Tail Probabilities for Randomized Program Runtimes via Martingales for Higher Moments

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Abstract. Programs with randomization constructs is an active research topic, especially after the recent introduction of martingale-based analysis methods for their termination and runtimes. Unlike most of the existing works that focus on proving almost-sure termination or estimating the expected runtime, in this work we study the tail probabilities of runtimes—such as “the execution takes more than 100 steps with probability at most 1%.” To this goal, we devise a theory of supermartingales that overapproximate higher moments of runtime. These higher moments, combined with a suitable concentration inequality, yield useful upper bounds of tail probabilities. Moreover, our vector-valued formulation enables automated template-based synthesis of those supermartingales. Our experiments suggest the method’s practical use.

1 Introduction

The important roles of randomization in algorithms and software systems are nowadays well-recognized. In algorithms, randomization can bring remarkable speed gain at the expense of small probabilities of imprecision. In cryptography, many encryption algorithms are randomized in order to conceal the identity of plaintexts. In software systems, randomization is widely utilized for the purpose of fairness, security and privacy.

Embracing randomization in programming languages has therefore been an active research topic for a long time. Doing so does not only offer a solid infrastructure that programmers and system designers can rely on, but also opens up the possibility of language-based, static analysis of properties of randomized algorithms and systems.

The current paper’s goal is to analyze imperative programs with randomization constructs—the latter come in two forms, namely probabilistic branching and assignment from a designated, possibly continuous, distribution. We shall refer to such programs as randomized programs.\footnote{With the rise of statistical machine learning, probabilistic programs attract a lot of attention. Randomized programs can be thought of as a fragment of probabilistic programs without conditioning (or observation) constructs. In other words, the Bayesian aspect of probabilistic programs is absent in randomized programs.}
Runtime and Termination Analysis of Randomized Programs  The runtime of a randomized program is often a problem of our interest; so is almost-sure termination, that is, whether the program terminates with probability 1. In the programming language community, these problems have been taken up by many researchers as a challenge of both practical importance and theoretical interest.

Most of the existing works on runtime and termination analysis follow either of these two methods.

- Martingale-based methods, initiated with a notion of ranking supermartingale in [6] and extended [1, 7, 12, 15], have their origin in the theory of stochastic processes. They can also be seen as a probabilistic extension of ranking functions, a standard proof method for termination of (non-randomized) programs. Martingale-based methods have seen remarkable success in automated synthesis using templates and constraint solving (like LP or SDP).

- The predicate-transformer approach, pursued in [3, 19, 20], uses a more syntax-guided formalism of program logic and emphasizes reasoning by invariants.

The essential difference between the two approaches is not big: an invariant notion in the latter is easily seen to be an adaptation of a suitable notion of supermartingale. The work [33] presents a comprehensive account on the order-theoretic foundation behind these techniques.

These existing works are mostly focused on the following problems: deciding almost-sure termination, computing termination probabilities, and computing expected runtime. (Here “computing” includes giving upper/lower bounds.) See [33] for a comparison of some of the existing martingale-based methods.

Our Problem: Tail Probabilities for Runtimes  In this paper we focus on the problem of tail probabilities that is not studied much so far. We present a method for overapproximating tail probabilities; here is the problem we solve.

Input: a randomized program \( \Gamma \), and a deadline \( d \in \mathbb{N} \)

Output: an upper bound of the tail probability \( \Pr(T_{\text{run}} \geq d) \), where \( T_{\text{run}} \) is the runtime of \( \Gamma \)

Our target language is an imperative language that features randomization (probabilistic branching and random assignment). We also allow nondeterminism; this makes the program’s runtime depend on the choice of a scheduler (i.e. how nondeterminism is resolved). In this paper we study the longest, worst-case runtime (therefore our scheduler is demonic). In the technical sections, we use the presentation of these programs as probabilistic control graphs (pCFGs)—this is as usual in the literature. See e.g. [1, 33].

An example of our target program is in Fig. 1.

It is an imperative program with randomization: in Line 3, the value of \( z \) is sampled from the uniform distribution over the interval \([-2,1]\). The symbol in the line 4 stands for a nondeterministic Boolean value; in our analysis, it is resolved so that the runtime becomes the longest.

Fig. 1: An example program

An exception is [6]; see [7] for comparison with the current work.
a randomized program $\Gamma$

**step 1:** template-based synthesis of vector-valued supermartingales (§3, §5)

upper bounds of higher moments $E[T_{\text{run}}], \ldots, E[(T_{\text{run}})^K]$

a deadline $d$ → **step 2:** calculation via a concentration inequality (§4)

an upper bound of the tail probability $\Pr(T_{\text{run}} \geq d)$

Fig. 2: Our workflow

Given the program in Fig. 1 and a choice of a deadline (say $d = 400$), we can ask the question “what is the probability $\Pr(T_{\text{run}} \geq d)$ for the runtime $T_{\text{run}}$ of the program to exceed $d = 400$ steps?” As we show in §6 our method gives a guaranteed upper bound 0.0684. This means that, if we allow the time budget of $d = 400$ steps, the program terminates with the probability at least 93%.

**Our Method: Concentration Inequalities, Higher Moments, and Vector-Valued Supermartingales** Towards the goal of computing tail probabilities, our approach is to use concentration inequalities, a technique from probability theory that is commonly used for overapproximating various tail probabilities. There are various concentration inequalities in the literature, and each of them is applicable in a different setting, such as a nonnegative random variable (Markov’s inequality), known mean and variance (Chebyshev’s inequality), a difference-bounded martingale (Azuma’s inequality), and so on. Some of them were used for analyzing randomized programs [6] (see §7 for comparison).

In this paper, we use a specific concentration inequality that uses higher moments $E[T_{\text{run}}], \ldots, E[(T_{\text{run}})^K]$ of runtimes $T_{\text{run}}$, up to a choice of the maximum degree $K$. The concentration inequality is taken from [4]; it generalizes Markov’s and Chebyshev’s. We observe that a higher moment yields a tighter bound of the tail probability, as the deadline $d$ grows bigger. Therefore it makes sense to strive for computing higher moments.

For computing higher moments of runtimes, we systematically extend the existing theory of ranking supermartingales, from the expected runtime (i.e. the first moment) to higher moments. The theory features a vector-valued supermartingale, which not only generalizes easily to degrees up to arbitrary $K \in \mathbb{N}$, but also allows automated synthesis much like usual supermartingales.

We also claim that the soundness of these vector-valued supermartingales is proved in a mathematically clean manner. Following our previous work [33], our arguments are based on the order-theoretic foundation of fixed points (namely the Knaster-Tarski, Cousot-Cousot and Kleene theorems), and we give upper bounds of higher moments by suitable least fixed points.

Overall, our workflow is as shown in Fig. 2. We note that the step 2 in Fig. 2 is computationally much cheaper than the step 1: in fact, the step 2 yields a symbolic expression for an upper bound in which $d$ is a free variable. This makes it possible to draw graphs like the ones in Fig. 3. It is also easy to find a deadline $d$ for which $\Pr(T_{\text{run}} \geq d)$ is below a given threshold $p \in [0, 1]$. 
We implemented a prototype that synthesizes vector-valued supermartingales using linear and polynomial templates. The resulting constraints are solved by LP and SDP solvers, respectively. Experiments show that our method can produce nontrivial upper bounds in reasonable computation time. We also experimentally confirm that higher moments are useful in producing tighter bounds.

**Our Contributions** Summarizing, the contribution of this paper is as follows.

- We extend the existing theory of ranking supermartingales from expected runtimes (i.e. the first moment) to higher moments. The extension has a solid foundation of order-theoretic fixed points. Moreover, its clean presentation by vector-valued supermartingales makes automated synthesis as easy as before. Our target randomized programs are rich, embracing nondeterminism and continuous distributions.

- We study how these vector-valued supermartingales (and the resulting upper bounds of higher moments) can be used to yield upper bounds of tail probabilities of runtimes. We identify a concentration lemma that suits this purpose. We show that higher moments indeed yield tighter bounds.

- Overall, we present a comprehensive language-based framework for overapproximating tail probabilities of runtimes of randomized programs (Fig. 2). It has been implemented, and our experiments suggest its practical use.

**Organization** We give preliminaries in §2. In §3 we review the order-theoretic characterization of ordinary ranking supermartingales and present an extension to higher moments of runtimes. In §4 we discuss how to obtain an upper bound of the tail probability of runtimes. In §5 we explain an automated synthesis algorithm for our ranking supermartingales. In §6 we give experimental results. In §7 we discuss related work. We conclude and give future work in §8. Some proofs and details are deferred to the appendices.

## 2 Preliminaries

We present some preliminary materials, including the definition of pCFGs (we use them as a model of randomized programs) and the definition of runtime.

Given topological spaces \( X \) and \( Y \), let \( \mathcal{B}(X) \) be the set of Borel sets on \( X \) and \( \mathcal{B}(X,Y) \) be the set of Borel measurable functions \( X \to Y \). We assume that the set \( \mathbb{R} \) of reals, a finite set \( L \) and the set \([0,\infty]\) are equipped with the usual topology, the discrete topology, and the order topology, respectively. We use the induced Borel structures for these spaces. Given a measurable space \( X \), let \( \mathcal{D}(X) \) be the set of probability measures on \( X \). For any \( \mu \in \mathcal{D}(X) \), let \( \text{supp}(\mu) \) be the support of \( \mu \). We write \( \mathbb{E}[X] \) for the expectation of a random variable \( X \).

Our use of pCFGs follows recent works including [1].

**Definition 2.1 (pCFG).** A probabilistic control flow graph (pCFG) is a tuple \( \Gamma = (L, V, l_{\text{init}}, x_{\text{init}}, \rightarrow, \text{Up}, \text{Pr}, G) \) that consists of the following.

