check required by Theorem 5.23.

program	pre-cond.	termination		bounds by my tool	bounds by Wang et al. [154]
Bitcoin Mining	$x \geq 1$	$\mathbb{E}[T] < \infty$ (deg 1, 0.080s)	ub.	$-1.475x$ (deg 1, 0.078s)	$-1.475x + 1.475$ (deg 2, 3.705s)
			lb.	$-1.5x$ (deg 1, 0.088s)	$-1.5x$ (deg 2, 3.485s)
Bitcoin Pool	$y \geq 0$	$\mathbb{E}[T^2] < \infty$ (deg 4, 0.168s)	ub.	$-7.375y^2 - 66.375y$ (deg 2, 0.127s)	$-7.375y^2 - 41.625y + 49$ (deg 2, 5.936s)
			lb.	$-7.5y^2 - 67.5y$ (deg 2, 0.134s)	$-7.5y^2 - 67.5y$ (deg 2, 6.157s)
Queueing Network	$n > 0$	$\mathbb{E}[T^2] < \infty$ (deg 2, 0.208s)	ub.	$0.0531n$ (deg 2, 0.134s)	$0.0492n$ (deg 3, 69.669s)
			lb.	$0.028n$ (deg 2, 0.139s)	$0.0384n$ (deg 3, 68.849s)
Running Example	$x \geq 0$	$\mathbb{E}[T^2] < \infty$ (deg 2, 0.064s)	ub.	$0.3333(x^2 + x)$ (deg 2, 0.063s)	$0.3333(x^2 + x)$ (deg 2, 3.766s)
			lb.	$0.3333(x^2 + x)$ (deg 2, 0.059s)	$0.3333(x^2 + x) - 0.6667$ (deg 2, 3.555s)
Nested Loop	$i \geq 0$	$\mathbb{E}[T^2] < \infty$ (deg 4, 0.127s)	ub.	$0.3333i^2 + i$ (deg 2, 0.117s)	$0.3333i^2 + i$ (deg 2, 28.398s)
			lb.	$0.3333i^2 + i$ (deg 2, 0.115s)	$0.3333i^2 - i$ (deg 2, 7.299s)
Random Walk	$x \leq n$	$\mathbb{E}[T] < \infty$ (deg 1, 0.063s)	ub.	$2.5x - 2.5n - 2.5$ (deg 1, 0.064s)	$2.5x - 2.5n$ (deg 2, 4.536s)
			lb.	$2.5x - 2.5n - 2.5$ (deg 1, 0.068s)	$2.5x - 2.5n - 2.5$ (deg 2, 4.512s)
2D Robot	$x \geq y$	$\mathbb{E}[T^2] < \infty$ (deg 2, 0.145s)	ub.	$1.7280(x-y)^2 + 31.4539(x-y) + 126.5167$ (deg 2, 0.132s)	$1.7280(x-y)^2 + 31.4539(x-y) + 126.5167$ (deg 2, 7.133s)
			lb.	$1.7280(x-y)^2 + 31.4539(x-y) + 29.7259$ (deg 2, 0.121s)	$1.7280(x-y)^2 + 31.4539(x-y)$ (deg 2, 7.040s)
Good Discount	$d \leq 30 \wedge n \geq 1$	$\mathbb{E}[T^2] < \infty$ (deg 2, 0.093s)	ub.	$-0.5n - 3.6667d + 117.3333$ (deg 2, 0.093s)	$0.0067dn - 0.7n - 3.8035d + 0.0022d^2 + 119.4351$ (deg 2, 5.272s)
			lb.	$-0.005n^2 - 0.5n$ (deg 2, 0.092s)	$0.0067dn - 0.7133n - 3.8123d + 0.0022d^2 + 112.3704$ (deg 2, 5.323s)
Pollutant Disposal	$n \geq 0$	$\mathbb{E}[T^2] < \infty$ (deg 2, 0.091s)	ub.	$-0.2n^2 + 50.2n$ (deg 2, 0.092s)	$-0.2n^2 + 50.2n$ (deg 2, 5.851s)
			lb.	$-0.2n^2 + 50.2n - 435.6$ (deg 2, 0.094s)	$-0.2n^2 + 50.2n - 482$ (deg 2, 5.215s)
Species Fight	$a \geq 5 \wedge b \geq 5$	$\mathbb{E}[T^2] < \infty$ (deg 2, 0.042s)	ub.	$40ab - 180a - 180b + 810$ (deg 2, 0.045s)	$40ab - 180a - 180b + 810$ (deg 3, 5.545s)
			lb.	N/A	N/A

Chapter 6

DMKAT: Deterministic Markov-Kleene Algebra with Tests

In Chapter 4, I have proposed a general framework PMAF for static analysis of probabilistic programs, but later in Chapter 5 I did *not* use PMAF in the development of the central-moment analysis framework. One reason for this is that the analysis algorithm of PMAF (see §4.2.3) is *iteration* based, whereas the central-moment analysis algorithm (see §5.2.4) is *constraint* based. In this chapter, I summarize my progress towards bridging the gap between PMAF and central moment reasoning, namely the *Deterministic Markov-Kleene Algebra with Tests* (DMKAT) framework, which can be seen as a conservative extension of PMAF, except that I get rid of nondeterminism and procedure calls from the framework. I also discuss some avenues for future research on enhancing the DMKAT framework.

The linear expectation-invariant analysis (LEIA)—presented in §4.3.3 as an instantiation of PMAF—is able to derive expectation invariants over program variables, thus it is already able to reason about moments, by instrumenting a program with auxiliary variables that track powers of variables. For example, Fig. 6.1(a) presents a simple one-dimensional biased random walk program, where the **tick**(1) statement indicates that the accumulated cost is the number of steps before the random walk terminates. Fig. 6.1(b) then instruments the program by explicitly using a program variable *tick* to accumulate costs, as well as introducing x_2, $tick_2$, and xt to reflect the values of x^2, $tick^2$, and $x \cdot tick$, respectively. Note that the instrumented program—which keeps track of values of nonlinear expressions—is actually linear, in the sense that all arithmetic expressions are linear. Interestingly, such an instrumentation technique can *linearize* nonlinear programs in a way that one can apply static analysis for linear programs (e.g., [44]). Two linear expectation invariants for Fig. 6.1(b), where variables with primes denote their values at the end of the program, are $\mathbb{E}[tick'] \leq tick + 20$ and $\mathbb{E}[tick_2'] \leq tick_2 + 40 \cdot tick + 460$, which give bounds to the first and second moments of the accumulated cost, respectively. However, LEIA *cannot* derive the desired expectation invariants about $\mathbb{E}[tick']$ or $\mathbb{E}[tick_2']$, because, as I discussed in §4.3.3 and also elaborated in §5.3.3, probabilistic termination complicates the analysis of expectations and I have to make many conservative design choices for LEIA.

Inspired by the development of central moment analysis, especially the use of Optional Stopping Theorems that reason about expectation invariants through stochastic processes (e.g., a Markov chain whose transitions are determined by a loop body), I observe that it is more natural to think

```
x := 0;
while x < 10 do
  if prob(0.75) then
    x := x + 1
  else
    x := x − 1
  fi;
  tick(1)
od
```

(a)

```
(x, x2, xt) := (0, 0, 0);
while x < 10 do
  if prob(0.75) then
    (x, x2, xt) := (x + 1, x2 + 2x + 1, xt + tick)
  else
    (x, x2, xt) := (x − 1, x2 − 2x + 1, xt − tick)
  fi;
  (tick, tick2, xt) := (tick + 1, tick2 + 2tick + 1, xt + x)
od
```

(b)

Fig. 6.1: (a) A simple one-dimensional biased random walk program, and (b) its instrumented version for moment tracking.

of *summarizing loops directly* instead of iterating the loop-body transformer to obtain a fixed point. For non-probabilistic programs, people have been successful to avoid iteration-based solving algorithms by using *Kleene algebras*—rather than lattices—as the algebraic foundation of the static analysis (e.g., [53, 54, 89, 92, 133, 157]). The intuition is that a Kleene algebra is equipped explicitly with a *Kleene-star* operation that corresponds to loops; in this way, the analysis designer has the opportunity to develop a non-iterative loop summarization algorithm to abstract Kleene-stars. Even better, for non-probabilistic programs represented as control-flow graphs, one can apply Tarjan's path-expression algorithm [142] to obtain a regular expression (i.e., an expression in a semantic Kleene algebra) that encodes all possible program executions.

However, I cannot directly adapt existing results on algebraic static analysis for non-probabilistic programs. The major gap here is that PMAF uses *hyper-graphs* to encode control-flow graphs, and Kleene algebras, in essence, provide a theory on regular sets of execution paths, rather than execution *hyper-paths*. Therefore, in this chapter, I first develop a theory on regular hyper-paths (see §6.1). The intuition is that a hyper-path is a concatenation of hyper-edges—each of which has one source node and multiple destination nodes—thus represents a *tree*, on which every root-to-leaf path corresponds to a program execution path. Thus, I adapt and adopt the theory on *regular-tree languages* and *regular-tree expressions* [31], as a generalization of the theory on regular languages and regular expressions. The key challenge is that for probabilistic programs, I have to consider *infinite* execution paths (to account for probabilistic termination), so a hyper-path might have an infinite height. My solution is to model hyper-paths as *possibly-infinite trees* and develop a theory on possibly-infinite trees based on *coinduction*.

Using the theory on regular hyper-paths, I am able to extract a *regular hyper-path expression*—as a finite representation—of a possibly-infinite hyper-path that leads from the entry node of a control-flow hyper-graph. Following the recipe of algebraic static analysis, in §6.2, I develop a new family of algebraic structures that can be used to reinterpret regular hyper-path expressions, namely the *Deterministic Markov-Kleene Algebra with Tests* (DMKAT). As the name suggests, I integrate a deterministic fragment of the Markov Algebra framework (developed in §3.3) with ideas from Kleene Algebra with Tests (KAT) framework [101]. A KAT combines a Kleene algebra with a Boolean algebra, thus enables algebraic reasoning of programs with sequencing, branching, and iteration constructs. I then formulate an algebraic interpretation of regular hyper-path expressions

with respect to DMKATs, and prove that the tree-based model (i.e., the interpretation of regular hyper-path expressions as possibly-infinite trees) is *sound* for any DMKAT. I also demonstrate two concrete DMKATs for reasoning about probabilistic programs (without nondeterminism): one for the relations among input and output states, and the other for transition kernels on states.

Finally, in §6.3, I present some preliminary results on building a static-analysis framework for probabilistic programs based on DMKAT. The first direction is to adapt existing abstract domains for analyzing non-probabilistic programs. The intuition is that if we are not concerned about the probabilities (i.e., probabilistic branching is treated as nondeterministic branching), we can achieve a hyper-path analysis by decomposing the hyper-path as a collection of rooted paths (recall that a hyper-path is a possibly-infinite tree), abstracting each rooted path, and joining the path-wise analysis results. Thus, I sketch an algorithm for computing an abstraction of a regular hyper-path expression, with respect to any non-probabilistic abstract domain that can be formulated as a regular algebra. The second direction is to consider the probabilistic aspects in analyses, e.g., the expectation-invariant analysis. When I developed PMAF in §4.2, I introduced *Pre-Markov Algebras* (PMAs) that are very similar to the *Markov Algebras* (which are usually used as concrete semantic algebras), but PMAs admit a different set of axioms that are more suitable for static analysis. Similarly, I provide a family of algebraic structures, namely *Deterministic Pre-Markov Algebras* (DPMAs), which are very similar to DMKATs, but DPMAs admit a different set of axioms. Instead of relying on iteration-until-fixed-point algorithms (which PMAF is based on), I argue that the use of regular hyper-path expressions enables the flexibility of adapting loop-summarization techniques. Intuitively, when abstracting a regular hyper-path expression that stands for a loop, my approach is to let the static-analysis developer determine how to discover an *invariant* for the loop. To achieve this, I sketch a declarative derivation system for abstract interpretations of regular hyper-path expressions. The actual theoretical development for §6.3 is left for future work, but I show some examples that demonstrate how DPMA-based analyses would work, including an analysis of the moment-tracking program in Fig. 6.1(b).

6.1 A Theory on Regular Hyper-Paths

My development in this section is largely inspired by the theory on regular-tree languages and regular-tree expressions [31]. However, I have to tackle a technical challenge that a hyper-path can correspond to a tree with an infinite height. Induction is a well-established proof principle for reasoning about inductively defined datatypes (e.g., finite lists and finite trees), but does not work for infinite datatypes in general. Thus, in this section, I rely on a principle of *coinduction*, which, as shown in prior work (e.g. [81, 102]), is indeed a well-founded principle for reasoning about coinductive datatypes (e.g., infinite streams and infinite trees).

6.1.1 Possibly-Infinite Trees

A *ranked alphabet* is a pair $(\mathcal{F}, \mathit{Arity})$ where $\mathcal{F}$ is a finite set and Arity is a map from $\mathcal{F}$ to $\mathbb{Z}^+$. The *arity* of a symbol $f \in \mathcal{F}$ is $\mathit{Arity}(f)$. The set of symbols of arity n is denoted by $\mathcal{F}_n$. For simplicity, we use parentheses and commas to specify symbols with their arity; for example, $f(,)$ specifies a binary symbol f.

Let $\mathcal{K}$ be a set of constants (i.e., symbols with arity zero) called *holes*. I assume that the sets $\mathcal{K}$ and $\mathcal{F}_0$ are disjoint, and there is a distinguished symbol $\ominus \notin \mathcal{F}_0 \cup \mathcal{K}$ with arity zero. Intuitively, a hole symbol in $\mathcal{K}$ represents a placeholder for later substitution with trees, and the $\ominus$ symbol indicates a "yet unknown subtree." A *possibly-infinite tree* $t \in \mathsf{Tree}^{\infty}(\mathcal{F}, \mathcal{K})$ over the ranked alphabet $\mathcal{F}$ and the set of variables $\mathcal{K}$ is a partial map $t : \mathbb{N}^* \rightharpoonup \mathcal{F} \cup \mathcal{K} \cup \{\ominus\}$ with domain $\mathrm{dom}(t) \subseteq \mathbb{N}^*$ satisfying the following property:

Property 6.1.

(i) $\mathrm{dom}(t)$ is non-empty and prefix-closed (thus $\epsilon \in \mathrm{dom}(t)$);

(ii) for any $p \in \mathrm{dom}(t)$, if $t(p) \in \mathcal{F}_n$ for some $n > 0$, then $\{j \mid pj \in \mathrm{dom}(t)\} = \{1, \cdots, n\}$;

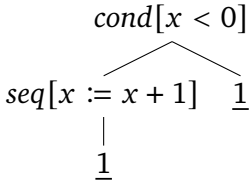
(iii) for any $p \in \mathrm{dom}(t)$, if $t(p) \in \mathcal{F}_0 \cup \mathcal{K} \cup \{\ominus\}$, then $\{j \mid pj \in \mathrm{dom}(t)\} = \emptyset$.

For brevity, we denote by a the finite tree $\{\epsilon \mapsto a\}$, for any $a \in \mathcal{F}_0 \cup \mathcal{K} \cup \{\ominus\}$. We also denote by $f(s_1, \cdots, s_n)$ the possibly-infinite tree

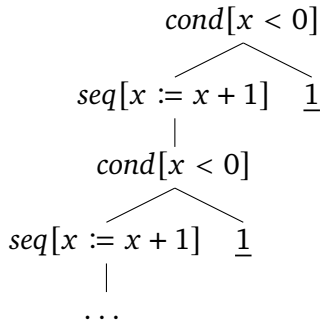
$$\{\epsilon \mapsto f\} \cup \textstyle\bigcup_{j \in \{1,\cdots,n\}} \{jp \mapsto s_j(p) \mid p \in \mathrm{dom}(s_j)\},$$

for any $f \in \mathcal{F}_n$ with $n > 0$ and $s_1, \cdots, s_n$ are possibly-infinite trees.

*Example 6.2. Let $\mathcal{F} = \{seq[x := x+1](), cond[x < 0](,), \underline{1}\}$. Recall the definition of control-flow hyper-graphs and control-flow actions in §2.2. Intuitively, $seq[x := x+1]$ is a unary symbol, representing the composition of the statement $x := x+1$ and the only argument of the symbol; $cond[x < 0]$ is a binary symbol, representing a conditional branch with predicate $x < 0$, such that the first and second arguments correspond to the then and else branches, respectively; and $\underline{1}$ is a constant, representing program termination. For example, the program "***if*** $x < 0$ ***then*** $x := x+1$ ***fi***" can be encoded as the following finite tree:*



*Encoding loops—for example, "***while*** $x < 0$ ***do*** $x := x+1$ ***od***"—requires infinite trees. Intuitively, the loop can be encoded as the following infinite tree:*



Formally, the tree t for the loop is defined in a way that $\mathrm{dom}(t) = 1^* \cup (11)^*2$*, and*

$$\begin{cases} t(1^{2k}) = cond[x < 0] & \text{for any } k \in \mathbb{Z}^+, \\ t(1^{2k+1}) = seq[x := x+1] & \text{for any } k \in \mathbb{Z}^+, \\ t((11)^k 2) = \underline{1} & \text{for any } k \in \mathbb{Z}^+. \end{cases}$$

In §6.1.2, I will develop a mechanism to finitely represent such infinite trees.

