Tail Bound Analysis for Probabilistic Programs via Central Moments

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Abstract
For probabilistic programs, it is usually not possible to automatically derive exact information about their properties, such as the distribution of states at a given program point. Instead, one can attempt to derive approximations, such as upper bounds on tail probabilities. Such bounds can be obtained via concentration inequalities, which rely on the moments of a distribution, such as the expectation (the first raw moment) or the variance (the second central moment). Tail bounds obtained using central moments are often tighter than the ones obtained using raw moments, but automatically analyzing higher moments is more challenging.

This paper presents an analysis for probabilistic programs that automatically derives symbolic over- and under-approximations for variances, as well as higher central moments. To overcome the challenges of higher-moment analysis, it generalizes analyses for expectations with an algebraic abstraction that simultaneously analyzes different moments, utilizing relations between them. The analysis is proved sound with respect to a trace-based, small-step model that maps programs to Markov chains. A key innovation is the notion of semantic optional stopping, and a generalization of the classical optional-stopping theorem.

The analysis has been implemented using a template-based technique that reduces the inference of polynomial approximations to linear programming. Experiments with our prototype central-moment analyzer show that, despite the analyzer’s over-/under-approximations of various quantities, it obtains tighter tail bounds than a prior system that uses only raw moments, such as expectations.

1 Introduction
Probabilistic programs [18, 23, 27] can be used to manipulate uncertain quantities modeled by probability distributions and random control-flows. Uncertainty arises naturally in Bayesian networks that capture statistical dependencies (e.g., for diagnosis of diseases [21]), randomized algorithms (e.g., cryptographic protocols [1] and privacy mechanisms [2]), and cyber-physical systems that are subject to sensor errors and peripheral disturbances (e.g., airborne collision-avoidance systems [26]). A probabilistic program propagates uncertainty through a computation, and produces a distribution over results, instead of a single value that can be determined by executing a deterministic program. In general, it is not tractable to automatically and precisely compute the result distributions of probabilistic programs, because composing simple distributions can quickly complicate the result distribution, and randomness in the control flow can easily lead to state explosion. Monte-Carlo simulation [33] is a common approach to study the result distributions, but the technique does not provide formal guarantees, and can sometimes be inefficient [3].

In this work, we study a static-analysis approach that leverages aggregate information, such as the expected result \( E[X] \) of program (e.g., \( X \)'s "first moment"), to answer queries about tail bounds of \( X \), e.g., the probability of assertions of the form \( P[X \geq d] \). The intuition why it is more promising to compute aggregate information than more fine-grained distributions, is that aggregate measures like expectations abstract distributions to a single number, while still indicating non-trivial properties. Moreover, (pre-)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 [27]. With the aggregate information in hand, we can employ concentration-of-measure inequalities [14] to reason about tail bounds.

In this paper, we focus on a specific yet important kind of uncertain quantity—cost accumulators, which are program variables that can only be increased or decreased through the program execution. A canonical example of such an accumulator is termination time, which is also the most studied one for probabilistic programs [3, 11, 12, 22, 29]. Rewards in Markov decision processes (MDPs) [32] can also be seen as accumulators. Recent work has shown that accumulator-like quantities can also be used to keep position information in control systems [6], and to model the cash flow during bitcoin mining [37].

Recent work has successfully automated inference on over- [28] and under-approximations [37] of the expected cost for probabilistic programs. Kura et al. [24] study higher moments (e.g., \( E[X^2] \). \( X \)'s "second moment") of runtimes to derive upper bounds on tail probabilities of the form \( P[X \geq d] \), where the random variable \( X \) stands for the runtime. However, prior work has considered only raw moments (i.e., \( E[X^k] \) for any \( k \geq 1 \), while central moments (i.e., \( E[(X - E[X])^k] \) for any \( k \geq 2 \) could provide more information about a distribution.
For example, the variance $\mathbb{V}[X]$ (i.e., $\mathbb{E}[(X - \mathbb{E}[X])^2]$), $X$‘s “second central moment”) of a random variable $X$ indicates how $X$ can deviate from its mean. With central moments, we not only find an opportunity to obtain more precise tail bounds, but also become able to derive bounds on tail probabilities of the form $\mathbb{P}[|X - \mathbb{E}[X]| \geq d]$.

In this paper, we present a technique for analyzing probabilistic programs to obtain aggregate information such as variances, and higher central moments of cost accumulators, which is then used in concentration inequalities to obtain tail-probability bounds. Our approach decomposes central moments of $\mathbb{E}[(X - \mathbb{E}[X])^2]$ to polynomials of raw moments $\mathbb{E}[X], \mathbb{E}[X^2], \ldots, \mathbb{E}[X^k]$ and over-approximates central moments via bounds on raw moments. For example, the variance $\mathbb{V}[X] = \mathbb{E}[(X - \mathbb{E}[X])^2]$ can be rewritten as $\mathbb{E}[X^2] - \mathbb{E}^2[X]$, i.e., you have to perform a subtraction. To over-approximate the result of a subtraction, a static analyzer also has to have an under-approximation of the value subtracted, i.e., the raw moment $\mathbb{E}[X]$.

Recently, Wang et al. [37] studied over- and under-approximation of expected cost, i.e., the first moment. In contrast, our approach is able to derive both over- and under-approximations of higher moments, by adapting the idea of ranking functions (aka ranking martingales or potential functions) [9, 11, 28]. The results are obtained via a novel notion of semantic optional stopping, which is an extension of the classic optional-stopping theorem from probability theory to the context of probabilistic programming. Intuitively, semantic optional stopping indicates when the locally-defined ranking function can imply a sound bound on the moments of the global accumulated cost. Moreover, we develop a template-based method for ranking-function inference that can be efficiently reduced to linear programming (LP).

In this work, we present and implement the first fully automatic analysis for deriving symbolic over- and under-approximations of higher moments for accumulated costs of probabilistic programs with general recursion and continuous sampling. One challenge is to support compositional reasoning to reuse analysis results for functions. Our 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 [25]. We use the technique to systematically extend a frame principle from [28] that enables compositional analysis of expectations to higher moments.

We implement our analysis for imperative probabilistic programs that feature recursive functions, continuous distributions, unstructured control-flow, and local variables. We evaluate our tool on a broad suite of benchmarks from the literature. We also conduct a case study of a timing-attack analysis for a program provided by DARPA during engagements of the STAC program [38]. Our experimental results show that on a variety of examples, our central-moment-based analyzer obtains tighter bounds than the system of [24], which uses only over-approximations of raw moments.

**Contributions.** Our work makes four main contributions.

- We describe a novel tail-bound analysis for probabilistic programs by deriving symbolic over- and under-approximations of higher (central) moments.
- We introduce a notion of semantic optional stopping for probabilistic programs. We use it to generalize the classical optional-stopping theorem, and to prove the soundness of our analysis method.
- We propose a family of algebraic structures—the moment monoids—to compose the moments of the accumulated costs for two computations, and to enable compositional reasoning about higher moments.
- We implement our technique by reducing the bound-inference problem to efficient LP solving. We show the effectiveness of the technique on a broad suite of benchmarks from prior work, and a case study of a timing-attack analysis.

## 2 Overview

We first review related work on static analysis for raw moments and sketch a moment-based analysis of tail bounds on the runtime of a simple random-walk program (§2.1). We then formalize the problem that our work addresses, and summarize the technical ideas used in our approach (§2.2).

### 2.1 Tail-Probability Analysis for a Random Walk

Tab. 1 summarizes the features of related work on moment analysis for probabilistic programs [6, 24, 28, 37]. The columns “loop”, “recur”, “cont”, and “non-mono” indicate supported programming features of the approaches. Non-monotonicity means that the accumulator can be either increased or decreased during the program execution, i.e., the stepwise costs can be positive or negative.\(^1\) The columns “higher mom.” and “intvl. approx” indicate supported analyses of the approaches. Interval approximations mean that both over- and under-approximations of the moments are derived. Note that our approach supports both higher moments and interval approximations, because they are required for the central-moment analysis. To compare prior approaches with ours, we use a simple random-walk program as an example.

\(^1\) Some approaches [24, 28] assume monotonicity because the goal is to reason about running time, which is indeed monotone.
Example 2.1. Consider the program shown in Fig. 1, which implements a bounded, biased random walk. The quantity we are interested in is the number of loop iterations, which is accumulated by the statement \texttt{tick} in the program. We denote this accumulator by \texttt{tick}. Suppose that we want to reason about the probability of the assertion (\texttt{tick} \geq 4N) at the exit of the program, where \( N > 0 \) is an integer-valued constant.

Chakarov et al. [6]'s technique is not applicable because it does not support unbounded loops, which arise in this example because the probabilistic-choice statement can always execute the else-branch, and as a result, the number of loop iterations can be unbounded. The methods from [28, 37] are both able to analyze this program, and derive the following over-approximation of the expected value \( E[\text{tick}] \) (i.e., the first raw moment of \( \text{tick} \)):

\[
E[\text{tick}] \leq 2N.
\]

There are a lot of concentration-of-measure inequalities in probability theory that derive bounds on the probability that a random variable deviates “far” from some some quantity [14]. Among those, one of the most important inequalities is Markov’s inequality:

Proposition 2.2 (Markov’s inequality). If \( X \) is a nonnegative random variable and \( a > 0 \), then \( P[X \geq a] \leq \frac{E[X]}{a} \). Moreover, if \( E[X^k] \) exists, then \( P[X \geq a] \leq \frac{E[X^k]}{a^k} \).

With Markov’s inequality, we derive the following tail bound:

\[
P[\text{tick} \geq 4N] \leq \frac{E[\text{tick}]}{4N} \leq \frac{2N}{4N} = \frac{1}{2}.
\] (1)

Beside the first raw moment, the algorithm of Kura et al. [24] is also capable of deriving over-approximations of higher moments of runtimes. It can produce the following bound on the second raw moment \( E[\text{tick}^2] \) of the accumulator \( \text{tick} \):

\[
E[\text{tick}^2] \leq 4N^2 + 6N,
\]

and then a tail bound by Markov’s inequality is

\[
P[\text{tick} \geq 4N] \leq \frac{E[\text{tick}^2]}{(4N)^2} \leq \frac{2N^2 + 3N}{8N^2} \xrightarrow{n \to \infty} \frac{1}{4}.
\] (2)

Note that for all \( N \geq 2 \), (2) provides a more precise bound on the probability of the assertion (\texttt{tick} \geq 4N) than (1) does.

Our central-moment analysis can obtain an even more precise tail bound. Besides the over-approximation of \( E[\text{tick}] \), our approach derives the following over-approximation of the variance \( V[\text{tick}] \) (i.e., the second central moment of \( \text{tick} \)):

\[
V[\text{tick}] \leq 6N.
\]

We can now employ concentration inequalities that involve variances of random variables. Recall Cantelli’s inequality:

Proposition 2.3 (Cantelli’s inequality). If \( X \) is a random variable and \( a > 0 \), then \( P[X - E[X] \geq a] \leq \frac{V[X]}{V[X] + a^2} \) and \( P[X - E[X] \leq -a] \leq \frac{V[X]}{V[X] + a^2} \).

With Cantelli’s inequality, we obtain the following tail bound:

\[
P[\text{tick} \geq 4N] = P[\text{tick} - 2N \geq 2N] \leq P[\text{tick} - E[\text{tick}] \geq 2N] \leq \frac{V[\text{tick}]}{V[\text{tick}] + (2N)^2} = \frac{E[\text{tick}^2]}{E[\text{tick}^2] + (2N)^2} \xrightarrow{n \to \infty} 0.
\] (3)

For all \( N \geq 2 \), (3) gives a more precise bound than both (1) and (2). It is clear from Fig. 2, where we plot the three tail bounds (1), (2), and (3), that the most precise bound is the one obtained via variances.

2.2 Problem Statement

The desire to use variances, and even higher central moments, inspired our research on automatic central-moment analysis for probabilistic programs. We want an automatic analyzer because (i) the analyzed programs might be quite complex, and (ii) traditional manual analysis can become cumbersome even for simple programs such as random walks [28].

Observing that a central moment \( E[(X - E[X])^k] \) can be rewritten as a polynomial of raw moments \( E[X], \ldots, E[X^k] \), we reduce the problem of bounding central moments to reasoning about raw moments. For example, the variance can be written as \( V[X] = E[X^2] - E[X]^2 \), so it suffices to analyze the over-approximation of the second moment \( E[X^2] \) and...
the under-approximation of the first moment $\mathbb{E}[X]$. For even higher central moments, this approach requires over- and under-approximations of higher raw moments. Consider the fourth central moment of a nonnegative random variable $X$:

$$
\mathbb{E}[(X-\mathbb{E}[X])^4] = \mathbb{E}[X^4] - 4\mathbb{E}[X^3] \mathbb{E}[X] + 6\mathbb{E}[X^2] \mathbb{E}[X] - 3\mathbb{E}[X]^3 - 3\mathbb{E}[X]^4.
$$

Deriving an over-approximation of the fourth central moment requires under-approximations of the first ($\mathbb{E}[X]$) and third ($\mathbb{E}[X^3]$) raw moments.

This paper addresses the following problem:

We adapt and extend the idea of ranking functions [16], which have been widely used to prove termination and to analyze to higher-moment analysis systematically. §7 describes moment monoids §5 proposes semantic optional stopping for probabilistic programs. §4 reviews ranking-function-based expected-cost-bound analysis. §3 introduces probabilistic programs. §6 presents semantic optional stopping for probabilistic programs. §7 describes an algorithm for moment-bound inference. §8 presents experimental results. §9 concludes.

3 Probabilistic Programs

This paper uses an imperative arithmetic probabilistic programming language AppL that supports general recursion and continuous sampling, where program variables are real-valued. We use the following notational conventions. Natural numbers $\mathbb{N}$ exclude 0, i.e., $\mathbb{N} = \{1, 2, 3, \cdots\} \subseteq \{0, 1, 2, \cdots\} \equiv \mathbb{Z}^+$. The Iverson brackets $[\cdot]$ are defined by $[\varphi] = 1$ if $\varphi$ is true and otherwise $[\varphi] = 0$. We denote updating an existing probability measure by $\|\cdot\|$. We also use the following standard notions from probability theory: $\sigma$-algebras, measurable spaces, measurable functions, random variables, probability measures, and expectations. Appendix A provides a review of those notions.

Syntax. Fig. 3 presents the syntax of AppL, where $p \in [0, 1]$, $a, b, c \in \mathbb{R}$, $a < b$, $x \in \text{VID}$ is a variable, and $f \in \text{FID}$ is a function identifier.

| Develop a static-analysis algorithm to infer symbolic over- and under-approximations of higher raw moments of the accumulated cost, for probabilistic programs that support general recursion and continuous sampling. |

$S := \text{skip} | \text{tick}(c) | x := E | x \sim D | \text{call } f$

$| \text{if } \text{prob}(p) \text{ then } S_1 \text{ else } S_2 \text{ fi } | \text{if } S \text{ then } S_1 \text{ else } S_2 \text{ fi}$

$| \text{while } L \text{ do } S \text{ od } | S_1 | S_2$

$L := \text{tt} | \text{not } L_1 | L_1 \text{ and } L_2 | E_1 \iff E_2$

$E := x | c | E_1 \ast E_2 | E_1 \star E_2$

$D := \text{uniform}(a, b) \cdots$

$K := \text{Kstop} | \text{Kloop } L S K | \text{Kseq } S K$

Figure 3. Syntax of AppL, where $p \in [0, 1]$, $a, b, c \in \mathbb{R}$, $a < b$, $x \in \text{VID}$ is a variable, and $f \in \text{FID}$ is a function identifier.
We use a pair \((S_{\text{main}}, \emptyset)\) to represent an APPL program, where \(S_{\text{main}}\) is the body of the main function and \(\emptyset : \text{FID} \rightarrow S\) is a map from function identifiers to their bodies.