- A finite set of locations \( L = L_D \cup L_P \cup L_N \cup L_A \). It is the union of four mutually disjoint sets of deterministic, probabilistic, nondeterministic and assignment locations, respectively.
- A finite set $V$ of program variables.
- An initial location $l_{init} \in L$. An initial valuation $x_{init} \in \mathbb{R}^V$.
- A transition relation $\rightarrow \subseteq L \times L$ which is total (i.e. $\forall l. \exists l'. l \rightarrow l'$).
- An update function $U_p : L_D \rightarrow V \times (B(\mathbb{R}^V, \mathbb{R}) \cup D(\mathbb{R}) \cup B(\mathbb{R}))$ for assignment.
- A family $\Pr = (\Pr_l)_{l \in L_P}$ of probability distributions, where $\Pr_l \in D(L)$, for probabilistic locations. We require that $l' \in \text{supp}(\Pr_l)$ implies $l \rightarrow l'$.
- A guard function $G : L_D \times L \rightarrow B(\mathbb{R}^V)$ such that for each $l \in L_D$ and $x \in \mathbb{R}^V$, there exists a unique location $l' \in L$ satisfying $l \rightarrow l'$ and $x \in G(l, l')$. The update function can be decomposed into three functions $U_{pD} : L_{AD} \rightarrow V \times B(\mathbb{R}^V, \mathbb{R})$, $U_{pP} : L_{AP} \rightarrow V \times D(\mathbb{R})$ and $U_{pN} : L_{AN} \rightarrow V \times B(\mathbb{R})$, under a suitable decomposition $L_A = L_{AD} \cup L_{AP} \cup L_{AN}$ of assignment locations. The elements of $L_{AD}$, $L_{AP}$ and $L_{AN}$ represent deterministic, probabilistic and nondeterministic assignments, respectively.

An example of a pCFG is shown on the right. It models the program in Fig. 1. The node $l_4$ is a nondeterministic location. $\text{Unif}(-2,1)$ is the uniform distribution on the interval $[-2, 1]$.

A configuration of a pCFG $\Gamma$ is a pair $(l, x) \in L \times \mathbb{R}^V$ of a location and a valuation. We regard the set $S = L \times \mathbb{R}^V$ of configurations as a topological space by assuming that $L$ is equipped with the discrete topology and $S$ is equipped with the product topology. We say a configuration $(l', x')$ is a successor of $(l, x)$, if $l \rightarrow l'$ and the following hold:

- If $l \in L_D$, then $x' = x$ and $x \in G(l, l')$.
- If $l \in L_N \cup L_P$, then $x' = x$.
- If $l \in L_A$, then $x' = x(x_j \leftarrow a)$, where $x(x_j \leftarrow a)$ denotes the vector obtained by replacing the $x_j$-component of $x$ by $a$. Here $x_j$ is such that $U_p(l) = (x_j, u)$, and $a$ is chosen as follows: 1) $a = u(x)$ if $u \in B(\mathbb{R}^V, \mathbb{R})$; 2) $a \in \text{supp}(u)$ if $u \in D(\mathbb{R})$; and 3) $a = u$ if $u \in B(\mathbb{R})$.

An invariant of a pCFG $\Gamma$ is a measurable set $I \in B(S)$ such that $(l_{init}, x_{init}) \in I$ and $I$ is closed under taking successors (i.e. if $c \in I$ and $c' \in I$ then $c' \in I$). Use of invariants is a common technique in automated synthesis of supermartingales [11]: it restricts configuration spaces and thus the constraints on supermartingales weaker. A run of $\Gamma$ is an infinite sequence of configurations $c_0c_1 \ldots$ such that $c_0$ is the initial configuration $(l_{init}, x_{init})$ and $c_{i+1}$ is a successor of $c_i$ for each $i$. Let $\text{Run}(\Gamma)$ be the set of runs of $\Gamma$.

A scheduler resolves nondeterminism: at a location in $L_N \cup L_{AN}$, it chooses a distribution of next configurations depending on the history of configurations visited so far. Given a pCFG $\Gamma$ and a scheduler $\sigma$ of $\Gamma$, a probability measure $\nu_{\sigma}^\Gamma$ on $\text{Run}(\Gamma)$ is defined in the usual manner. See Appendix 13 for details.

**Definition 2.2 (reaching time $T_{C,\sigma}^\Gamma, T_{E,\sigma}^\Gamma$).** Let $\Gamma$ be a pCFG and $C \subseteq S$ be a set of configurations called a destination. The reaching time to $C$ is a function $T_E^\Gamma : \text{Run}(\Gamma) \rightarrow [0, \infty]$ defined by $T_E^\Gamma(c_0c_1 \ldots) = \arg\min_{i \in \mathbb{N}}(c_i \in C)$. Fixing a scheduler $\sigma$ makes $T_E^\Gamma$ a random variable, since $\sigma$ determines a probability measure $\nu_{\sigma}^\Gamma$ on $\text{Run}(\Gamma)$. It is denoted by $T_{E,\sigma}^\Gamma$. 

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Runtimes of pCFGs are a special case of reaching times, namely to the set of terminating configurations.

The following higher moments are central to our framework. Recall that we are interested in demonic schedulers, i.e. those which make runtimes longer.

**Definition 2.3** \((\mathcal{M}^{\Gamma,k}_{C,\sigma} and \mathcal{M}^{\Gamma,k}_{c})\). Assume the setting of Def. 2.2 and let \(k \in \mathbb{N}\) and \(c \in S\). We write \(\mathcal{M}^{\Gamma,k}_{C,\sigma}(c)\) for the \(k\)-th moment of the reaching time of \(\Gamma\) from \(c\) to \(C\) under the scheduler \(\sigma\), i.e. that is, \(\mathcal{M}^{\Gamma,k}_{C,\sigma}(c) = \mathbb{E}[(T^{\Gamma}_{C,\sigma})^k] = \int(T^{\Gamma}_{C})^k d\nu^\sigma_{\Gamma}\), where \(T_{\Gamma}\) is a pCFG obtained from \(\Gamma\) by changing the initial configuration to \(c\). Their supremum under varying \(\sigma\) is denoted by \(\mathcal{M}^{\Gamma,k}_{C} := \sup_{\sigma} \mathcal{M}^{\Gamma,k}_{C,\sigma}\).

### 3 Ranking Supermartingale for Higher Moments

We introduce one of the main contributions in the paper, a notion of ranking supermartingale that overapproximates higher moments. It is motivated by the following observation: martingale-based reasoning about the second moment must concur with one about the first moment. We conduct a systematic theoretical extension that features an order-theoretic foundation and vector-valued supermartingales. The theory accommodates nondeterminism and continuous distributions, too. We omit some details and proofs; they are in Appendix C.

Prior to these, we review the existing theory of ranking supermartingales, through the lens of order-theoretic fixed points. In doing so we follow [33].

**Definition 3.1** (“nexttime” operation \(\mathcal{X}\) (pre-expectation)). Given \(\eta : S \to [0,\infty]\), let \(\mathcal{X}\eta : S \to [0,\infty]\) be the function defined as follows.

- If \(l \in L_D\) and \(x \equiv G(l,l')\), then \((\mathcal{X}\eta)(l,x) = \eta(l',x)\).
- If \(l \in L_P\), then \((\mathcal{X}\eta)(l,x) = \sum_{l \rightarrow l'} \mathbb{P}_{l'}(l') \eta(l',x)\).
- If \(l \in L_N\), then \((\mathcal{X}\eta)(l,x) = \sup_{l \rightarrow l'} \eta(l',x)\).
- If \(l \in L_A\), \(\text{Up}(l) = (x,u)\) and \(l \rightarrow l'\),
  - if \(u \in B(\mathbb{R}^d, \mathbb{R})\), then \((\mathcal{X}\eta)(l,x) = \eta(l',x(x_j \leftarrow u(x)))\);
  - if \(u \in D(\mathbb{R})\), then \((\mathcal{X}\eta)(l,x) = \int_{u} \eta(l',x(x_j \leftarrow y)) \, dy\);
  - if \(u \in B(\mathbb{R})\), then \((\mathcal{X}\eta)(l,x) = \sup_{y \in \eta} \eta(l',x(x_j \leftarrow y))\).

Intuitively, \(\mathcal{X}\eta\) is the expectation of \(\eta\) after one transition. Nondeterminism is resolved by the maximal choice.

We define \(F_1 : (S \to [0,\infty]) \to (S \to [0,\infty])\) as follows.

\[
(F_1(\eta))(c) = \begin{cases} 
1 + (\mathcal{X}\eta)(c) & c \in I \setminus C \\
0 & \text{otherwise}
\end{cases}
\]

(Here “1+” accounts for time elapse)

The function space \((S \to [0,\infty])\) is a complete lattice structure, because \([0,\infty]\) is; moreover \(F_1\) is easily seen to be monotone. It is not hard to see either that the expected reaching time \(\mathcal{M}^{\Gamma,1}_{C}\) to \(C\) coincides with the least fixed point \(\mu F_1\).

The following theorem is fundamental in theoretical computer science.
Theorem 3.2 (Knaster–Tarski, see e.g. [35]). Let \((L, \leq)\) be a complete lattice and \(f : L \to L\) be a monotone function. The least fixed point \(\mu f\) is the least prefixed point, i.e. \(\mu f = \min\{l \in L \mid f(l) \leq l\}\).

The significance of the Knaster-Tarski theorem in verification lies in the induced proof rule: \(f(l) \leq l \Rightarrow \mu f \leq l\). Instantiating to the expected reaching time \(\bar{M}_{\Gamma, 1}\), it means \(F_1(\eta) \leq \eta \Rightarrow \bar{M}_{\Gamma, 1} \leq \eta\), i.e. an arbitrary prefixed point of \(F_1\) —which coincides with the notion of ranking supermartingale [5]—overapproximates the expected reaching time. This proves soundness of ranking supermartingales.