Let $t \in \mathsf{Tree}^\infty(\mathcal{F}, \mathcal{K})$ be a possibly-infinite tree. Every element in $\mathrm{dom}(t)$ is called a *position*. A *leaf position* is a position p such that $pj \notin \mathrm{dom}(t)$ for any $j \in \mathbb{N}$. We denote by $root(t)$ the *root symbol* of t, defined by $root(t) \stackrel{\text{def}}{=} t(\epsilon)$. A *subtree* $t|_p$ of a tree t at position p is the tree defined by the following:

- $\mathrm{dom}(t|_p) = \{q \mid pq \in \mathrm{dom}(t)\}$, and
- $\forall q \in \mathrm{dom}(t|_p) : t|_p(q) = t(pq)$.

A tree t can then be decomposed as $f(t|_1, \cdots, t|_n)$, where $f = root(t)$ with arity n.

To compare two possibly-infinite trees, I define a *refinement relation* $\sqsubseteq_{\mathcal{T}} \subseteq \mathsf{Tree}^\infty(\mathcal{F}, \mathcal{K}) \times \mathsf{Tree}^\infty(\mathcal{F}, \mathcal{K})$ as the *maximum* binary relation satisfying the following property:

Property 6.3. If $t_1 \sqsubseteq_{\mathcal{T}} t_2$, then either

(i) $t_1 = \ominus$, or

(ii) $root(t_1) = f$ and $root(t_2) = f$ for some $f \in \mathcal{F} \cup \mathcal{K}$, and for all $i \in \{1, \cdots, Arity(f)\}$, it holds that $t_1|_i \sqsubseteq_{\mathcal{T}} t_2|_i$.

This property formulates the idea that the symbol $\ominus$ indicates a "yet unknown subtree." Because the relation $\sqsubseteq_{\mathcal{T}}$ is maximum, the converse of the Property 6.3 also holds. Therefore, the relation $\sqsubseteq_{\mathcal{T}}$ can be characterized by the *greatest* fixed point of the operator below.

$$T_{\sqsubseteq_{\mathcal{T}}}(R) \stackrel{\text{def}}{=} \{\langle \ominus, t\rangle \mid t \in \mathsf{Tree}^\infty(\mathcal{F}, \mathcal{K})\} \cup \{\langle f(s_1, \cdots, s_n), f(t_1, \cdots, t_n)\rangle \mid f \in \mathcal{F} \cup \mathcal{K}, Arity(f) = n, \forall j \in \{1, \cdots, n\} : \langle s_j, t_j\rangle \in R\}.$$

Lemma 6.4. *The relation $\sqsubseteq_{\mathcal{T}}$ is a partial order on $\mathsf{Tree}^\infty(\mathcal{F}, \mathcal{K})$.*

Proof. The relation $\sqsubseteq_{\mathcal{T}}$ is reflexive because $\{\langle t, t\rangle \mid t \in \mathsf{Tree}^\infty(\mathcal{F}, \mathcal{K})\}$ satisfies Property 6.3, and the relation $\sqsubseteq_{\mathcal{T}}$ is maximum by definition.

We claim that $\sqsubseteq_{\mathcal{T}}$ is antisymmetric, i.e., if $t_1 \sqsubseteq_{\mathcal{T}} t_2$ and $t_2 \sqsubseteq_{\mathcal{T}} t_1$, then $t_1 = t_2$. If $root(t_1) = \ominus$, then by $t_2 \sqsubseteq_{\mathcal{T}} t_1$ we also have $root(t_2) = \ominus$, thus $t_1 = t_2$. Otherwise, we know that $root(t_1) = f$ for some $f \in \mathcal{F} \cup \mathcal{K}$, then by $t_1 \sqsubseteq_{\mathcal{T}} t_2$ we have $root(t_2) = f$, and for all $i \in \{1, \cdots, Arity(f)\}$, it holds that $t_1|_i \sqsubseteq_{\mathcal{T}} t_2|_i$. By $t_2 \sqsubseteq_{\mathcal{T}} t_1$, we also have $t_2|_i \sqsubseteq_{\mathcal{T}} t_1|_i$ for all $i \in \{1, \cdots, Arity(f)\}$. Therefore, by coinduction hypothesis[11], we have $t_1|_i = t_2|_i$ for all $i \in \{1, \cdots, Arity(f)\}$, thus $t_1 = t_2$.

We claim that $\sqsubseteq_{\mathcal{T}}$ is transitive, i.e., if $t_1 \sqsubseteq_{\mathcal{T}} t_2$ and $t_2 \sqsubseteq_{\mathcal{T}} t_3$, then $t_1 \sqsubseteq_{\mathcal{T}} t_3$. If $root(t_1) = \ominus$, then we have $t_1 \sqsubseteq_{\mathcal{T}} t_3$ by definition. Otherwise, we know that $root(t_1) = f$ for some $f \in \mathcal{F} \cup \mathcal{K}$. By $t_1 \sqsubseteq_{\mathcal{T}} t_2$, we know that $root(t_2) = f$ and for all $i \in \{1, \cdots, Arity(f)\}$, it holds that $t_1|_i \sqsubseteq_{\mathcal{T}} t_2|_i$. By $t_2 \sqsubseteq_{\mathcal{T}} t_3$, we know that $root(t_3) = f$ and for all $i \in \{1, \cdots, Arity(f)\}$, it holds that $t_2|_i \sqsubseteq_{\mathcal{T}} t_3|_i$. Thus, by coinduction hypothesis, for all $i \in \{1, \cdots, Arity(f)\}$, it holds that $t_1|_i \sqsubseteq_{\mathcal{T}} t_3|_i$. Therefore, by definition, we conclude that $t_1 \sqsubseteq_{\mathcal{T}} t_3$. □

The next lemma justifies that the order $\sqsubseteq_{\mathcal{T}}$ stands for refinements, in the sense that if $t_1 \sqsubseteq_{\mathcal{T}} t_2$, it must hold that t_2 is obtained by substituting some $\ominus$ symbols in t_1 with trees.

[11] As pointed out by Kozen and Silva [102], we can use the coinduction hypothesis as long as there is progress in observing the roots of trees, and there is no further investigation of the children of the trees.

LEMMA 6.5. *If* $t_1 \sqsubseteq_{\mathscr{T}} t_2$, *then* $\mathrm{dom}(t_1) \subseteq \mathrm{dom}(t_2)$, *and for all* $p \in \mathrm{dom}(t_1)$, *it holds that* $t_1(p) = \ominus$ *or* $t_1(p) = t_2(p)$.

PROOF. If $root(t_1) = \ominus$, then $\mathrm{dom}(t_1) = \{\epsilon\}$ and the lemma holds obviously. Otherwise, we know that $root(t_1) = f$ for some $f \in \mathcal{F} \cup \mathcal{K}$, and by $t_1 \sqsubseteq_{\mathscr{T}} t_2$, we have $root(t_2) = f$ and for all $i \in \{1, \cdots, Arity(f)\}$, it holds that $t_1|_i \sqsubseteq_{\mathscr{T}} t_2|_i$. By coninduction hypothesis, for all $i \in \{1, \cdots, Arity(f)\}$, we know that the lemma holds for $t_1|_i \sqsubseteq_{\mathscr{T}} t_2|_i$. Thus, we have

$$\begin{aligned}\mathrm{dom}(t_1) &= \bigcup_{i\in\{1,\cdots,Arity(f)\}} \{ip \mid p \in \mathrm{dom}(t_1|_i)\} \\ &\subseteq \bigcup_{i\in\{1,\cdots,Arity(f)\}} \{ip \mid p \in \mathrm{dom}(t_2|_i)\} \\ &= \mathrm{dom}(t_2).\end{aligned}$$

For any $p \in \mathrm{dom}(t_1)$, either $p = \epsilon$, or there exists i such that $p = ip'$ and $p' \in \mathrm{dom}(t_1|_i)$. In the former case, we have $t_1(\epsilon) = f = t_2(\epsilon)$. In the latter case, we know that either $t_1|_i(p') = \ominus$ or $t_1|_i(p') = t_2|_i(p')$. Therefore, we conclude that either $t_1(p) = t_1(ip') = t_1|_i(p') = \ominus$, or $t_1(p) = t_1(ip') = t_1|_i(p') = t_2|_i(p') = t_2(ip') = t_2(p)$. □

LEMMA 6.6. *The relation* $\sqsubseteq_{\mathscr{T}}$ *is an* ω*-continuous partial order on* $\mathsf{Tree}^{\infty}(\mathcal{F}, \mathcal{K})$ *with* $\ominus$ *as the least element.*

PROOF. Fix an ω-chain $\{t_k\}_{k\in\mathbb{N}}$ of possibly-infinite trees with respect to the partial order $\sqsubseteq_{\mathscr{T}}$ (Lemma 6.4). We then try to construct the least upper bound of the chain, and call it t'. We set $\mathrm{dom}(t')$ to be $\bigcup_{k\in\mathbb{N}} \mathrm{dom}(t_k)$. By Lemma 6.5, we know that $\{\mathrm{dom}(t_k)\}_{k\in\mathbb{N}}$ is a $\subseteq$-chain. For a position $p \in \mathrm{dom}(t')$, we set $t'(p)$ to be

- $\ominus$, if there exists $K \in \mathbb{N}$ such that $t_k(p) = \ominus$ for all $k \geq K$;
- $t_{k_p}(p)$, if there exists $k_p \in \mathbb{N}$ satisfying $p \in \mathrm{dom}(t_{k_p})$ and $t_{k_p}(p) \neq \ominus$.

The well-definedness of t' is guaranteed by Lemma 6.5. If t' is an upper bound on $\{t_k\}_{k\in\mathbb{N}}$, then t' is the least one as $\mathrm{dom}(t')$ is the least upper bound on $\{\mathrm{dom}(t_k)\}_{k\in\mathbb{N}}$. Thus, it remains to prove that t' is indeed an upper bound.

We then proceed the proof by coinduction. For any $\ell \in \mathbb{N}$, if $root(t_\ell) = \ominus$, then $t_\ell \sqsubseteq_{\mathscr{T}} t'$. Thus, without loss of generality, we can assume that $t_1 \neq \ominus$. Let $f = root(t_1) \in \mathcal{F} \cup \mathcal{K}$. Thus, by definition, we know that $root(t_k) = f$ for all $k \in \mathbb{N}$, and also $root(t') = f$. Let $n = Arity(f)$. Then for each $j \in \{1, \cdots, n\}$, it holds that $\{t_k|_j\}_{k\in\mathbb{N}}$ is an ω-chain, and by coinduction hypothesis, we know that $t'|_j$ is an upper bound on $\{t_k|_j\}_{k\geq\mathbb{N}}$. Therefore, $f(t'|_1, \cdots, t'|_n)$ is an upper bound of $\{f(t_k|_1, \cdots, t_k|_n)\}_{k\in\mathbb{N}}$. □

I now formulate a mechanism to define functions on possibly-infinite trees. Note that the standard definition of inductive functions does *not* work because of the existence of infinite trees. Let $(D, \sqsubseteq_D)$ be an ω-cpo with a least element $\bot_D$. To define a function from possibly-infinite trees in $\mathsf{Tree}^{\infty}(\mathcal{F}, \mathcal{K})$ to D, I require a map $\mathsf{base} : \mathcal{F}_0 \cup \mathcal{K} \to D$ and a family of maps into ω-continuous functions $\mathsf{ind}_n : \mathcal{F}_n \to [D^n \to D]$ for all $n > 0$ such that $\mathcal{F}_n \neq \emptyset$. I then introduce an ω-chain of functions $\{h_i\}_{i\geq 0}$ as follows, and define the target function by $h \stackrel{\text{def}}{=} \bigsqcup_{i\geq 0} h_i$ with respect to the

pointwise extension of $\sqsubseteq_D$.

$$h_0 \stackrel{\text{def}}{=} \lambda t.\ \bot,$$
$$h_{i+1} \stackrel{\text{def}}{=} \lambda t.\ \begin{cases} \bot & \text{if } root(t) = \ominus, \\ \mathsf{base}(root(t)) & \text{if } root(t) \in \mathcal{F}_0 \cup \mathcal{K}, \\ \mathsf{ind}_n(root(t))(h_i(t|_1), \cdots, h_i(t|_n)) & \text{if } root(t) \in \mathcal{F}_n \text{ for some } n > 0. \end{cases}$$

LEMMA 6.7. *Let $h : \mathsf{Tree}^\infty(\mathcal{F}, \mathcal{K}) \to D$ be a function from possibly-infinite trees to an ω-cpo $(D, \sqsubseteq_D)$ with a least element $\bot_D$. Then $h(\ominus) = \bot_D$.*

PROOF. By definition, we know that there exists an ω-chain of functions $\{h_j\}_{j\geq 0}$ defined as above such that $h = \bigsqcup_{j\geq 0} h_j$. Also, it is obvious that for each $j \geq 0$, $h_j(\ominus) = \bot_D$. Thus, we conclude that $h(\ominus) = \bigsqcup_{j\geq 0} h_j(\ominus) = \bigsqcup_{j\geq 0} \bot_D = \bot_D$. □

LEMMA 6.8. *Let $h : \mathsf{Tree}^\infty(\mathcal{F}, \mathcal{K}) \to D$ be a function from possibly-infinite trees to an ω-cpo $(D, \sqsubseteq_D)$ with a least element $\bot_D$, induced by maps base and ind_n for $n > 0$. Then h is ω-continuous with respect to the pointwise extension of $\sqsubseteq_D$.*

PROOF. We know that there exists an ω-chain of functions $\{h_j\}_{j\geq 0}$ defined as above such that $h = \bigsqcup_{j\geq 0} h_j$. We claim that for each $j \geq 0$, the function h_j is ω-continuous. We proceed by induction on j.

When $j = 0$:

By definition, we have $h_0 \stackrel{\text{def}}{=} \lambda t.\ \bot$, which is obviously ω-continuous.

When $j = k + 1$:

By definition, we have

$$h_j \stackrel{\text{def}}{=} \lambda t.\ \begin{cases} \bot & \text{if } root(t) = \ominus, \\ \mathsf{base}(root(t)) & \text{if } root(t) \in \mathcal{F}_0 \cup \mathcal{K}, \\ \mathsf{ind}_n(root(t))(h_k(t|_1), \cdots, h_k(t|_n)) & \text{if } root(t) \in \mathcal{F}_n \text{ for some } n > 0. \end{cases}.$$

Consider an ω-chain of trees $\{t_i\}_{i\geq 0}$. Without loss of generality, we assume that $root(t_0) \neq \ominus$ (because $h_j(\{\epsilon \mapsto \ominus\}) = \bot$).

Then by the definition of the refinement order $\sqsubseteq_{\mathscr{T}}$, we know that $\{root(t_i) \mid i \geq 0\}$ is a singleton set.

If the singleton set contains a symbol $a \in \mathcal{F}_0 \cup \mathcal{K}$, we know that $h_j(t_i) = \mathsf{base}(a)$ for all $i \geq 0$, thus $h_j(\bigsqcup_{i\geq 0} t_i) = h_j(a) = \bigsqcup_{i\geq 0} h_j(a) = \bigsqcup_{i\geq 0} h_j(t_i)$.

If the singleton set contains a symbol $f \in \mathcal{F}_n$ for some $n > 0$, then by the assumption that

$\mathsf{ind}_n(f)$ is ω-continuous and by induction hypothesis that h_k is ω-continuous, we can derive

$$\begin{aligned}
h_j(\bigsqcup_{i\geq 0} t_i) &= \mathsf{ind}_n(f)(h_k((\bigsqcup_{i\geq 0} t_i)|_1), \cdots, h_k((\bigsqcup_{i\geq 0} t_i)|_n)) \\
&= \mathsf{ind}_n(f)(h_k(\bigsqcup_{i\geq 0}(t_i|_1)), \cdots, h_k(\bigsqcup_{i\geq 0}(t_i|_n))) \\
&= \mathsf{ind}_n(f)(\bigsqcup_{i\geq 0} h_k(t_i|_1), \cdots, \bigsqcup_{i\geq 0} h_k(t_i|_n)) \\
&= \bigsqcup_{i_1\geq 0}\cdots\bigsqcup_{i_n\geq 0} \mathsf{ind}_n(f)(h_k(t_{i_1}|_1), \cdots, h_k(t_{i_n}|_n)) \\
&\quad (\sqsupseteq\text{: obvious}) \\
&\quad (\sqsubseteq\text{: } \forall i_1, \cdots i_n\text{, the LHS item is bounded by the } \max(i_1, \cdots, i_n)\text{-th RHS item}) \\
&= \bigsqcup_{i\geq 0} \mathsf{ind}_n(f)(h_k(t_i|_1), \cdots, h_k(t_i|_n)) \\
&= \bigsqcup_{i\geq 0} h_j(t_i).
\end{aligned}$$

Thus, we conclude the proof of the claim that h_j is ω-continuous for all $j \geq 0$.