**Semantics.** We adopt a small-step operational semantics with continuations and Borgström et al.’s distribution-based semantics for probabilistic lambda calculus [5] to define an operational cost semantics for APPL. Full details of the semantics are included in appendix B. A program configuration \(\sigma \in \Sigma\) is a quadruple \((y, S, K, \alpha)\) where \(y : \text{VID} \rightarrow \mathbb{R}\) is a program state that maps variables to values, \(S\) is the statement being executed, \(K\) is a continuation that described what remains to be done after the execution of \(S\), and \(\alpha \in \mathbb{R}\) is the global cost accumulator. A continuation \(K\) is either an empty continuation \(\text{Kstop}\), a loop continuation \(\text{Kloop} \, L \, S \, K\), or a sequence continuation \(\text{Kseq} \, S \, K\). Note that there does not exist a continuation for function calls, because we assume that functions only manipulate global program variables. Nevertheless, it is a common approach to include a continuation component in the program configurations if functions have local variables. An execution of an APPL program is initialized with \((\lambda \_0, S_{\text{main}}, \text{Kstop}, 0)\), and the termination configurations have the form \((\_, \text{skip}, \text{Kstop}, \_\_\_)\).

Different from a standard semantics where each program configuration steps to at most one new configuration, a probabilistic semantics may pick several different new configurations. The evaluation relation for APPL has the form \(\sigma \xrightarrow{\mu} \mu\) where \(\mu \in \mathcal{D}(\Sigma)\) is a probability measure over configurations. Below are two example rules. The rule (E-Prob) constructs a distribution whose support has exactly two elements, which stand for the two branches of the probabilistic choice. We write \(\delta(\sigma)\) for the Dirac measure at \(\sigma\), defined as \(\lambda \alpha.\{\sigma \in A\}\) where \(A\) is a measurable subset of \(\Sigma\). We also write \(p: \mu_1 + (1-p) \mu_2\) for a convex combination of measures \(\mu_1\) and \(\mu_2\) where \(p \in [0, 1]\), defined as \(\lambda A.\mu_1(A) + (1-p)\mu_2(A)\).

The rule (E-Sample) "pushes" the probability distribution of \(D\) to a distribution over post-sampling program configurations.

\[
\begin{align*}
\text{(E-Prob)} & \quad S = \text{if} \, \text{prob}(p) \, \text{then} \, S_1 \, \text{else} \, S_2 \, \text{fi} \\
& \quad \langle y, S, K, \alpha \rangle \rightarrow p \cdot \delta(y, S_1, K, \alpha) + (1-p) \cdot \delta(y, S_2, K, \alpha)
\end{align*}
\]

\[
\begin{align*}
\text{(E-Sample)} & \quad \langle y, x \rightarrow D, K, \alpha \rangle \rightarrow \lambda A.\mu_D([r \mid \langle y[x \rightarrow r], \text{skip}, K, \alpha \rangle \in A])
\end{align*}
\]

**Example 3.1.** Suppose that a random sampling statement is being executed, i.e., the current configuration is \(\{r \rightarrow r_0\}, (r \sim \text{uniform}(-1, 2)), K_0, \alpha_0\). The probability measure for the uniform distribution is \(\lambda A.\int_{-1}^{2} \frac{1}{3} dr\). Thus by the rule (E-Sample), we derive the post-sampling probability measure over configurations via the following density function:

\[
\lambda \langle y, S, K, \alpha \rangle.\frac{1 - y(r) \leq 2}{3} \cdot [S = \text{skip} \land K = K_0 \land \alpha = \alpha_0].
\]

**Trace-Based Semantics.** In this work, we harness Markov-chain-based reasoning [22, 29] to develop a trace-based semantics for APPL, based on the evaluation relation \(\sigma \mapsto \mu\). An advantage of the trace-based approach is that it allows us to study how the cost of every single evaluation step contributes to the accumulated cost at the exit of the program. Details of the trace semantics are included in appendix C.

Let \((\Omega, \mathcal{F}, \mathbb{P})\) be the probability space where \(\Omega = \Sigma^N\) is the set of all infinite traces over program configurations, \(\mathcal{F}\) is a \(\sigma\)-algebra on \(\Omega\), and \(\mathbb{P}\) is a probability measure on \((\Omega, \mathcal{F})\) obtained by the evaluation relation \(\sigma \mapsto \mu\) and the initial configuration \((\lambda \_0, S_{\text{main}}, \text{Kstop}, 0)\). Intuitively, \(\mathbb{P}\) specifies the probability distribution over all possible executions of a probabilistic program. The probability of an assertion \(\theta\) with respect to \(\mathbb{P}\), written \(\mathbb{P}[\theta]\), is defined as \(\mathbb{P}([\omega \mid \theta(\omega)\text{ is true}])\).

### 4 Expected-Cost Bound Analysis

In this section, we review the ranking-function-based approach that underlies several expected-cost bound analyses [24, 28, 37]. The basic idea is to study how stepwise costs contribute to the accumulated cost at the termination configurations, via the trace-based semantics introduced in §3. More formally, if \(\{A_n\}_{n \in \mathbb{Z}^+}\) is a sequence of accumulated costs at the \(n\)-th evaluation step, and \(A_T\) is the accumulated cost at the termination configurations, we wish to establish that the sequence of stepwise approximations \(\{\mathbb{E}[A_n]\}_{n \in \mathbb{Z}^+}\) converges to \(\mathbb{E}[A_T]\). The bound analysis is divided into two sub-problems: (i) how to use ranking functions to capture the probabilistic invariants in the stepwise approximations, and (ii) when do the stepwise approximations converge to the expected cost at the termination configurations.

First, we define the stopping time \(T : \Omega \rightarrow \mathbb{Z}^+ \cup \{\infty\}\) of a probabilistic program as a random variable on the probability space \((\Omega, \mathcal{F}, \mathbb{P})\) of program traces:

\[
T(\omega) \overset{\text{def}}{=} \inf\{n \in \mathbb{Z}^+ \mid \omega_n = (\_, \text{skip}, \text{Kstop}, \_\_\_)\}
\]

i.e., \(T(\omega)\) is the number of evaluation steps before the trace \(\omega\) reaches some termination configuration \((\_, \text{skip}, \text{Kstop}, \_\_\_)\). We define the accumulated cost \(A_T : \Omega \rightarrow \mathbb{R}\) with respect to the stopping time \(T\) as

\[
A_T(\omega) \overset{\text{def}}{=} A_T(\omega, T(\omega)),
\]

where \(A_n : \Omega \rightarrow \mathbb{R}\) captures the accumulated cost at the \(n\)-th evaluation step for \(n \in \mathbb{Z}^+\), which is defined as

\[
A_n(\omega) \overset{\text{def}}{=} \alpha_n \, \text{where} \, \omega_n = (\_, \_, \_, \alpha_n).
\]

In this paper, we focus on accumulated costs at termination configurations, so we define \(A_\infty(\omega) \overset{\text{def}}{=} 0\). The expected accumulated cost is then given by the expectation \(\mathbb{E}[A_T]\) with respect to the probability measure \(\mathbb{P}\).

A ranking function \(\phi\), or ranking martingale [9, 10, 24], or potential function [28] is a measurable map from \(\Sigma\) to \(\mathbb{R}\) such that \(\phi(\sigma)\) is the expected accumulated cost of the computation that continues from the configuration \(\sigma\), or more...
formally, \( \phi((\_, \text{skip}, \text{Kstop}, \_)) = 0 \) and for any program configuration \( \sigma \in \Sigma \), it holds that

\[
\phi(\sigma) = \mathbb{E}_{\sigma \sim \mu}(\phi(\alpha') + \phi(\sigma')) \tag{4}
\]

where \( \sigma = (\_, \_, \_, \_) \), \( \sigma' = (\_, \_, \_, \_\sigma' \_\), and \( \sim \) is the probability measure after one evaluation step from the configuration \( \sigma \). The notation \( \mathbb{E}_{x \sim \mu}[f(x)] \) represents the expected value of \( f(x) \), where \( x \) is drawn from a distribution \( \mu \). Intuitively, the sum of the accumulated cost to reach a configuration \( \sigma \) and the ranking function at \( \sigma \) should be an invariant.

Let \( \Phi_\mu(\omega) \) be the ranking function at step \( n \). We define cost invariants \( \mathcal{Y}_0(\omega) = A_\mu(\omega) + \Phi_\mu(\omega) \) as the sum of accumulated cost and the ranking function at step \( n \). Then \( \mathcal{Y}_0(\omega) = A_\mu(\omega) + \Phi_\mu(\omega) = 0 + \phi(\omega_0) \) is the ranking function at the initial configuration, i.e., \( \mathcal{Y}_0 = \Phi_0 \). Similar to the definition of the accumulated cost \( A_T \) at termination configurations, we assume \( \Phi_\mu(\omega) \) is 0 and define \( \Phi(\omega) \) as well as \( \mathcal{Y}_T(\omega) \) as the sum of \( Y_T(\omega) \) at a termination configuration, we have \( \Phi(\omega) = 0 \) and \( Y_T(\omega) = A_T \).

In the expected-cost bound analysis, instead of establishing a bound on \( \mathbb{E}[A_T] \) directly, we establish a bound on \( \mathbb{E}[Y_T] \), which gives us the following leverage:

We reason about \( \mathbb{E}[\mathcal{Y}_n] \) and then prove that \( \mathbb{E}[Y_T] = \mathbb{E}[Y_0] \).

We can prove that \( \mathbb{E}[\mathcal{Y}_n] \) is an invariant for expectations of stepwise approximations. Therefore, if we could show that \( \mathbb{E}[Y_T] = \lim_{n \to \infty} \mathbb{E}[\mathcal{Y}_n] \), then we would conclude that \( \mathbb{E}[A_T] = \mathbb{E}[Y_T] = \mathbb{E}[Y_0] = \Phi_0 \), i.e., the ranking function at the initial configuration captures the expected accumulated cost at termination configurations.

However, the property \( \mathbb{E}[Y_T] = \lim_{n \to \infty} \mathbb{E}[\mathcal{Y}_n] \) does not necessarily hold. In Ex. 4.1, we analyze the random walk in Ex. 2.1, assuming this convergence property. Then in Counterexample 4.2, we analyze a variant random walk where this convergence property does not hold, and ranking-function-based reasoning would be unSound.

Example 4.1. Recall the random walk in Ex. 2.1. We assume that there is a map \( \rho : \mathbb{Z}^+ \to \mathbb{Z}^+ \), such that \( \rho(k) \) records the evaluation step at the end of the \( k \)-th loop iteration, with respect to the trace-based semantics. For simplicity, we define \( A'_k \overset{\text{def}}{=} A_{\rho(k)} \), \( \Phi'_k \overset{\text{def}}{=} \Phi_{\rho(k)} \), \( Y'_k \overset{\text{def}}{=} Y_{\rho(k)} \) as random variables for accumulated costs, ranking functions, cost invariants, respectively, at the end of the \( k \)-th loop iteration.

We want to show that the expected accumulated cost \( \mathbb{E}[A_T] \) is \( 2 \cdot N \), where \( N \) is the initial value of \( x \). We define a ranking function \( \phi \) as \( \phi((\_, \_, \_, \_)) = 2 \cdot y(x) \), or \( 2 \cdot x \) for simplicity. We need to show that property (4) holds for the loop body \( \text{if } \text{prob}(y) \text{ then } x := x + 1 \text{ else } x + 1 \text{ tick(1)} \). If the program executes the then-branch, then \( x \) is incremented and the ranking function becomes \( 2 \cdot (x + 1) \). Otherwise, \( x \) is incremented and the ranking function evaluates to \( 2 \cdot (x + 1) \). Thus, the expected value of the ranking function after the branching statement is \( \gamma \cdot 2 \cdot (x - 1) + \gamma \cdot 2 \cdot (x + 1) = 2 \cdot x - 1 \). No matter which branch is executed, the loop body increases the cost accumulator by one. Thus, the right-hand-side of (4) is \( 2 \cdot (x - 1) + 1 \), which equals the left-hand-side of (4).

As we will show shortly after Prop. 4.3, the convergence property \( \mathbb{E}[Y_T] = \lim_{n \to \infty} \mathbb{E}[\mathcal{Y}_n] \) holds for this example; thus, we can also show that \( \mathbb{E}[Y_T] = \lim_{k \to \infty} \mathbb{E}[Y'_k] \). We then conclude that the expected accumulated cost \( \mathbb{E}[A_T] = \mathbb{E}[Y'_0] = \mathbb{E}[\Phi'_0] = 2 \cdot N \), where \( N \) is the initial value of \( x \).

Counterexample 4.2. Consider the following program that describes an unbiased random walk that terminates with probability one:

\[
\begin{align*}
&x \leftarrow 0; \\
&\text{while } x < 1 \text{ do} \\
&\quad \text{if } \text{prob(0.5)} \text{ then } x \leftarrow x + 1; \text{ tick(1)} \\
&\quad \text{else } x \leftarrow x - 1; \text{ tick(-1)} \text{ fi} \\
&\text{od}
\end{align*}
\]

Similar to Ex. 4.1, we define \( A'_k \), \( \Phi'_k \), \( Y'_k \) as random variables at the end of the \( k \)-th loop iteration. Intuitively, the cost accumulator should be the same as the value of \( x \) at any time of the execution. At the termination of the program, the value of \( x \) should be at least one, thus \( A_T \geq 1 \) and \( \mathbb{E}[A_T] \neq 0 \).

However, we are able to define a ranking function as the constant function \( \phi(\_ ) \overset{\text{def}}{=} 0 \), because in each loop iteration, the expected cost is \( 0.5 \cdot 1 + 0.5 \cdot (-1) = 0 \). Then \( \mathbb{E}[Y'_k] = \mathbb{E}[A'_k] + \mathbb{E}[\Phi'_k] = 0 \) for all \( k \in \mathbb{Z}^+ \). Because we already showed that \( \mathbb{E}[A_T] \geq 1 \), we have \( \mathbb{E}[Y'_T] \geq 1 \). Therefore, \( \mathbb{E}[Y'_T] \neq \lim_{k \to \infty} \mathbb{E}[Y'_k] \), and also \( \mathbb{E}[Y'_T] \neq \lim_{n \to \infty} \mathbb{E}[\mathcal{Y}_n] \).

It has been shown that the convergence property holds if all the stepwise costs are nonnegative and the analysis only considers over-approximations [24, 28]. To handle negative costs or to derive under-approximations while ruling out sound ranking functions, like the one in Counterexample 4.2, recent research [19, 37] has adapted the Optional Stopping Theorem (OST) from probability theory:

**Proposition 4.3** (Doob’s OST [40, Thm. 10.10]). If \( \mathbb{E}[\mathcal{Y}_n] < \infty \) for all \( n \in \mathbb{Z}^+ \), then \( \mathbb{E}[Y_T] \) exists and \( \mathbb{E}[Y_T] = \mathbb{E}[Y_0] \) in each of the following situations:

(a) \( T \) is bounded;
(b) \( \mathbb{E}[T] < \infty \) and for some \( C \geq 0 \), \( |Y_{n+1} - Y_n| \leq C \) for all \( n \in \mathbb{Z}^+ \);
(c) \( \mathbb{P}[T < \infty] = 1 \) and for some \( C \geq 0 \), \( |Y_n| \leq C \) for all \( n \in \mathbb{Z}^+ \).

Note that from item (a) to item (c) in Prop. 4.3, the constraint on the stopping time \( T \) is getting weaker while the constraint on \( \{ \mathcal{Y}_n \}_{n \in \mathbb{Z}^+} \) is getting stronger. Prop. 4.3(a) corresponds to an analogy we will present in Ex. 5.1 about non-probabilistic programs: one does not need extra constraints on the costs or ranking functions if the program terminates.

For the random walk in Ex. 4.1, the expected value \( \mathbb{E}[T] \) of the stopping time has been shown to be finite [28], and meanwhile, \( |Y'_{k+1} - Y'_k| \leq |A'_{k+1} - A'_k| + |\Phi'_{k+1} - \Phi'_k| \), the
If the program is non-probabilistic, then the nontermination:

\[ \text{Example 5.1.} \]

\[ \text{Example 5.2.} \]

In this section, we present a semantic characterization of optional stopping for probabilistic programs. Proofs for this section are included in appendix D.

Recall the problem: we want to establish the convergence property \( \lim_{n \to \infty} E[Y_n] = E[Y_T] \). To start with, let us consider the case for non-probabilistic programs.

\[ \text{Example 5.1.} \]

\[ \text{Example 5.2.} \]

The three situations in the classic OST (Prop. 4.3) can be interpreted as sufficient conditions for the "product-of-probability-and-expected-gap-approach-zero" principle.