3.1 Ranking Supermartingales for the Second Moments

We extend ranking supermartingales to the second moments. It paves the way to a fully general theory (up to the \(K\)-th moments) in §3.2.

The key in the martingale-based reasoning of expected reaching times (i.e. first moments) was that they are characterized as the least fixed point of a function \(F_1\). Here it is crucial that for an arbitrary random variable \(T\), we have \(E[T + 1] = E[T] + 1\) and therefore we can calculate \(E[T + 1]\) from \(E[T]\). However, this is not the case for second moments. As \(E[(T + 1)^2] = E[T^2] + 2E[T] + 1\), calculating the second moment requires not only \(E[T^2]\) but also \(E[T]\). This encourages us to define a vector-valued supermartingale.

Definition 3.3 (time-elapse function \(El_1\)). A function \(El_1 : [0, \infty]^2 \to [0, \infty]^2\) is defined by \(El_1(x_1, x_2) = (x_1 + 1, x_2 + 2x_1 + 1)\).

Then, an extension of \(F_1\) for second moments can be defined as a combination of the time-elapse function \(El_1\) and the pre-expectation \(\overline{X}\).

Definition 3.4 \((F_2)\). Let \(I\) be an invariant and \(C \subseteq I\) be a Borel set. We define \(F_2 : (S \to [0, \infty]^2) \to (S \to [0, \infty]^2)\) by

\[
(F_2(\eta))(c) = \begin{cases} 
(\overline{X}(El_1 \circ \eta))(c) & c \in I \setminus C \\
(0, 0) & \text{otherwise.} 
\end{cases}
\]

Here \(\overline{X}\) is applied componentwise: \((\overline{X}(\eta_1, \eta_2))(c) = ((\overline{X}\eta_1)(c), (\overline{X}\eta_2)(c))\).

We can extend the complete lattice structure of \([0, \infty]\) to the function space \(S \to [0, \infty]^2\) in a pointwise manner. It is a routine to prove that \(F_2\) is monotone with respect to this complete lattice structure. Hence \(F_2\) has the least fixed point. In fact, while \(\bar{M}_{\Gamma, 1}^{F_2} = \mu F_2\) was characterized as the least fixed point of \(F_1\), a tuple \((\bar{M}_{\Gamma, 1}^{F_2}, \bar{M}_{\Gamma, 2}^{F_2})\) is not the least fixed point of \(F_2\) (cf. Example 3.8 and Thm. 3.9). However, the least fixed point of \(F_2\) overapproximates the tuple of moments.

Theorem 3.5. For any configuration \(c \in I\), \((\mu F_2)(c) \geq (\bar{M}_{\Gamma, 1}^{F_2}(c), \bar{M}_{\Gamma, 2}^{F_2}(c))\). □
Let $T_{C,\sigma,n}^L = \min\{n, T_{C,\sigma}^L\}$. To prove the above theorem, we inductively prove
\[(F_2)^n(\downarrow)(c) \geq \left( \int T_{C,\sigma,n}^L \, d\nu_\sigma^L, \int (T_{C,\sigma,n}^L)^2 \, d\nu_\sigma^L \right)\]
for each $\sigma$ and $n$, and take the supremum. See Appendix C for more details.

Like ranking supermartingale for first moments, ranking supermartingale for second moments is defined as a prefixed point of $F_2$, i.e. a function $\eta$ such that $\eta \geq F_2(\eta)$. However, we modify the definition for the sake of implementation.

**Definition 3.6 (ranking supermartingale for second moments).** A ranking supermartingale for second moments is a function $\eta : S \to \mathbb{R}^2$ such that: i) $\eta(c) \geq (\mathbb{E}(E_{l_1} \circ \eta))(c)$ for each $c \in I \setminus C$; and ii) $\eta(c) \geq 0$ for each $c \in I$.

Even though we only have inequality in Thm. 3.5, we can prove the following desired property of our supermartingale notion.

**Theorem 3.7.** If $\eta : S \to \mathbb{R}^2$ is a supermartingale for second moments, then $(\mathbb{M}_C^{1,1}(c), \mathbb{M}_C^{1,2}(c)) \leq \eta(c)$ for each $c \in I$. \hfill $\square$

The following example and theorem show that we cannot replace $\leq$ with $=$ in Thm. 3.5 in general, but it is possible in the absence of nondeterminism.

**Example 3.8.** The figure on the right shows a pCFG such that $l_2 \in L_D$ and all the other locations are in $L_N$, the initial location is $l_0$ and $l_{12}$ is a terminating location. For the pCFG, the left-hand side of the inequality in Thm. 3.5 is $\mu F_2(l_0) = (6, 37.5)$. In contrast, if a scheduler $\sigma$ takes a transition from $l_1$ to $l_2$ with probability $p$, $(\mathbb{M}_C^{1,1}(l_0), \mathbb{M}_C^{1,2}(l_0)) = (6 - \frac{1}{2}p, 36 - \frac{5}{2}p)$. Hence the right-hand side is $(\mathbb{M}_C^{1,1}(l_0), \mathbb{M}_C^{1,2}(l_0)) = (6, 36)$.

**Theorem 3.9.** If $L_N = L_{AN} = \emptyset$, $\forall c \in I, (\mu F_2)(c) = (\mathbb{M}_C^{1,1}(c), \mathbb{M}_C^{1,2}(c))$. \hfill $\square$

### 3.2 Ranking Supermartingales for the Higher Moments

We extend the result in 3.1 to moments higher than second.

Firstly, the time-elapse function $E_{l_1}$ is generalized as follows.

**Definition 3.10 (time-elapse function $E_{l_1^{K,k}}$).** For $K \in \mathbb{N}$ and $k \in \{1, \ldots, K\}$, a function $E_{l_1^{K,k}} : [0, \infty]^K \to [0, \infty]$ is defined by $E_{l_1^{K,k}}(x_1, \ldots, x_K) = 1 + \sum_{j=1}^k \binom{k}{j} x_j$. Here $\binom{k}{j}$ is the binomial coefficient.

Again, a monotone function $F_K$ is defined as a combination of the time-elapse function $E_{l_1^{K,k}}$ and the pre- expectation $\mathbb{I}$.

**Definition 3.11 ($F_K$).** Let $I$ be an invariant and $C \subseteq I$ be a Borel set. We define $F_K : (S \to [0, \infty]^K) \to (S \to [0, \infty])$ by $F_K(\eta)(c) = (F_{K,1}(\eta))(c), \ldots, F_{K,K}(\eta)(c))$, where $F_{K,K} : (S \to [0, \infty]^K) \to (S \to [0, \infty])$ is given by

\[
(F_{K,K}(\eta))(c) = \begin{cases} \mathbb{E}(E_{l_1^{K,k}} \circ \eta))(c) & c \in I \setminus C \\ 0 & \text{otherwise.} \end{cases}
\]
As in Def. 3.6, we define a supermartingale as a prefixed point of $F_K$.

**Definition 3.12 (ranking supermartingale for $K$-th moments).** We define $\eta_1, \ldots, \eta_K : S \to \mathbb{R}$ by $(\eta_1(c), \ldots, \eta_K(c)) = \eta(c)$. A ranking supermartingale for $K$-th moments is a function $\eta : S \to \mathbb{R}^K$ such that for each $k$, i) $\eta_k(c) \geq (\mathbb{E}(\mathcal{E}^{K,k}_1 \circ \eta_k))(c)$ for each $c \in I \setminus C$; and ii) $\eta_k(c) \geq 0$ for each $c \in I$.

For higher moments, we can prove an analogous result to Thm. 3.7.

**Theorem 3.13.** If $\eta$ is a supermartingale for $K$-th moments, then for each $c \in I$, $\min_{0 \leq k \leq K} \frac{u_k}{d^k}$.

\[ \eta(c) \leq \eta(c). \]

\[ \square \]

## 4 From Moments to Tail Probabilities via Concentration Inequalities

We discuss how to obtain upper bounds of tail probabilities of runtimes from upper bounds of higher moments of runtimes. Combined with the result in §3, it induces a martingale-based method for overapproximating tail probabilities.

We use a concentration inequality. There are many choices of concentration inequalities (see e.g. [4]), and we use a variant of Markov’s inequality. We prove that the concentration inequality is not only sound but also complete in a sense.

Formally, our goal is to calculate an upper bound of $\text{Pr}(T_{C,\sigma}^f \geq d)$ for a given deadline $d > 0$, under the assumption that we know upper bounds $u_1, \ldots, u_K$ of moments $\mathbb{E}[T_{C,\sigma}^f], \ldots, \mathbb{E}[(T_{C,\sigma}^f)^K]$. In other words, we want to over-approximate $\sup_{\mu} \mu([d, \infty])$ where $\mu$ ranges over the set of probability measures on $[0, \infty]$ satisfying $\left(\int x \, d\mu(x), \ldots, \int x^K \, d\mu(x)\right) \leq (u_1, \ldots, u_K)$.

To answer the above problem, we make use of the following generalized form of Markov’s inequality.

**Proposition 4.1 (see e.g. [4, §2.1]).** Let $X$ be a real-valued random variable and $\phi$ be a nondecreasing and nonnegative function. For any $d \in \mathbb{R}$ with $\phi(d) > 0$,

\[ \text{Pr}(X \geq d) \leq \frac{\mathbb{E}\phi(X)}{\phi(d)}. \]

\[ \square \]

By letting $\phi(x) = x^k$ in Prop 4.1, we obtain the following inequality. It gives an upper bound of the tail probability that is “tight.”