Let us now consider an ω-chain of trees $\{t_i\}_{i\geq 0}$. Then we can conclude the proof by

$$\begin{aligned}
h(\bigsqcup_{i\geq 0} t_i) &= (\bigsqcup_{j\geq 0} h_j)(\bigsqcup_{i\geq 0} t_i) \\
&= \bigsqcup_{j\geq 0} h_j(\bigsqcup_{i\geq 0} t_i) \\
&= \bigsqcup_{j\geq 0}\bigsqcup_{i\geq 0} h_j(t_i) \\
&= \bigsqcup_{i\geq 0}\bigsqcup_{j\geq 0} h_j(t_i) \\
&= \bigsqcup_{i\geq 0}(\bigsqcup_{j\geq 0} h_j)(t_i) \\
&= \bigsqcup_{i\geq 0} h(t_i).
\end{aligned}$$

□

I end this section by demonstrating a function that maps possibly-infinite trees to collections of *rooted paths* on trees. I define $\mathit{paths}(t) \subseteq \mathsf{Path}^\infty(\mathcal{F},\mathcal{K}) \stackrel{\text{def}}{=} (\mathcal{F}\cup\mathcal{K})\cdot(\mathbb{N}\cdot(\mathcal{F}\cup\mathcal{K}))^\infty$ with the following base and induction steps:

$$\begin{aligned}
\mathit{paths} &: \mathsf{Tree}^\infty(\mathcal{F},\mathcal{K}) \to \mathsf{Path}^\infty(\mathcal{F},\mathcal{K}) \\
\mathit{paths}(a) &\stackrel{\text{def}}{=} \{a\} \quad \text{for } a \in \mathcal{F}_0 \cup \mathcal{K} \\
\mathit{paths}(f(s_1,\cdots,s_n)) &\stackrel{\text{def}}{=} \{f\,j\,w \mid j = 1,\ldots,n \wedge w \in \mathit{paths}(s_j)\} \quad \text{for } f \in \mathcal{F}_n \text{ for some } n > 0
\end{aligned}$$

Note that the set $\mathsf{Path}^\infty(\mathcal{F},\mathcal{K})$ of possibly-infinite paths admits an ω-cpo with the following ordering

$$A \sqsubseteq_\mathsf{P} B \stackrel{\text{def}}{=} (A \cap \mathsf{Path}^+(\mathcal{F},\mathcal{K}) \subseteq B \cap \mathsf{Path}^+(\mathcal{F},\mathcal{K})) \wedge (A \cap \mathsf{Path}^\omega(\mathcal{F},\mathcal{K}) \supseteq B \cap \mathsf{Path}^\omega(\mathcal{F},\mathcal{K})),$$

and the least element $\bot_\mathsf{P} \stackrel{\text{def}}{=} \mathsf{Path}^\omega(\mathcal{F},\mathcal{K})$, where $\mathsf{Path}^+(\mathcal{F},\mathcal{K}) \stackrel{\text{def}}{=} (\mathcal{F}\cup\mathcal{K})\cdot(\mathbb{N}\cdot(\mathcal{F}\cup\mathcal{K}))^*$ is the set of finite paths, and $\mathsf{Path}^\omega(\mathcal{F},\mathcal{K}) \stackrel{\text{def}}{=} (\mathcal{F}\cup\mathcal{K})\cdot(\mathbb{N}\cdot(\mathcal{F}\cup\mathcal{K}))^\omega$ is the set of infinite paths. We can again see that the $\ominus$ symbol indicates a "yet unknown tree," because $\mathit{paths}(\ominus)$, by Lemma 6.7, equals $\bot_\mathsf{P}$, i.e., the set of all infinite paths.

$$\frac{}{a \in \mathsf{RegExp}^{\infty}(\mathcal{F},\mathcal{K})}\ (\textsc{Leaf})\ a \in \mathcal{F}_0 \cup \mathcal{K} \qquad \frac{}{f(E_1,\cdots,E_n) \in \mathsf{RegExp}^{\infty}(\mathcal{F},\mathcal{K})}\ (\textsc{Node})\ f \in \mathcal{F}_n \quad n > 0 \quad \forall i = 1,\cdots,n\colon E_i \in \mathsf{RegExp}^{\infty}(\mathcal{F},\mathcal{K})$$

$$\frac{}{(E_1 \cdot_{\square} E_2) \in \mathsf{RegExp}^{\infty}(\mathcal{F},\mathcal{K})}\ (\textsc{Concatenation})\ E_1 \in \mathsf{RegExp}^{\infty}(\mathcal{F},\mathcal{K} \cup \{\square\}) \quad E_2 \in \mathsf{RegExp}^{\infty}(\mathcal{F},\mathcal{K}) \qquad \frac{}{E^{\infty_{\square}} \in \mathsf{RegExp}^{\infty}(\mathcal{F},\mathcal{K})}\ (\textsc{Iteration})\ E \in \mathsf{RegExp}^{\infty}(\mathcal{F},\mathcal{K} \cup \{\square\})$$

Fig. 6.2: Generation rules for regular hyper-path expressions.

6.1.2 Regular Hyper-Path Expressions

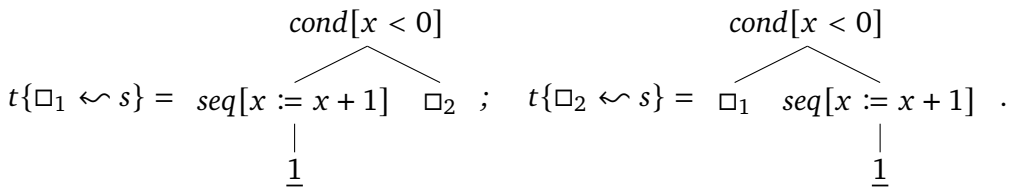
Recall that a regular expression gives a finite representation of a (possibly infinite) regular set of finite words, and a regular-tree expression gives a finite representation of a (possibly infinite) regular set of finite trees [31]. Because in this chapter, I focus on probabilistic programs *without nondeterminism*, each program should correspond to exactly one hyper-path (recall Example 6.2). As a consequence, instead of identifying regular sets of hyper-paths, I identify regular hyper-paths in this section. Intuitively, a hyper-path is a possibly-infinite tree, and my goal in this section is develop a finite representation for such possibly-infinite trees, namely *regular hyper-path expressions*.

Let $\mathsf{RegExp}^{\infty}(\mathcal{F},\mathcal{K})$ denote the set of regular hyper-path expressions over a ranked alphabet $\mathcal{F}$ and a set $\mathcal{K}$ of holes symbols. The set is defined to be inductively generated from the inference rules listed in Fig. 6.2. In other words, a regular hyper-path expression in $\mathsf{RegExp}^{\infty}(\mathcal{F},\mathcal{K})$ takes one of the syntactic forms: a, $f(E_1,\cdots,E_n)$, $(E_1 \cdot_{\square} E_2)$, and $E^{\infty_{\square}}$, where E's are regular hyper-path expressions. Each regular hyper-path expression should correspond to exactly one hyper-path, i.e., one possibly-infinite tree in $\mathsf{Tree}^{\infty}(\mathcal{F},\mathcal{K})$. The rules (Leaf) and (Node) are the basic operations for constructing leaf nodes and internal nodes of a tree, respectively. Intuitively, a hole $\square \in \mathcal{K}$ represents a *substitution* placeholder: $(E_1 \cdot_{\square} E_2)$ represents a tree obtained by substituting the tree encoded by E_2 for the any leaf with symbol $\square$ in the tree encoded by E_1. Then the iteration operator $E^{\square_\infty}$ represents a tree obtained by $(E \cdot_{\square} E \cdot_{\square} \cdots \cdot_{\square} E \cdot_{\square} \cdots)$, i.e., self-substituting E for the hole $\square$ for an infinite number of times.

To formally interpret regular hyper-path expressions as possibly-infinite trees, I first introduce a *substitution* operator, defined as a function on possibly-infinite trees with the following base and induction steps, where $-_1$ and $-_2$ indicates the two arguments of the substitution operator, and the function is defined coinductively on the first argument:

$$\begin{aligned}
(-_1)\{\square \leftsquigarrow -_2\} &: \mathsf{Tree}^{\infty}(\mathcal{F},\mathcal{K}) \times \mathsf{Tree}^{\infty}(\mathcal{F},\mathcal{K} \setminus \{\square\}) \to \mathsf{Tree}^{\infty}(\mathcal{F},\mathcal{K} \setminus \{\square\}) \\
\square\{\square \leftsquigarrow t\} &\stackrel{\text{def}}{=} t \\
a\{\square \leftsquigarrow t\} &\stackrel{\text{def}}{=} a \quad \text{for } a \neq \square \\
f(s_1,\cdots,s_n)\{\square \leftsquigarrow t\} &\stackrel{\text{def}}{=} f(s_1\{\square \leftsquigarrow t\},\cdots,s_n\{\square \leftsquigarrow t\})
\end{aligned}$$

Example 6.9. Let $\mathcal{F} = \{seq[x := x+1](), cond[x < 0](,), \underline{1}\}$ *and* $\mathcal{K} = \{\square_1, \square_2\}$. *Let* $t = cond[x < 0](\square_1, \square_2)$ *and* $s = seq[x := x+1](\underline{1})$. *Then*

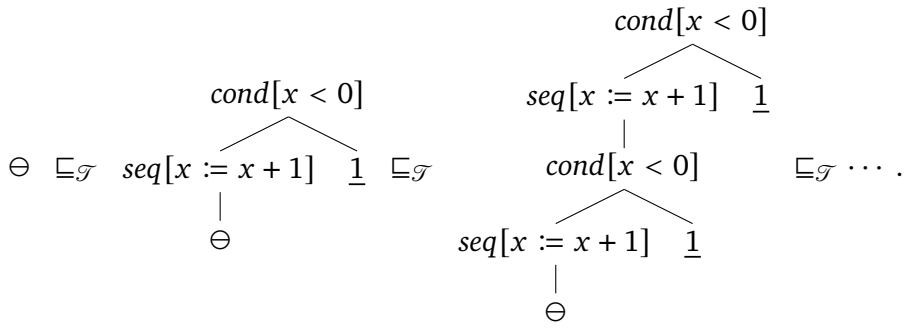


Proposition 6.10. *The substitution operator is ω-continuous in its second argument.*

I now define an interpretation from regular hyper-path expressions to possibly-infinite trees via the map $\mathscr{T}_{\mathcal{K}}[\![-]\!]$ inductively defined on the structure of regular hyper-path expressions as follows.

$$\begin{aligned}
\mathscr{T}_{\mathcal{K}}[\![-]\!] &: \mathsf{RegExp}^{\infty}(\mathcal{F},\mathcal{K}) \to \mathsf{Tree}^{\infty}(\mathcal{F},\mathcal{K}) \\
\mathscr{T}_{\mathcal{K}}[\![a]\!] &\stackrel{\text{def}}{=} a \\
\mathscr{T}_{\mathcal{K}}[\![f(E_1,\cdots,E_n)]\!] &\stackrel{\text{def}}{=} f(\mathscr{T}_{\mathcal{K}}[\![s_1]\!],\cdots,\mathscr{T}_{\mathcal{K}}[\![s_n]\!]) \\
\mathscr{T}_{\mathcal{K}}[\![E_1 \cdot_{\Box} E_2]\!] &\stackrel{\text{def}}{=} \mathscr{T}_{\mathcal{K}\cup\{\Box\}}[\![E_1]\!]\{\Box \leftsquigarrow \mathscr{T}_{\mathcal{K}}[\![E_2]\!]\} \\
\mathscr{T}_{\mathcal{K}}[\![E^{\infty_{\Box}}]\!] &\stackrel{\text{def}}{=} \mathrm{lfp}^{\sqsubseteq_{\mathscr{T}}}_{\ominus}\ \lambda X.\ (\mathscr{T}_{\mathcal{K}\cup\{\Box\}}[\![E]\!]\{\Box \leftsquigarrow X\})
\end{aligned}$$

*Example 6.11. The regular hyper-path expression $E \stackrel{\text{def}}{=} (cond[x < 0](seq[x := x + 1](\Box), \underline{1}))^{\infty_{\Box}}$ gives a finite representation of the infinite hyper-path presented in Example 6.2, i.e., the loop "***while*** $x < 0$ ***do*** $x := x + 1$ ***od***." Intuitively, the map $\mathscr{T}_{\emptyset}[\![E]\!]$ constructs the following ω-chain of trees and obtains the least upper bound as the interpretation of E:*



6.1.3 Solving Regular Equations

In this section, I study the correspondence between regular hyper-path expressions and control-flow hyper-graphs without nondeterminism, i.e., hyper-graphs where every non-exit node has exactly one outgoing hyper-edge. Recall that a hyper-graph H is a quadruple $(V, E, v^{\mathsf{entry}}, v^{\mathsf{exit}})$, where each hyper-edge $e \in E$ is associated with a control-flow action $Ctrl(e)$. Consider a ranked alphabet $\mathcal{F} \stackrel{\text{def}}{=} \{Ctrl(e) \mid e \in E\} \cup \{\underline{1}\}$ with a distinguished symbol $\underline{1}$ with arity zero, where for each $e = (v, \{u_1, \cdots, u_k\}) \in E$, the arity of e is $Arity(e) = k$. Let X_v for each $v \in V$ be a variable denoting some possibly-infinite tree. Intuitively, we can treat each hyper-edge $e = (v, \{u_1, \cdots, u_k\}) \in E$ as an *equation* $X_v = e(X_{u_1}, \cdots, X_{u_k})$, where the right-hand-side is a regular hyper-path expression in $\mathsf{RegExp}^{\infty}(\mathcal{F}, \{X_v \mid v \in V\})$. Thus, we can extract the following equation system from a

Algorithm 1 Gaussian elimination for regular hyper-path equations

Input: An equation system $\{X_i = R_i\}_{i=1}^n$ where each $R_i \in \mathsf{RegExp}^\infty(\mathcal{F}, \{X_i \mid i = 1, \cdots, n\})$
Output: A closed-form solution $\{X_i = E_i\}_{i=1}^n$ where each $E_i \in \mathsf{RegExp}^\infty(\mathcal{F}, \emptyset)$

```
for i ← 1 to n do                                              ▷ Front-solving
    if X_i appears in R_i then
        Let R'_i be such that R'_i{□_i ↜ X_i} = R_i and X_i does not appear in R'_i
        R_i ← (R'_i)^{∞□_i}                                    ▷ Loop-solving
    end if
    for each j > i do
        R_j ← R_j{X_i ↜ R_i}
    end for
end for
for i ← n to 2 do                                              ▷ Back-solving
    for each j < i do
        R_j ← R_j{X_i ↜ R_i}
    end for
end for
return {X_i = R_i}_{i=1}^n
```

hyper-graph:

$$X_v = Ctrl(e)\ (X_{u_1}, \cdots, X_{u_k}), \qquad e = (v, \{u_1, \cdots, u_k\}) \in E,$$
$$X_{v^{\mathsf{exit}}} = \underline{1},$$

where each variable X_v appears exactly once as a left-hand-side, because every non-exit node has exactly one outgoing edge. In the rest of this section, I outline an algorithm for computing a regular hyper-path expression $E_v \in \mathsf{RegExp}^\infty(\mathcal{F}, \emptyset)$ for each variable X_v ($v \in V$), such that

$$\mathscr{T}_\emptyset[\![E_v]\!] = \mathscr{T}_\emptyset[\![Ctrl(e)\ (E_{u_1}, \cdots, E_{u_k})]\!], \qquad e = (v, \{u_1, \cdots, u_k\}) \in E,$$
$$\mathscr{T}_\emptyset[\![E_{v^{\mathsf{exit}}}]\!] = \mathscr{T}_\emptyset[\![\underline{1}]\!],$$

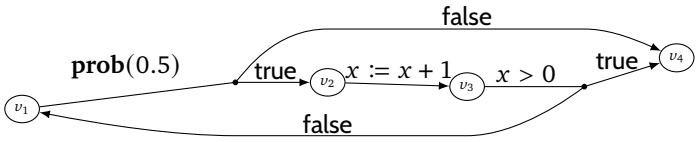
as well as $\{X_v = E_v\}_{v \in V}$ is a least solution to the equation system with respect to the tree refinement order $\sqsubseteq_{\mathscr{T}}$.

The algorithm can be seen as a variation of Gaussian elimination, given in Algorithm 1. The front-solving phase eliminates variables in $\{X_i \mid i = 1, \cdots, n\}$ one-by-one, in the sense that after the i-th step, the variable X_i does *not* appear in the right-hand-side of any equation $X_j = R_j$ for $j \geq i$. The back-solving phase then eliminates all variable occurrences from right-hand-sides by, at the i-th step, substituting the closed-form R_i for the symbol X_i in the equation $X_j = R_j$ for $j < i$. The key ingredient of this algorithm is the loop-solving step, which solves a single recursive equation $X_i = R'_i\{\square_i \leftsquigarrow X_i\}$ using the iteration operator and takes $(R'_i)^{\infty_{\square_i}}$ to be the solution.