In practice, the criteria of Prop. 4.3 can be too restrictive to derive bounds on the expected cost of probabilistic programs. In Ex. 5.2, we present a variant of random walks, where we cannot apply Prop. 4.3. Later, in §6, we will also show that those criteria are not so useful for reasoning about higher moments.

\[ \text{Example 5.2.} \]

\[ \text{Example 5.2.} \]

As shown by Ex. 5.1, nontermination is the reason that the convergence property may fail to hold. Probabilistic programs can exhibit a mixed behavior of termination and nontermination: even though the two programs in Ex. 4.1 and Counterexample 4.2 terminate with probability one, they have some traces that are nonterminating. Because we focus on the accumulated cost at termination configurations, nonterminating traces finally have zero contribution to the expectation \( E[Y_T] \), but they do affect \( E[Y_n] \) for finite \( n \). Intuitively, to establish the convergence property, we need to put a limit on the contribution of nonterminating traces to \( E[Y_n] \), which should approach zero when \( n \) approaches infinity.
reason is that for the assignments $x := x - 1$ and $x := x + 1$, the accumulated cost is unchanged, but the change of the ranking function cannot be bounded by a constant. We have $|(x - 1)^2 + (x - 1) - (x^2 + x)| = 2x$, $|(x + 1)^2 + (x + 1) - (x^2 + x)| = 2x + 2$, where $x$ can be arbitrarily large during an execution.

To address the issue in Ex. 5.2, we propose an extension of OST that we use as the soundness criterion for the bound-inference algorithm developed in §7.

**Theorem 5.3** (An extension of OST). If $E[Y_n] < \infty$ for all $n \in \mathbb{Z}^+$, then $E[Y_T] = E[Y_n]$ in the following situation:

1. **There exist $\ell \in \mathbb{N}$ and $C \geq 0$ such that $E[T^\ell] < \infty$ and for all $n \in \mathbb{Z}^+$, $|Y_n| \leq C \cdot (n + 1)^\ell$ almost surely.**

Thm. 5.3 allows the process $\{Y_n\}_{n \in \mathbb{Z}}$ to be bounded by a polynomial of degree $\ell$ in $n$, which relaxes the bounded-difference property in Prop. 4.3(b), while the theorem requires that $E[T^\ell] < \infty$, which is a stronger property than the finite expected-stopping time in Prop. 4.3(b). Note that the recent extension of OST proposed by Wang et al. [37] is not as strong as ours, because their theorem assumes that the probability $P[T \geq n]$ drops exponentially in $n$, which implies that $E[T^\ell] < \infty$ for all finite $\ell$.

**Example 5.4.** Recall the random walk in Ex. 5.2. We apply Thm. 5.3 to prove the soundness of the ranking function $\phi(y, \ldots, -s, -s) \overset{\text{def}}{=} y(x)^2 + y(x)$. Because in each iteration of the outer loop, the variable can be either incremented or decremented, we know that after $k$ iterations, the value of $x$ is bounded by $N + k$, where $N$ is a constant. Therefore, the random variable $Y_k'$ is bounded by $(N + k)^2 + (N + k)$. At the same time, the cost of the $k$-th iteration is also bounded by $N + k$, so the random variable $A_k'$ is bounded by $k \cdot (N + k)$. Thus $Y_k' = A_k' + \phi_k'$ is bounded by $C \cdot (k + 1)^2$ for some constant $C$. By Thm. 5.3, the soundness of $\phi$ is reduced to proving $E[T^2] < \infty$ where $T$ is the runtime of the program.

Note that $E[T^2]$ for $\ell \in \mathbb{N}$ is a higher moment of the termination time. To avoid our algorithm having a circular dependence, we use a different technique to reason about $E[T^2]$, taking into account the monotonicity of runtimes. Because upper-bound analysis of higher moments of runtimes has been studied by Kura et al. [24], we skip the details here, but include them in appendix E.

### 6 Higher Moments via Moment Monoids

In this section, we introduce moment monoids to compose accumulated costs for two computations (§6.1). Then we use the moment monoids to systematically lift the expected-cost bound analysis in §4 to reason about over- and under-approximations for higher moments of the accumulated cost (§6.2). Proofs for this section are included in appendix F.
We now define
\[ I = \{(a', a) \mid a' \leq a\} \subseteq T \oplus T \oplus T \oplus T \oplus T \text{,} \]
where the identity element is then defined as \( I \triangleq (1, 0, 0, 0, 0) \).

Algebraic higher-order moment monoids. We extend the first- and second-order moment monoids to higher moments. Instead of restricting the elements of monoids to be vectors of numbers, we propose algebraic moment monoids that can be instantiated to describe vectors of intervals, which we need for the interval-bound analysis in §6.2.

**Definition 6.1.** The m-th order moment monoid \( M^{(m)} \) parametrized by a partially ordered semiring \( R = (\{\mathbb{R}\}, \triangleq, \otimes, \oplus, 0) \), is defined as \( M^{(m)} \triangleq (\{\mathbb{R}\}^{m+1}, \otimes_M, 1_M) \), where
\[
(\mathbf{u} \otimes_M \mathbf{v})_k \triangleq \binom{k}{i}(u_i \otimes v_{k-i}),
\]
\( \binom{k}{i} \) is the binomial coefficient, the scalar product \( n \cdot u \) is an abbreviation for \( \bigoplus_{i=1}^{n} u_i \), for \( n \in \mathbb{Z}^+ \), \( u \in R \), and \( 1_M \triangleq (1, 0, \ldots, 0) \). We define the partial order \( \subseteq_M \) as the pointwise extension of the partial order \( \subseteq \) on the semiring \( R \).

Intuitively, the definition of \( \otimes_M \) in (5) can be seen as the multiplication of two moment-generating polynomials with coefficients \( u \) and \( v \), respectively. We prove the following fundamental composition property for moment monoids.

**Lemma 6.2.** For all \( u, v \in R \), it holds that
\[
(1, u \oplus v, (u \oplus v)^2, \ldots, (u \oplus v)^m) \otimes_M (1, v \oplus u, v^2, \ldots, v^m)
\]
where \( u^n \) is an abbreviation for \( \bigoplus_{i=1}^{n} u \) for \( n \in \mathbb{Z}^+ \), \( u \in R \).

### 6.2 Interval-Valued Ranking Functions and OST

In practice, it is not always feasible to come up with a precise ranking function that captures the exact accumulated cost for a probabilistic program. Instead, we allow ranking functions to be interval-valued, i.e., to keep track of over- and under-approximations of the accumulated cost.

We achieve this by instantiating moment monoids with the interval semiring \( I \triangleq ([a, b] \mid a \leq b) \subseteq T \oplus T \oplus T \oplus T \oplus T \), where \( [a_1, b_1] \otimes [a_2, b_2] \triangleq [a_1 + a_2, b_1 + b_2] \) is the pointwise addition, \( 0_I \triangleq [0, 0] \), \( 1_I \triangleq [1, 1] \) are singletons, and
\[
[a_1, b_1] \oplus [a_2, b_2] \triangleq [\min S_{a_1, b_1, a_2, b_2}, \max S_{a_1, b_1, a_2, b_2}],
\]
where \( S_{a_1, b_1, a_2, b_2} \triangleq \{a_1 a_2, a_1 b_2, a_2 b_1, b_1 b_2\} \). The partial order \( \subseteq_I \triangleq \subseteq \) is defined as set inclusion.

We fix a degree \( m \in \mathbb{N} \) and let \( M^{(m)} \) be the m-th order moment monoid instantiated with the interval semiring \( I \). We now define \( M^{(m)} \)-valued ranking functions.

**Definition 6.3.** A measurable map \( \phi : \Sigma \to M^{(m)} \) is said to be a ranking function if

\begin{align*}
(\text{i}) \quad & \phi(\sigma) = 1_M \text{ if } \sigma = (\_, \text{skip}, \text{Kstop}, \_), \\
(\text{ii}) \quad & \exists_M \mathbf{E}_{\sigma \to \sigma'}[[\alpha' - \alpha]^k, (\alpha' - \alpha)^k] \otimes_M \phi(\sigma')
\end{align*}

where \( \sigma = (\_, \_, \_, \alpha), \sigma' = (\_, \_, \_, \alpha') \) for all \( \sigma \in \Sigma \).

Intuitively, \( \phi(\sigma) \) is an interval bound for the moments of the accumulated cost for the computation that continues from the configuration \( \sigma \). Similar to the expected-cost bound analysis, we define \( A_n, \Phi_n, Y_n \), where \( n \in \mathbb{Z}^+ \), to be random variables on the probability space \( (\Omega, \mathcal{F}, \mathbb{P}) \) of the trace-based semantics as
\[
A_n(\omega) \triangleq [a_n^k, a_n^k] \text{ where } a_n = (\_, \_, \_, n), \quad \Phi_n(\omega) \triangleq \phi(\omega),
\]
\[
Y_n(\omega) \triangleq A_n(\omega) \otimes_M \Phi_n(\omega).
\]

In the definition of cost invariants \( Y_n \), we use \( \otimes_M \) to compose the powers of the accumulated cost at step \( n \) and the ranking function that stands for the moments of the accumulated cost of the rest of the computation.

We extend Thm. 5.3 to interval-valued ranking functions. Let \( \|a_k^i, b_k^i\|_{\text{max}} \triangleq \max_k \{\max\{|a_k^i|, |b_k^i|\}\} \).

**Theorem 6.4.** If \( \mathbb{E}[\|Y_n\|_{\text{max}}] < \infty \) for all \( n \in \mathbb{N} \), then \( \mathbb{E}[Y_{T'}] \) exists and \( \mathbb{E}[Y_T] \leq \mathbb{E}[E_Y] \mathbb{E}[Y_{T'}] \) in the following situation:

There exist \( \ell \in \mathbb{N} \) and \( C \geq 0 \) such that \( \mathbb{E}[T^\ell] < \infty \) and for all \( n \in \mathbb{Z}^+ \), \( \|Y_n\|_{\text{max}} \leq C \cdot (n + 1)^\ell \) almost surely.

When reasoning about higher moments, Thm. 6.4 becomes more effective than the classic OST (Prop. 4.3), because higher-degree arithmetic involved in \( Y_n = A_n \otimes_M \Phi_n \) makes it difficult to bound \( |Y_n - Y_{n+1}| \) uniformly by a constant.

### 7 Derivation System for Bound Inference

In this section, we describe the inference system used by our analysis. To automate ranking-function-based bound inference, we use templates to fix the shape of ranking functions. We present the derivation system as a declarative program logic that enables compositional reasoning. Finally, we show the soundness of the analysis with respect to the trace semantics. Details and proofs for this section are included in appendix G.

**Template-Based Ranking Functions.** The basic approach to automated bound inference using ranking functions is to fix the shape, i.e., a template, of the ranking functions. Because we use \( M^{(m)} \)-valued ranking functions whose range is vectors of intervals, the templates should be of vectors of intervals whose ends are represented symbolically. In this paper, we represent the ends of intervals by polynomials in \( \mathbb{R}_d[\text{VID}] \) over program variables up to some fixed degree \( d \in \mathbb{N} \). In the implementation, we adopt the technique from prior work \([28, 37]\), where manipulations of polynomials are reduced to efficient linear-algebra operations in the coefficients of the monomials.

More formally, we lift the interval semiring \( I \) to a symbolic interval semiring \( P_I \) by representing the ends of the \( k \)-th interval by piecewise polynomials in \( \mathbb{R}_d[\text{VID}] \). We formulate
\(P\) with piecewise polynomials to define the \(\otimes_{P^T}\) operation, which involves min and max. In the implementation, we assume one operand of \(\otimes_{P^T}\) has the form \([c, c]\) with \(c \in \mathbb{R}\) to avoid manipulation of piecewise functions. We fix a degree \(m \in \mathbb{N}\) and let \(M_{P^T}^{(m)}\) be the \(m\)-th order moment monoid instantiated with the symbolic interval semiring. Let \(Q = [L_k, U_k] \in M_{P^T}^{(m)}\) where \(L_k\)'s and \(U_k\)'s are polynomials in \(\mathbb{R}_{kd}[VID]\). It defines an \(\mathcal{M}_{I}^{(m)}\)-valued ranking function \(\phi_Q(y) \triangleq [L_k(y), U_k(y)]\) where \(y\) is a program state.

**Inference Rules.** We formalize our derivation system for the bound inference in a Hoare-logic style. The main judgment has the form \(\Delta \vdash \{\Gamma; Q\} S \{\Gamma'; Q'\}\), where \(S\) is a program statement, \(\{\Gamma; Q\}\) is a precondition, \(\{\Gamma'; Q'\}\) is a postcondition, and \(\Delta\) is a context for function specifications. The *logical context* \(\Gamma \in (VID \rightarrow R) \rightarrow \{\top, \bot\}\) is a predicate on program states that describes reachable states at a program point. The *quantitative context* \(Q \in M_{P^T}^{(m)}\) specifies a map from program states to the moment monoid that is used to define interval-valued ranking functions. The logical contexts have the same meaning as in Hoare logic. The semantics of the triple \(\{\vdash; Q\} S \{\vdash; Q'\}\) 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 \(\phi_Q\).

Fig. 4 presents some of the inference rules. The rule (Q-Sample) accounts for sampling statements. To compute the expectation of the post-condition \(Q'\), where \(x\) is drawn from distribution \(D\), i.e., \(E_x_{\mu_0}[Q']\), we assume the moments for \(D\) up to degree \(d\) are well-defined and computable, and substitute \(x^1, \ldots, x^d\) with the corresponding moments in \(Q'\).

The other probabilistic rule (Q-Prob) deals with probabilistic branching. Intuitively, if the moments of the accumulated cost of the computation after the branching and the execution of \(S_1, S_2\) are bounded by \(\phi_Q\) and \(q_1, q_2\), respectively, then the moments for the whole computation should be bounded by a "weighted average" of \((q_1 \otimes_{M} \phi_Q)\) and \((q_2 \otimes_{M} \phi_Q)\), with respect to the branching probability \(p\). We implement the weighted average by the pointwise extension of the \(\otimes_{P^T}\) operator applied to \([\{p, p\}, \{0, 0\}, \ldots, \{0, 0\}] \otimes_{M} q_1 \otimes_{M} \phi_Q\) and \(([1 - p, 1 - p], \{0, 0\}, \ldots, \{0, 0\}] \otimes_{M} q_2 \otimes_{M} \phi_Q\).

The rule (Q-Tick) is the only rule that deals with costs in a program. To accumulate the cost to the moments, we use the \(\otimes_{M}\) operation in the moment monoid \(M_{P^T}^{(m)}\). The rule (Q-Call) handles function calls. We fetch the pre- and post-condition for the function \(f\) from the specification context \(\Delta\). Then we compose a constant frame \([c_k, c_k] \in M_{I}^{(m)}\) to the function specification. The frame is used to account for the cost of the computation after the function call for most non-tail-recursive programs.

**Example 7.1.** The annotated function rdwalk in Fig. 5 models a biased random walk where the length of each step is randomly sampled from a uniform distribution on the interval \([-1, 2]\). Let us reason about the *under-approximation* of the second moment of the accumulated cost and omit the over-approximations of the moments. The annotations in the figure justify the following specification

\[ \{x < n + 2; (1, 2(n-x), 4(n-x)^2 + 6(n-x) - 4)\}, \{\top; (1, 0, 0)\}\].

To reason about the sampling statement, we apply the rule (Q-Sample) with the fact that \(E[q] = 1/2\) and \(E[q^2] = 1\). To justify the statement *call* rdwalk with the post-condition \(\{\top; (1, 1, 1)\}\), we apply the rule (Q-Call) with \(\mathcal{M}_I\) instantiated by \((1, 1, 1)\), and then obtain the quantitative context of the pre-condition as

\[
(1, 2(n-x), 4(n-x)^2 + 6(n-x) - 4) \otimes_{M} (1, 1, 1) = (1, 2(n-x)+1, 4(n-x)^2 + 6(n-x) - 4 + 2 \cdot 2(n-x) + 1) = (1, 2(n-x)+1, 4(n-x)^2 + 10(n-x) - 3).
\]

**Soundness.** The soundness of the derivation system is proved with respect to the trace-based semantics.

**Theorem 7.2.** Suppose \(\Delta \vdash \{\Gamma; Q\} S_{\text{main}} \{\Gamma'; 1_{M}\}\), where \(Q \in M_{P^T}^{(m)}\) and the ends of the \(k\)-th interval in \(Q\) are polynomials in \(\mathbb{R}_{kd}[VID]\). Let \(\{Y_n\}_{n \in \mathbb{Z}^+}\) be a sequence of cost invariants extracted from the derivation of \(\Delta \vdash \{\Gamma; Q\} S_{\text{main}} \{\Gamma'; 1_{M}\}\). If the following conditions hold:

(i) \(E[T^{md}] < \infty\), and

(ii) there exists \(C \geq 0\) such that for all \(n \in \mathbb{Z}^+\), \(\|Y_n\|_{\infty} \leq C \cdot (n + 1)^{md}\) almost surely.