**Proposition 4.2.** Let $X$ be a nonnegative random variable. Assume $\mathbb{E}[X^k] \leq u_k$ for each $k \in \{0, \ldots, K\}$. Then, for any $d > 0$,

\[ \text{Pr}(X \geq d) \leq \min_{0 \leq k \leq K} \frac{u_k}{d^k}. \]  

Moreover, this upper bound is tight: for any $d > 0$, there exists a probability measure such that the above equation holds.

\[ \text{Proof.} \] The former part is immediate from Prop 4.1. For the latter part, consider $\mu = p\delta_d + (1-p)\delta_0$ where $\delta_x$ is the Dirac measure at $x$ and $p$ is the value of the right-hand side of (1).  

\[ \square \]
By combining Thm. 3.13 with Prop. 4.2, we obtain the following corollary. We can use it for overapproximating tail probabilities.

**Corollary 4.3.** Let \( \eta : S \to \mathbb{R}^k \) be a ranking supermartingale for \( k \)-th moments. For each scheduler \( \sigma \) and a deadline \( d > 0 \),

\[
\Pr(T_{C,\sigma}^r \geq d) \leq \min_{0 \leq k \leq K} \frac{\eta_k(l_{\text{init}}, x_{\text{init}})}{d^k}.
\]

Here \( \eta_0, \ldots, \eta_K \) are defined by \( \eta_0(c) = 1 \) and \( \eta(c) = (\eta_1(c), \ldots, \eta_K(c)) \).

For each \( K \) there exists \( d > 0 \) such that

\[
\eta_K(l_{\text{init}}, x_{\text{init}}) = \min_{0 \leq k \leq K} \frac{\eta_k(l_{\text{init}}, x_{\text{init}})}{d^k}.
\]

Hence higher moments become useful in overapproximating tail probabilities as \( d \) gets large. Later in [4] we demonstrate this fact experimentally.

## 5 Template-Based Synthesis Algorithm

We discuss an automated synthesis algorithm that calculates an upper bound for the \( k \)-th moment of the runtime of a pCFG using a supermartingale in Def. 3.6 or Def. 3.12. It takes a pCFG \( \Gamma \), an invariant \( I \), a set \( C \subseteq I \) of configurations, and a natural number \( K \) as input and outputs an upper bound of \( K \)-th moment.

Our algorithm is adapted from existing template-based algorithms for synthesizing a ranking supermartingale (for first moments) [5, 7, 8]. It fixes a linear or polynomial template with unknown coefficients for a supermartingale and using numerical methods like linear programming (LP) or semidefinite programming (SDP), calculate a valuation of the unknown coefficients so that the axioms of ranking supermartingale for \( K \)-th moments are satisfied.

We hereby briefly explain the algorithms. See Appendix [D] for details.

**Linear Template** Our linear template-based algorithm is adapted from [5, 8]. We should assume that \( \Gamma \), \( I \) and \( C \) are all “linear” in the sense that expressions appearing in \( \Gamma \) are all linear and \( I \) and \( C \) are represented by linear inequalities. To deal with assignments from a distribution like \( x := \text{Norm}(0, 1) \), we also assume that expected values of distributions appearing in \( \Gamma \) are known.

The algorithm first fixes a template for a supermartingale: for each location \( l \), it fixes a \( K \)-tuple \( (\sum_{j=1}^{V} a_{j,j,l} x_j + b_{l,1}, \ldots, \sum_{j=1}^{V} a_{j,K,l} x_j + b_{l,K}) \) of linear formulas. Here each \( a_{j,j,l} \) and \( b_{l,i} \) are unknown variables called parameters. The algorithm next collects conditions on the parameters so that the tuples constitute a ranking supermartingale for \( K \)-th moments. It results in a conjunction of formulas of a form \( \varphi_1 \geq 0 \land \cdots \land \varphi_m \geq 0 \Rightarrow \psi \geq 0 \). Here \( \varphi_1, \ldots, \varphi_m \) are linear formulas without parameters and \( \psi \) is a linear formula where parameters linearly appear in the coefficients. By Farkas’ lemma (see e.g. [29] Cor. 7.1h) we can turn such formulas into linear inequalities over parameters by adding new variables. Its feasibility is efficiently solvable with an LP solver. We naturally wish to minimize an upper bound of the \( K \)-th moment, i.e. the last component of \( \eta(l_{\text{init}}, x_{\text{init}}) \). We can minimize it by setting it to the objective function of the LP problem.
**Polynomial Template**  The polynomial template-based algorithm is based on [7]. This time, \( \Gamma, I \) and \( C \) can be “polynomial.” To deal with assignments of distributions, we assume that the \( n \)-th moments of distributions in \( \Gamma \) are easily calculated for each \( n \in \mathbb{N} \). It is similar to the linear template-based one.

It first fixes a polynomial template for a supermartingale, i.e. it assigns each location \( l \) a \( K \)-tuple of polynomial expressions with unknown coefficients. Likewise the linear template-based algorithm, the algorithm reduces the axioms of supermartingale for higher moments to a conjunction of formulas of a form \( \varphi_1 \geq 0 \land \cdots \land \varphi_m \geq 0 \Rightarrow \psi \geq 0 \). This time, each \( \varphi_i \) is a polynomial formula without parameters and \( \psi \) is a polynomial formula whose coefficients are linear formula over the parameters. In the polynomial case, a conjunction of such formula is reduced to an SDP problem using a theorem called Positivstellensatz (we used a variant called Schmüdgen’s Positivstellensatz [28]). We solve the resulting problem using an SDP solver setting \( \eta(l_{\text{init}}, x_{\text{init}}) \) as the objective function.

### 6 Experiments

We implemented two programs in OCaml to synthesize a supermartingale based on a) a linear template and b) a polynomial template. The programs translate a given randomized program to a pCFG and output an LP or SDP problem as described in [5]. An invariant \( I \) and a terminal configuration \( C \) for the input program are specified manually. See e.g. [21] for automatic synthesis of an invariant. For linear templates, we have used GLPK (v4.65) [13] as an LP solver. For polynomial templates, we have used SOSTOOLS (v3.03) [31] (a sums of squares optimization tool that internally uses an SDP solver) on Matlab (R2018b). We used SDPT3 (v4.0) [30] as an SDP solver. The experiments were carried out on a Surface Pro 4 with an Intel Core i5-6300U (2.40GHz) and 8GB RAM. We tested our implementation for the following two programs and their variants, which were also used in the literature [8, 20]. Their code is in Appendix E.

**Coupon collector’s problem.** A probabilistic model of collecting coupons enclosed in cereal boxes. There exist \( n \) types of coupons, and one repeatedly buy cereal boxes until all the types of coupons are collected. We consider two cases: (1-1) \( n = 2 \) and (1-2) \( n = 4 \). We tested the linear template program for them.

**Random walk.** We used three variants of 1-dimensional random walks: (2-1) integer-valued one, (2-2) real-valued one with assignments from continuous distributions, (2-3) with adversarial nondeterminism; and two variants of 2-dimensional random walks (2-4) and (2-5) with assignments from continuous distributions and adversarial nondeterminism. We tested both the linear and the polynomial template programs for these examples.

**Experimental results**  We measured execution times needed for Step 1 in Fig. 2. The results are in Table 1. Execution times are less than 0.2 seconds for linear template programs and several minutes for polynomial template programs. Upper bounds of tail probabilities obtained from Prop. 4.2 are in Fig. 3.

We can see that our method is applicable even with nondeterministic branching ((2-3), (2-4) and (2-5)) or assignments from continuous distributions ((2-2), (2-3), (2-4) and (2-5)).
(2-4) and (2-5)). We can use a linear template for bounding higher moments as long as there exists a supermartingale for higher moments representable by linear expressions ((1-1), (1-2) and (2-3)). In contrast, for (2-1), (2-2) and (2-4), only a polynomial template program found a supermartingale for second moments.

It is expectable that the polynomial template program gives a better bound than the linear one because a polynomial template is more expressive than a linear one. However, it did not hold for some test cases, probably because of numerical errors of the SDP solver. For example, (2-1) has a supermartingale for third moments that can be checked by a hand calculation, but the SDP solver returned “infeasible” in the polynomial template program. It appears that our program fails when large numbers are involved (e.g. the third moments of (2-1), (2-2) and (2-3)). We have also tested a variant of (2-1) where the initial position is multiplied by 10000. Then the SDP solver returned “infeasible” in the polynomial template program while the linear template program returns a nontrivial bound. Hence it seems that numerical errors are likely to occur to the polynomial template program when large numbers are involved.

Fig. 3 shows that the bigger the deadline \(d\) is, the more useful higher moments become (cf. a remark just after Cor. 4.3). For example, in (1-2), an upper bound of \(\Pr(T^f_{C,\sigma} \geq 100)\) calculated from the upper bound of the first moment is \(\Pr(T^f_{C,\sigma} \geq 100) \leq 0.680\), while we obtain \(\Pr(T^f_{C,\sigma} \geq 100) \leq 0.105\) from the upper bound of the fifth moment.

To show the merit of our method compared with sampling-based methods, we calculated a tail probability bound for a variant of (2-2) (shown in Fig. 4 on p. 13) with a deadline \(d = 10^{11}\). Because of its very long expected runtime, a sampling-based method would not work for it. In contrast, the linear template-based program gave an upper bound \(\Pr(T^f_{C,\sigma} \geq 10^{11}) \leq 5000000025/10^{11} \approx 0.05\) in almost the same execution time as (2-2) (< 0.02 seconds).

7 Related Work

Martingale-Based Analysis of Randomized Programs  Martingale-based methods are widely studied for the termination analysis of randomized programs. One of the first is ranking supermartingales, introduced in \([5]\) for proving almost sure termination. The theory of ranking supermartingales has since been extended actively: accommodating nondeterminism \([1, 7, 8, 12]\), syntax-oriented composition of supermartingales \([12]\), proving properties beyond termination/reachability \([15]\), and so on. Automated template-based synthesis of supermartingales by constraint solving has been pursued, too \([1, 5, 7, 8]\).