Example 6.12. Consider the unstructured probabilistic program in Fig. 6.3(a), whose corresponding control-flow hyper-graph is presented in Fig. 6.3(b), where v_1 is the entry node and v_4 is the exit node. We can extract an equation system from the CFHG as follows, using the ranked alphabet

```
while prob(0.5) do
  x := x + 1;
  if x > 0 then break
  else continue
  fi
od
```

(a)



(b)

Fig. 6.3: (a) An example unstructured probabilistic program and (b) its CFHG.

$\mathcal{F} \stackrel{\text{def}}{=} \{prob[0.5](,), seq[x := x+1](), cond[x > 0](,), \underline{1}\}$ *and hole symbols* $\mathcal{K} \stackrel{\text{def}}{=} \{X_{v_1}, X_{v_2}, X_{v_3}, X_{v_4}\}$.

$$X_{v_1} = prob[0.5](X_{v_2}, X_{v_4}), \qquad X_{v_2} = seq[x := x+1](X_{v_3}),$$
$$X_{v_3} = cond[x > 0](X_{v_4}, X_{v_1}), \qquad X_{v_4} = \underline{1}.$$

Solving the equation system via Algorithm 1 leads to the following closed-form solution:

$$X_{v_1} = prob[0.5]\left(seq[x := x+1]\left(\left(cond[x > 0](\underline{1}, prob[0.5](seq[x := x+1](\square), \underline{1}))\right)^{\infty_\square}\right), \underline{1}\right),$$
$$X_{v_2} = seq[x := x+1]\left(\left(cond[x > 0](\underline{1}, prob[0.5](seq[x := x+1](\square), \underline{1}))\right)^{\infty_\square}\right),$$
$$X_{v_3} = \left(cond[x > 0](\underline{1}, prob[0.5](seq[x := x+1](\square), \underline{1}))\right)^{\infty_\square},$$
$$X_{v_4} = \underline{1}.$$

The Gaussian-elimination-based Algorithm 1 on a CFHG has a cubic time complexity in terms of the size of the CFHG. In the non-probabilistic case, i.e., where control flow graphs and standard directed graphs, the connection between Gaussian elimination and graph algorithms inspired Tarjan's path-expression algorithm [142], which can achieve a nearly linear time complexity on reducible control-flow graphs. Designing a more efficient algorithm to solve regular hyper-path equations is an interesting future research direction.

6.2 Deterministic Markov-Kleene Algebra with Tests

Recall that for a control-flow hyper-graph, its algebraic denotational semantics is obtained by composing $Ctrl(e)$ (the control action associated with e) operations along hyper-edges. The semantics of a program is determined by an interpretation, which consists of (i) a semantic algebra, which defines a set of possible program meanings, and which is equipped with operators to compose these meanings, and (ii) a semantic function, which assigns a meaning to each data action $\mathsf{act} \in \mathsf{Act}$. As I discussed in §6.1, a hyper-graph (without nondeterminism) can be finitely represented by a regular hyper-path expression with the alphabet set to be the control-flow actions attached to the hyper-edges in the graph, plus a distinguished constant $\underline{1}$ standing for program termination. Thus, in this section, I assume the ranked alphabet $\mathcal{F}$ is a finite subset of

$$\{\underline{1}\} \cup \{seq[\mathsf{act}]() \mid \mathsf{act} \in \mathsf{Act}\} \cup \{cond[\varphi](,) \mid \varphi \in \mathcal{L}\} \cup \{prob[p](,) \mid p \in [0,1]\},$$

where Act is the set of data actions (assignments, sampling, etc.), and $\mathcal{L}$ is the set of logical conditions. Note that I followed a similar setup to §4.2 to distinguish standard logical conditions

and purely probabilistic conditions. Meanwhile, I also remove procedure calls because I do not consider multiple procedures in this chapter.

I now define the *Deterministic Markov-Kleene Algebra with Tests* (DMKAT), which can be seen as a variant of the Markov algebra developed in §3.3.

Definition 6.13. A DMKAT over a set $\mathcal{L}$ of logical conditions (also called *tests*) is a 7-tuple $\mathcal{M} = (M, \sqsubseteq_M, \otimes_M, {}_{\varphi}\Diamond_M, {}_{p}\oplus_M, \bot_M, 1_M)$, where $(M, \sqsubseteq_M)$ forms a dcpo with $\bot_M$ as its least element; $(M, \otimes_M, 1_M)$ forms a monoid (i.e., $\otimes_M$ is an associative binary operator with 1_M as its identity element); ${}_{\varphi}\Diamond_M$ is a binary operator parametrized by a condition $\varphi \in \mathcal{L}$; ${}_{p}\oplus_M$ is a binary operator parameterized by $p \in [0,1]$; and $\otimes_M, {}_{\varphi}\Diamond_M, {}_{p}\oplus_M$ are Scott-continuous.

Definition 6.14. An *interpretation* is a pair $\mathscr{M} = (\mathcal{M}, [\![\cdot]\!]^{\mathscr{M}})$, where $\mathcal{M}$ is a DMKAT and $[\![\cdot]\!]^{\mathscr{M}} : \mathsf{Act} \to \mathcal{M}$. We call $\mathcal{M}$ the *semantic algebra* of the interpretation and $[\![\cdot]\!]^{\mathscr{M}}$ the *semantic function*.

Given a regular hyper-path expression $E \in \mathsf{RegExp}^{\infty}(\mathcal{F}, \mathcal{K})$, an interpretation $\mathscr{M} = (\mathcal{M}, [\![\cdot]\!]^{\mathscr{M}})$, and a *hole-valuation* $\gamma : \mathcal{K} \to \mathcal{M}$ (which, intuitively, gives an interpretation for each hole symbol), I define the interpretation of E under γ, denoted by $\mathscr{M}_\gamma[\![E]\!]$, as follows.

$$
\begin{aligned}
\mathscr{M}_\gamma[\![-]\!] &: \mathsf{RegExp}^{\infty}(\mathcal{F}, \mathcal{K}) \to \mathcal{M} \\
\mathscr{M}_\gamma[\![\underline{1}]\!] &\stackrel{\text{def}}{=} 1_M \\
\mathscr{M}_\gamma[\![seq[\mathsf{act}](E_1)]\!] &\stackrel{\text{def}}{=} [\![\mathsf{act}]\!]^{\mathscr{M}} \otimes_M \mathscr{M}_\gamma[\![E_1]\!] \\
\mathscr{M}_\gamma[\![cond[\varphi](E_1, E_2)]\!] &\stackrel{\text{def}}{=} \mathscr{M}_\gamma[\![E_1]\!] \; {}_{\varphi}\Diamond_M \; \mathscr{M}_\gamma[\![E_2]\!] \\
\mathscr{M}_\gamma[\![prob[p](E_1, E_2)]\!] &\stackrel{\text{def}}{=} \mathscr{M}_\gamma[\![E_1]\!] \; {}_{p}\oplus_M \; \mathscr{M}_\gamma[\![E_2]\!] \\
\mathscr{M}_\gamma[\![\square]\!] &\stackrel{\text{def}}{=} \gamma(\square), \quad \text{where } \square \in \mathcal{K} \\
\mathscr{M}_\gamma[\![E_1 \cdot_\square E_2]\!] &\stackrel{\text{def}}{=} \mathscr{M}_{\gamma[\square \mapsto \mathscr{M}_\gamma[\![E_2]\!]]}[\![E_1]\!] \\
\mathscr{M}_\gamma[\![(E_1)^{\infty_\square}]\!] &\stackrel{\text{def}}{=} \mathrm{lfp}^{\sqsubseteq_M}_{\bot_M} \lambda X.\, \mathscr{M}_{\gamma[\square \mapsto X]}[\![E_1]\!]
\end{aligned}
$$

The interesting cases are the rules for interpreting concatenation $(E_1 \cdot_\square E_2)$ and iteration $(E_1)^{\infty_\square}$. For $(E_1 \cdot_\square E_2)$, by the rule (Concatenation) in Fig. 6.2, we can see that the hole symbol $\square$ does *not* appear in E_2, but it might appear in E_1. Thus, we can already interpret E_2 under the hole-valuation γ, and to interpret E_1, we need to extend γ with an interpretation for the hole $\square$. Recall the interpretation of regular hyper-path expressions as possibly-infinite trees: $(E_1 \cdot_\square E_2)$ is intended to represent a tree obtained by substituting E_2 for $\square$ in E_1. Thus, to interpret E_1, we extend γ by mapping $\square$ to the interpretation of E_2. For $(E_1)^{\infty_\square}$, by the rule (Iteration) in Fig. 6.2, we can see that the hole symbol $\square$ might appear in E_1. In this case, we should find an interpretation X for the iteration expression, in a way that $X = \mathscr{M}_{\gamma[\square \mapsto X]}[\![E_1]\!]$. Because the semantic algebra $\mathcal{M}$ admits a dcpo, I define the interpretation for iteration expressions using fixed points.

The key theoretical result I will establish in this section is that the tree-based interpretation (developed in §6.1.2) is *sound* for any DMKAT interpretation, i.e., regular hyper-path expressions with the same tree-based interpretation also yield the same interpretation under any DMKAT.

Theorem 6.15. *Let $E, F \in \mathsf{RegExp}^{\infty}(\mathcal{F}, \mathcal{K})$. If $\mathscr{T}_{\mathcal{K}}[\![E]\!] = \mathscr{T}_{\mathcal{K}}[\![F]\!]$, then for any DMKAT interpretation $\mathscr{M} = (\mathcal{M}, [\![\cdot]\!]^{\mathscr{M}})$ and any hole-valuation $\gamma : \mathcal{K} \to \mathcal{M}$, it holds that $\mathscr{M}_\gamma[\![E]\!] = \mathscr{M}_\gamma[\![F]\!]$.*

Before proving the theorem, I define an interpretation map from possibly-infinite trees $\mathsf{Tree}^{\infty}(\mathcal{F},\mathcal{K})$ into a semantic algebra $\mathcal{M}$ equipped with an interpretation $\mathscr{M} = (\mathcal{M}, [\![\cdot]\!]^{\mathscr{M}})$. Because $\mathcal{M}$ admits a dcpo, thus it also admits an ω-cpo, I can follow the coinductive principle for function definitions on trees (developed in §6.1.1). Below gives the base and induction steps for an interpretation map $r_{\gamma}^{\mathscr{M}}$, parameterized by a hole-valuation $\gamma : \mathcal{K} \to \mathcal{M}$. The interpretation is well-defined because the operators $\otimes_M$, ${}_{\varphi}\Diamond_M$, ${}_{p}\oplus_M$ are all Scott-continuous, thus they are also ω-continuous.

$$r_{\gamma}^{\mathscr{M}}(\underline{1}) \stackrel{\text{def}}{=} 1_M$$
$$r_{\gamma}^{\mathscr{M}}(seq[\mathsf{act}](s_1)) \stackrel{\text{def}}{=} [\![\mathsf{act}]\!]^{\mathscr{M}} \otimes_M r_{\gamma}^{\mathscr{M}}(s_1)$$
$$r_{\gamma}^{\mathscr{M}}(cond[\varphi](s_1,s_2)) \stackrel{\text{def}}{=} r_{\gamma}^{\mathscr{M}}(s_1)\ {}_{\varphi}\Diamond_M\ r_{\gamma}^{\mathscr{M}}(s_2)$$
$$r_{\gamma}^{\mathscr{M}}(prob[p](s_1,s_2)) \stackrel{\text{def}}{=} r_{\gamma}^{\mathscr{M}}(s_1)\ {}_{p}\oplus_M\ r_{\gamma}^{\mathscr{M}}(s_2)$$
$$r_{\gamma}^{\mathscr{M}}(\Box) \stackrel{\text{def}}{=} \gamma(\Box)$$

I then prove the following property of $r_{\gamma}^{\mathscr{M}}$ about substitutions.

Lemma 6.16. *For any $t \in \mathsf{Tree}^{\infty}(\mathcal{F},\mathcal{K}\cup\{\Box\})$, $u \in \mathsf{Tree}^{\infty}(\mathcal{F},\mathcal{K})$, and $\gamma : \mathcal{K} \to \mathcal{M}$, it holds that $r^{\mathscr{M}}_{\gamma[\Box\mapsto r_{\gamma}^{\mathscr{M}}(u)]}(t) = r_{\gamma}^{\mathscr{M}}(t\{\Box \leftsquigarrow u\})$.*

Proof. Let $\gamma' \stackrel{\text{def}}{=} \gamma[\Box \mapsto r_{\gamma}^{\mathscr{M}}(u)]$. Then $\gamma' : (\mathcal{K}\cup\{\Box\}) \to \mathcal{M}$.

We proceed by induction on the structure of t.

Case $t = \underline{1}$**:**

By definition, we have $r_{\gamma'}^{\mathscr{M}}(\underline{1}) = 1_M$.

By definition, we have $\underline{1}\{\Box \leftsquigarrow u\} = \underline{1}$, and also $r_{\gamma}^{\mathscr{M}}(\underline{1}) = 1_M$.

Thus, we conclude that $r_{\gamma'}^{\mathscr{M}}(\underline{1}) = r_{\gamma}^{\mathscr{M}}(\underline{1}\{\Box \leftsquigarrow u\})$.

Case $t = seq[\mathsf{act}](s)$**:**

By induction hypothesis, we have $r_{\gamma'}^{\mathscr{M}}(s) = r_{\gamma}^{\mathscr{M}}(s\{\Box \leftsquigarrow u\})$.

By definition, we have $r_{\gamma'}^{\mathscr{M}}(seq[\mathsf{act}](s)) = [\![\mathsf{act}]\!]^{\mathscr{M}} \otimes_M r_{\gamma'}^{\mathscr{M}}(s)$.

By definition, we have $seq[\mathsf{act}](s)\{\Box \leftsquigarrow u\} = seq[\mathsf{act}](s\{\Box \leftsquigarrow u\})$, and also $r_{\gamma}^{\mathscr{M}}(seq[\mathsf{act}](s\{\Box \leftsquigarrow u\})) = [\![\mathsf{act}]\!]^{\mathscr{M}} \otimes_M r_{\gamma}^{\mathscr{M}}(s\{\Box \leftsquigarrow u\})$.

Thus, we conclude that $r_{\gamma'}^{\mathscr{M}}(seq[\mathsf{act}](s)) = r_{\gamma}^{\mathscr{M}}(seq[\mathsf{act}](s)\{\Box \leftsquigarrow u\})$.

Case $t = cond[\varphi](s_1,s_2)$**:**

By induction hypothesis on s_1 and s_2, respectively, we have $r_{\gamma'}^{\mathscr{M}}(s_1) = r_{\gamma}^{\mathscr{M}}(s_1\{\Box \leftsquigarrow u\})$ and $r_{\gamma'}^{\mathscr{M}}(s_2) = r_{\gamma}^{\mathscr{M}}(s_2\{\Box \leftsquigarrow u\})$, respectively.

By definition, we have $r_{\gamma'}^{\mathscr{M}}(cond[\varphi](s_1,s_2)) = r_{\gamma'}^{\mathscr{M}}(s_1)\ {}_{\varphi}\Diamond_M\ r_{\gamma'}^{\mathscr{M}}(s_2)$.

By definition, we have $cond[\varphi](s_1,s_2)\{\Box \leftsquigarrow u\} = cond[\varphi](s_1\{\Box \leftsquigarrow u\}, s_2\{\Box \leftsquigarrow u\})$, and also

$$r_{\gamma}^{\mathscr{M}}(cond[\varphi](s_1\{\Box \leftsquigarrow u\}, s_2\{\Box \leftsquigarrow u\})) = r_{\gamma}^{\mathscr{M}}(s_1\{\Box \leftsquigarrow u\})\ {}_{\varphi}\Diamond_M\ r_{\gamma}^{\mathscr{M}}(s_2\{\Box \leftsquigarrow u\}).$$

Thus, we conclude that $r_{\gamma'}^{\mathscr{M}}(cond[\varphi](s_1,s_2)) = r_{\gamma}^{\mathscr{M}}(cond[\varphi](s_1,s_2)\{\Box \leftsquigarrow u\})$.

Case $t = prob[p](s_1, s_2)$**:**

By induction hypothesis on s_1 and s_2, respectively, we have $r^{\mathscr{M}}_{\gamma'}(s_1) = r^{\mathscr{M}}_{\gamma}(s_1\{\Box \leftsquigarrow u\})$ and $r^{\mathscr{M}}_{\gamma'}(s_2) = r^{\mathscr{M}}_{\gamma}(s_2\{\Box \leftsquigarrow u\})$, respectively.

By definition, we have $r^{\mathscr{M}}_{\gamma'}(prob[p](s_1, s_2)) = r^{\mathscr{M}}_{\gamma'}(s_1) \ {}_p\oplus_M \ r^{\mathscr{M}}_{\gamma'}(s_2)$.