Then \(E[Y_T] \subseteq_{M} E[Y_0]\) and \(E[A_T] \subseteq_{M} \phi_Q(\lambda_0)\).

The intuitive meaning of \(E[A_T] \subseteq_{M} \phi_Q(\lambda_0)\) is that the moments \(E[A_T]\) of the accumulated cost upon program termination are bounded by intervals in \(\phi_Q(\lambda_0)\) where \(Q\) is the quantitative context and \(\lambda_0\) is the initial state.

We reduce the soundness proof to the extended OST (Thm. 6.4) for interval-valued bounds. Thm. 7.2(i) and (ii) correspond to the constraints on the stopping time \(T\) and the cost invariants \(\{Y_n\}_{n \in \mathbb{Z}^+}\) required by the extended OST. Operationally, we implement the routine discussed in §5 to check if \(E[T^{md}]\) is finite. To ensure the almost-sure boundedness of \(\{Y_n\}_{n \in \mathbb{Z}^+}\), we assume the bounded-update property: every (deterministic or probabilistic) assignment to a program variable updates the variable with an almost surely bounded change. As observed in [37], bounded updates are common in practice.

### 8 Implementation and Experiments

In this section, we first describe the implementation of our automatic moment-analysis tool. We then evaluate the performance of the tool, compared with state-of-the-art analysis tools for higher moments.

**Implementation.** Our tool is implemented in OCaml, and consists of about 3200 LOC. The tool works on imperative arithmetic probabilistic programs using a CFG-based IR [36].
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we implemented an interprocedural numeric analysis to infer

Evaluation Setup.

that satisfy the pre-condition.

obtained symbolic bounds are sound for all concrete inputs

are inferred with respect to the pre-condition; therefore, the

unknown coefficients as the objective. In our implementa-

tion, we allow symbolic inputs with optional pre-conditions

the concrete inputs, and use the obtained linear function over

checks the satisfiability of the constraints, but is also able

GLPK [39] to solve the constraints. The LP solver not only

ner. Our tool generates linear constraints over the unknown

coefficients of the monomials in polynomials. The bound-

lyzed moment, and a maximal degree for the polynomials to

mode (over- or under-approximation), the order of the ana-

cost for a program, the user needs to specify an analysis

infer the bounds on the central moments of the accumulated

under-approximation of the second moment.

Figure 4. Selected inference rules of the derivation system.

(Q-Tick)

\[ Q = \{k^p c^q \} \otimes M \]

\[ \Delta \vdash \{ \Gamma; Q \} \textbf{tick}(c) \{ \Gamma; Q' \} \]

(Q-Sample)

\[ \Gamma = \forall x \in \text{supp}(\mu_D); \Gamma' \]

\[ Q = \mathbb{E}_{x \sim \mu_D}[Q'] \]

\[ \Delta \vdash \{ \Gamma; Q \} x \sim D \{ \Gamma'; Q' \} \]

(Q-Prob)

\[ \Delta \vdash \{ \Gamma; Q \} S_1 \{ \Gamma'; Q' \} \]

\[ P = \{[p, 1, [0, 0], \cdots, [0, 0]] \otimes M \} \]

\[ Q_k = P_k \otimes_{\mathbb{R}} R_k \]

\[ \Delta \vdash \{ \Gamma; Q \} \text{if prob}(p) \text{ then } S_1 \text{ else } S_2 \text{ fi } \{ \Gamma'; Q' \} \]

\[ \text{func rdwalk() begin} \]

\[ \{x < n + 2; (1, 2(n-x), 4(n-x)^2 + 6(n-x) - 4)\} \]

\[ \text{if } x < n \text{ then} \]

\[ \{x < n; (1, 2(n-x), 4(n-x)^2 + 6(n-x) - 4)\} \]

\[ r \sim \text{uniform}(-1, 2); \]

\[ \{x < n \land r \leq 2; (1, 2(n-x-r) + 1, 4(n-x-r)^2 + 10(n-x-r) - 3)\} \]

\[ x := x + r; \]

\[ \{x < n + 2; (1, 2(n-x) + 1, 4(n-x)^2 + 10(n-x) - 3)\} \]

\[ \text{call rdwalk}; \{T; (1, 1, 1)\} \textbf{tick}(1) \{T; (1, 0, 0)\} \]

\[ \text{fi } \{T; (1, 0, 0)\} \]

end

Figure 5. The rdwalk function with annotations for the under-approximation of the second moment.

The language supports recursive functions, continuous distribu-

tions, unstructured control-flow, and local variables. To infer

the bounds on the central moments of the accumulated cost for a program, the user needs to specify an analysis mode (over- or under-approximation), the order of the an-

alyzed moment, and a maximal degree for the polynomials to be used in ranking-function templates. Using APRON [20], we implemented an interprocedural numeric analysis to infer the logical contexts used in the derivation system.

Our tool represents ranking functions by the unknown coefficients of the monomials in polynomials. The bound-

inference rules are implemented in a syntax-directed manner. Our tool generates linear constraints over the unknown coefficients on-the-fly and uses the off-the-shelf LP solver GLPK [39] to solve the constraints. The LP solver not only checks the satisfiability of the constraints, but is also able to optimize a linear objective function. For example, if the analyzed program is supplied with concrete inputs, we can instantiate the template at the beginning of the program with the concrete inputs, and use the obtained linear function over unknown coefficients as the objective. In our implementation, we allow symbolic inputs with optional pre-conditions (e.g., \(x < n + 2\) in Ex. 7.1) and to generate a concrete input that satisfies the condition. Note that the logical contexts are inferred with respect to the pre-condition; therefore, the obtained symbolic bounds are sound for all concrete inputs that satisfy the pre-condition.

Evaluation Setup. We evaluated our tool to answer to follow-

ing two research questions:

1. How does the raw-moment inference part of our tool compare to existing techniques for expected-cost bound analysis [28, 37]?

2. How does our tool compare to the state of the art in tail-probability analysis (which is based only on higher raw moments [24])?

For the first question, we collected a broad suite of challenge-

ing examples from related work [24, 28, 37] with different loop and recursion patterns, as well as probabilistic branching, discrete sampling, and continuous sampling. Our tool achieved comparable precision and efficiency with the prior work on expected-cost bound analysis [28, 37]. The details are included in appendix I.

For the second question, we evaluated our tool on the complete benchmarks from Kura el al. [24]. We also con-

ducted a case study of a timing-attack analysis, where central moments are more useful than raw moments to bound the success probability of an attacker. We include the case study in appendix I.

The experiments were performed on a machine with an Intel Core i7 3.6GHz processor and 16GB of RAM.

Results. The results of the evaluation to answer the second research question are presented in Tab. 2. The program (1-

and (1-2) describe the coupon-collector problems with a total of two and four coupons, respectively. The other five are variants of random walks. The first three are 1-

dimensional random walks: (2-1) is integer-valued, (2-2) is real-valued with continuous sampling, and (2-3) exhibits adversarial nondeterminism. The program (2-4) and (2-5) are 2-

dimensional random walks. The table contains the inferred over-approximations of the moments for runtimes of these programs, and the running times of the analyses. We compared our results with Kura et al.’s inference tool for higher moments [24]. Our tool is as precise as, and sometimes more precise than the prior work on all the benchmark programs. Meanwhile, our tool is able to infer an over-approximation of 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 ef-

ficiency, our tool processed all the analyses in less than 30

seconds, while the prior work took more than a few minutes on some programs. One reason why our tool is more
efficient is that we always reduce the higher-moment inference with non-linear polynomial templates to LP solving, but the prior work requires semidefinite programming (SDP) for polynomial templates.

Besides the raw moments, our tool is also capable of inferring over-approximations of the central moments of runtimes for the benchmarks. To evaluate the quality of the inferred central moments, Fig. 6 plots the upper bounds of tail probabilities on runtimes \( T \) obtained by Kura et al. [24], and those by our central-moment analysis. Specifically, the prior work uses Markov’s inequality (Prop. 2.2), while we are also able to apply Cantelli’s inequality (Prop. 2.3) with central moments. For both raw and central moments, the tail bounds \( \Pr(T \geq d) \) become more precise when the constant \( d \) is large. Our tool outperforms the prior work on program (1-1), (2-3), (2-5) and derives better tail bounds when \( d \) is large on program (2-2), (2-4), while it obtains similar curves on program (1-2), (2-1). Because our central-moment analysis involves over- and under-approximations of raw moments, the tail bounds obtained from central moments are significantly tighter if our tool can infer very precise over- and under-approximations of raw moments.

Beyond the precision and efficiency, our tool is also capable of deriving symbolic approximations of higher moments. Tab. 3 presents the inferred over-approximations of the second moments given by raw moments of degree up to four inferred by [24]. Each red line is the minimum of tail bounds given by \( x \geq y \). Each gray line is the minimum of tail bounds given by \( x \geq y \) compared to [24]. Each red line is the minimum of tail bounds given by [24].

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9 Conclusion

We have presented a tail-bound analysis of probabilistic programs that support general recursion and continuous sampling, by deriving symbolic over-/under-approximations of higher raw/central moments for the accumulated costs, and employing concentration-of-measure inequalities. We have proposed semantic optional stopping for probabilistic programs and moment monoids for compositional reasoning, as well as extended the classic Optional Stopping Theorem to prove soundness of our technique. The effectiveness of our
technique has been demonstrated with our prototype implementation and the analysis of a broad suite of benchmarks, as well as a case study of a timing-attack analysis.

In the future, we plan to go beyond arithmetic programs and add support for more datatypes, e.g., Booleans and lists. We will also work on other kinds of uncertain quantities for probabilistic programs. Another research direction is to apply our analysis to higher-order functional programs.

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A Preliminaries on Measure Theory

Interested readers can refer to textbooks and notes in the literature [4, 35] for more details.

A.1 Basics

A measurable space is a pair (|X|, $\Sigma_X$) where |X| is a nonempty set and $\Sigma_X$ is an $\sigma$-algebra over |X|, i.e., a subset of its powerset $\mathcal{P}(|X|)$ that contains $\emptyset$ and is closed under complement and countable union. For simplicity, most of the time we will write X for the pair. The smallest $\sigma$-algebra that contains $\mathcal{S} \subseteq \mathcal{P}(|X|)$ as a subset is said to be generated by $\mathcal{S}$, denoted by $\sigma(\mathcal{S})$. Every topological space $X$ admits a Borel $\sigma$-algebra, denoted by $\mathcal{B}(X)$, which is generated by its open sets. This gives a canonical $\sigma$-algebra on $\mathbb{R}$. A measurable function $f : X \to Y$ is a function from |X| to |Y| such that for all $B \in \Sigma_Y$, it holds that $f^{-1}(B) \in \Sigma_X$. Measurable functions from $X$ to $\mathbb{R}$ are called random variables on $X$.

A measure $\mu$ on a measurable space $X$ is a function from $\Sigma_X$ to $[0, +\infty]$ such that (i) $\mu(\emptyset) = 0$, and (ii) for all pairwise-disjoint $\omega$-chains $(A_n)_{n \in \mathbb{N}} \subseteq \Sigma_X$, it holds that $\sum_{n \in \mathbb{N}} \mu(A_n) = \mu(\bigcup_{n \in \mathbb{N}} A_n)$. For any measures $\mu, \nu$, we write $\mu + \nu$ for the measure $\lambda \mu(A) + \nu(A)$. For any measure $\mu$ and scalar $c \geq 0$, we write $c \cdot \mu$ for the measure $\lambda c \cdot \mu(A)$. For all $x \in |X|$, the Dirac measure $\delta(x)$ is defined as $\lambda A[x \in A]$. A measure $\mu$ on $X$ is called a probability measure if $\mu(\{x\}) = 1$. We denote the collection of probability measures on $X$ by $\mathcal{D}(X)$.

The integral of a random variable $f$ with respect to a measure $\mu$ on $X$ is defined following Lebesgue’s theory and denoted by $\int_A f \, d\mu$, or $\int_X f(x) \, d\mu(dx)$ where $A \in \Sigma_X$. If $A = X$, we also call the integration as the expectation of $f$, written $\mathbb{E}_X[f(x)]$, or simply $\mathbb{E}[f]$ when the scope is clear.

A kernel from a measurable space $X$ to another measurable space $Y$ is a function $\kappa : |X| \to \Sigma_Y \to [0, +\infty]$ such that:
1. $\kappa$ is $\mathcal{A}$-measurable, $\kappa(x)$ is a measure on $Y$, and
2. for all $B \in \Sigma_Y$, the function $\lambda \kappa \lambda B \kappa(x) \kappa$ is measurable.

Sometimes we will write $\kappa : X \rightsquigarrow Y$ to declare $\kappa$ as a kernel from $X$ to $Y$. We can “push” a measure $\mu$ on $X$ to a measure on $Y$ through a kernel $\kappa : X \to Y$ by integration with respect to $\mu^X(\mu \kappa \kappa x \kappa) \kappa \kappa (x) \kappa \kappa (dx)$. A kernel $\kappa$ is called a probability kernel if $\kappa(x)(|Y|) = 1$ for all $x \in |X|$.

A.2 Product Measures

The product of two measurable spaces $X$ and $Y$ is defined as $X \otimes Y \triangleq \{(x, y) \mid x \in X, y \in Y\}$, where $\rho_1$ is the $i$-the coordinate map (i.e., $\rho_1(x, y) = x$ and $\rho_2(x, y) = y$). The product measurable space carries the smallest $\sigma$-algebra that makes $\rho_1$ and $\rho_2$ measurable. If $\mu_1$ and $\mu_2$ are two probability measures on $X$ and $Y$, respectively,

then there exists a unique probability measure $\mu$ on $X \otimes Y$, called the product measure of $\mu_1$ and $\mu_2$, written $\mu_1 \otimes \mu_2$, such that $\mu(A \times B) = \mu_1(A) \cdot \mu_2(B)$ for all $A \in \Sigma_X$ and $B \in \Sigma_Y$.

If $\mu$ is a probability measure on $X$ and $\kappa : X \rightsquigarrow Y$ is a probability kernel, then we can construct the a probability measure on $X \otimes Y$ that captures all transitions from $\mu$ via $\kappa$:

$$ (\mu \otimes \kappa)((A, B)) \triangleq \int_A \kappa(x)(B) \mu(dx). $$

If $\mu$ is a probability measure on $X_0$ and $k_1 : X_{i-1} \rightsquigarrow X_i$ is a probability kernel for $i = 1, \cdots, n$ with $n \in \mathbb{N}$, then we can construct a probability measure on $\bigotimes_{i=1}^n X_i$, i.e., sequences of $n$ transitions by inductively applying $k_i$ to $\mu$:

$$ \mu \otimes \bigotimes_{i=1}^k k_i \triangleq (\mu \otimes \bigotimes_{i=1}^{k-1} k_i) \otimes k_k, \quad 0 < k \leq n. $$

It is also possible to define infinite products of measurable spaces. Let $X_i = (|X_i|, \Sigma_i), i \in I$ be a family of measurable spaces. Their product, denoted by $\bigotimes_{i \in I} X_i = (\prod_{i \in I} |X_i|, \bigotimes_{i \in I} \Sigma_i)$, is the product space with the smallest $\sigma$-algebra such that for every $i \in I$, the coordinate map $\rho_i$ is measurable. The following theorem is widely used to construct a probability measures over an infinite product via a kernel.