Other martingale-based methods that are fundamentally different from ranking supermartingales have been devised, too. They include: different notions of repulsing supermartingales for refuting termination (in \([9, 33]\); also studied in control theory \([32]\)); and multiply-scaled submartingales for underapproximating reachability probabilities \([33, 37]\). See \([33]\) for an overview.

In the literature on martingale-based methods, the one closest to this work is \([6]\). Among its contribution is the analysis of tail probabilities. It is done by
| moment | a) linear template | b) polynomial template |
|--------|-------------------|------------------------|
|        | upper bound | time (sec) | upper bound | time (sec) |
| (1-1) | 1st | 13 | 0.012 | |
|        | 2nd | 21 | 0.019 | |
|        | 3rd | 3829 | 0.023 | |
|        | 4th | 1204976 | 0.126 | |
|        | 5th | 1048131068 | 0.191 | |
| (1-2) | 1st | 68 | 0.024 | |
|        | 2nd | 3124 | 0.054 | |
|        | 3rd | 171532 | 0.089 | |
|        | 4th | 1953418052 | 0.101 | |
| (2-1) | 1st | 20 | 0.024 | 24.980 | 2 |
|        | 2nd | - | 0.013 | 37.609 | 2 |
|        | 3rd | - | 0.011 | 40.746 | 2 |
| (2-2) | 1st | 25 | 0.009 | 75.0 | 2 |
|        | 2nd | - | 0.014 | 83.434 | 2 |
|        | 3rd | - | 0.021 | 100 | 4 |
| (2-3) | 1st | 62 | 0.020 | 62.0 | 2 |
|        | 2nd | 28605.4 | 0.038 | 70.156 | 2 |
|        | 3rd | 19267843.96 | 0.057 | 97.442 | 3 |
| (2-4) | 1st | 90 | 0.020 | 95.95 | 2 |
|        | 2nd | - | 0.029 | 10944.0 | 2 |
|        | 3rd | - | 0.022 | 143.055 | 2 |
|        | 4th | - | 0.032 | 327.202 | 3 |

Table 1: Upper bounds of the moments of runtimes. ‘-’ indicates that the LP or SDP solver returned “infeasible”. The “degree” column shows the degree of the polynomial template used in the experiments.

```
1 x := 200000000;
2 while true do
3   if prob(0.7) then
4     z := Unif(0,1);
5     x := x - z
6   else
7     z := Unif(0,1);
8     x := x + z
9   fi;
10  refute (x < 0)
11 od
```

Fig. 4: A variant of (2-2).

```
13
```

Fig. 3: Upper bounds of the tail probabilities (except (2-5)). Each gray line is the value of $\frac{1}{d_k}$ where $u_k$ is the best upper bound in Table 1 of $k$-th moments and $d$ is a deadline. Each black line is the minimum of gray lines, i.e. the upper bound by Prop. 4.2. The red lines in (1-1), (1-2) and (2-1) show the true tail probabilities calculated analytically. The red points in (2-2) show tail probabilities calculated by Monte Carlo sampling where the number of trials is 100000000. We did not calculate the true tail probabilities nor approximate them for (2-4) and (2-5) because these examples seem difficult to do so due to nondeterminism.
either of the following combinations: 1) difference-bounded ranking supermartingales and the corresponding Azuma’s martingale concentration inequality; and 2) (not necessarily difference-bounded) ranking supermartingales and Markov’s concentration inequality. When we compare these two methods with ours, the first method requires repeated martingale synthesis for different parameter values, which can pose a performance challenge. The second method corresponds to the restriction of our method to the first moment; recall that we showed the advantage of use of higher moments, theoretically (§4) and experimentally (§6).

See Appendix F.1 for detailed discussions. Implementation is lacking in [6], too.

The work [1] is also close to ours in that their supermartingales are vector-valued. The difference is in the orders: in [1] they use the lexicographic order between vectors, and they aim to prove almost sure termination. In contrast, we use the pointwise order between vectors, for overapproximating higher moments.

The Predicate-Transformer Approach to Runtime Analysis In the runtime/termination analysis of randomized programs, another principal line of work uses predicate transformers [3, 19, 20], following the precedent works on probabilistic predicate transformers such as [22, 25]. In fact, from the mathematical point of view, the main construct for witnessing runtime/termination in those predicate transformer calculi (called invariants, see e.g. in [20]) is essentially the same thing as ranking supermartingales. Therefore the difference between the martingale-based and predicate-transformer approaches is mostly the matter of presentation—the predicate-transformer approach is more closely tied to program syntax and has a stronger deductive flavor. It also seems that there is less work on automated synthesis in the predicate-transformer approach.

In the predicate-transformer approach, the work [19] is the closest to ours, in that it studies variance of runtimes of randomized programs. The main differences are as follows: 1) computing tail probabilities is not pursued [19]; 2) their extension from expected runtimes to variance involves an additional variable $\tau$, which poses a challenge in automated synthesis as well as in generalization to even higher moments; and 3) they do not pursue automated analysis. See Appendix F.2 for further details.

Higher Moments of Runtimes Computing and using higher moments of runtimes of probabilistic systems—generalizing randomized programs—has been pursued before. In [10], computing moments of runtimes of finite-state Markov chains is reduced to a certain linear equation. In the study of randomized algorithms, the survey [11] collects a number of methods, among which are some tail probability bounds using higher moments. Unlike ours, none of these methods are language-based static ones. They do not allow automated analysis.

Other Potential Approaches to Tail Probabilities We discuss potential approaches to estimating tail probabilities, other than the martingale-based one.

Sampling is widely employed for approximating behaviors of probabilistic systems; especially so in the field of probabilistic programming languages, since exact symbolic reasoning is hard in presence of conditioning. See e.g. [36]. We also used sampling to estimate tail probabilities in (2-2), Fig. 8. The main advantages of our current approach over sampling are threefold: 1) our upper bounds
come with a mathematical guarantee, while the sampling bounds can always be erroneous; 2) it requires ingenuity to sample programs with nondeterminism; and 3) programs whose execution can take millions of years can still be analyzed by our method in a reasonable time, without executing them. The latter advantage is shared by static, language-based analysis methods in general; see e.g. [3].

Another potential method is probabilistic model checkers such as PRISM [23]. Their algorithms are usually only applicable to finite-state models, and thus not to randomized programs in general. Nevertheless, fixing a deadline d can make the reachable part $S_{\leq d}$ of the configuration space $S$ finite, opening up the possibility of use of model checkers. It is an open question how to do so precisely, and the following challenges are foreseen: 1) if the program contains continuous distributions, the reachable part $S_{\leq d}$ becomes infinite; 2) even if $S_{\leq d}$ is finite, one has to repeat (supposedly expensive) runs of a model checker for each choice of $d$.

In contrast, in our method, an upper bound for the tail probability $\Pr(T_{\text{run}} \geq d)$ is symbolically expressed as a function of $d$ (Prop. 4.2). Therefore, estimating tail probabilities for varying $d$ is computationally cheap.

8 Conclusions and Future Work

We provided a technique to obtain an upper bound of the tail probability of runtimes given a randomized algorithm and a deadline. We first extended the ordinary ranking supermartingale notion using the order-theoretic characterization so that it can calculate upper bounds of higher moments of runtimes for randomized programs. Then by using a suitable concentration inequality, we introduced a method to calculate an upper bound of tail probabilities from upper bounds of higher moments. Our method is not only sound but also complete in a sense. Our method was obtained by combining our supermartingale and the concentration inequality. We also implemented an automated synthesis algorithm and demonstrated the applicability of our framework.

Future Work Example 3.8 shows that our supermartingale is not complete: it sometimes fails to give a tight bound for higher moments. Studying and improving the incompleteness is one possible direction of future work. For example, the following questions would be interesting: Can the bound given by our supermartingale be arbitrarily bad? Can we remedy the completeness by restricting the type of nondeterminism? Can we define a supermartingale that is complete?

We are also interested in improving the implementation. The polynomial template program failed to give an upper bound for higher moments because of numerical errors (see §6). We wish to remedy this situation. There exist several studies for using numerical solvers for verification without affected by numerical errors [16,18,26,27]. We might make use of these works for improvements.

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Appendix

A Preliminaries on Measure Theory

In this section, we review some results from measure theory that is needed in the rest of the paper. For more details, see e.g. [2,34].

Definition A.1. Let $\phi : X \to Y$ be a measurable function and $\mu$ be a probability measure on $X$. A pushforward measure $(\phi)_* \mu$ is a measure on $Y$ defined by $(\phi)_* \mu(E) = \mu(\phi^{-1}(E))$ for each measurable set $E \subseteq Y$.

Lemma A.2. Let $\phi : X \to Y$ and $f : Y \to [0, \infty]$ be measurable functions and $\mu$ be a probability measure on $X$.
\[
\int f \, d((\phi)_* \mu) = \int (f \circ \phi) \, d\mu
\]
where $f \circ \phi$ denotes the composite function of $f$ and $\phi$. $\square$

Lemma A.3. Let $(X, \mathcal{B}_X)$ and $(Y, \mathcal{B}_Y)$ be measurable spaces and $\mu_x$ be a probability measure on $Y$ for each $x \in X$. The following conditions are equivalent.

1. For each $E \in \mathcal{B}_Y$, a mapping $x \mapsto \mu_x(E)$ is measurable.
2. For each measurable function $f : X \times Y \to [0, \infty]$, $x \mapsto \int_Y f(x, y) \, d\mu_x(y)$ is measurable.