By definition, we have $prob[p](s_1, s_2)\{\Box \leftsquigarrow u\} = prob[p](s_1\{\Box \leftsquigarrow u\}, s_2\{\Box \leftsquigarrow u\})$, and also

$$r^{\mathscr{M}}_{\gamma}(prob[p](s_1\{\Box \leftsquigarrow u\}, s_2\{\Box \leftsquigarrow u\})) = r^{\mathscr{M}}_{\gamma}(s_1\{\Box \leftsquigarrow u\}) \ {}_p\oplus_M \ r^{\mathscr{M}}_{\gamma}(s_2\{\Box \leftsquigarrow u\}).$$

Thus, we conclude that $r^{\mathscr{M}}_{\gamma'}(prob[p](s_1, s_2)) = r^{\mathscr{M}}_{\gamma}(prob[p](s_1, s_2)\{\Box \leftsquigarrow u\})$.

Case $t = \Box$**:**

By definition, we have $r^{\mathscr{M}}_{\gamma'}(\Box) = \gamma'(\Box) = r^{\mathscr{M}}_{\gamma}(u)$.

By definition, we have $\Box\{\Box \leftsquigarrow u\} = u$.

Thus, we conclude that $r^{\mathscr{M}}_{\gamma'}(\Box) = r^{\mathscr{M}}_{\gamma}(\Box\{\Box \leftsquigarrow u\})$.

Case $t = \Box'$ where $\Box' \neq \Box$**:**

By definition, we have $r^{\mathscr{M}}_{\gamma'}(\Box') = \gamma'(\Box') = \gamma(\Box')$.

By definition, we have $\Box'\{\Box \leftsquigarrow u\} = \Box'$, and also $r^{\mathscr{M}}_{\gamma}(\Box') = \gamma(\Box')$.

Thus, we conclude that $r^{\mathscr{M}}_{\gamma'}(\Box') = r^{\mathscr{M}}_{\gamma}(\Box'\{\Box \leftsquigarrow u\})$.

□

I can now present the proof of Theorem 6.15.

Proof of Theorem 6.15. Fix $E, F \in \mathsf{RegExp}^{\infty}(\mathcal{F}, \mathcal{K})$ such that $\mathscr{T}_{\mathcal{K}}[\![E]\!] = \mathscr{T}_{\mathcal{K}}[\![F]\!]$. Fix an interpretation $\mathscr{M} = (\mathcal{M}, [\![\cdot]\!]^{\mathscr{M}})$ and a hole-valuation $\gamma : \mathcal{K} \to \mathcal{M}$. The theorem requires us to show that $\mathscr{M}_{\gamma}[\![E]\!] = \mathscr{M}_{\gamma}[\![F]\!]$. We claim that for any expression E, it holds that $\mathscr{M}_{\gamma}[\![E]\!] = r^{\mathscr{M}}_{\gamma}(\mathscr{T}_{\mathcal{K}}[\![E]\!])$. If this is true, we can conclude the proof by

$$\mathscr{M}_{\gamma}[\![E]\!] = r^{\mathscr{M}}_{\gamma}(\mathscr{T}_{\mathcal{K}}[\![E]\!]) = r^{\mathscr{M}}_{\gamma}(\mathscr{T}_{\mathcal{K}}[\![F]\!]) = \mathscr{M}_{\gamma}[\![F]\!].$$

To prove the claim, we fix an expression E and proceed by induction on the structure of E.

Case $E = \underline{1}$**:**

By definition, we have $\mathscr{M}_{\gamma}[\![\underline{1}]\!] = 1_M$.

By definition, we have $\mathscr{T}_{\mathcal{K}}[\![\underline{1}]\!] = \underline{1}$, and also $r^{\mathscr{M}}_{\gamma}(\underline{1}) = 1_M$.

Thus, we conclude that $\mathscr{M}_{\gamma}[\![\underline{1}]\!] = r^{\mathscr{M}}_{\gamma}(\mathscr{T}_{\mathcal{K}}[\![\underline{1}]\!])$.

Case $E = seq[\mathsf{act}](E_1)$**:**

By induction hypothesis, we have $\mathscr{M}_{\gamma}[\![E_1]\!] = r^{\mathscr{M}}_{\gamma}(\mathscr{T}_{\mathcal{K}}[\![E_1]\!])$.

By definition, we have $\mathscr{M}_{\gamma}[\![seq[\mathsf{act}](E_1)]\!] = [\![\mathsf{act}]\!]^{\mathscr{M}} \otimes_M \mathscr{M}_{\gamma}[\![E_1]\!]$.

By definition, we have $\mathscr{T}_{\mathcal{K}}[\![seq[\mathsf{act}](E_1)]\!] = seq[\mathsf{act}](s_1)$, where $s_1 \stackrel{\text{def}}{=} \mathscr{T}_{\mathcal{K}}[\![E_1]\!]$, and also $r^{\mathscr{M}}_{\gamma}(seq[\mathsf{act}](s_1)) = [\![\mathsf{act}]\!]^{\mathscr{M}} \otimes_M r^{\mathscr{M}}_{\gamma}(s_1)$.

Thus, we conclude that $\mathscr{M}_{\gamma}[\![seq[\mathsf{act}](E_1)]\!] = r^{\mathscr{M}}_{\gamma}(\mathscr{T}_{\mathcal{K}}[\![seq[\mathsf{act}](E_1)]\!])$.

Case $E = cond[\varphi](E_1, E_2)$**:**

By induction hypothesis on E_1 and E_2, respectively, we have $\mathscr{M}_\gamma[\![E_1]\!] = r_\gamma^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}}[\![E_1]\!])$ and $\mathscr{M}_\gamma[\![E_2]\!] = r_\gamma^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}}[\![E_2]\!])$, respectively.

By definition, we have $\mathscr{M}_\gamma[\![cond[\varphi](E_1, E_2)]\!] = \mathscr{M}_\gamma[\![E_1]\!] \ {}_\varphi\Diamond_M \ \mathscr{M}_\gamma[\![E_2]\!]$.

By definition, we have $\mathscr{T}_{\mathcal{K}}[\![cond[\varphi](E_1, E_2)]\!] = cond[\varphi](s_1, s_2)$, where $s_1 \stackrel{\text{def}}{=} \mathscr{T}_{\mathcal{K}}[\![E_1]\!]$, $s_2 \stackrel{\text{def}}{=} \mathscr{T}_{\mathcal{K}}[\![E_1]\!]$, and also $r_\gamma^{\mathscr{M}}(cond[\varphi](s_1, s_2)) = r_\gamma^{\mathscr{M}}(s_1) \ {}_\varphi\Diamond_M \ r_\gamma^{\mathscr{M}}(s_2)$.

Thus, we conclude that $\mathscr{M}_\gamma[\![cond[\varphi](E_1, E_2)]\!] = r_\gamma^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}}[\![cond[\varphi](E_1, E_2)]\!])$.

Case $E = prob[p](E_1, E_2)$**:**

By induction hypothesis on E_1 and E_2, respectively, we have $\mathscr{M}_\gamma[\![E_1]\!] = r_\gamma^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}}[\![E_1]\!])$ and $\mathscr{M}_\gamma[\![E_2]\!] = r_\gamma^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}}[\![E_2]\!])$, respectively.

By definition, we have $\mathscr{M}_\gamma[\![prob[p](E_1, E_2)]\!] = \mathscr{M}_\gamma[\![E_1]\!] \ {}_p\oplus_M \ \mathscr{M}_\gamma[\![E_2]\!]$.

By definition, we have $\mathscr{T}_{\mathcal{K}}[\![prob[p](E_1, E_2)]\!] = prob[p](s_1, s_2)$, where $s_1 \stackrel{\text{def}}{=} \mathscr{T}_{\mathcal{K}}[\![E_1]\!]$, $s_2 \stackrel{\text{def}}{=} \mathscr{T}_{\mathcal{K}}[\![E_1]\!]$, and also $r_\gamma^{\mathscr{M}}(prob[p](s_1, s_2)) = r_\gamma^{\mathscr{M}}(s_1) \ {}_p\oplus_M \ r_\gamma^{\mathscr{M}}(s_2)$.

Thus, we conclude that $\mathscr{M}_\gamma[\![prob[p](E_1, E_2)]\!] = r_\gamma^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}}[\![prob[p](E_1, E_2)]\!])$.

Case $E = \square$ for some $\square \in \mathcal{K}$**:**

By definition, we have $\mathscr{M}_\gamma[\![\square]\!] = \gamma(\square)$.

By definition, we have $\mathscr{T}_{\mathcal{K}}[\![\square]\!] = \square$, and also $r_\gamma^{\mathscr{M}}(\square) = \gamma(\square)$.

Thus, we conclude that $\mathscr{M}_\gamma[\![\square]\!] = r_\gamma^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}}[\![\square]\!])$.

Case $E = E_1 \cdot_\square E_2$**:**

By induction hypothesis on E_2, we have $\mathscr{M}_\gamma[\![E_2]\!] = r_\gamma^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}}[\![E_2]\!])$.

Let $\gamma' \stackrel{\text{def}}{=} \gamma[\square \mapsto \mathscr{M}_\gamma[\![E_2]\!]]$. Then $\gamma' : (\mathcal{K} \cup \{\square\}) \to \mathcal{M}$.

By induction hypothesis on E_1 (which is an expression in $\mathsf{RegExp}^\infty(\mathcal{F}, \mathcal{K} \cup \{\square\})$), we have $\mathscr{M}_{\gamma'}[\![E_1]\!] = r_{\gamma'}^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}\cup\{\square\}}[\![E_1]\!])$.

By definition, we have $\mathscr{M}_\gamma[\![E_1 \cdot_\square E_2]\!] = \mathscr{M}_{\gamma'}[\![E_1]\!]$.

By definition, we have $\mathscr{T}_{\mathcal{K}}[\![E_1 \cdot_\square E_2]\!] = \mathscr{T}_{\mathcal{K}\cup\{\square\}}[\![E_1]\!]\{\square \leftsquigarrow \mathscr{T}_{\mathcal{K}}[\![E_2]\!]\}$.

By Lemma 6.16, we know that for any $s \in \mathsf{Tree}^\infty(\mathcal{F}, \mathcal{K} \cup \{\square\})$, it holds that $r_{\gamma'}^{\mathscr{M}}(s) = r_\gamma(s\{\square \leftsquigarrow \mathscr{T}_{\mathcal{K}}[\![E_2]\!]\})$. Therefore, we have

$$r_\gamma^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}\cup\{\square\}}[\![E_1]\!]\{\square \leftsquigarrow \mathscr{T}_{\mathcal{K}}[\![E_2]\!]\}) = r_{\gamma'}^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}\cup\{\square\}}[\![E_1]\!]).$$

Thus, we conclude that $\mathscr{M}_\gamma[\![E_1 \cdot_\square E_2]\!] = r_\gamma^{\mathscr{M}}(\mathscr{T}_{\mathcal{K}}[\![E_1 \cdot_\square E_2]\!])$.

Case $E = (E_1)^{\infty_\square}$**:**

By definition, we have $\mathscr{M}_\gamma[\![(E_1)^{\infty_\square}]\!] = \mathrm{lfp}_{\bot_M}^{\sqsubseteq_M} \lambda X.\ \mathscr{M}_{\gamma[\square\mapsto X]}[\![E_1]\!]$.

By definition, we have $\mathscr{T}_{\mathcal{K}}[\![(E_1)^{\infty_\square}]\!] = \mathrm{lfp}_{\ominus}^{\sqsubseteq_{\mathscr{T}}} \lambda X.\ (\mathscr{T}_{\mathcal{K}\cup\{\square\}}[\![E_1]\!]\{\square \leftsquigarrow X\})$.

Let $F \stackrel{\text{def}}{=} \lambda X.\ \mathscr{M}_{\gamma[\square\mapsto X]}[\![E_1]\!]$ and $G \stackrel{\text{def}}{=} \lambda X.\ (\mathscr{T}_{\mathcal{K}\cup\{\square\}}[\![E_1]\!]\{\square \leftsquigarrow X\})$. By the Kleene fixed-point theorem (Proposition 3.4), it suffices to show that for any $n \geq 0$, $F^n(\bot_M) = r_\gamma^{\mathscr{M}}(G^n(\ominus))$. We prove the claim by induction on n.

When $n = 0$**:**

By definition, we have $F^0(\bot_M) = \bot_M$.
By definition, we have $G^0(\ominus) = \ominus$, and also $r^{\mathscr{M}}_{\gamma}(\ominus) = \bot_M$.
Thus, we conclude this that $F^0(\bot_M) = r^{\mathscr{M}}_{\gamma}(G^0(\ominus))$.

When $n = k + 1$**:**
By induction hypothesis (on n), we have $F^k(\bot_M) = r^{\mathscr{M}}_{\gamma}(G^k(\ominus))$.
Let $\gamma' \stackrel{\text{def}}{=} \gamma[\square \mapsto F^k(\bot_M)]$. Then $\gamma' : (\mathcal{K} \cup \{\square\}) \to \mathcal{M}$.
By definition, we have $F^n(\bot_M) = \mathscr{M}_{\gamma'}[\![E_1]\!]$.
By definition, we have $G^n(\ominus) = \mathscr{T}_{\mathcal{K}\cup\{\square\}}[\![E_1]\!]\{\square \leftarrow G^k(\ominus)\}$, and also by Lemma 6.16, we have $r^{\mathscr{M}}_{\gamma}(\mathscr{T}_{\mathcal{K}\cup\{\square\}}[\![E_1]\!]\{\square \leftarrow G^k(\ominus)\}) = r^{\mathscr{M}}_{\gamma'}(\mathscr{T}_{\mathcal{K}\cup\{\square\}}[\![E_1]\!])$.
By induction hypothesis (on E_1), we have $\mathscr{M}_{\gamma'}[\![E_1]\!] = r^{\mathscr{M}}_{\gamma'}(\mathscr{T}_{\mathcal{K}\cup\{\square\}}[\![E_1]\!])$.
Thus, we conclude that $F^n(\bot_M) = r^{\mathscr{M}}_{\gamma}(G^n(\ominus))$.

□

In the rest of §6.2, I demonstrate two concrete DMKAT-based interpretations for reasoning about probabilistic programs.

6.2.1 A Relational Interpretation

This subsection gives a DMKAT-based interpretation as binary relations, a common model of input-output behavior for a probabilistic programming language. Note that this interpretation does not keep track of probabilities; instead, it treats probabilistic branching as nondeterministic branching. Let $\iota = (\Sigma, \mathsf{eval}, \mathsf{sat})$ be a triple of a set Σ of *states*, a binary relation $\mathsf{eval}(\mathsf{act}) \subseteq \Sigma \times \Sigma$ for each data action $\mathsf{act} \in \mathsf{Act}$, and a set of states $\mathsf{sat}(\varphi) \subseteq \Sigma$ for each logical condition $\varphi \in \mathcal{L}$. Intuitively, the set of states that satisfy φ is given by $\mathsf{sat}(\varphi)$, and it holds that $\mathsf{sat}(\neg\varphi) = \Sigma \setminus \mathsf{sat}(\varphi)$. To reason about divergence, I assume there is a symbol $\circlearrowleft$ such that $\circlearrowleft \notin \Sigma$.

The DMKAT $\mathcal{R} = (R, \sqsubseteq_R, \otimes_R, {}_{\varphi}\Diamond_R, {}_{p}\oplus_R, \bot_R, 1_R)$ for the *relational interpretation* $\mathscr{R} = (\mathcal{R}, [\![\cdot]\!]^{\mathscr{R}})$ with respect to ι is defined as follows.

- $R \stackrel{\text{def}}{=} \Sigma \times (\Sigma \cup \{\circlearrowleft\})$.
- $A \sqsubseteq_R B \stackrel{\text{def}}{=} (A \cap (\Sigma \times \Sigma) \subseteq B \cap (\Sigma \times \Sigma)) \wedge (A \cap (\Sigma \times \{\circlearrowleft\}) \supseteq B \cap (\Sigma \times \{\circlearrowleft\}))$.
- $A \otimes_R B \stackrel{\text{def}}{=} \{\langle\sigma, \circlearrowleft\rangle \mid \langle\sigma, \circlearrowleft\rangle \in A\} \cup \{\langle\sigma, \sigma''\rangle \mid \exists\sigma' : \langle\sigma, \sigma'\rangle \in A \wedge \langle\sigma', \sigma''\rangle \in B\}$.
- $A \,{}_{\varphi}\Diamond_R\, B \stackrel{\text{def}}{=} \{\langle\sigma, \sigma'\rangle \mid \sigma \in \mathsf{sat}(\varphi) \wedge \langle\sigma, \sigma'\rangle \in A\} \cup \{\langle\sigma, \sigma'\rangle \mid \sigma \in \mathsf{sat}(\neg\varphi) \wedge \langle\sigma, \sigma'\rangle \in B\}$.
- $A \,{}_{p}\oplus_R\, B = A \cup B$.
- $\bot_R \stackrel{\text{def}}{=} \{\langle\sigma, \circlearrowleft\rangle \mid \sigma \in \Sigma\}$.
- $1_R \stackrel{\text{def}}{=} \{\langle\sigma, \sigma\rangle \mid \sigma \in \Sigma\}$.