Proposition A.1 (Ionescu-Tulcea). Let $S_0 = (|S_0|, \Sigma_0)$ be a measurable space and $\mu_0$ be a probability measure on $S_0$. Let $S_i = (|S_i|, \Sigma_i)$ be a sequence of measurable spaces for all $i \in \mathbb{N}$. For each $i \in \mathbb{N}$, let $k_i : S^{i-1} \rightsquigarrow S_i$ be a probability kernel, where $S^i \triangleq \bigotimes_{k=0}^i S_k$. Then there exists a sequence of probability measures $\mu_i \triangleq \mu_0 \otimes \bigotimes_{k=i}^{\infty} k_k$, and there exists a uniquely defined probability measure $\mu$ on $\bigotimes_{k=i}^{\infty} S_k$ such that $\mu(A) = \mu_0 \otimes \prod_{k=i}^{\infty} S_k = \mu_0 \otimes \bigotimes_{k=i}^{\infty} k_k$, for all $i \in \mathbb{N}$ and $A \in \Sigma_i$.

A.3 Conditional Expectations

Let $(\Omega, \mathcal{F}, \mu)$ be a measure space. Let $X : \Omega \to \mathbb{R}$ be an integrable random variable and $\mathcal{G} \subseteq \mathcal{F}$ be a sub-$\sigma$-algebra of $\mathcal{F}$. Then there exists a random variable $Y : \Omega \to \mathbb{R}$ such that:
1. $Y$ is $\mathcal{G}$-measurable, (ii) $Y$ is integrable, i.e., $\mathbb{E}[|Y|] < \infty$, and
3. for every set $G$ of $\mathcal{G}$, it holds that $\int_G Y \, d\mu = \int_G X \, d\mu$. Such a random variable $Y$ is said to be a version of conditional expectation $\mathbb{E}[X \mid \mathcal{G}]$ of $X$ given $\mathcal{G}$. Conditional expectations admit almost-sure uniqueness.

Intuitively, for some $\omega \in \Omega$, $Y(\omega) = \mathbb{E}[X \mid \mathcal{G}](\omega)$ is the expectation of $X$ given the set of values $Z(\omega)$ for every $\mathcal{G}$-measurable random variable $Z$. For example, if $\mathcal{G} = \{\emptyset, \Omega\}$, which contains no information, then $\mathbb{E}[X \mid \mathcal{G}](\omega) = \mathbb{E}[X]$ for all $\omega \in \Omega$.

We review some useful properties of conditional expectations.

Proposition A.2. Suppose $X : \Omega \to \mathbb{R}$ is an integrable random variable.
(a) If $Y$ is any version of $\mathbb{E}[X \mid \mathcal{G}]$, then $\mathbb{E}[Y] = \mathbb{E}[X]$.
(b) If $X$ is $\mathcal{G}$-measurable, then $\mathbb{E}[X \mid \mathcal{G}] = X$, a.s.
(c) If $Z$ is $\mathcal{G}$-measurable, then $E[Z \cdot X | \mathcal{G}] = Z \cdot E[X | \mathcal{G}]$, a.s.

### A.4 Convergence Theorems

We review two important convergence theorems for series of random variables.

**Proposition A.3** (Monotone convergence theorem). If \( \{f_n\}_{n \in \mathbb{Z}^+} \) is a non-decreasing sequence of nonnegative $\Sigma_X$-measurable functions in a measure space $X = ([X], \Sigma_X, \mu)$ and $\{f_n\}_{n \in \mathbb{Z}^+}$ converges to $f$ pointwise, then $f$ is also $\Sigma_X$-measurable and
\[
\lim_{n \to \infty} \int_X f_n(x) \mu(dx) = \int_X f(x) \mu(dx).
\]

**Proposition A.4** (Dominated convergence theorem). If $\{f_n\}_{n \in \mathbb{Z}^+}$ is a sequence of $\Sigma_X$-measurable functions in a measure space $X = ([X], \Sigma_X)$, $\{f_n\}_{n \in \mathbb{Z}^+}$ converges to $f$ pointwise, and $\{f_n\}_{n \in \mathbb{Z}^+}$ is dominated by a nonnegative integrable function $g$, i.e., $f_n(x) \leq g(x)$ for each $n \in \mathbb{Z}^+$ and $x \in [X]$ where $\int_X gd\mu < \infty$, then $f$ is integrable and
\[
\lim_{n \to \infty} \int_X f_n(x) \mu(dx) = \int_X f(x) \mu(dx).
\]

Further, the theorem is still true if the domination holds almost everywhere and $f$ is chosen as a measurable function that agrees almost everywhere with the almost everywhere existing pointwise limit.

### B Operational Cost Semantics

We follow Borgström et al.’s distribution-based small-step operational semantics for probabilistic lambda calculus [5] to define reduction rules for the semantics of APPL. A probabilistic semantics steps a program configuration to a probability distribution over configurations. To formally describe these distributions, we need to construct a measurable space of program configurations. Our 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** $\gamma : \text{VID} \to \mathbb{R}$ are finite real-valued maps, so we define $X_V \defeq ([X_V], \Sigma_{X_V})$ as the canonical structure for finite-dimensional spaces:
\[
[X_V] \subseteq \mathbb{R}^{\text{VID}}, \quad \Sigma_{X_V} \defeq \sigma(\mathcal{B}(\mathbb{R})^{\text{VID}}).
\]
- **The executing statement $S$ can contain real numbers**, so we need to “lift” the Borel $\sigma$-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, we achieve this by constructing a metric space over statements and then extracting a Borel $\sigma$-algebra from the metric space. Fig. 7 presents a recursively defined metric $d_S$ over statements, as well as metrics $d_E$, $d_1$, and $d_D$ over expressions, conditions, and distributions, respectively, as they are required by $d_S$. We denote the result measurable space by $X_S$.
- **Similarly**, we construct a measurable space $X_K$ over continuations by extracting from a metric space. Fig. 7 shows the definition of a metric $d_K$ over continuations.
- **The cost accumulator $\alpha \in \mathbb{R}$ is a real number**, so we define $X_A \defeq (\mathbb{R}, \mathcal{B}(\mathbb{R}))$ as the canonical measurable space on $\mathbb{R}$.

Then the semantic domain is defined as the product measurable space of the four components: $\Sigma \defeq X_V \otimes X_S \otimes X_K \otimes X_A$.

Fig. 8 presents the rules of the evaluation relation $\rightarrow$ for APPL where $\sigma$ is a configuration and $\mu$ is a probability distribution over configurations. Note that in APPL, expressions $E$ and conditions $L$ are deterministic, so we define a standard big-step evaluation relation for them, written $\gamma \vdash E \downarrow r$ and $\gamma \vdash L \downarrow b$, where $\gamma$ is a valuation, $r \in \mathbb{R}$, and $b \in \{2\}$. Most of the rules in Fig. 8, except (E-SAMPLE) and (E-PROB), are also deterministic as they step to a Dirac measure.

The evaluation relation $\rightarrow$ can be interpreted as a distribution transformer. Indeed, $\rightarrow$ can be seen as a probability kernel.

**Lemma B.1.** Let $\gamma : \text{VID} \to \mathbb{R}$ 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 $b \in \{2\}$ such that $\gamma \vdash L \downarrow b$.

**Proof.** By induction on the structure of $E$ and $L$.

**Lemma B.2.** For every configuration $\sigma \in \Sigma$, there exists a unique $\mu \in \mathcal{D}(\Sigma)$ such that $\sigma \vdash \mu$.

**Proof.** Let $\sigma = \langle y, S, K, a \rangle$. Then by case analysis on the structure of $S$, followed by a case analysis on the structure of $K$ is $S = \text{skip}$. The rest of the proof appeals to Lem. B.1.

**Theorem B.3.** The evaluation relation $\rightarrow$ defines a probability kernel over program configurations.

**Proof.** Lem. B.2 tells us that $\rightarrow$ can be seen as a function $\rightarrow$ defined as follows:
\[
\rightarrow(\sigma)(A) \defeq \mu(A) \quad \text{where} \quad \sigma \vdash \mu.
\]

It is clear that $\rightarrow(\sigma)$ is a probability measure. On the other hand, to show that $\lambda \sigma. \rightarrow(\sigma)(A)$ is measurable for any measurable $A$, we need to prove that $O(A, B) \defeq (\lambda \sigma. \rightarrow(\sigma)(A))^{-1}(B)$ is a measurable set of configurations whenever $B$ is a measurable set of real numbers.

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

\[
\begin{align*}
\hat{S} & : \text{skip} | \text{tick}(\square) | x := \hat{E} | x \sim \hat{D} | \text{call } f \\
& | \text{if } \text{prob}(\square) \text{ then } \hat{S}_1 \text{ else } \hat{S}_2 | \text{if } \hat{L} \text{ then } \hat{S}_1 \text{ else } \hat{S}_2 \\
& | \text{while } \hat{L} \text{ do } \hat{S} \text{ od } | \hat{S}_1 | \hat{S}_2 \\
\hat{L} & : \texttt{tt} | \text{not } \hat{L} | \hat{L}_1 \text{ and } \hat{L}_2 | \hat{E}_1 <= \hat{E}_2 \\
\hat{E} & : x | \square \ell \ | \hat{E}_1 + \hat{E}_2 | \hat{E}_1 \ast \hat{E}_2 \\
\hat{D} & : \text{gaussian}(\square \ell_1, \square \ell_2) | \text{uniform}(\square \ell_1, \square \ell_2)
\end{align*}
\]
\[ d_E(x, x) \overset{\text{def}}{=} 0 \]
\[ d_E(c_1, c_2) \overset{\text{def}}{=} |c_1 - c_2| \]
\[ d_E(E_{11} \ast E_{12}, E_{21} \ast E_{22}) \overset{\text{def}}{=} d_E(E_{11}, E_{21}) + d_E(E_{12}, E_{22}) \]
\[ d_E(E_{11} \ast E_{12}, E_{21} \ast E_{22}) \overset{\text{def}}{=} d_E(E_{11}, E_{21}) + d_E(E_{12}, E_{22}) \]
\[ d_E(E_1, E_2) \overset{\text{def}}{=} \infty \text{ otherwise} \]

\[ d_D(\text{uniform}(a_1, b_1), \text{uniform}(a_2, b_2)) \overset{\text{def}}{=} |a_1 - a_2| + |b_1 - b_2| \]
\[ d_D(D_1, D_2) \overset{\text{def}}{=} \infty \text{ otherwise} \]

\[ d_S(\text{skip}, \text{skip}) \overset{\text{def}}{=} 0 \]
\[ d_S(\text{tick}(c_1), \text{tick}(c_2)) \overset{\text{def}}{=} |c_1 - c_2| \]
\[ d_S(x := E_1, x := E_2) \overset{\text{def}}{=} d_E(E_1, E_2) \]
\[ d_S(x - D_1, x - D_2) \overset{\text{def}}{=} d_D(D_1, D_2) \]
\[ d_S(\text{call } f, \text{call } f) \overset{\text{def}}{=} 0 \]
\[ d_S(\text{if } \text{prob}(p_1) \text{ then } S_{11} \text{ else } S_{12} \text{ fi}, \text{if } \text{prob}(p_2) \text{ then } S_{21} \text{ else } S_{22} \text{ fi}) \overset{\text{def}}{=} \left| p_1 - p_2 \right| + d_S(S_{11}, S_{21}) + d_S(S_{12}, S_{22}) \]
\[ d_S(\text{if } L_1 \text{ then } S_{11} \text{ else } S_{12} \text{ fi}, \text{if } L_2 \text{ then } S_{21} \text{ else } S_{22} \text{ fi}) \overset{\text{def}}{=} d_L(L_1, L_2) + d_S(S_{11}, S_{21}) + d_S(S_{12}, S_{22}) \]
\[ d_S(\text{while } L_1 \text{ do } S_1 \text{ od}, \text{while } L_2 \text{ do } S_2 \text{ od}) \overset{\text{def}}{=} d_L(L_1, L_2) + d_S(S_1, S_2) \]
\[ d_S(S_{11}; S_{12}; S_{21}; S_{22}) \overset{\text{def}}{=} d_S(S_{11}, S_{21}) + d_S(S_{12}, S_{22}) \]
\[ d_S(S_1, S_2) \overset{\text{def}}{=} \infty \text{ otherwise} \]

\[ d_K(\text{Kseq } S_1 K_1, \text{Kseq } S_2 K_2) \overset{\text{def}}{=} d_S(S_1, S_2) + d_K(K_1, K_2) \]
\[ d_K(K_1, K_2) \overset{\text{def}}{=} \infty \text{ otherwise} \]

\[ d_K(\text{Kloop } L_1 S_1 K_1, \text{Kloop } L_2 S_2 K_2) \overset{\text{def}}{=} d_L(L_1, L_2) + d_S(S_1, S_2) + d_K(K_1, K_2) \]
\[ d_K(\text{Kstop}, \text{Kstop}) \overset{\text{def}}{=} 0 \]

\[ \hat{K} := K_{\text{stop}} \mid K_{\text{loop }} L \hat{S} \hat{K} \mid \text{Kseq } \hat{S} \hat{K} \]

Figure 7. Metrics for expressions, conditions, distributions, statements, and continuations.

The holes \( \Box_l \) are placeholders for real numbers parameterized by locations \( l \in \mathcal{L} \). We assume that the holes in a program structure are always pairwise distinct. Let \( \eta : \mathcal{L} \to \mathbb{R} \) be a map from holes to real numbers and \( \eta \hat{S}, \eta \hat{L}, \eta \hat{E}, \eta \hat{D}, \eta \hat{K} \) the instantiation of a statement (resp., condition, expression, distribution, continuation) skeleton by substituting \( \eta(l) \) for \( \Box_l \). 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. 7.

Observe that:
\[ \mathcal{O}(A, B) = \bigcup_{\hat{S}, \hat{K}} \mathcal{O}(A, B) \cap \{ \gamma, \eta \hat{S}, \eta \hat{L}, \eta \hat{E}, \eta \hat{D}, \eta \hat{K}, \alpha \mid \text{any } \gamma, \alpha, \eta \} \]
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 \( \hat{C}(\hat{S}, \hat{K}) \) later in the proof, is measurable. Note that \( C(\hat{S}, \hat{K}) \) 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 \( \overset{\text{det}}{=} \) by getting rid of the \( \delta(\cdot) \) notations in the rules in Fig. 8 except probabilistic ones (E-SAMPLE) and (E-PROB). Obviously, \( \overset{\text{det}}{=} \) can be interpreted as a measurable function over configurations.

- If the evaluation rule is deterministic, then we have:
\[ \mathcal{O}(A, B) \cap \hat{C}(\hat{S}, \hat{K}) = \{ \sigma \mid \sigma \mapsto \mu, \mu(A) \in B \} \cap \hat{C}(\hat{S}, \hat{K}) \]
The expression $E$ evaluates to a real value $r$ under the valuation $\gamma$.

The condition $L$ evaluates to a Boolean value $b$ under the valuation $\gamma$.