Proof. $(1 \Rightarrow 2)$ We write $\mathcal{B}_{X \times Y}$ for the product $\sigma$-algebra of $\mathcal{B}_X$ and $\mathcal{B}_Y$. By the monotone convergence theorem (see e.g. [2, Theorem 1.6.2]) and the linearity of integration, it suffices to prove that for each $E \in \mathcal{B}_{X \times Y}$, $f = 1_E : X \times Y \to [0, \infty]$ satisfies the condition 2. Let $M = \{E \in \mathcal{B}_{X \times Y} \mid 1_E \text{ satisfies the condition 2}\}$. By the monotone class theorem (see e.g. [2, Theorem 1.3.9]), to prove $M = \mathcal{B}_{X \times Y}$, it suffices to prove that $M$ is a monotone class and contains a Boolean algebra
\[
\{\bigcup_{i=1}^n (E_i \times F_i) \mid E_i \in B_X, F_i \in B_Y\}.
\]
The rest of the proof is easy.

$(2 \Rightarrow 1)$ Given $E \in B_Y$, consider $f = 1_{X \times E}$. $\square$

For any $f : A \to B$ and any set $X$, $X^f : X^B \to X^A$ denotes a precomposition of $f$ i.e. $X^f(u) = u \circ f$. If $A \subseteq B$, we write $X^A \subseteq B$ for $X^i : X^B \to X^A$ where $i : A \to B$ is the inclusion mapping.

In [34] we use the following corollary of the Kolmogorov extension theorem (see [34, §2.4]).

Corollary A.4. Let $(X, \mathcal{B}_X)$ be a measurable space and $\mu_n$ be an inner regular probability measure on $X^n$ for each $n < \omega$. Assume $(X^{n \leq n+1})_m \mu_{n+1} = \mu_n$. There exists a unique probability measure $\mu_\omega$ on $X^\omega$ such that $(X^{n \leq \omega})_m \mu_\omega = \mu_n$. $\square$
B \ K\text{-th moments of runtimes and rewards}

We define a probably measure on the set of runs of a pCFG given a scheduler. We then define the \(k\)-th moment of runtimes. Here we slightly generalize runtime model by considering a reward function and redefine some of the notions to accommodate the reward function. However, this generalization is not essential, and therefore the readers can safely assume that we are just counting the number of steps until termination (by taking the constant function \(1\) as a reward function).

Let \(\Gamma = (L, V, l_{\text{init}}, x_{\text{init}}, \rightarrow, U_p, P_t, G)\) be a pCFG. A reward function on \(\Gamma\) is a measurable function \(\text{Rew} : S \to [0, \infty]\). Recall that we regard the set \(S = L \times \mathbb{R}^V\) of configurations as the product measurable space of \((L, 2^L)\) and \((\mathbb{R}^V, \mathcal{B}(\mathbb{R}^V))\). A scheduler of \(\Gamma\) resolves two types of nondeterminism: nondeterministic transition and nondeterministic assignment.

**Definition B.1 (scheduler).** A scheduler \(\sigma = (\sigma_1, \sigma_2)\) of \(\Gamma\) consists of the following components.

- A function \(\sigma_1 : (L \times \mathbb{R}^V)^{\ast}(L_N \times \mathbb{R}^V) \to \mathcal{D}(L)\) such that
  - if \(\pi \in (L \times \mathbb{R}^V)^{\ast}(L_N \times \mathbb{R}^V)\) and \(l \in L_N\) is the last location of \(\pi\), then \(l' \in \text{supp}(\sigma_1(\pi))\) implies \(l \rightarrow l'\), and
  - for each \(l \in L\), the mapping \(\pi \mapsto \sigma_1(\pi)(\{l\}) : (L \times \mathbb{R}^V)^{\ast}(L_N \times \mathbb{R}^V) \to [0, 1]\) is measurable.
- A function \(\sigma_2 : (L \times \mathbb{R}^V)^{\ast}(L_{AN} \times \mathbb{R}^V) \to \mathcal{D}(\mathbb{R})\) such that
  - if \(\pi \in (L \times \mathbb{R}^V)^{\ast}(L_{AN} \times \mathbb{R}^V)\), \(l \in L_{AN}\) is the last location of \(\pi\) and \((x_j, u) = U_p(l)\), then \(\text{supp}(\sigma_2(\pi)) \subseteq u\), and
  - for each \(A \in \mathcal{B}(\mathbb{R})\), the mapping \(\pi \mapsto \sigma_2(\pi)(A)\) is measurable.

Note that if \(L_N = \emptyset\) and \(L_{AN} = \emptyset\), then there exists only one scheduler that is trivial.

In the rest of the paper, the concatenation of two finite sequences \(\rho_1, \rho_2\) is denoted by \(\rho_1 \rho_2\) or by \(\rho_1 \cdot \rho_2\).

Given a scheduler \(\sigma\) and a history of configurations \(\rho \in S^+\), let \(\mu_\rho^\sigma\) be a probability distribution of the next configurations determined by \(\sigma\).

**Definition B.2.** Let \(\sigma\) be a scheduler and \(\rho \in S^+\). A probability measure \(\mu_\rho^\sigma\) on \(S\) is defined as follows.

- If \(l \in L_D\) and \(x \vdash G(l, l')\), \(\mu_\rho^\sigma(l, x) = \delta(l', x)\).
- If \(l \in L_P\), \(\mu_\rho^\sigma(l, x) = \sum_{l'} \Pr_t(l') \delta(l', x)\).
- If \(l \in L_N\), \(\mu_\rho^\sigma(l, x) = \sum_{l'} \sigma_1(\rho \cdot (l, x))(\{l'\}) \delta(l', x)\).
- Assume \(l \in L_A\), \(U_p(l) = (x_j, u)\) and \(l \rightarrow l'\).
  - If \(u \in \mathcal{B}(\mathbb{R}^V, \mathbb{R})\), \(\mu_\rho^\sigma(l, x) = \delta(l', x_j \leftarrow u(x))\).
  - If \(u \in \mathcal{D}(\mathbb{R})\), \(\mu_\rho^\sigma(l, x) = (\lambda y. (l', x(x_j \leftarrow y)))_u\).
  - If \(u \in B(\mathbb{R})\), \(\mu_\rho^\sigma(l, x) = (\lambda y. (l', x(x_j \leftarrow y)))\sigma_a(\rho \cdot (l, x))\).

**Lemma B.3.** For each \(E \in \mathcal{B}(S)\), a mapping \(\rho \mapsto \mu_\rho^\sigma(E) : S^+ \to [0, 1]\) is measurable.
Proof. Let \( f : S^+ \to [0, 1] \) be a function defined by \( f(\rho) = \mu_\sigma^\rho(E) \). It suffices to prove that for each \( n < \omega \) and \( l \in L \), \( f_{|S^n_\rho \times \{l\} \times \mathbb{R}^V} : S^n \times \{l\} \times \mathbb{R}^V \to [0, 1] \) is measurable, that is, a function \( g_{n,l} : S^n_\rho \times \mathbb{R}^V \to [0, 1] \) defined by \( g_{n,l}(\rho, x) = \mu_{\sigma^\rho(l, x)}(E) \) is measurable.

- Assume \( l \in L_D \).
  \[ g_{n,l}(\rho, x) = \delta_{l,x}(E) = 1_E(l, x) \]

- Assume \( l \in L_P \).
  \[ g_{n,l}(\rho, x) = \sum_{l \to l'} \Pr(l'|l)1_E(l', x) \]

- Assume \( l \in L_N \).
  \[ g_{n,l}(\rho, x) = \sum_{l \to l'} \sigma_t(\rho \cdot (l, x))(\{l'\})1_E(l', x) \]

- Assume \( l \in L_A \), \( \Up(l) = (x_j, u) \) and \( l \mapsto l' \).
  - Assume \( u \in \mathcal{B}(\mathbb{R}^V, \mathbb{R}) \).
    \[ g_{n,l}(\rho, x) = 1_E(l', x(x_j \leftarrow u(x))) \]
  - Assume \( u \in \mathcal{D}(\mathbb{R}) \).
    \[ g_{n,l}(\rho, x) = \int_{\mathbb{R}} 1_E(l', x(x_j \leftarrow y)) \, du(y) \]
  - Assume \( u \in \mathcal{B}(\mathbb{R}) \).
    \[ g_{n,l}(\rho, x) = \int_{\mathbb{R}} 1_E(l', x(x_j \leftarrow y)) \, d(\sigma_a(\rho \cdot (l, x)))(y) \]

In each case, it easily follows that \( g_{n,l} \) is measurable. Note that \( \delta_{l,-}(E) = 1_E \) and \( (x, y) \mapsto x(x_j \leftarrow y) \) are measurable functions. We use Lemma A.3 for the last two cases.

Given an initial configuration \( c_0 \), let \( \nu_{c_0,n}^\sigma \) be a probability measure on the set \( \{c_0 \rho \mid \rho \in S^n\} \cong S^n \) of paths.

**Definition B.4.** For each \( n \in \omega \), \( \nu_{c_0,n}^\sigma \) is a probability measure on \( S^n \) defined as

\[
\nu_{c_0,n}^\sigma(E) = \begin{cases} 
\int_S \cdots \int_S 1_E(c_1, \ldots, c_n) \, d\mu_{c_0 \cdots c_{n-1}}^\sigma(c_n) \cdots d\mu_{c_0}^\sigma(c_1) & \text{if } n > 0 \\
\delta_* & \text{if } n = 0
\end{cases}
\]

where * is the element of \( S^0 = \{\ast\} \).

**Definition B.4** is well-defined by Lemma A.3 and Lemma B.3.

The following lemma is a fundamental property of \( \nu_{c_0,n}^\sigma \).

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Lemma B.5. Assume \( n > 0 \). For any measurable function \( f : S^n \to [0, \infty] \),
\[
\int f \, d\nu_{c_0,n}^\sigma = \int \cdots \int f(c_1, \ldots, c_n) \, d\mu_{c_0,\ldots,c_{n-1}}^\sigma(c_n) \ldots d\mu_{c_0}^\sigma(c_1).
\]

Proof. By the monotone convergence theorem and the linearity of integration. \( \square \)

Lemma B.6. For each \( n \in \mathbb{N} \), \( (S^{\leq n+1})_*\nu_{c_0,n+1}^\sigma = \nu_{c_0,n}^\sigma \).