I then define the semantic function for the relational interpretation as $[\![\mathsf{act}]\!]^{\mathscr{R}} = \mathsf{eval}(\mathsf{act})$.

Proposition 6.17. *$\mathscr{R}$ is a DMKAT.*

*Example 6.18. Consider the simple program "***while prob**(0.5) **do** $x \coloneqq x+1$ **od***." One regular hyper-path expression encoding the program is $(prob[0.5](seq[x \coloneqq x+1](\square), \underline{1}))^{\infty_\square}$. We can then interpret the expression under the relational interpretation $\mathscr{R}$ to extract the input-output behavior of the program, with $\Sigma \stackrel{\text{def}}{=} \mathsf{Var} \to \mathbb{R}$:*

$$
\begin{aligned}
&\mathscr{R}_{\{\}}[\![(prob[0.5](seq[x \coloneqq x+1](\square), \underline{1}))^{\infty_\square}]\!] \\
&= \mathrm{lfp}^{\sqsubseteq_R}_{\bot_R} \lambda A.\ \mathscr{R}_{\{\square \mapsto A\}}[\![prob[0.5](seq[x \coloneqq x+1](\square), \underline{1})]\!] \\
&= \mathrm{lfp}^{\sqsubseteq_R}_{\bot_R} \lambda A.\ \left(\mathscr{R}_{\{\square \mapsto A\}}[\![seq[x \coloneqq x+1](\square)]\!] \cup \{\langle \sigma, \sigma\rangle \mid \sigma \in \Sigma\}\right) \\
&= \mathrm{lfp}^{\sqsubseteq_R}_{\bot_R} \lambda A.\ ((\{\langle \sigma, \sigma[x \mapsto \sigma(x)+1]\rangle \mid \sigma \in \Sigma\} \otimes_R A) \cup \{\langle \sigma, \sigma\rangle \mid \sigma \in \Sigma\}) \\
&= \{\langle \sigma, \sigma[x \mapsto \sigma(x)+k]\rangle \mid \sigma \in \Sigma \wedge k \in \mathbb{Z}^+\} \cup \{\langle \sigma, \circlearrowleft\rangle \mid \sigma \in \Sigma\}.
\end{aligned}
$$

6.2.2 A Kernel Interpretation

This subsection gives a DMKAT-based interpretation in terms of sub-probability kernels (reviewed in §2.1), a common model for probabilistic programming languages without nondeterminism. This interpretation is intended to define a denotational semantics that is equivalent to the operational semantics developed in §2.3. Let $\iota = ((\Sigma, \mathcal{O}), \mathsf{eval}, \mathsf{sat})$ be a triple of a measurable space $(\Sigma, \mathcal{O})$ of *states*, a probability kernel $\mathsf{eval}(\mathsf{act}) : (\Sigma, \mathcal{O}) \rightsquigarrow (\Sigma, \mathcal{O})$ for each data action $\mathsf{act} \in \mathsf{Act}$, and a measurable map $\mathsf{sat}(\varphi) : \Sigma \to \mathbb{2}$ for each logical condition $\varphi \in \mathcal{L}$, where $\mathbb{2} = \{\top, \bot\}$ is the set of Boolean values, equipped with a standard σ-algebra $\wp(\{\top, \bot\})$. Intuitively, sat evaluates logical conditions, and it holds that $\mathsf{sat}(\neg\varphi)(\sigma) = \neg\mathsf{sat}(\varphi)(\sigma)$ for any $\varphi \in \mathcal{L}$ and $\sigma \in \Sigma$.

The DMKAT $\mathscr{P} = (\mathcal{P}, \sqsubseteq_P, \otimes_P, {}_\varphi\Diamond_P, {}_p\oplus_P, \bot_P, 1_P)$ for the *kernel interpretation* $\mathscr{P} = (\mathcal{P}, [\![\cdot]\!]^{\mathscr{P}})$ with respect to ι is defined as follows.

- $\mathcal{P}$ is the set of sub-probability kernels on the state space $(\Sigma, \mathcal{O})$.
- $\kappa \sqsubseteq_P \rho \stackrel{\text{def}}{=} \forall \sigma \in \Sigma, U \in \mathcal{O} : \kappa(\sigma, U) \leq \rho(\sigma, U)$.
- $\kappa \otimes_P \rho \stackrel{\text{def}}{=} \kappa \fatsemi \rho$, i.e., kernel composition.
- $\kappa\ {}_\varphi\Diamond_P\ \rho \stackrel{\text{def}}{=} \lambda(\sigma, U).\ [\mathsf{sat}(\varphi)(\sigma)] \cdot \kappa(\sigma, U) + [\mathsf{sat}(\neg\varphi)(\sigma)] \cdot \rho(\sigma, U)$.
- $\kappa\ {}_p\oplus_p\ \rho \stackrel{\text{def}}{=} \lambda(\sigma, U).\ p \cdot \kappa(\sigma, U) + (1-p) \cdot \rho(\sigma, U)$.
- $\bot_P \stackrel{\text{def}}{=} \lambda(\sigma, U).\ 0$.
- $1_P \stackrel{\text{def}}{=} \lambda(\sigma, U).\ [\sigma \in U]$.

I then define the semantic function for the kernel interpretation as $[\![\mathsf{act}]\!]^{\mathscr{P}} \stackrel{\text{def}}{=} \mathsf{eval}(\mathsf{act})$.

Proposition 6.19. *$\mathscr{P}$ is a DMKAT.*

*Example 6.20. Consider the simple program "***while prob**(0.5) **do** $x \coloneqq x+1$ **od***," which can be encoded as the regular hyper-path expression* $(prob[0.5](seq[x \coloneqq x+1](\square), \underline{1}))^{\infty_\square}$*. We can then interpret the expression under the kernel interpretation* $\mathscr{P}$ *to extract the transition kernel of the program, with* $\Sigma \overset{\text{def}}{=} \mathsf{Var} \to \mathbb{R}$*:*

$$
\begin{aligned}
& \mathscr{P}_{\{\}}[\![(prob[0.5](seq[x \coloneqq x+1](\square), \underline{1}))^{\infty_\square}]\!] \\
= \ & \mathrm{lfp}^{\sqsubseteq_P}_{\bot_P} \lambda\kappa.\ \mathscr{P}_{\{\square \mapsto \kappa\}}[\![prob[0.5](seq[x \coloneqq x+1](\square), \underline{1})]\!] \\
= \ & \mathrm{lfp}^{\sqsubseteq_P}_{\bot_P} \lambda\kappa.\ \left(0.5 \cdot \mathscr{P}_{\{\square \mapsto \kappa\}}[\![seq[x \coloneqq x+1](\square)]\!] + 0.5 \cdot \lambda\sigma.\ \delta(\sigma)\right) \\
= \ & \mathrm{lfp}^{\sqsubseteq_P}_{\bot_P} \lambda\kappa.\ (0.5 \cdot (\lambda\sigma.\delta(\sigma[x \mapsto \sigma(x)+1]) \gg\!= \kappa) + 0.5 \cdot \lambda\sigma.\ \delta(\sigma)) \\
= \ & \textstyle\sum_{k \in \mathbb{Z}^+} 0.5^k \cdot (1-0.5) \cdot \lambda\sigma.\ \delta(\sigma[x \mapsto \sigma(x)+k]).
\end{aligned}
$$

Note that $\mathbb{Z}^+$ *includes* 0 *and I use the curried version of kernels in the derivation. We can see that the program terminates with probability one by the fact that* $\sum_{k \in \mathbb{Z}^+} 0.5^k \cdot (1-0.5) = 1$*.*

6.3 Towards Abstract Interpretations for DMKAT

In §6.1 and §6.2, I have developed an algebraic foundation for reasoning about probabilistic programs without nondeterminism. In this section, I present my progress towards building a static-analysis framework based on DMKAT. Kincaid et al. [92] summarized a recipe for algebraic static analysis, which consists of the following three steps:

1. *(Modeling)* Express the concrete semantics as the least solution to an equation system. In this chapter, the modeling step amounts to extracting an equation system from a control-flow hyper-graph (§6.1.3) and designing a DMKAT for concrete semantics (e.g., the relational interpretation in §6.2.1 or the kernel interpretation in §6.2.2).

2. *(Closed forms)* Design a language for "closed-form solutions" and an algorithm for computing them. In this chapter, I use regular hyper-path expressions (§6.1.2) as the closed forms and develop a Gaussian-elimination algorithm to solve a regular equation system (Algorithm 1).

3. *(Interpretation)* Design an abstract interpretation of the closed-form language and a soundness relation between the concrete and abstract interpretations. Thus, in this section, I focus on building abstract interpretations for DMKAT.

6.3.1 Non-Probabilistic Abstract Interpretations

To show that the DMKAT framework is a generalization of the KAT framework, in this section, I sketch an approach for adapting existing algebraic abstract domains for analyzing non-probabilistic programs to the DMKAT framework. Recall that in the Kleene-algebra-based framework, the building blocks are regular languages and regular expressions, thus the abstract interpretation happens at the *path* level rather than the *hyper-path* level. Intuitively, to abstract the meaning of a hyper-path, i.e., a possibly-infinite tree, we can abstract each rooted path on the tree individually, and then *join* all the path abstractions to obtain an abstraction of the hyper-path.

To demonstrate the idea, I use the *transition-formula abstraction* as an example in this section. Consider a finite set of program variables Var. A transition formula is then a two-vocabulary logical formula $F(\mathsf{Var}, \mathsf{Var}')$ over Var and a set Var' of "primed" versions of the program variables. A transition formula is intended to approximate the input-output behavior of a program by expressing a relation between the input states (the Var variables) and the output states (the Var' variables). For example, the transition formula $(x < 0 \wedge x' = x + 1 \wedge \mathit{tick}' = \mathit{tick})$ asserts that a program has a pre-condition $x < 0$, and if the program terminates, the value of x is incremented by one and the value of *tick* is unchanged. We can define a regular algebra $\mathcal{T} = (T, +_T, \cdot_T, {}^{*_T}, 0_T, 1_T)$ on the universe T of transition-formulas as follows (note that this algebra is *not* a Kleene algebra):

$$
\begin{aligned}
F +_T G &\stackrel{\text{def}}{=} F \vee G \\
F \cdot_T G &\stackrel{\text{def}}{=} \exists \mathsf{Var}'' : F(\mathsf{Var}, \mathsf{Var}'') \wedge G(\mathsf{Var}'', \mathsf{Var}') \\
0_T &\stackrel{\text{def}}{=} \mathit{false} \\
1_T &\stackrel{\text{def}}{=} \bigwedge_{x \in \mathsf{Var}} (x' = x)
\end{aligned}
$$

The notation $F(\mathsf{Var}, \mathsf{Var}'')$ denotes the formula obtained by substituting all the Var' variables with "double primed" versions in Var''. Thus, the composition $F \cdot_T G$ performs a relational composition of the input-output behavior specified by F and the input-output behavior specified by G. To compute F^{*_T}, which encodes a loop whose body is expressed as the transition formula F, there are many techniques for approximating the reflexive transitive closure of F (e.g., [3, 54, 90, 91, 103, 121]). In this section, I use a technique based on *recurrence analysis* [54]. Let us consider arithmetic programs and denote by $\mathbf{x}$ and $\mathbf{x}'$ the vectors for the program variables Var and Var', respectively. For a transition formula F, a *linear recurrence inequality* of F takes the form $\mathbf{a}^T\mathbf{x}' \leq \mathbf{a}^T\mathbf{x} + b$ and is entailed by F. To compute F^{*_T}, the idea is to extract a collection of recurrence inequalities $\{\mathbf{a}_i^T\mathbf{x}' \leq \mathbf{a}_i^T\mathbf{x} + b_i\}_{i \in \mathcal{I}}$ of F, and then use the closed form of the recurrence relations to approximate the reflexive transitive closure of F, where k stands for the number of loop iterations:

$$
F^{*_T} \stackrel{\text{def}}{=} \exists k \in \mathbb{Z} : k \geq 0 \wedge \bigwedge_{i \in \mathcal{I}} \mathbf{a}_i^T\mathbf{x}' \leq \mathbf{a}_i^T\mathbf{x} + kb_i
$$

Example 6.21. Consider the following non-probabilistic program:

while $i > 0$ **do**
  if $x < y$ **then** $x := x + 1$ **else** $y := y + 1$ **fi**;
  $i := i - 1$
od

The loop exhibits the following linear recurrence inequalities

$$
\begin{aligned}
i' &\leq i - 1 & \qquad -i' &\leq -i + 1 \\
(x' + y') &\leq (x + y) + 1 & \qquad (-x' - y') &\leq (-x - y) - 1 \\
x' &\leq x + 1 & \qquad y' &\leq y + 1
\end{aligned}
$$

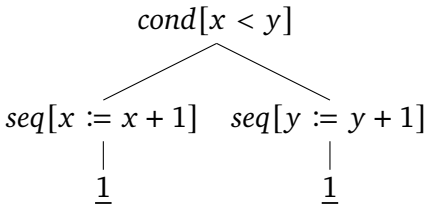
which yield the following transition formula that summarizes the loop:

$$
\exists k \in \mathbb{Z} : k \geq 0 \wedge i' = i - k \wedge (x' + y') = (x + y) + k \wedge x' \leq x + k \wedge y' \leq y + k.
$$

Taking the loop guard $i > 0$ into account, we can simplify the transition formula above to a formula that approximates the whole program:

$$(i \leq 0 \wedge i' = i \wedge x' = x \wedge y' = y) \vee (i > 0 \wedge i' = 0 \wedge (x' + y') = (x + y) + i \wedge x' \leq x + i \wedge y' \leq y + i).$$

I now lift the transition-formula domain from path-level abstractions to hyper-path-level abstractions. The idea is that we can obtain a transition formula F_p for each rooted path p on a hyper-path (i.e., a possibly-infinite tree), then take their join $\bigvee_p F_p$ as an abstraction for the hyper-path. For example, the finite tree below corresponds to the program "**if** $x < y$ **then** $x := x+1$ **else** $y := y+1$."



For the rooted path to the left leaf, the transition formula is $F_1 \stackrel{\text{def}}{=} (x < y \wedge x' = x + 1 \wedge y' = y)$. For the rooted path to the right leaf, the transition formula is $F_2 \stackrel{\text{def}}{=} (x \geq y \wedge x' = x \wedge y' = y + 1)$. Their join $F_1 \vee F_2$ then entails $((x' + y') = (x + y) + 1 \wedge x' \leq x + 1 \wedge y' \leq y + 1)$, which leads to some of the recurrence inequalities shown in Example 6.21.

Based on the hyper-path-as-a-collection-of-paths approach, I can apply a non-probabilistic abstract domain in the DMKAT framework. Let $\mathcal{A} = (A, +_A, \cdot_A, {}^{*_A}, 0_A, 1_A)$ be a regular algebra that represents an abstract domain, and $\mathscr{A} = (\mathcal{A}, [\![\cdot]\!]^{\mathscr{A}})$ be an abstract interpretation with a semantic function $[\![\cdot]\!]^{\mathscr{A}} : \mathsf{Act} \cup \mathcal{L} \to \mathcal{A}$ that abstracts data actions and logical conditions. Using the same setup for DMKAT (§6.2), to analyze a probabilistic program, I extract a ranked alphabet $\mathcal{F}$ to be the collection of control-flow actions in the program. For a regular hyper-path expression $E \in \mathsf{RegExp}^{\infty}(\mathcal{F}, \mathcal{K})$, I use the judgment $\vdash_{\mathcal{K}} E : a \mid \gamma$ to express that the abstract interpretation of E is a pair of $a \in \mathcal{A}$ and $\gamma : \mathcal{K} \to \mathcal{A}$. The element a is intended to abstract all the rooted paths of the tree represented by E that do *not* end with a hole leaf. The map γ is then intended to abstract rooted paths ending with hole symbols, i.e., for $\square \in \mathcal{K}$, the element $\gamma(\square)$ abstracts all the rooted paths of E ending with $\square$. Fig. 6.4 presents the syntax-directed rules for deriving $\vdash_{\mathcal{K}} E : a \mid \gamma$. One interesting rule is the (ITERATION) rule. Consider the closure expression $(E_1)^{\infty_\square} \in \mathsf{RegExp}^{\infty}(\mathcal{F}, \mathcal{K})$. The premise $\vdash_{\mathcal{K} \cup \{\square\}} E_1 : a_1 \mid \gamma_1$ computes an abstraction for E_1. Intuitively, the closure expression represents a loop with $\square$ as the self-concatenation point, thus the element a_1 abstracts all paths that lead to non-hole leaves, i.e., that exit the loop. Also, the element $\gamma_1(\square)$ abstracts all paths that lead to $\square$, i.e., that express the loop body. Therefore, to summarize the loop, I use the closure operator ^{*_A} on the loop body ($b = \gamma_1(\square)$) and then extend it with the loop-exit abstraction (a_1), i.e., I use $b^{*_A} \cdot_A a_1$ as the loop summarization.