The configuration $(y, S, K, \alpha)$ steps to a probability distribution $\mu$ over $(y', S', K', \alpha')$'s.

\[
\langle y, S, K, \alpha \rangle \mapsto \delta(\langle y, S, K, \alpha \rangle)
\]

\[
\langle y, \text{skip, Kstop}, \alpha \rangle \mapsto \delta(\langle y, \text{skip, Kstop}, \alpha \rangle)
\]

\[
\langle y, \text{tick}(c), K, \alpha \rangle \mapsto \delta(\langle y, \text{tick}, K, \alpha + c \rangle)
\]

\[
\langle y, x := E, K, \alpha \rangle \mapsto \delta(\langle y[x := r], \text{skip}, K, \alpha \rangle)
\]

\[
\langle y, \text{if prob}(\alpha) \text{ then } S_1 \text{ else } S_2 \text{ fi, K, } \alpha \rangle \mapsto \delta(\langle y, \text{if prob}(\alpha) \text{ then } S_1 \text{ else } S_2 \text{ fi, K, } \alpha \rangle + (1 - p) \delta(\langle y, S_2, K, \alpha \rangle))
\]

\[
\langle y, \text{if } L \text{ then } S_1 \text{ else } S_2 \text{ fi, K, } \alpha \rangle \mapsto \delta(\langle y, \text{if } L \text{ then } S_1 \text{ else } S_2 \text{ fi, K, } \alpha \rangle + [\neg b] \delta(\langle y, S_2, K, \alpha \rangle))
\]

\[
\langle y, \text{while } L \text{ do } S \text{ od, K, } \alpha \rangle \mapsto \delta(\langle y, \text{while } L \text{ do } S \text{ od, K, } \alpha \rangle)
\]

Figure 8. Rules of the operational semantics of Appl.

$$
\begin{align*}
\exists \sigma [\sigma &\xrightarrow{\text{det}} \sigma', [\sigma' \in A] \in B] \cap C(\hat{S}, \hat{K}) \\
C(\hat{S}, \hat{K}) &= \begin{cases}
\{0, 1\} & \text{if } B = \emptyset \\
\left\{(A) \cap C(\hat{S}, \hat{K}) \right\} & \text{if } 1 \in B \\
\left\{(A') \cap C(\hat{S}, \hat{K}) \right\} & \text{if } 0 \in B \\
\emptyset & \text{if } 0, 1 \cap B = \emptyset
\end{cases}
\end{align*}
$$

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

- (E-Prob): Consider $B$ with the form $(-\infty, t]$ with $t \in \mathbb{R}$. Similar to the previous case, we assume that $t < 1$. Let $\hat{S} = x \sim \text{uniform}(\square t, \square t)$, without loss of generality. Then we have

$$
O(A, B) \cap C(\hat{S}, \hat{K}) = \{[\sigma, \mu(A) \in B] \cap C(\hat{S}, \hat{K})
$$

\[
\begin{align*}
\exists \sigma [\sigma &\xrightarrow{\text{det}} \mu, [\mu(A) \in B] \cap C(\hat{S}, \hat{K}) \\
\{[\sigma, \mu(A) &\in B] \cap C(\hat{S}, \hat{K})
\end{align*}
\]
whose, there is a sub-probability kernel \( \kappa_D : \mathbb{R}^{\mathbb{R}} \to \mathbb{R} \).
For example, \( \kappa_{\text{uniform}}(a, b) \) is defined to be \( \ell_{\text{uniform}}(a, b) \) if \( a < b \), or \( 0 \) otherwise. Therefore, \( \lambda(a, b, k_{\text{uniform}}(a, b))(r | \langle y | x \to r, \text{skip}, K, a \rangle \in A) \) is measurable, and its inversion on \( (-\infty, t) \) is a measurable set over distribution parameters \((a, b)\). Hence the set above is measurable.

\[ \square \]

C Trace-Based Cost Semantics
To reason about moments of the accumulated cost, we follow the Markov-chain-based reasoning [22, 29] to develop a trace-based cost semantics for AppL. Let \((\Omega, \mathcal{F}) \cong \Sigma^N\) be a measurable space of infinite traces over 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-\(\sigma\)-algebras in \( \mathcal{F} \), generated by coordinate maps \( X_n(\omega) \) for \( n \in \mathbb{Z}^+ \). Let \( \mu_0 \cong \delta((\lambda_0, 0, S_{\text{main}}, K_{\text{stop}}, 0)) \) be the initial distribution. Let \( \mathbb{P} \) be the probability measure over infinite traces induced by Prop. A.1 and Thm. B.3. Then \((\Omega, \mathcal{F}, \mathbb{P})\) forms a probability space over infinite traces for a program.

D Trace-Based Reasoning on Expectations
Recall that we define a stopping time \( T : \Omega \to \mathbb{Z}^+ \cup \{\infty\} \) as
\[
T(\omega) \cong \inf\{n \in \mathbb{Z}^+ \mid \omega_n = (\_ \_ \_ \_ \text{skip}, K_{\text{stop}}, \_ \_ \) \},
\]
and random variables \( \{A_n\}_{n \in \mathbb{Z}^+}, \{\Phi_n\}_{n \in \mathbb{Z}^+}, \{Y_n\}_{n \in \mathbb{Z}^+} \) as
\[
A_n(\omega) \cong \alpha_n \text{ where } \omega_n = (\_ \_ \_ \_ \_),
\]
\[
\Phi_n(\omega) \cong \phi(\omega_n),
\]
\[
Y_n(\omega) \cong A_n(\omega) + \Phi_n(\omega),
\]
where \( \phi : \Sigma \to \mathbb{R} \) is a ranking function for expected cost bound analysis. We also define \( A_{\infty}(\omega) \cong 0, \Phi_{\infty}(\omega) \cong 0, \) and thus \( Y_{\infty}(\omega) \cong 0 \). Taking the stopping time into consideration, we define the stopped version for these random variables as
\[
A_T(\omega) \cong A_T(\omega), \Phi_T(\omega) \cong \Phi_T(\omega), Y_T(\omega) \cong Y_T(\omega).
\]
Lemma D.1. If \( \mathbb{P}[T < \infty] = 1 \), i.e., the program terminates almost surely, then \( \mathbb{P}[\lim_{n \to \infty} A_n = A_T] = 1 \). Further, if \( \{A_n\}_{n \in \mathbb{Z}^+} \) is pointwise non-decreasing, then \( \lim_{n \to \infty} \mathbb{E}[A_n] = \mathbb{E}[A_T] \).

Proof. By the property of the operational semantics, for each \( \omega \in \Omega \), we have \( A_n(\omega) = A_T(\omega) \) for all \( n \geq T(\omega) \). Then we have
\[
\mathbb{P}[\lim_{n \to \infty} \mathbb{E}[A_n] = \mathbb{E}[A_T]] = \mathbb{P}(\{\omega \mid \mathbb{E}[A_n(\omega) = A_T(\omega)]\})
\geq \mathbb{P}(\{\omega \mid \lim_{n \to \infty} A_n(\omega) = A_T(\omega) \wedge T(\omega) < \infty\})
= \mathbb{P}(\{\omega \mid A_T(\omega) = A_T(\omega) \wedge T(\omega) < \infty\})
= \mathbb{P}(\{\omega \mid T(\omega) < \infty\})
= 1.
\]
Now let us assume that \( \{A_n\}_{n \in \mathbb{Z}^+} \) is pointwise non-decreasing. By the property of the operational semantics, we know that \( A_0 = 0 \). Therefore, \( A_n \)'s are nonnegative random variables, and their expectations \( \mathbb{E}[A_n] \)'s are well-defined. By Prop. A.3, we have \( \lim_{n \to \infty} \mathbb{E}[A_n] = \mathbb{E}[\lim_{n \to \infty} A_n] \). We then conclude by the fact that \( \lim_{n \to \infty} A_n = A_T, a.s. \), which is just proved.

We reformulate the martingale property using the filtration \( \{\mathcal{F}_n\}_{n \in \mathbb{Z}^+} \).

Lemma D.2. For all \( n \in \mathbb{Z}^+ \), it holds that
\[
\mathbb{E}[Y_{n+1} | \mathcal{F}_n] = Y_n, a.s.,
\]
i.e., the expectation of \( Y_n \) conditioned on the execution history is an invariant for \( n \in \mathbb{Z}^+ \).

Proof. We say that a sequence of random variables \( \{X_n\}_{n \in \mathbb{Z}^+} \) is 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 \( \omega_n \). Then we have
\[
\mathbb{E}[Y_{n+1} | \mathcal{F}_n](\omega) = \mathbb{E}[A_{n+1} + \Phi_{n+1} | \mathcal{F}_n](\omega)
= \mathbb{E}[(A_{n+1} - A_n) + \Phi_{n+1} + A_n | \mathcal{F}_n](\omega)
= \mathbb{E}[(A_{n+1} - A_n) + \Phi_{n+1} | \mathcal{F}_n](\omega) + A_n(\omega)
= \mathbb{E}[(A_{n+1} - A_n) + \Phi(\omega_n) | \mathcal{F}_n] + A_n(\omega)
= \mathbb{E}[\sigma'=\sigma(\omega_n)[(\alpha' - \alpha_n) + \phi(\sigma')] + A_n(\omega)]
= \phi(\omega_n) + A_n(\omega)
= \Phi_n(\omega) + A_n(\omega)
= Y_n(\omega).
\]
Furthermore, we have the following corollary:
\[
\mathbb{E}[Y_{n+1}] = \mathbb{E}[(\mathbb{E}[Y_{n+1} | \mathcal{F}_n])] = \mathbb{E}[Y_n],
\]
for each \( n \in \mathbb{Z}^+ \), thus \( \mathbb{E}[Y_n] = \mathbb{E}[Y_0] \) for all \( n \in \mathbb{Z}^+ \).

Now we can prove soundness of the extended OST.

Theorem (Thm. 5.3). If \( \mathbb{P}[Y_n < \infty] = 1 \) for all \( n \in \mathbb{Z}^+ \), then \( \mathbb{P}[Y_T] \) exists and \( \mathbb{E}[Y_T] = \mathbb{E}[Y_0] \) in the following situation:
There exist \( \ell \in [0, 1] \) and \( C \geq 0 \) such that \( \mathbb{E}[T^\ell] < \infty \) and for all \( n \in \mathbb{Z}^+, |Y_n| \leq C \cdot (n + 1)^\ell \) almost surely.

Proof. By \( \mathbb{E}[T^\ell] < \infty \) where \( \ell \geq 1 \), we know that \( \mathbb{P}[T < \infty] = 1 \). Then similar to the proof of Lem. D.1, we know that \( \mathbb{P}[\lim_{n \to \infty} Y_n = Y_T] = 1 \). On the other hand, we have
\[
|Y_n| = |\min(T, n + 1)| \leq C \cdot (n + 1)^\ell \leq C \cdot (T + 1)^\ell, a.s.
\]
Recall that \( \mathbb{E}[T^\ell] < \infty \). Then \( \mathbb{E}[T^\ell + 1] = \mathbb{E}[T^\ell + O(T^{\ell-1})] < \infty \). By Prop. A.4, with the function \( g \) set to \( \lambda(\omega) \cdot C \cdot (T^\ell + 1)^\ell \), we know that \( \lim_{n \to \infty} \mathbb{E}[Y_n] = \mathbb{E}[Y_T] \). By Lem. D.2, we have \( \mathbb{E}[Y_n] = \mathbb{E}[Y_0] \) for all \( n \in \mathbb{Z}^+ \) thus we conclude that \( \mathbb{E}[Y_n] = \mathbb{E}[Y_T] \).

\[ \square \]

E Termination Analysis
In this section, we develop a technique to reason about upper bounds on higher moments \( \mathbb{E}[T^m] \) of the stopping time \( T \). We adapt the idea of ranking functions, but rely
on a simpler convergence proof. In this section, we assume \( \mathcal{R} = \{(0, \infty], \leq, +, 0, 1\} \) to be a partially ordered semiring on extended nonnegative real numbers.

**Definition E.1.** A map \( \psi : \Sigma \to \mathcal{M}_\mathcal{R} \) is said to be a ranking function for upper bounds on stopping time if

(i) \( \psi(\sigma)_0 = 1 \) for all \( \sigma \in \Sigma \),

(ii) \( \psi(\sigma) = 1_M \) if \( \sigma = (\_ , \text{skip, Kstop, } _) \), and

(iii) \( \psi(\sigma) \sqsupseteq_M \mathbb{E}_{\sigma^{-}\prec}(1, 1, \cdots, 1) \otimes_M \psi(\sigma') \) 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 \( \sigma \). We define \( A_n \) and \( \Psi_n \), where \( n \in \mathbb{Z^+} \) to be random variables on the probability space \((\Omega, \mathcal{F}, P)\) of the trace semantics as \( A_n(\omega) \triangleq n^k \) and \( \Psi_n(\omega) \triangleq \psi(\omega) \). Then we define \( A_T(\omega) \triangleq A_T(\omega) \). Note that here we define \( A_{\infty}(\omega) = \lim_{n \to \infty} A_n(\omega) = (0, \infty, \cdots, \infty) \). Note that \( T_T = T_k \).

We now show that a valid ranking function for stopping time always gives a sound upper bound.

**Theorem E.2.** \( E[A_T] \subseteq_M E[\Psi] \).

**Proof.** Let \( C_n(\omega) \triangleq (1, 1, \cdots, 1) \) if \( n < T(\omega) \), otherwise \( C_n(\omega) \triangleq (1, 0, \cdots, 0) \). Then \( A_T = \bigotimes_{i=0}^{\infty} C_i \) for all \( n \in \mathbb{Z^+} \). By Prop. A.3, we know that \( E[A_T] = \lim_{n \to \infty} \mathbb{E}_{(\bigotimes_{i=0}^{n} C_i)} \). Thus it suffices to show that for all \( n \in \mathbb{Z^+} \), \( \mathbb{E}_{(\bigotimes_{i=0}^{n} C_i)} \subseteq_M \mathbb{E}[\Psi] \).

Observe that \( \{C_n\}_{n \in \mathbb{Z^+}} \) is adapted to \( \{\mathcal{F}_n\}_{n \in \mathbb{Z^+}} \), because the event \( \{T \leq n\} \) is \( \mathcal{F}_n \)-measurable. Then we have

\[
E[C_0 \otimes_M \Psi_{n+1} | \mathcal{F}_n] = E[C_0 \otimes_M \Psi_{n+1} | \mathcal{F}_n] = \mathbb{E}_{(\bigotimes_{i=0}^{n} C_i)} \subseteq_M \mathbb{E}[\Psi].
\]

Therefore, \( \mathbb{E}_{(\bigotimes_{i=0}^{n} C_i)} \subseteq_M \mathbb{E}[\Psi] \) for all \( n \in \mathbb{Z^+} \) by a simple induction. Because \( \Psi_{n+1} \sqsupseteq_M 1_M \), we conclude that

\[
\mathbb{E}_{(\bigotimes_{i=0}^{n} C_i)} \subseteq_M \mathbb{E}[\Psi].
\]

\( \square \)

## F Trace-Based Reasoning on Moments

We start with the fundamental composition property for moment monoids.

**Lemma (Lem. 6.2).** For all \( u, v \in \mathcal{R} \), it holds that

\[
(1_{\mathcal{R}}, (u \oplus v), (u \oplus v)^2, \ldots, (u \oplus v)^m)
= (1_{\mathcal{R}}, u^r, \cdots, u^m) \otimes_M (1_{\mathcal{R}}, v^r, \cdots, v^m),
\]

where \( u^r \) is an abbreviation for \( \bigotimes_{i=1}^{n} u \) for \( n \in \mathbb{Z^+} \).

**Proof.** Observe that

\[
RHS_k = \bigoplus_{i=0}^{k} (k \choose i) \cdot (u^i \otimes v^{k-i}).
\]

We prove by induction on \( k \) that \( (u \oplus v)^k = RHS_k \).

- \( k = 0 \): Then \( (u \oplus v)^0 = \_ \). On the other hand, we have \( RHS_0 = \_ \).

- Suppose that \( (u \oplus v)^k = RHS_k \). Then \( (u \oplus v)^{k+1} = (u \oplus v) \otimes (u \oplus v)^k \)

\[
= (u \oplus v) \otimes \bigoplus_{i=0}^{k} (k \choose i) \cdot (u^i \otimes v^{k-i})
= \bigoplus_{i=0}^{k} (k \choose i) \cdot (u^i \otimes v^{k-i} + v^i \otimes u^{k-i})
= \bigoplus_{i=0}^{k+1} (k \choose i) \cdot (u^i \otimes v^{k-i})
= RHS_{k+1}.
\]

We also show that \( \otimes_M \) is monotone if the operations of the underlying semiring are monotone.

**Lemma F.1.** Let \( \mathcal{R} = ([\mathcal{R}], \sqsubseteq, \circledast, \ominus, 0, 1) \) be a partially ordered semiring. If \( \circledast \) and \( \ominus \) are monotone with respect to \( \sqsubseteq \), then \( \otimes_M \) in the moment monoid \( \mathcal{M}_\mathcal{R} \) is also monotone with respect to \( \sqsubseteq_M \).

**Proof.** Without loss of generality, we show that \( \overline{u} \otimes_M \overline{v} \subseteq_M \overline{u} \circledast_M \overline{v} \). By the definition of \( \sqsubseteq_M \), we know that \( v_k \sqsubseteq w_k \) for all \( k = 0, 1, \cdots, m \). Then for each \( k \), we have

\[
(u \otimes v)^k = \bigoplus_{i=0}^{k} (k \choose i) \cdot (u^i \otimes v^{k-i})
= \bigoplus_{i=0}^{k} (k \choose i) \cdot (u^i \otimes w^{k-i})
= (u \otimes_M \overline{v})^k.
\]

Then we conclude by the definition of \( \sqsubseteq_M \).