Proof.
\[
((S^{\leq n+1})_*\nu_{c_0,n+1}^\sigma)(E) = \nu_{c_0,n+1}^\sigma(E \times S)
= \int \cdots \int 1_{E \times S}(c_1, \ldots, c_{n+1}) \, d\mu_{c_0,\ldots,c_n}^\sigma(c_{n+1}) \ldots d\mu_{c_0}^\sigma(c_1)
= \int \cdots \int (\int 1_{S}(c_{n+1}) \, d\mu_{c_0,\ldots,c_n}(c_{n+1})) \cdot 1_{E}(c_1, \ldots, c_n) \, d\mu_{c_0,\ldots,c_{n-1}}^\sigma(c_n) \ldots d\mu_{c_0}^\sigma(c_1)
= \int \cdots \int 1_{E}(c_1, \ldots, c_n) \, d\mu_{c_0,\ldots,c_{n-1}}^\sigma(c_n) \ldots d\mu_{c_0}^\sigma(c_1)
= \nu_{c_0,n}^\sigma(E) \quad \square
\]

By Corollary A.3, we define a probability measure on \( S^\omega \). Note that \( (S, \mathcal{B}(S)) \) is a Polish space (a separable completely metrizable topological space), and hence a Radon space. Therefore, \( \nu_{c_0,n}^\sigma \) is inner regular.

Definition B.7. Let \( \nu_{c_0}^\sigma \) be the probability measure defined as a unique measure such that \( (S^{\leq \omega})_*\nu_{c_0}^\sigma = \nu_{c_0,n}^\sigma \).

Definition B.8 (accumulated reward \( \text{Rew}_C^0 \)). Given a reward function \( \text{Rew} : S \to [0, \infty] \), let \( \text{Rew}_C^0 : S^\omega \to [0, \infty] \) be a measurable function defined by the sum of the rewards from the initial configuration \( c_0 \) to the last configuration before entering \( C \). That is,
\[
\text{Rew}_C^0(c_1c_2 \ldots) = \begin{cases} 
\sum_{j=0}^{N-1} \text{Rew}(c_j) & \text{if } N \geq 0 \text{ s.t. } c_N \in C \land (0 \leq j < N \Rightarrow c_j \notin C) \\
\sum_{j=0}^{\infty} \text{Rew}(c_j) & \text{otherwise (i.e. for each } i, c_i \notin C). 
\end{cases}
\]

Note that \( \text{Rew}(c_0) \) is included in the sum.

Definition B.9 (k-th moment of rewards). We define two functions \( M_{C,\sigma}^{\text{Rew},k}, \overline{M}_C^{\text{Rew},k} : S \to [0, \infty] \) as follows.
\[
M_{C,\sigma}^{\text{Rew},k}(c_0) = \int (\text{Rew}_C^0)^k \, d\nu_{c_0}^\sigma \quad \overline{M}_C^{\text{Rew},k}(c_0) = \sup_{\sigma} M_{C,\sigma}^{\text{Rew},k}(c_0)
\]

Note that \( M_{C,\sigma}^{\text{Rew},k} \) is measurable by Lemma A.3.

The correspondence of the notations in \( \mathbb{E} \) and in \( \mathbb{H} \) is as follows.

| \( \mathbb{E} \) | \( \mathbb{H} \) |
|-----------------|-----------------|
| \( \nu_{c_0}^\sigma \) | \( \nu_{c_0}^\sigma \) where \( c_0 = (l_{\text{init}}, \mathbf{x}_{\text{init}}) \) |
| \( T^{\text{Rew},k}_C, \sigma \) | \( \text{Rew}_C^0 \) where \( c_0 = (l_{\text{init}}, \mathbf{x}_{\text{init}}) \) |
| \( M_{C,\sigma}^{\text{Rew},k} \), \( \overline{M}_C^{\text{Rew},k} \) | \( M_{C,\sigma}^{\text{Rew},k} \), \( \overline{M}_C^{\text{Rew},k} \) where \( \text{Rew}(c) = 1 \) for each \( c \) |
C Omitted Details and Proofs in §3

The ultimate goal of this section is to prove Theorem 3.13. In §C.1-C.2 we prove some lemmas regarding to $X$ (Definition 3.1) and $E_{1,k}^1$ (Definition 3.10). In §C.3 we prove analogous theorem to Theorem 3.7, Theorem 3.9 and Theorem 3.13. In §C.4, we prove Theorem 3.13. We prove them in a generalized way so that an arbitrary reward function is allowed as in §B.

C.1 Basic properties of the pre-expectation

We prove several lemmas for $\overline{X}$ in Definition 3.1.

The next lemma claims that we can ignore outside of an invariant $I$.

Lemma C.1. Let $I$ be an invariant. If $\eta(c) = \eta'(c)$ for any $c \in I$, then $(\overline{X}\eta)(c) = (\overline{X}\eta')(c)$ for any $c \in I$. □

The complete lattice $[0, \infty]$ has the following properties as an $\omega$-cpo, and the set of functions $S \to [0, \infty]^K$ inherits the same properties.

- Let $\{\eta_n\}_{n<\omega}$ and $\{\eta'_n\}_{n<\omega}$ be $\omega$-chains. Then we have
  \[ \sup_{n \in \omega} \eta_n + \sup_{n \in \omega} \eta'_n = \sup_{n \in \omega} (\eta_n + \eta'_n). \]  \hspace{1cm} (4)

  That is, the addition $+$ is $\omega$-continuous.

- Let $\{\eta_n\}_{n<\omega}$ be a $\omega$-chain and $a \geq 0$. Then we have
  \[ a \cdot \sup_{n \in \omega} \eta_n = \sup_{n \in \omega} (a \cdot \eta_n). \]  \hspace{1cm} (5)

  That is, $a \cdot (\cdot)$ is $\omega$-continuous.

These properties are often used in the proofs of $\omega$-continuity in the rest of the paper.

Lemma C.2. $\overline{X}$ is $\omega$-continuous.

Proof. Let $\{\eta_n : S \to [0, \infty]\}_{n \in \omega}$ be an $\omega$-chain. We prove $(\overline{X}(\sup_{n \in \omega} \eta_n))(l, x) = \sup_{n \in \omega}(\overline{X}\eta_n)(l, x)$ for each $(l, x) \in L \times \mathbb{R}^V$.

- Assume $l \in L_D$ and $x \models G(l, l')$.
  \[ (\overline{X}(\sup_{n \in \omega} \eta_n))(l, x) = (\sup_{n \in \omega} \eta_n)(l', x) = (\sup_{n \in \omega} \eta_n(l', x)) = (\overline{X}\eta_n)(l, x) \]

- Assume $l \in L_P$.
  \[ (\overline{X}(\sup_{n \in \omega} \eta_n))(l, x) = \sum_{l \rightarrow l'} \Pr_l(l') (\sup_{n \in \omega} \eta_n)(l', x) \]
  \[ = \sup_{n \in \omega} \sum_{l \rightarrow l'} \Pr_l(l') \eta_n(l', x) \]
  \[ = \sup_{n \in \omega}(\overline{X}\eta_n)(l, x) \]
– Assume \( l \in L_N \).
\[
\left( \mathcal{X}(\sup_{n \in \omega} \eta_n) \right)(l, x) = \sup_{n \in \omega} \eta_n(l', x) = \sup_{n \in l \rightarrow l'} \eta_n(l', x) = \sup_{n \in \omega} \eta_n(l, x).
\]

– Assume \( l \in L_A \). \( \text{Up}(l) = (x_j, u) \) and \( l \mapsto l' \).

  • Assume \( u \in B(R^V, R) \).
\[
\left( \mathcal{X}(\sup_{n \in \omega} \eta_n) \right)(l, x) = \sup_{n \in \omega} \eta_n(l', x(x_j \leftarrow u(x))) = \sup_{n \in \omega} \eta_n(l, x)
\]

  • Assume \( u \in D(R) \).
\[
\left( \mathcal{X}(\sup_{n \in \omega} \eta_n) \right)(l, x) = \int_R (\sup_{n \in \omega} \eta_n(l', x(x_j \leftarrow y)) \, du(y)
\]
\[
= \sup_{n \in \omega} \int_R \eta_n(l', x(x_j \leftarrow y)) \, du(y)
\]
\[
= \sup_{n \in \omega} \eta_n(l, x)
\]
by the monotone convergence theorem.

  • Assume \( u \in D(R) \).
\[
\left( \mathcal{X}(\sup_{n \in \omega} \eta_n) \right)(l, x) = \sup_{n \in \omega} \eta_n(l', x(x_j \leftarrow y))
\]
\[
= \sup_{n \in \omega} \eta_n(l', x(x_j \leftarrow y))
\]
\[
= \sup_{n \in \omega} \eta_n(l, x)
\]

The next lemma is a justification of the name “pre-expectation”.