Example 6.22. Consider the following probabilistic program:

while $i > 0$ **do**
  if prob(0.5) **then** $x := x + 1$ **else** $y := y + 1$ **fi**;
  $i := i - 1$
od

A regular hyper-path expression that encodes the program above could be

$$(cond[i > 0](prob[0.5](seq[x := x + 1](\square_2), seq[y := y + 1](\square_2)) \cdot_{\square_2} seq[i := i - 1](\square_1), \underline{1}))^{\infty_{\square_1}}.$$

$$\text{(Skip)}\quad \frac{}{\vdash_{\mathcal{K}} \underline{1} : 1_A \mid \{\square \mapsto 0_A\}_{\square\in\mathcal{K}}} \qquad \text{(Action)}\quad \frac{\vdash_{\mathcal{K}} E_1 : a_1 \mid \gamma}{\vdash_{\mathcal{K}} seq[\mathsf{act}](E_1) : [\![\mathsf{act}]\!]^{\mathscr{A}} \cdot_A a_1 \mid \{\square \mapsto [\![\mathsf{act}]\!]^{\mathscr{A}} \cdot_A \gamma(\square)\}_{\square\in\mathcal{K}}}$$

$$\text{(Condition)}\quad \frac{\vdash_{\mathcal{K}} E_1 : a_1 \mid \gamma_1 \qquad \vdash_{\mathcal{K}} E_2 : a_2 \mid \gamma_2}{\vdash_{\mathcal{K}} cond[\varphi](E_1,E_2) : ([\![\varphi]\!]^{\mathscr{A}} \cdot_A a_1) +_A ([\![\neg\varphi]\!]^{\mathscr{A}} \cdot_A a_2) \mid \{\square \mapsto ([\![\varphi]\!]^{\mathscr{A}} \cdot_A \gamma_1(\square)) +_A ([\![\neg\varphi]\!]^{\mathscr{A}} \cdot_A \gamma_2(\square))\}_{\square\in\mathcal{K}}}$$

$$\text{(Probability)}\quad \frac{\vdash_{\mathcal{K}} E_1 : a_1 \mid \gamma_1 \qquad \vdash_{\mathcal{K}} E_2 : a_2 \mid \gamma_2}{\vdash_{\mathcal{K}} prob[p](E_1,E_2) : a_1 +_A a_2 \mid \{\square \mapsto \gamma_1(\square) +_A \gamma_2(\square)\}_{\square\in\mathcal{K}}}$$

$$\text{(Concatenation)}\quad \frac{\vdash_{\mathcal{K}\cup\{\square\}} E_1 : a_1 \mid \gamma_1 \qquad b = \gamma_1(\square) \qquad \vdash_{\mathcal{K}} E_2 : a_2 \mid \gamma_2}{\vdash_{\mathcal{K}} E_1 \cdot_\square E_2 : a_1 +_A (b \cdot_A a_2) \mid \{\square' \mapsto \gamma_1(\square') +_A (b \cdot_A \gamma_2(\square'))\}_{\square'\in\mathcal{K}}}$$

$$\text{(Iteration)}\quad \frac{\vdash_{\mathcal{K}\cup\{\square\}} E_1 : a_1 \mid \gamma_1 \qquad b = \gamma_1(\square)}{\vdash_{\mathcal{K}} (E_1)^{\infty_\square} : b^{*_A} \cdot_A a_1 \mid \{\square' \mapsto b^{*_A} \cdot_A \gamma_1(\square')\}_{\square'\in\mathcal{K}}} \qquad \text{(Hole)}\quad \frac{}{\vdash_{\mathcal{K}} \square : 0_A \mid \{\square \mapsto 1_A\} \cup \{\square' \mapsto 0_A\}_{\square'\in\mathcal{K}\setminus\{\square\}}}$$

Fig. 6.4: The non-probabilistic abstract interpretation of regular hyper-path expressions.

First, for the three assignments, we can interpret them under the transition-formula domain as

$$\vdash_{\{\square_1,\square_2\}} seq[x := x+1](\square_2) : false \mid \{\square_1 \mapsto false, \square_2 \mapsto (x' = x+1 \wedge y' = y \wedge i' = i)\},$$
$$\vdash_{\{\square_1,\square_2\}} seq[y := y+1](\square_2) : false \mid \{\square_1 \mapsto false, \square_2 \mapsto (x' = x \wedge y' = y+1 \wedge i' = i)\},$$
$$\vdash_{\{\square_1\}} seq[i := i-1](\square_1) : false \mid \{\square_1 \mapsto (x' = x \wedge y' = y \wedge i' = i-1)\}.$$

Let us denote the three assignment statements by S_1, S_2, S_3, respectively. Let $S_4 \stackrel{\text{def}}{=} prob[0.5](S_1, S_2)$. By the (Probability) rule, we have

$$\vdash_{\{\square_1,\square_2\}} S_4 : false \mid \{\square_1 \mapsto false, \square_2 \mapsto ((x'+y') = (x+y)+1 \wedge x' \le x+1 \wedge y' \le y+1 \wedge i' = i)\}.$$

Then by the (Concatenation) rule, we can derive

$$\vdash_{\{\square_1\}} S_4 \cdot_{\square_2} S_3 : false \mid \{\square_1 \mapsto ((x'+y') = (x+y)+1 \wedge x' \le x+1 \wedge y' \le y+1 \wedge i' = i-1)\}.$$

Let $S_5 \stackrel{\text{def}}{=} cond[i>0](S_4 \cdot_{\square_2} S_3, \underline{1})$. By the (Condition) rule, we obtain a loop-body summary:

$$\vdash_{\{\square_1\}} S_5 : (i \le 0 \wedge x' = x \wedge y' = y \wedge i' = i)$$
$$\mid \{\square_1 \mapsto (i > 0 \wedge (x'+y') = (x+y)+1 \wedge x' \le x+1 \wedge y' \le y+1 \wedge i' = i-1)\}$$

Let $F_1 \stackrel{\text{def}}{=} (i \le 0 \wedge x' = x \wedge y' = y \wedge i' = i)$ and $F_2 \stackrel{\text{def}}{=} (i > 0 \wedge (x'+y') = (x+y)+1 \wedge x' \le x+1 \wedge y' \le y+1 \wedge i' = i-1)$. Finally, by the (Iteration) rule, we know that the transition formula for $(S_5)^{\infty_{\square_1}}$ is $F_2^{*_T} \cdot_T F_1$. Recall the recurrence-based analysis in Example 6.21. In the same way, we obtain the formula below that approximates the whole program:

$$(i \le 0 \wedge i' = i \wedge x' = x \wedge y' = y) \vee (i > 0 \wedge i' = 0 \wedge (x'+y') = (x+y)+i \wedge x' \le x+i \wedge y' \le y+i).$$

Proving the soundness of the rules in Fig. 6.4 is left for future work.

6.3.2 Probabilistic Abstract Interpretations

One major principle in my thesis is that probabilistic programs are naturally represented by control-flow hyper-graphs, and this principle indicates that a static analysis of probabilistic programs is essentially a hyper-path analysis. For static analyses that take probabilities into consideration, e.g., the expectation-invariant analysis, the method sketched in §6.3.1 does *not* work, because in general, it might be intractable to obtain the analysis result of a hyper-path as the join of the analysis results of the rooted paths on the hyper-path. In this section, I discuss some preliminary results on probabilistic abstract interpretations for the DMKAT framework.

Recall the definition of *Pre-Markov Algebras* (PMAs) that I developed in §4.2. I use a variant of PMAs below, where the nondeterministic operator is removed.

Definition 6.23. A *deterministic pre-Markov algebra* (DPMA) over a set of logical conditions $\mathcal{L}$ (also called *tests*) is a 7-tuple $\mathcal{M} = (M, \sqsubseteq_M, \otimes_M, {}_\varphi\Diamond_M, {}_p\oplus_M, \bot_M, 1_M)$, where $(M, \sqsubseteq_M)$ forms a complete lattice with $\bot_M$ as its least element; $(M, \otimes_M, 1_M)$ forms a monoid (i.e., $\otimes_M$ is an associative binary operator with 1_M as its identity element); ${}_\varphi\Diamond_M$ is a binary operator parameterized by a condition $\varphi \in \mathcal{L}$; ${}_p\oplus_M$ is a binary operator parameterized by $p \in [0,1]$; and $\otimes_M$, ${}_\varphi\Diamond_M$, ${}_p\oplus_M$ are monotone with respect to $\sqsubseteq_M$.

Definition 6.24. An *abstract interpretation* is a pair $\mathscr{M} = (\mathcal{M}, [\![\cdot]\!]^{\mathscr{M}})$, where $\mathcal{M}$ is a DPMA for an abstract domain and $[\![\cdot]\!]^{\mathscr{M}} : \mathsf{Act} \to \mathcal{M}$. We call $\mathcal{M}$ the *semantic algebra* of the interpretation and $[\![\cdot]\!]^{\mathscr{M}}$ the *semantic function*.

Note that the structure of DPMAs is almost the same as the structure of DMKATs; the different is only that I use a different set of axioms for DPMAs. In this way, it is straightforward to develop an iteration-based analysis framework based on the fixed-point-based interpretation of DMKATs (§6.2). However, the whole development around regular hyper-path expressions in this chapter allows me to apply *loop-summarization* techniques. To see this, let $E \in \mathsf{RegExp}^{\infty}(\mathcal{F}, \mathcal{K})$ be a regular hyper-path expression. I use the judgment $\gamma \vdash_{\mathcal{K}} E : a$ to express that the abstract interpretation of E is an abstract element $a \in \mathcal{M}$, *given* that all the hole symbols in $\mathcal{K}$ are interpreted with respect to the map $\gamma : \mathcal{K} \to \mathcal{M}$. Fig. 6.5 presents the rules of a declarative derivation system for $\gamma \vdash_{\mathcal{K}} E : a$. Most of the rules are syntax-directed, except (Iteration) and (Relax). The (Iteration) rule works very similarly to *loop-invariant verification*. For an iteration expression $(E_1)^{\infty_\square} \in \mathsf{RegExp}^{\infty}(\mathcal{F}, \mathcal{K})$, we know that the hole $\square$ is the self-concatenation point in the tree of E_1. We say $a \in \mathcal{M}$ is an invariant for the iteration expression, if assuming the abstraction for $\square$ is a leads to that the abstraction of the loop body E_1 is also a. The advantage of such a (Iteration) rule is that it allows the analysis developer to implement an algorithm to discover such invariants, whereas the original PMAF framework always uses an iteration-until-fixed-point algorithm for loops (see §4.2). The (Relax) rule can apply to any regular hyper-path expression, and it essentially strengthens the hole-abstraction map γ and weakens the analysis result of the expression E.

I will end this section by two examples showing that different loop-invariant-generation strategies for the (Iteration) rule can lead to better analysis results than PMAF. The proof of the soundness for the rules in Fig. 6.5 and a complete development of an expectation-invariant abstract domain for DMKAT are left for future work.

$$\text{(Skip)}\ \frac{}{\gamma \vdash_{\mathcal{K}} \underline{1} : 1_M} \qquad \text{(Action)}\ \frac{\gamma \vdash_{\mathcal{K}} E_1 : a}{\gamma \vdash_{\mathcal{K}} seq[\mathsf{act}](E_1) : [\![\mathsf{act}]\!]^{\mathscr{M}} \otimes_M a} \qquad \text{(Condition)}\ \frac{\gamma \vdash_{\mathcal{K}} E_1 : a_1 \qquad \gamma \vdash_{\mathcal{K}} E_2 : a_2}{\gamma \vdash_{\mathcal{K}} cond[\varphi](E_1, E_2) : a_1 \ {}_{\varphi}\Diamond_{M}\ a_2}$$

$$\text{(Probability)}\ \frac{\gamma \vdash_{\mathcal{K}} E_1 : a_1 \qquad \gamma \vdash_{\mathcal{K}} E_2 : a_2}{\gamma \vdash_{\mathcal{K}} prob[p](E_1, E_2) : a_1 \ {}_{p}\oplus_{M}\ a_2} \qquad \text{(Concatenation)}\ \frac{\gamma\{\square \mapsto a_2\} \vdash_{\mathcal{K} \cup \{\square\}} E_1 : a_1 \qquad \gamma \vdash_{\mathcal{K}} E_2 : a_2}{\gamma \vdash_{\mathcal{K}} E_1 \cdot_{\square} E_2 : a_1}$$

$$\text{(Iteration)}\ \frac{\gamma\{\square \mapsto a\} \vdash_{\mathcal{K} \cup \{\square\}} E_1 : a}{\gamma \vdash_{\mathcal{K}} (E_1)^{\infty_{\square}} : a} \qquad \text{(Hole)}\ \frac{}{\gamma \vdash_{\mathcal{K}} \square : \gamma(\square)} \qquad \text{(Relax)}\ \frac{\gamma' \vdash_{\mathcal{K}} E : a' \qquad a' \sqsubseteq_M a \qquad \gamma \mathrel{\dot{\sqsubseteq}}_M \gamma'}{\gamma \vdash_{\mathcal{K}} E : a}$$

Fig. 6.5: The probabilistic abstract interpretation of regular hyper-path expressions.

Example 6.25. Consider the one-dimensional random-walk program in Fig. 6.1(b), which can be expressed by the following regular hyper-path expression:

$$seq[S_1]((cond[x < 10](prob[0.75](seq[S_2](\square_2), seq[S_3](\square_2)) \cdot_{\square_2} seq[S_4](\square_1), \underline{1}))^{\infty_{\square_1}}),$$

where the assignment statements are defined as $S_1 \stackrel{\text{def}}{=} (x, x_2, xt) := (0, 0, 0)$, $S_2 \stackrel{\text{def}}{=} (x, x_2, xt) := (x{+}1, x_2{+}2x{+}1, xt{+}tick)$, $S_3 \stackrel{\text{def}}{=} (x, x_2, xt) := (x{-}1, x_2{-}2x{+}1, xt{-}tick)$, *and* $S_4 \stackrel{\text{def}}{=} (tick, tick_2, xt) := (tick + 1, tick_2 + 2tick + 1, xt + x)$. *Imagine that we have a DPMA that keeps track of expectation invariants (like the LEIA domain developed in §4.3.3 or the modular expected-value analysis proposed by Avanzini et al. [4]). Inspired by Optional Stopping Theorems (recall that I used them to prove soundness of central moment analysis in §5.3.3), we now extract expectation invariants of the form* $\mathbb{E}[\mathcal{E}'] \leq \mathcal{E}$ *for the loop, where* $\mathcal{E}$ *is an arithmetic expression on variables.*

For the loop body, we temporarily set the interpretation of $\square_1$ *(i.e., the self-concatenation point for the loop) to be the identity element, which should consist of the following invariants:*

$$\mathbb{E}[x'] = x \wedge \mathbb{E}[x_2'] = x_2 \wedge \mathbb{E}[tick'] = tick \wedge \mathbb{E}[tick_2'] = tick_2 \wedge \mathbb{E}[xt'] = xt.$$

Following the rules in Fig. 6.5, we might derive the following abstraction for the loop body:

$$\begin{aligned}&(x \geq 10 \wedge \mathbb{E}[x'] = x \wedge \mathbb{E}[x_2'] = x_2 \wedge \mathbb{E}[tick'] = tick \wedge \mathbb{E}[tick_2'] = tick_2 \wedge \mathbb{E}[xt'] = xt)\\ \vee\ &(x < 10 \wedge \mathbb{E}[x'] = x + 0.5 \wedge \mathbb{E}[x_2'] = x_2 + x + 1 \wedge \mathbb{E}[tick'] = tick + 1\\ &\wedge \mathbb{E}[tick_2'] = tick_2 + 2tick + 1 \wedge \mathbb{E}[xt'] = xt + x + 0.5 \cdot tick + 0.5).\end{aligned}$$

Intuitively, because we set the interpretation of $\square_1$ *to identity, the invariants above should hold for zero iterations* as well as *for one iteration. We then extract linear inequalities of the form* $\mathbb{E}[\mathcal{E}'] \leq \mathcal{E}$, *using linearity of expectations:*

$$\mathbb{E}[tick' - 2x'] \leq tick - 2x \wedge \mathbb{E}[tick_2' + 4x_2' - 4xt' - 6x'] \leq tick_2 + 4x_2 - 4xt - 6x. \tag{6.1}$$

To establish that those inequalities in (6.1) *are expectation invariants of the entire loop, the implementation of the (Iteration) rule should consider the termination behavior of the loop (possibly via*