As we allow ranking functions to be interval-valued, we show that the interval semiring \( \mathcal{I} \) satisfies the monotonicity required in Lem. F.1.

**Lemma F.2.** The operations \( \otimes_\mathcal{I} \) and \( \otimes_\mathcal{I} \) are monotone with respect to \( \sqsubseteq_\mathcal{I} \).
Proof. It is straightforward to show \( \Theta \) is monotone. For the rest of the proof, it suffices to show that \([a, b] \otimes [c, d] \subseteq [a', b'] \otimes [c, d]\) if \([a, b] \subseteq [a', b']\), i.e., \([a, b] \subseteq [a', b']\) or \(a \geq a', b \leq b'\).

We claim that \(\min S_{a,b,c,d} \geq \min S_{a',b,c,d}\). i.e., \(\min \{a', b', c', d'\} \geq \min \{a', b', c', d'\}\).

- If \(0 \leq c \leq d\): Then \(a \leq c, a \leq b, a \leq c, b \leq d\).
  
  Then it suffices to show that \(a \leq b, a \leq c, a \leq d\).

- Because \(d \geq c \geq 0\) and \(a \geq a'\), we conclude that \(a \geq a' c\) and \(a \leq d\).

- If \(c < 0 \leq d\): Then \(a \leq c, a \leq b, a \leq c, b \leq d\).
  
  Then it suffices to show that \(a \leq b, a \leq c, a \leq d\).

- Because \(d \geq c \geq 0\) and \(a \geq a'\), we conclude that \(a \geq a' c\) and \(a \leq d\).

In a similar way, we can also prove that \(\max S_{a,b,c,d} \leq \max S_{a',b,c,d}\).

Lemma F.3. If \(\{[a_n, b_n]\}_{n \in \mathbb{Z}^+}\) is a montone sequence in \(\mathbb{Z}^+\), i.e., \([a_n, b_n] \subseteq [a_{n+1}, b_{n+1}] \subseteq [a_{n+2}, b_{n+2}] \subseteq \cdots\) and \([a_n, b_n] \subseteq [c, d]\) 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 \([a, b] \subseteq [c, d]\).

Proof. By the definition of \(\subseteq\), we know that \([a_n]\) is non-increasing and \([b_n]\) is non-decreasing. Because \(a_n \geq c\) for all \(n \in \mathbb{Z}^+\), we conclude that \(\lim_{n \to \infty} a_n \geq c\). Because \(b_n \leq d\) for all \(n \in \mathbb{Z}^+\), we conclude that \(\lim_{n \to \infty} b_n \leq d\). Thus we conclude that \([a, b] \subseteq [c, d]\).

Recall that we extend the notions of \(A_n, \Phi_n, Y_n\) with intervals for higher moments as follows:

\[
A_n(\omega) = \{a^n_k, a^n_n\} \text{ where } \omega_n = \langle \ldots, a^n_0, a^n_n \rangle, \\
\Phi_n(\omega) = \varphi(\omega_n), \\
Y_n(\omega) = A_n(\omega) \otimes_M \Phi_n(\omega).
\]

Note that in the definition of \(Y_n\), we use \(\otimes_M\) to compose the powers of the accumulated cost at step \(n\) and the ranking function that stands for the moments of the accumulated cost of the rest of the computation.

We now extend some of the previous results on first moments to higher moments with intervals.

Lemma F.4. If \(X: \Omega \to \mathcal{M}_2\) is \(\mathcal{G}\)-measurable and \(X(\omega) = [a_k(\omega), a_k(\omega)]\) for all \(\omega \in \Omega\), then \(\mathbb{E}[X \otimes_M Y \mid \mathcal{G}] = \mathbb{E}[X \otimes_M Y \mid \mathcal{G}]\) almost surely.

Proof. Fix \(\omega \in \Omega\). Let \(Y(\omega) = [b_k(\omega), c_k(\omega)]\). Then we have \(\mathbb{E}[X \otimes_M Y \mid \mathcal{G}] = \mathbb{E}[a_k \otimes_M b_k \mid \mathcal{G}]\).

Lemma F.5. For all \(n \in \mathbb{Z}^+\), it holds that

\[
\mathbb{E}[Y_n \mid F_n] = \mathbb{E}[A_{n+1} \otimes_M \Phi_n \mid F_n] = \mathbb{E}[A_{n+1} \otimes_M \Phi_n \mid F_n] = \mathbb{E}[A_n \otimes_M \Phi_{n+1} \mid F_n] = \mathbb{E}[A_{n+1} \otimes_M \Phi_n \mid F_n]
\]

Proof. Similar to the proof of Lem. D.2, we know that \(\{A_n\}_{n \in \mathbb{Z}^+}\) and \(\{\Phi_n\}_{n \in \mathbb{Z}^+}\) are adapted to \(\{F_n\}_{n \in \mathbb{Z}^+}\). Then we have

\[
\mathbb{E}[Y_{n+1} \mid F_n] = \mathbb{E}[A_{n+1} \otimes_M \Phi_n \mid F_n] = \mathbb{E}[A_{n+1} \otimes_M \Phi_n \mid F_n] = \mathbb{E}[A_n \otimes_M \Phi_{n+1} \mid F_n] = \mathbb{E}[A_{n+1} \otimes_M \Phi_n \mid F_n]
\]
As a corollary, we have 

$$\Delta \vdash \phi_{\omega_{n+1}}(\omega_{n+1}) \Rightarrow \phi_{\omega_n}(\omega_n)$$

Recall the property of the ranking function $\phi$ in Defn. 6.3. Then by Lem. F.1 with Lem. F.2, we have 

$$E[Y_{n+1}] \subseteq M E[\phi_{\omega_n}(\omega_n)]$$

As a corollary, we have $E[Y_n] \subseteq M E[Y_0]$ for all $n \in \mathbb{Z}^+$. □

Now we prove the following extension of OST to deal with interval-valued ranking functions.

**Theorem** (Thm. 6.4). Let $||a_k, b_k||_{\infty} \leq \max_{i,j} \{\max(|a_{ki}|, |b_{kj}|)\}$.

If $E[\|Y_n\|_{\infty}] < \infty$ for all $n \in \mathbb{Z}^+$, then $E[Y_T] \exists$ and $E[Y_T] \subseteq M E[Y_0]$ in the following situation:

There exist $\ell \in \mathbb{N}$ and $C \geq 0$ such that $E[T^{\ell}] < \infty$ and for all $n \in \mathbb{Z}^+$, $\|Y_n\|_{\infty} \leq C \cdot (n+1)^{\ell}$ almost surely.

**Proof:** By $E[T^{\ell}] < \infty$ where $\ell \geq 1$, we know that $P[T < \infty] = 1$. Then similar to the proof of Lem. D.1, we know that $P[\lim_{n \to \infty} Y_n = Y_T] = 1$. 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 $E[\|Y_n\|_{\infty}] < \infty$ and $\|Y_n\|_{\infty} \leq C \cdot (n+1)^{\ell}$ almost surely, we know that $E[|a_n|] \leq E[\|Y_n\|_{\infty}] < \infty$ and $|a_n| \leq \|Y_n\|_{\infty} \leq C \cdot (n+1)^{\ell}$ almost surely. Therefore,

$$|a_n| = |a_{\min(T,n)}| \leq C \cdot (\min(T,n) + 1)^{\ell} \leq C \cdot (T + 1)^{\ell}, \text{a.s.}$$

Recall that $E[T^{\ell}] < \infty$. Then $E[T^{\ell+1}] = E[T^{\ell}] + O(T^{\ell-1})$ almost surely. By Prop. A.4, with the function $g$ set to $\lambda_0 \cdot C \cdot T^{(\ell+1)}$, we know that $\lim_{n \to \infty} E[a_n] = E[\gamma_T]$. Because $a_n$ is an arbitrary real-valued component in $Y_n$, we know that $\lim_{n \to \infty} E[Y_n] = E[Y_T]$. By Lem. F.5, we know that $E[Y_n] \subseteq M E[Y_0]$ for all $n \in \mathbb{Z}^+$. By Lem. F.3, we conclude that $\lim_{n \to \infty} E[Y_n] \subseteq M E[Y_0]$, i.e., $E[Y_T] \subseteq M E[Y_0]$. □

## G Soundness of Bound Inference

Fig. 6 presents the inference rules of the derivation system. *Function specifications* are valid pairs of pre- and post-conditions for all declared functions in a program. Valid specifications are justified by the judgment $\Delta \vdash \{\Gamma; Q\} \mathcal{D}(f) \{\Gamma'; Q'\}$. The validity of a context $\Delta$ for function specifications is then established by the validity of all specifications in $\Delta$, denoted by $\vdash \Delta$. Note that to perform context-sensitive analysis, a function can have multiple specifications.

In addition to rules of the judgments for statements and function specifications, we also include rules for continuations and configurations that are used in the operational semantics. A continuation $K$ is valid with a pre-condition $\{\Gamma; Q\}$, written $\Delta \vdash \{\Gamma; Q\} K$, if $\phi_Q$ describes a bound on the moments of the accumulated cost of the computation represented by $K$ on the condition that the valuation before $K$ satisfies $\Gamma$. Validity for configurations, written $\Delta \vdash \{\Gamma; Q\} \{\gamma, S, K, \alpha\}$, is established by validity of the statement $S$ and the continuation $K$, as well as the requirement that the valuation $\gamma$ satisfies the pre-condition $\Gamma$. Here $\phi_Q$ also describes an interval bound on the moments of the accumulated cost of the computation that continues from the configuration $\{\gamma, S, K, \alpha\}$.

The rule (Q-Weaken) and (QK-Weaken) are used to strengthen the pre-condition and relax the post-condition. In terms of the bounds on moments of the accumulated cost, if the triple $\{\cdot; Q\} S \{\cdot; Q'\}$ is valid, then we can safely narrow the intervals in the pre-condition $Q$ and widen the intervals in the post-condition $Q'$. In the implementation, we borrow the idea of rewrite functions from [8, 28] to handle the judgment $\Gamma \vdash Q \equiv M Q'$. Intuitively, to check that $[L_1, U_1] \equiv_{PI} [L_2, U_2]$ under the logical context $\Gamma$, where $L_1, U_1, L_2, U_2$ are polynomials, we find rewrite polynomials $T_1, T_2$ that are always nonnegative under $\Gamma$ such that $L_1 = L_2 + T_1$ and $U_1 = U_2 - T_2$. For example, if $\Gamma$ is a set of linear constraints of the form $E \geq 0$, then we can represent $T_1, T_2$ by conic combinations of monomials of the linear expressions $E$ in $\Gamma$.

**Example G.1** (An instance of the (Q-Sample) rule). For example, if $D = \text{uniform}(-1, 2)$ and $d = 3$, we know the following facts

$$E_{x-\mu_D}[x^0] = 1, E_{x-\mu_D}[x^1] = \frac{1}{2}, E_{x-\mu_D}[x^2] = 1, E_{x-\mu_D}[x^3] = \frac{5}{4}.$$ 

Then if $Q' = \{(1, 1), (1 + x^2, xy^2 + x^3 y^2)\}$, by the linearity of expectations, we compute the pre-condition $Q$ as follows:

$$E_{x-\mu_D}[Q'] = \{(1, 1), [E_{x-\mu_D}[1 + x^2], E_{x-\mu_D}[xy^2 + x^3 y^2]]\} = \{(1, 1), [1 + E_{x-\mu_D}[x^2], y^2 E_{x-\mu_D}[x] + y E_{x-\mu_D}[x^3]]\} = \{(1, 1), [1, 2, \frac{y^2}{2} + \frac{5}{4}]\}.$$ 

To reduce the soundness proof to the extended OST for interval-valued bounds, we construct an annotated transition kernel from validity judgements $\vdash \Delta$ and $\Delta \vdash \{\Gamma; Q\} S_{\text{main}} (\Gamma'; Q')$.

**Lemma G.2.** Suppose $\vdash \Delta$ and $\Delta \vdash \{\Gamma; Q\} S_{\text{main}} (\Gamma'; Q')$.

An annotated program configuration has the form $(\Gamma, Q, \gamma, S, K, \alpha)$ such that $\Delta \vdash \{\Gamma; Q\} \{\gamma, S, K, \alpha\}$. Then there exists a probability kernel $\kappa$ over annotated program configurations such that:

For all $\sigma = (\Gamma, Q, \gamma, S, K, \alpha) \in \text{dom}(\kappa)$, it holds that

(i) $\kappa$ is the same as the evaluation relation $\mapsto$ if the annotations are omitted, i.e.,

$$\kappa(\sigma) = \lambda(\ldots, \gamma, S', K', \alpha') \Delta((\gamma', S', K', \alpha')) = \mapsto((\gamma, S, K, \alpha)),$$

and
Lemma G.3. Suppose \( \vdash \Delta \). If \( \vdash \{ \Gamma; Q \} S \{ \Gamma'; Q' \} \), then for all \( \gamma' \in \mathbb{R}^{m+1} \), the judgment \( \vdash \{ \Gamma; Q \} \bowtie \gamma' \{ \Gamma'; Q' \} \) is derivable.

Proof: By induction on the derivation of \( \vdash \{ \Gamma; Q \} S \{ \Gamma'; Q' \} \).

- \( \vdash \{ \Gamma; Q \} \text{skip} \{ \Gamma; Q \} \)
  - By (Q-Skip), we immediately have \( \vdash \{ \Gamma; Q \} \bowtie \gamma' \{ \Gamma'; Q' \} \).

- \( \vdash \{ \Gamma; Q \} \text{tick}(c) \{ \Gamma'; Q' \} \)
  - By associativity, we have \( \{c^k, c^k\} \bowtie \gamma' \{ \Gamma'; Q' \} \) and \( \{c^k, c^k\} \bowtie \gamma' \{ \Gamma'; Q' \} \).

Because \( \gamma' \in \mathbb{R}^{m+1} \) is a constant, we know that \( \{E/x\}[Q' \bowtie \gamma' \{c^k, c^k\}] = [E/x][Q' \bowtie \gamma' \{c^k, c^k\}] = [E/x][Q' \bowtie \gamma' \{c^k, c^k\}] \bowtie \gamma' \{ \Gamma'; Q' \} \).

The inference rules of the derivation system are shown in Figure 9.
By induction hypothesis, we have $\Delta \vdash \{ \Gamma \land \neg L; Q \} S \{ \Gamma; Q' \}$ and $\Delta \vdash \{ \Gamma \land \neg L; Q \} S \{ \Gamma; Q' \}$.

By induction hypothesis, we have $\Delta \vdash \{ \Gamma; Q \} S \{ \Gamma'; Q' \}$. By the premise, we know that $\Delta \vdash \{ \Gamma \land L; Q \} S \{ \Gamma; Q \}$. Then it remains to show that $\Delta \vdash \{ \Gamma; Q \} L S K$. By (Q-Loop), it suffices to show that $\Delta \vdash \{ \Gamma \land L; Q \} S \{ \Gamma; Q \}$ and $\Delta \vdash \{ \Gamma \land \neg L; Q \} K$. Then appeal to the premise.

If $b = \bot$, then $\mu = \delta((y, \text{skip}, K, \alpha))$. We set $\mu = \delta((\Gamma \land \neg L, Q, \gamma, \text{skip}(y, r), \alpha))$. By the premise, we know that $\Delta \vdash \{ \Gamma \land \neg L; Q \} S \{ \Gamma; Q \}$ and $\Delta \vdash \{ \Gamma \land \neg L; Q \} K$. Then appeal to the premise.

In both cases, $y$ and $Q$ do not change, thus we conclude that $\phi_Q(y) = 1_M \otimes_M \phi_Q(y)$.

By induction hypothesis, we have $\Delta \vdash \{ \Gamma; Q \} S \{ \Gamma'; Q' \}$ and $\Delta \vdash \{ \Gamma'; Q' \} K$. By the premise, we know that $\Delta \vdash \{ \Gamma \land \neg L; Q \} S \{ \Gamma; Q \}$ and $\Delta \vdash \{ \Gamma \land \neg L; Q \} K$. Then appeal to the premise.

We have $\nu = \delta((y, \text{skip}, K, \alpha + c))$. Then we set $\mu = \delta((\Gamma, Q', y, \text{skip}(K, \alpha + c)))$. We set $\mu = \delta((\Gamma', Q', y, \text{skip}(K, \alpha + c)))$. Then by the assumption, we have $\Delta \vdash \{ \Gamma; Q \} K$. It remains to show that $\phi_Q(y) = \phi_Q(y)$. We set $\phi_Q(y) = \phi_Q(y)$. By the premise, we have $\phi_Q(y) = \phi_Q(y)$. We set $\phi_Q(y) = \phi_Q(y)$. By the premise, we have $\phi_Q(y) = \phi_Q(y)$.

We have $\nu = \delta((y, \text{skip}(K, \alpha + c)))$. Then we set $\mu = \delta((\Gamma, Q', y, \text{skip}(K, \alpha + c)))$. We set $\mu = \delta((\Gamma', Q', y, \text{skip}(K, \alpha + c)))$. Then by the assumption, we have $\Delta \vdash \{ \Gamma; Q \} K$. It remains to show that $\phi_Q(y) = \phi_Q(y)$. By the premise, we have $\phi_Q(y) = \phi_Q(y)$. We set $\phi_Q(y) = \phi_Q(y)$. By the premise, we have $\phi_Q(y) = \phi_Q(y)$.
We have \( v = \delta(\langle y, \text{skip}, \text{Kloop} L S K, a \rangle) \). Then we set \( \mu = \delta(\langle \Gamma, Q, y, \text{skip}, \text{Kloop} L S K, a \rangle) \). By (Q-Skip), we have \( \Delta + \{ \Gamma; Q \} \text{ skip } \{ \Gamma; Q \} \). Then by the assumption \( \Delta + \{ \Gamma; \text{Kloop} L S K \} \) and the premise, we know that \( \Delta + \{ \Gamma; Q \} \text{Kloop} L S K \) by (Q-KLoop). Because \( y \) and \( Q \) do not change, we conclude that \( \phi_Q(y) = 1_M \otimes \mu \Phi_Q(y) \).

(Q-Seq)

\( \Delta + \{ \Gamma; Q \} S_1 \{ \Gamma'; Q' \} \quad \Delta + \{ \Gamma; Q \} S_2 \{ \Gamma''; Q'' \} \)

We have \( v = \delta(\langle y, S_1, \text{Kseq} S_2 K, a \rangle) \). Then we set \( \mu = \delta(\langle \Gamma, Q, y, S_1, \text{Kseq} S_2 K, a \rangle) \). By the first premise, we have \( \Delta + \{ \Gamma; Q \} S_1 \{ \Gamma'; Q' \} \). By the assumption \( \Delta + \{ \Gamma'; Q' \} \text{Kseq} S_2 K \) and the second premise, we know that \( \Delta + \{ \Gamma'; Q' \} \text{Kseq} S_2 K \) by (Q-KSeq). Because \( y \) and \( Q \) do not change, we conclude that \( \phi_Q(y) = 1_M \otimes \mu \Phi_Q(y) \).

(Q-Weaken)

\( \Delta + \{ \Gamma; Q \} S \{ \Gamma'; Q' \} \)

By \( y = \Gamma \) and \( \Gamma = \Gamma \), we know that \( y = \Gamma \). By the assumption \( \Delta + \{ \Gamma'; Q' \} \) and the premise \( \Gamma_0' \otimes Q' \subseteq M_Q' \), we derive \( \Delta + \{ \Gamma'_0; Q'_0 \} \) by (Q-Weaken). Thus let \( \mu_0 \) be obtained by the induction hypothesis on \( \Delta + \{ \Gamma_0; Q_0 \} S \{ \Gamma'_0; Q'_0 \} \). Then \( \phi_Q(y) \otimes \epsilon_M \sigma^{-\mu_0[a]\langle(a' - a)^k, (a'' - a'')^k \rangle} M_Q \Phi_Q(y') \), where \( \sigma = \langle \ldots, Q'', y', \ldots \rangle \). We set \( \mu = \mu_0 \). By the premise \( \Gamma \subseteq Q \otimes \mu_0 \) and \( y = \Gamma \), we conclude that \( \phi_Q(y) \otimes \mu \Phi_Q(y) \).

\( \Box \)

Therefore, we can use the annotated kernel \( \kappa \) above to re-construct the trace-based moment semantics in appendix C. Then we can define the ranking function on annotated program configurations as \( \phi(\sigma) \triangleq \phi_Q(y) \) where \( \sigma = \langle \ldots, Q, y, \ldots \rangle \).

The next step is to apply the extended OST for interval bounds (Thm. 6.4). Recall that the theorem requires that for some \( E \) \( \in \mathbb{N} \) and \( C \geq 0 \), \( ||\gamma||_E \leq C \cdot (n + 1)^E \) almost surely for all \( n \in \mathbb{N}^* \). 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 in [37], bounded updates are common in practice. We formulate the idea as follows.

**Lemma G.4.** If there exists \( C_0 \geq 0 \) such that for all \( n \in \mathbb{N}^* \) and \( \kappa \in \text{VID} \), it holds that \( \|\gamma_n(x) - \gamma_{n-1}(x)\|_E = C_0 \) where \( \omega \) is an infinite trace, \( \omega_n = \langle y_n, \ldots, \gamma_0 \rangle \), and \( \omega_{n+1} = \langle y_{n+1}, \ldots \rangle \), then there exists \( C \geq 0 \) such that for all \( n \in \mathbb{N}^* \), \( ||\gamma_n||_E \leq C \cdot (n + 1)^{md} \) almost surely.

**Proof.** Let \( C_1 \geq 0 \) be such that for all \( \text{tick}(c) \) statements in the program, \( |c| \leq C_1 \). Then for all \( \omega \), if \( \omega_n = \langle \ldots, \omega_0 \rangle \), then \( |\omega_n| \leq n \cdot C_1 \). On the other hand, we know that \( \|\gamma_n(x) - \gamma_{n-1}(x)\|_E \leq C_0 \cdot n \) for any variable \( x \). As we assume all
the program variables are initialized to zero, we know that $F[[y_n(x)]] = C_0 \cdot n = 1$. From the construction in the proof of Lem. G.2, we know that all the templates used to define the interval-valued ranking 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 $F_{k,d}[VID]$. Therefore, $\Phi_n(\omega) = \phi(\omega_n) = \phi_Q(y_n)$, and  
$$|\phi_Q(y_n)| \leq \sum_{i=0}^{kd} C_2 \cdot |VID|^i \cdot |C_0 \cdot n|^i \leq C_3 \cdot (n+1)^{kd}, \text{a.s.,}$$
for some sufficiently large constant $C_3$. Thus 
$$|(Y_n)_k| = |(A_n \cdot M \Phi_n)_k| = \left| \sum_{i=0}^{kd} \left( \frac{\partial}{\partial I} \right)_i (k) \cdot ((A_n; \cdot I)(\Phi_n)_k-i) \right|$$ 
$$\leq \sum_{i=0}^{kd} \left( \frac{\partial}{\partial I} \right)_i (k) \cdot (n \cdot C_3)_i \cdot (C_3 \cdot (n+1))^{k-i}$$ 
$$\leq C_4 \cdot (n+1)^{kd}, \text{a.s.,}$$
for some sufficiently large constant $C_4$. Therefore $\|Y_n\|_\infty \leq C_3 \cdot (n+1)^{md}$, a.s., for some sufficiently large constant $C_3$. $\Box$

Now we prove the soundness of bound inference.

**Theorem** (Thm. 7.2). Suppose $\bot \in \Delta$ and $\bot \in \{\Gamma; Q\}$. Then $E[Ar] \subseteq M[\phi_Q(\lambda_\bot)]$, i.e., the moments $E[Ar]$ of the accumulated cost upon program termination are bounded by intervals in $\phi_Q(\lambda_\bot)$ where $Q$ is the quantitative context and $\lambda_\bot$ is the initial valuation, if both of the following properties hold:

(i) $E[T^{md}] < \infty$, and

(ii) there exists $C_0 \geq 0$ such that for all $n \in \mathbb{Z}^+$ and $x \in V_ID$, it holds almost surely that $|y_{n+1}(x) - y_n(x)| \leq C_0$ where $\langle y_{n+1}, \ldots \rangle = o_n$ and $\langle y_{n+1}, \ldots \rangle = o_{n+1}$ of an infinite trace $\omega$.

**Proof.** By Lem. G.4, 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 $E[T^{md}] < \infty$. Thus by Thm. 6.4, we conclude that $E[Y_T] \subseteq M[E[0]]$, i.e., $E[Ar] \subseteq M[\phi_0] = \phi_Q(\lambda_\bot)$. $\Box$

## H Experimental Evaluation

Fig. 10 is the complete version of the plots in Fig. 6.

Tab. 4 compares our tool with Kura et al. [24] on their benchmarks for upper bounds on the first moments of runtimes. In the parentheses after the bounds, we record the degree of polynomials for the templates and the running time of the analysis. A special "unroll" tag means that our tool performs a loop-unrolling technique to obtain more precise results. All the analyses were processed in one second, and our tool can derive better bounds than the compared tool [24].

Tab. 5 compares our tool with **Absynth** by Ngo et al. [28] on their benchmarks for upper bounds on the first moments of monotone costs. Both tools are able to infer symbolic polynomial bounds. **Absynth** uses a finer-grained set of base functions, and it supports bounds of the form $|\langle x, y \rangle|$, which is defined as $\max(0, y-x)$. Our tool achieves the same precision as **Absynth** for most of the time, but it is less efficient than **Absynth**. One reason for this could be that we use GLPK as the LP backend, while **Absynth** employs CoinOr CLP, which seems to be more efficient than GLPK on large instances. Nevertheless, all the analyses were processed in around 10 seconds.

Tab. 6 compares our tool with Wang et al. [37] on their benchmarks for lower and upper bounds on the first moment of accumulated costs. All the benchmark programs satisfy the bounded-update property. To ensure soundness, our tool has to perform an extra termination check required by Thm. 7.2. Our tool derives similar symbolic lower- and upper-bounds, compared to the results of [37]. Meanwhile, our tool is more efficient than the compared tool. One source of slowdowns of [37] could be that they use Matlab as the LP backend and the initializations of Matlab have significant overheads.

## I Case Study: Timing-Attack Analysis

We motivate our work on central-moment analysis using 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 [38]. 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. 11(a) is the interface of the checker, and Fig. 11(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
Figure 10. Upper bounds of the tail probabilities, with comparison to [24]. Each gray line is the minimum of tail bounds given by raw moments of degree up to four inferred by [24]. Each red line is the minimum of tail bounds given by 2nd and 4th central moments inferred by our tool.

Table 5. Upper bounds of the expectations of monotone costs, with comparison to [28].
see shortly that such a countermeasure does not protect the program from a timing attack.

We now show how the moments of the running time of Bitcoin—the kind of information provided by our central-moment analysis (§7)—are useful for analyzing the success probability of the attack program given in Fig. 11(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 $\text{secret}[i+1]$ through $\text{secret}[N]$; we now guess that the next bit, $\text{secret}[i]$, is 1 and set $\text{guess}[i] := 1$. Theoretically, if the following two conditional expectations

$$E[T_i] \triangleq E[T \mid \bigwedge_{j=i+1}^N (\text{secret}[j] = \text{guess}[j]) \land (\text{secret}[i] = 1 \land \text{guess}[i] = 1)]$$

$$E[T_0] \triangleq E[T \mid \bigwedge_{j=i+1}^N (\text{secret}[j] = \text{guess}[j]) \land (\text{secret}[i] = 0 \land \text{guess}[i] = 1)]$$

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 $E[T]$, and choosing the value of $\text{guess}[i]$ according to whichever of (6) and (7) is closest to our estimate. However, if the difference between $E[T_i]$ and $E[T_0]$ 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 $\text{guess}[i]$ incorrectly, which happens when, due to an unfortunate fluctuation, the running-time estimate $\text{est}$ is closer to one of $E[T_i]$ and $E[T_0]$, but the truth is actually the other. For instance, suppose that $E[T_0] < E[T_i]$ and $\text{est} < E[T_i] + E[T_0]$, the attack program would pick $T_0$ as the truth, and set $\text{guess}[i]$ to 0. If such a choice is incorrect, then the actual distribution of $\text{est}$ on the $i^{th}$ round of the attack program satisfies $E[\text{est}] = E[T_i]$, and the probability of this failure event is

$$P[\text{est} < \frac{E[T_0] + E[T_i]}{2}] = P[\text{est} < E[T_i] - E[T_0] = \frac{E[T_0] - E[T_i]}{2}]$$

under the condition given by the conjunction in (6). This formula has exactly the same shape as a tail probability, which makes it possible to utilize moments and concentration of measure inequalities [14] 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. Assume that we have applied our central-moment-analysis technique (§7), 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 (6) and (7).

$$E[T_i] \geq 13N,$$

$$\forall T_i \leq 26N^2 + 42N,$$

$$E[T_0] \geq 13N - 5i,$$

$$\forall T_0 \leq 8N - 36i + 52Ni + 24i.$$

To bound the probability that the attack program makes an incorrect guess for the $i^{th}$ bit, we do case analysis:

- Suppose that $\text{secret}[i] = 1$, but the attack program assigns $\text{guess}[i] := 0$. The truth—with respect to the actual distribution of the running time $T$ of compare for the $i^{th}$ bit—is that $E[\text{est}] = E[T_i]$, but the attack program in Fig. 11(c) executes the then-branch of the conditional statement. Thus, our task reduces to that of bounding $P[\text{est} < 13N - 1.5i]$. The estimate $E[\text{est}]$ is the average of $K$ i.i.d. random variables drawn from a distribution with mean $E[T_i]$ and variance $V[T_i]$. We derive the following, using the inequalities from (8):

$$E[\text{est}] = E[T_i] \geq 13N,$$
Tail Bound Analysis for Prob. Prog. via Central Moments

\textbf{Figure 11.} (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.

\begin{equation}
\forall [\text{est}] = \frac{\mathbb{E}[T_i]}{K} \leq \frac{26N^2 + 42N}{K}. \quad (10)
\end{equation}

Recall a generalization of Chebyshev’s inequality that makes use of variances:

\textbf{Proposition (Cantelli’s inequality).} If $X$ is a random variable and $a > 0$, then we have $P[X - \mathbb{E}[X] \leq -a] \leq \frac{\mathbb{V}[X]}{\mathbb{V}[X] + a^2}$, and $P[X - \mathbb{E}[X] \geq a] \leq \frac{\mathbb{V}[X]}{\mathbb{V}[X] + a^2}$.

We are now able to derive an upper bound on $P[\text{est} < 13N - 1.5i]$ as follows:

\begin{itemize}
  \item The other case, in which $\text{secret}[i] = 0$ but the attack program chooses to set $\text{guess}[i] := 1$, can be analyzed in a similar way to the previous case, and the bound obtained is the following:
  \begin{align*}
P[\text{est} > 13N - 1.5i] &\leq P[\text{est} \geq 13N - 1.5i] \\
&\leq \frac{8N - 36i^2 + 52Ni + 24i}{8N - 36i^2 + 52Ni + 24i + 2.25Ki^2}.
\end{align*}
\end{itemize}

Let $F_i^1$ and $F_i^0$, respectively, denote the two upper bounds on the failure probabilities for the $i^{th}$ bit.

For the attack program to succeed, it has to succeed for all bits. If the number of bits is $N = 32$, and in each iteration the number of trials that the attack program uses to estimate the running time is $K = 10^9$, we derive a lower bound on the success rate of the attack program from the upper bounds on the failure probabilities derived above:

\begin{equation}
P[\text{Success}] \geq \prod_{i=1}^{32}(1 - \max(F_i^1, F_i^0)) \geq 0.219413,
\end{equation}

which is low, but not insignificant. However, the somewhat low probability is caused by a property of compare: if $\text{guess}$ and $\text{secret}$ share a very long prefix, then the running-time behavior on different values of $\text{guess}$ becomes indistinguishable. However, if instead we bound the success rate for all but the last six bits, we obtain:

\begin{equation}
P[\text{Success for all but the last six bits}] \geq 0.830561,
\end{equation}

which is a much higher probability! The attack program can enumerate all the possibilities to resolve the last six bits. (Moreover, by brute-forcing the last six bits, a total of 10,000×26+64 = 260,064 calls to check would be performed, rather than 320,000.)

Overall, our analysis concludes that the check and compare in Fig. 11 are vulnerable to a timing attack.