Optional Stopping Theorems). In this example, the loop simulates a biased one-dimensional random walk, which has been shown to have a finite expected termination time. Therefore, the inequalities in (6.1) *hold for the whole loop, and taking the initial value* $x = 0$ *and the final value* $x = 10$ *into consideration, we know* $x' = 10$, $x'_2 = 100$, $xt' = 10 \cdot tick'$, *and derive the following expectation invariants for the whole program:*

$$\begin{aligned}
\mathbb{E}[tick'] &\le 2 \cdot \mathbb{E}[x'] + tick - 2x \\
&= 2 \cdot 10 + tick - 2 \cdot 0 \\
&= tick + 20, \\
\mathbb{E}[tick'_2] &\le -4 \cdot \mathbb{E}[x'_2] + 4 \cdot \mathbb{E}[xt'] + 6 \cdot \mathbb{E}[x'] + tick_2 + 4x_2 - 4xt - 6x \\
&= -4 \cdot 100 + 4 \cdot 10 \cdot \mathbb{E}[tick'] + 6 \cdot 10 + tick_2 + 4 \cdot 0 - 4 \cdot 0 - 6 \cdot 0 \\
&\le -400 + 40 \cdot (tick + 20) + 60 + tick_2 \\
&= tick_2 + 40 \cdot tick + 460.
\end{aligned}$$

Example 6.26. Consider the following probabilistic program:

```
1 θ := 0;
2 i := 0;
3 while i < n do
4     tick := tick + 0.1 · θ;
5     z ~ a distribution whose first moment is 0 and second moment is 0.001;
6     θ := 0.8 · θ + z;
7     i := i + 1
8 od
```

The program is intended to model a simple lane-keeping controller: the cost accumulator keeps track of the distance between the vehicle and the middle of the lane, and in each iteration (i.e., a time unit), the vehicle changes its position with respect to an angle θ, *and then updates the angle in a stochastic way. Probabilistic programs have been used to model other cyber-physical systems [17]. The loop can be expressed by the following regular hyper-path expression:*

$$(cond[i < n](seq[S_4](seq[S_5](seq[S_6](seq[S_7](\square_2))))), \square_1))^{\infty_{\square_2}} \cdot_{\square_1} \underline{1},$$

where S_ℓ *represents the statement on line* ℓ *of the program.*

Because the termination behavior of the loop is totally deterministic, *i.e., the number of loop iterations before termination does not depend on the probabilistic aspect of the program. Thus, to analyze expectation invariants of this program, we can try a method that is similar to the non-probabilistic abstraction domain on transition formulas (see §6.3.1). For example, for the regular hyper-path expression above, we first set the interpretations of* $\square_1$ *and* $\square_2$ *in the loop body to be the bottom element and the identity element, respectively. In this way, we can obtain the following abstraction for one loop iteration:*

$$\begin{aligned}
F_1 \overset{\text{def}}{=}\ & i < n \wedge i' = i + 1 \wedge \mathbb{E}[\theta'] = 0.8 \cdot \theta \wedge \mathbb{E}[\theta'_2] = 0.64 \cdot \theta_2 + 0.001 \\
& \wedge \mathbb{E}[tick'] = tick + 0.1 \cdot \theta \wedge \mathbb{E}[tick'_2] = tick_2 + 0.2 \cdot tick \cdot \theta + 0.01 \cdot \theta_2,
\end{aligned}$$

where we implicitly instrument the program with $\theta_2, tick_2$ *tracking the values of nonlinear terms* θ^2, $tick^2$, *respectively. Because of the deterministic termination behavior, it should be sound for us to*

apply the recurrence analysis (similar to Example 6.21), in the sense that we treat a variable $\mathbb{E}[x']$ exactly the same as x'. Therefore, applying recurrence solving techniques that are capable of deriving nonlinear solutions (e.g., [90, 91]) can lead to the following loop summarization:

$$\begin{aligned} F_1^* \implies \exists k \in \mathbb{Z} : k \geq 0 \wedge i' = i + k \wedge \mathbb{E}[\theta'] = (\frac{4}{5})^k \cdot \theta \wedge \mathbb{E}[\theta_2'] = \frac{1}{360} + (\frac{16}{25})^k \cdot (\theta_2 - \frac{1}{360}) \\ \wedge \mathbb{E}[tick'] = tick + (\frac{1}{2} - \frac{1}{2}(\frac{4}{5})^k) \cdot \theta \\ \wedge \mathbb{E}[tick_2'] = tick_2 + (1 - (\frac{4}{5})^k) \cdot tick \cdot \theta + (\frac{1}{36} - \frac{1}{36}(\frac{16}{25})^k) \cdot \theta_2 \\ + (\frac{2}{9} + \frac{5}{18}(\frac{16}{25})^k - \frac{1}{2}(\frac{4}{5})^k) \cdot \theta^2 \\ + (\frac{1}{36000}k + \frac{1}{12960}(\frac{16}{25})^k - \frac{1}{12960}). \end{aligned}$$

We now go back to the original regular hyper-path expression with $\square_1$ and $\square_2$. We set the interpretation of $\square_1$ and $\square_2$ in the loop body to be the identity element and the bottom element, respectively. In this way, we can obtain the following abstraction for the case when the loop terminates:

$$F_2 \stackrel{\text{def}}{=} i \geq n \wedge i' = i \wedge \mathbb{E}[\theta'] = \theta \wedge \mathbb{E}[\theta_2'] = \theta_2 \wedge \mathbb{E}[tick'] = tick \wedge \mathbb{E}[tick_2'] = tick_2.$$

Therefore, the abstraction for the whole program can be obtained by $F_0 \cdot F_1^* \cdot F_2$, where F_0 abstracts two assignment statements before the loop. The whole-program abstraction can then yield the following expectation invariants:

$$\begin{aligned} \mathbb{E}[\theta'] = 0, \qquad & \mathbb{E}[\theta_2'] = \frac{1}{360} - \frac{1}{360}(\frac{16}{25})^n, \\ \mathbb{E}[tick'] = tick, \qquad & \mathbb{E}[tick_2'] = tick_2 + \frac{1}{36000}n + \frac{1}{12960}(\frac{16}{25})^n - \frac{1}{12960}. \end{aligned}$$

6.4 Discussion

In this section, I discuss some related work of the DMKAT framework.

Regular Tree Expressions and Finite Tree Automata Comon et al. [31] compiled a book on the theory and application of finite tree automata. They presented some fundamental properties about finite tree automata: (i) a tree language L, i.e., a set of finite trees over a fixed ranked alphabet, is *recognizable* by some finite tree automaton if and only if L is a *regular* tree language, and (ii) a tree language L is *regular* if and only if L can be finitely represented by a *regular tree expression*. Therefore, a finite tree automaton that recognizes a tree language L can be translated to a regular tree expression representing L, and vice versa. My development in this chapter follows a similar methodology; intuitively, a control-flow hyper-graph can be thought as an automaton, the language it recognizes it the control-flow hyper-path on the graph, and the possibly-infinite hyper-path can be finitely represented by a regular hyper-path expression. I take inspiration from regular tree expressions to develop regular hyper-path expressions; in particular, regular tree expressions can take the iteration form $E^{*\square}$, which means self-substituting E for the hole $\square$ for a

finite number of times. However, my work involves *infinite* trees, and the iteration operator $E^{\infty\square}$ denotes infinite self-substitution, thus most results in the book [31] do not necessarily carry over to my development.

There are multiple future directions for extending the theory of regular hyper-path expressions. First, I do not consider nondeterminism in this chapter, so each regular hyper-path expression correspond to exactly one hyper-path. It would be interesting research to add a combination operator (like the ones in regular expressions and regular tree expressions that denote set union) to regular hyper-path expressions, and as a result support finite representations of sets of possibly-infinite hyper-paths. Second, devising a suitable family of automata that recognize regular hyper-paths and establishing a formal correspondence between automata and regular hyper-path expressions would also be an interesting direction for theoretical research. Third, similar to Tarjan's path-expression algorithm [142] and its application to algebraic static analysis [92], it would be interesting research to develop an efficient algorithm that constructs regular hyper-path expressions from control-flow hyper-graphs and apply the algorithm to algebraic static analysis of probabilistic programs.

ω-Regular Expressions and Büchi Automata The theory of regular (word) languages has been lifted to languages that can contain infinite words and different kinds of automata. (Interested readers can referred to textbooks, e.g., the book by Pin and Perrin [129], for more details.) Regular languages for infinite words are called *ω-regular* languages, and their fundamental properties can be summarized as follows: (i) an ω-language L, i.e., a set of infinite words over a fixed alphabet, is *recognizable* by some *Büchi automaton* if and only if L is an ω-regular language, and (ii) an ω-language L is *regular* if and only if L can be finitely represented by an *ω-regular expression*. In the common formalism, an ω-regular expression is of the form $r_1 \cdot s_1^\omega + \cdots + r_n \cdot s_n^\omega$, where r_i, s_i's are standard regular expressions and each s_i denotes a nonempty language. The class of ω-regular expressions can also be defined *inductively* over standard regular expressions; that is, every ω-regular expression is either E^ω, $E \cdot F$, or $F_1 + F_2$, where E's are standard regular expressions and F's are ω-regular expressions. The capability of describing sets of infinite words makes ω-regular expressions suitable for reasoning about program *termination*. Zhu and Kincaid [157] proposed an algebraic termination analysis (for non-probabilistic programs) that uses ω-regular path expressions to represent sets of infinite execution paths in a control-flow graph.

My work in this chapter focuses on hyper-paths, i.e., possibly-infinite trees, which can be seen as a generalization of infinite words, so I need to develop a more general theory (i.e., §6.1) to handle infinite objects. On the other hand, for a probabilistic program without nondeterminism, i.e., the class of the programs considered in this chapter, one can extract an ω-regular expression that encodes all non-terminating execution paths, each of which is annotated with a probability. Such an approach would be a suitable basis for analyzing the termination probability of a probabilistic program without nondeterminism; however, static analyses that leverage *aggregate* information (e.g., the central-moment analysis developed in Chapter 5) need to consider both the terminating and non-terminating execution paths in a program. In addition, there seems to be an interesting connection between regular hyper-paths and ω-regular languages: I conjecture that the set of infinite rooted paths on a regular hyper-path can always be characterized by an ω-regular language. A more thorough and formal investigation is left for future work.

∞-Regular Expressions and Parity Automata Recently, Löding and Tollkötter [108] proposed ∞-*regular expressions*, which encode mixed sets of finite and infinite words. Their ∞-regular expressions are defined as standard regular expression plus one extra syntactic form E^∞, which means iterating E for a possibly infinite number of times. They proved that an ∞-regular language can always be separated into a regular language and an ω-regular language, and that a language L of both finite and infinite words can be recognized by a *parity automaton* if and only if L can be encoded as an ∞-regular expression.

The reason why I need a different theory for hyper-paths is exactly the same as my argument in the discussion about ω-regular expressions. On the other hand, for non-probabilistic programs (and also probabilistic programs without nondeterminism), it would be interesting future research to use ∞-regular path expressions to represent sets of both finite and infinite execution paths in a control-flow graph, and develop algebraic static analyses that account for *total-correctness* properties, because both the termination and non-termination behavior are captured by the ∞-regular path expressions.

Chapter 7

Conclusion

In this chapter, I reiterate the main contributions of the thesis and offer some concluding remarks.

7.1 Contributions

The main contributions of the research covered by this thesis are as follows.

- I developed a novel *hyper-graph*-based program model for low-level probabilistic programs with unstructured control-flow, general recursion, and nondeterminism. (See §2.2.) Control-flow hyper-graphs (CFHGs) turn out to be a natural representation of probabilistic programs with nondeterminism, because CFHGs allow different treatment for indeterminacy caused by *probabilistic*-branching (encoded as a hyper-edge with multiple destinations) and that caused by *nondeterministic*-branching (encoded as a bunch of hyper-edges starting from one source). In this sense, CFHGs precisely correspond to the intended meaning of a probabilistic program as a collection of probability distributions on executions. (See also the discussion at the beginning of Chapters 3 and 6.)

- I developed Markov algebras, which can describe the algebraic structure for control-flow hyper-graphs of probabilistic programs in a natural and general way. Based on Markov algebras, I devised an algebraic denotational semantics for low-level probabilistic programs. One notable advantage of the framework is that it can be instantiated with different models of nondeterminism. (See §3.3.)

- I presented a domain-theoretic development of a new model of nondeterminism for probabilistic programming, which is called *nondeterminism-first* and resolves nondeterminacy prior to program inputs, and thus achieves state-transformer-level nondeterminism, rather than the standard state-level nondeterminism. A potential application of nondeterminism-first would be refinement-based reasoning about relational properties. (See §3.2 and §3.4.3.)

- Based on the hyper-graph program model and the algebraic denotational semantics, I presented a new algebraic framework, which I call PMAF, for static analysis of probabilistic programs. The framework uses a variant of Markov algebras, namely the pre-Markov algebras, as the interface between the analysis framework and the abstract domains for concrete analyses. (See §4.1 and §4.2.)

- I demonstrated that PMAF can be instantiated to perform interprocedural versions of existing analyses such as Bayesian-inference analysis and expected-reward analysis for MDPs, as well as perform a novel linear expectation-invariant analysis. (See §4.3 and §4.4.)
- I developed the first fully automated analysis for deriving symbolic interval bounds on higher central moments for cost accumulators (such as running time) in probabilistic programs with general recursion and continuous distributions. For compositional derivation, I presented a new family of algebraic structures, namely the *moment semirings*, and a novel frame rule to handle procedure calls with moment-polymorphic recursion. (See §5.2.)
- I proved the (non-trivial) soundness of the central-moment analysis, incorporating Markov-chain-based semantics and Optional Stopping Theorems from probability theory. The proof establishes a general method to apply mathematical results about stochastic processes to analyses of probabilistic programs. (See §5.3.)
- I implemented the central-moment analysis, together with many practical enhancements, as an open-source tool and evaluated it on a broad suite of benchmark programs. (See §5.5.)
- I applied the central-moment analysis to tail-bound analysis via concentration inequalities. I also performed a case study on using tail bounds on program running time to analyze timing-leak vulnerabilities. (See §5.4 and §5.6.)
- I developed regular hyper-path expressions, which provide a finite representation of the possibly-infinite hyper-path obtained by composing hyper-edges on a control-flow hyper-graph for a probabilistic program without nondeterminism. My approach followed the "Kleene Algebras interpret regular expressions extracted from control-flow graphs" approach for algebraic static analysis of non-probabilistic programs. Notably, regular hyper-path expressions allow an *iteration operator*, which is similar to the Kleene-star. (See §6.1.)
- I presented some preliminary results on extending PMAF by using regular hyper-path expressions as the representation of probabilistic programs. To this end, I devised Deterministic Markov-Kleene Algebras with Tests (DMKATs) and developed a "DMKATs interpret regular hyper-path expressions extracted from control-flow hyper-graphs" approach. In this way, the analysis developer has an opportunity to specify how loops should be summarized via the iteration operator, rather than uses the built-in iteration algorithm of PMAF. I demonstrated how a DMKAT-based static-analysis framework would derive invariants on higher moments of program variables, including the cost accumulators. (See §6.2 and §6.3.)

7.2 Concluding Remarks

In this thesis, I have presented an algebraic approach for static analysis of probabilistic programs. Probabilistic programs are programs that can draw random samples from probability distributions and change the control flow at random. Probabilistic programs provide a general and flexible tool to implement and analyze probabilistic systems, which can be found in various applications including algorithm design, cryptographic protocols, uncertainty modeling, and statistical inference. The quantitative nature of probabilistic programs leads to non-trivial challenges to the development of

formal methods, including static analysis. Algebraic static analysis—the focus of the thesis—helps people reason about probabilistic programs at compile time in a compositional and versatile way, via a powerful framework based on the hyper-graph-based program model, the algebraic framework for denotational semantics and static analysis, as well as other techniques developed in this thesis.

This thesis also leaves and opens many directions for future research on static analysis of probabilistic programs. Besides those that are already mentioned in the discussion sections, I would like to emphasize extending the DMKAT framework. Recall that I proposed the DMKAT framework, mainly because the constraint-based central-moment analysis does not fit into the iteration-based analysis framework PMAF. I hope that in the future, DMKAT will be extended to a general, systematic, flexible, efficient, and non-iteration-based algebraic framework for static analysis of probabilistic programs, just like the algebraic framework for analyzing non-probabilistic programs developed by Kincaid et al. [92].

As probabilistic programming becomes increasingly popular in recent days, there are many opportunities to carry out impactful research on static analysis of probabilistic programs. Notably, probabilistic programs have been used for expressing and performing *probabilistic inference*, a method of inferring a statistical model from observed data, which is good at capturing uncertainty in model parameters and integrating domain knowledge. However, probabilistic inference requires considerable expertise from the practitioner [62], and it is not uncommon that people incorrectly program inference in a way that breaks convergence and leads to unsound learned model. Verifying properties of probabilistic programs that are used for data modeling, especially some statistical properties (such as convergence), brings new angles and challenges for programming-language research on static analysis of probabilistic programs. I hope that in the future more static-analysis techniques (ideally algebraic), which helps people diagnose inference-related bugs or optimize inference performance, can be developed and integrated in the toolchain of probabilistic inference to create a more reliable and efficient probabilisitic programming system.

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