**Lemma C.3.** For any configuration \( c_0 \), measurable function \( \eta : S \rightarrow [0, \infty] \), scheduler \( \sigma \),
\[
\mathcal{X}\eta(c_0) \geq \int_S \eta(c_1) \, d\mu_{\sigma, c_0}(c_1).
\]

**Proof.** Let \( (l_0, x_0) = c_0 \).

– Assume \( l_0 \in L_D \) and \( x_0 \vdash G(l_0, l_1) \).
\[
\int_S \eta(c_1) \, d\mu_{\sigma, c_0}(c_1) = \eta(l_1, x_0) = \mathcal{X}\eta(c_0)
\]

– Assume \( l_0 \in L_P \).
\[
\int_S \eta(c_1) \, d\mu_{\sigma, c_0}(c_1) = \sum_{l_0 \rightarrow l_1} \text{Pr}_{l_0}(l_1) \eta(l_1, x_0) = \mathcal{X}\eta(c_0)
\]

– Assume \( l_0 \in L_N \).
\[
\int_S \eta(c_1) \, d\mu_{\sigma, c_0}(c_1) = \sum_{l_0 \rightarrow l_1} \sigma_{l}(c_0)(l_1) \eta(l_1, x_0) \leq \sup_{l_0 \rightarrow l_1} \eta(l_1, x_0) = \mathcal{X}\eta(c_0)
\]
– Assume \( l_0 \in L_A \), \( \text{Up}(l_0) = (x_j, u) \) and \( l_0 \mapsto l_1 \).
  - Assume \( u \in B(\mathbb{R}^V, \mathbb{R}) \).
    \[
    \int_S \eta(c_1) d\mu_{c_0}^\sigma(c_1) = \int_R \eta(l_1, x_0(x_j \leftarrow u(x_0))) = \mathcal{X}\eta(c_0)
    \]
  - Assume \( u \in D(\mathbb{R}) \).
    \[
    \int_S \eta(c_1) d\mu_{c_0}^\sigma(c_1) = \int_R \eta(l_1, x_0(x_j \leftarrow y)) d\sigma_a(c_0)(y) \leq \sup_{y \in u} \eta(l_1, x_0(x_j \leftarrow y)) = \mathcal{X}\eta(c_0)
    \]

\[\Box\]

**Lemma C.4.** Assume \( L_N = \emptyset \) and \( L_{AN} = \emptyset \) and let \( \sigma \) be the unique scheduler that plays no role. For any configuration \( c_0 \) and any measurable function \( \eta : S \rightarrow [0, \infty] \),
\[
\mathcal{X}\eta(c_0) = \int_S \eta(c_1) d\mu_{c_0}^\sigma(c_1).
\]

**Proof.** Immediate from the proof of Lemma C.3 \[\Box\]

### C.2 Basic properties of the time-elapse function

We next prove lemmas for the time-elapse function in Definition 3.10. We redefine the time-elapse function for the generalized runtime model.

**Definition C.5 (time-elapse function).** For each \( a \in [0, \infty] \), natural number \( K \) and \( k \in \{1, \ldots, K\} \), \( \text{El}_{a}^{K,k} : [0, \infty]^K \rightarrow [0, \infty] \) is a function defined by
\[
\text{El}_{a}^{K,k}(x_1, \ldots, x_K) = a^k + \sum_{j=1}^{k} \binom{k}{j} a^{k-j} x_j
\]

**Lemma C.6.** \( \text{El}_{a}^{K,k} \) is \( \omega \)-continuous.

**Proof.** Immediate from (4) and (5). \[\Box\]

**Lemma C.7 (commutativity of \( \int \) and \( \text{El}_{a}^{K,k} \)).** For any probability measure \( \mu \) on \( X \), any measurable functions \( f_1, \ldots, f_n : X \rightarrow [0, \infty] \) and \( a \in [0, \infty] \), \( \text{El}_{a}^{K,n} \) and integrals commute. That is
\[
\int \text{El}_{a}^{K,k}(f_1(x), \ldots, f_n(x)) d\mu(x) = \text{El}_{a}^{K,k} \left( \int f_1(x) d\mu(x), \ldots, \int f_n(x) d\mu(x) \right).
\]

**Proof.** By the linearity of integration. \[\Box\]
C.3 Characterizing higher moments by $F_K$

We prove Theorem 3.7, Theorem 3.9 and Theorem 3.13 in the generalized runtime model. We first extend Definition 3.11 so that an arbitrary reward is allowed.

**Definition C.8.** Let $I$ be an invariant and $C \subseteq I$ be a Borel set. Let $F_K : (S \rightarrow [0, \infty]^K) \rightarrow (S \rightarrow [0, \infty]^K)$ be a function defined by $F_K(c) = (F_{K,1}(c), \ldots, F_{K,K}(c))$ where the $k$-th component $F_{K,k} : (S \rightarrow [0, \infty]^K) \rightarrow (S \rightarrow [0, \infty])$ of $F_K$ is defined by

$$F_{K,k}(\eta)(c) = \begin{cases} (\mathbb{E}(\text{Ex}^{K,k}_{\text{Rew}(c) \circ \eta})(c)) & c \in I \setminus C \\ 0 & \text{otherwise.} \end{cases}$$

**Lemma C.9.** $F_K$ is $\omega$-continuous.

**Proof.** Immediate from Lemma C.2 and Lemma C.6. \qed

The following theorems generalize Theorem 3.7, 3.13 and Theorem 3.9, respectively.

**Theorem C.10.**

$$\mu F_K \geq \langle \overline{\text{Rew}_1}, \ldots, \overline{\text{Rew}_K} \rangle$$

for any $c_0 \in I$.

**Theorem C.11.** If $L_N = \emptyset$ and $L_{AN} = \emptyset$,

$$\mu F_K = \langle \overline{\text{Rew}_1}, \ldots, \overline{\text{Rew}_K} \rangle$$

for any $c_0 \in I$.

Here a function $\langle f_1, \ldots, f_n \rangle$ is defined by $\langle f_1, \ldots, f_K \rangle(x) = (f_1(x), \ldots, f_K(x))$.

To prove Theorem C.10 and Theorem C.11 we consider an approximation of $k$-th moments of accumulated rewards up to finite steps.

**Definition C.12 (accumulated reward up to $n$ steps).** Let $\text{Rew}_{C,n}^{c_0} : S^n \rightarrow [0, \infty]$ be a measurable function defined by

$$\text{Rew}_{C,n}^{c_0}(c_1 \ldots c_n) = \begin{cases} \sum_{j=0}^{N-1} \text{Rew}(c_j) & \exists N \geq 0, c_i \in C \wedge (0 \leq j < N \Rightarrow c_j \notin C) \\ \sum_{j=0}^{n-1} \text{Rew}(c_j) & \text{otherwise} \end{cases}$$

The definition of $\text{Rew}_{C,n}^{c_0}$ is similar to $\text{Rew}_{C}^{c_0}$ except that the sum of the value of reward function is restricted to the first $n$ configurations. The next lemma shows a connection between $\text{Rew}_{C}^{c_0}$ and $\text{Rew}_{C,n}^{c_0}$.

**Lemma C.13.** $\{\text{Rew}_{C,n}^{c_0} \circ S^{n \leq \omega} : S^\omega \rightarrow [0, \infty]\}_n$ is an increasing sequence of functions and its limit is $\text{Rew}_{C}^{c_0}$.

**Proof.** Given $\rho = c_1 c_2 \cdot \in S^\omega$, there are two cases.
- Assume there exists $N \in \omega$ such that $c_N \in C$ and $0 \leq j < N \Rightarrow c_j \notin C$.

$$\text{Rew}_C^{c_0} \circ S^{n \leq \omega}(c_1 c_2 \ldots) = \begin{cases} 
\sum_{j=0}^{n-1} \text{Rew}(c_j) & \text{if } n < N - 1 \\
\sum_{j=0}^{N-1} \text{Rew}(c_j) & \text{if } N - 1 \leq n
\end{cases}$$

$$\text{Rew}_C^{c_0} (c_1 c_2 \ldots) = \sum_{j=0}^{N-1} \text{Rew}(c_j)$$

- Assume $\rho \in (S \setminus C)^\omega$.

$$\text{Rew}_C^{c_0} \circ S^{n \leq \omega}(c_1 c_2 \ldots) = \sum_{j=0}^{n-1} \text{Rew}(c_j)$$

$$\text{Rew}_C^{c_0} (c_1 c_2 \ldots) = \sum_{j=0}^{\infty} \text{Rew}(c_j)$$

In both cases, it is easy to prove $\text{Rew}_C^{c_0} \circ S^{n \leq \omega} \leq \text{Rew}_C^{c_0} \circ S^{n+1 \leq \omega}$ for each $n$, and $\text{Rew}_C^{c_0} = \sup_{n \in \omega} (\text{Rew}_C^{c_0} \circ S^{n \leq \omega})$. \hfill \Box

The $k$-th moment of $\text{Rew}_C^{c_0}$ is denoted by $M_{C,\sigma,n}^{\text{Rew},k}(c_0)$.

**Definition C.14 (k-th moment up to n steps).** A function $M_{C,\sigma,n}^{\text{Rew},k} : S \to [0, \infty]$ is defined as follows.

$$M_{C,\sigma,n}^{\text{Rew},k}(c_0) = \int (\text{Rew}_C^{c_0})^k d\nu_{c_0,n}$$

A connection between $M_{C,\sigma,n}^{\text{Rew},k}$ and $M_{C,\sigma}^{\text{Rew},k}$ is as follows.

**Lemma C.15.** A sequence $\{M_{C,\sigma,n}^{\text{Rew},k}\}_{n \in \omega}$ is increasing and its limit is $M_{C,\sigma}^{\text{Rew},k}$:

$$M_{C,\sigma}^{\text{Rew},k} = \sup_{n \in \omega} M_{C,\sigma,n}^{\text{Rew},k}.$$
Proof. The former part is immediate by Lemma C.13. The latter part is proved by the following calculation.

\[ M_{C,\sigma}^{\text{Rew},k}(c_0) = \int (\text{Rew}_{C}^{\sigma})^k \, d\nu_{c_0} \]
\[ = \int \sup_{n \in \omega} (\text{Rew}_{C, n}^{\sigma})^k \circ S^n \, d\nu_{c_0} \quad \text{(by Lemma C.13)} \]
\[ = \sup_{n \in \omega} \int (\text{Rew}_{C, n}^{\sigma})^k \circ S^n \, d\nu_{\pi_{c_0}} \quad \text{(by the monotone convergence theorem)} \]
\[ = \sup_{n \in \omega} \int (\text{Rew}_{C, n}^{\sigma})^k \, d((S^n \omega)_{\nu_{c_0}}) \quad \text{(by Lemma A.2)} \]
\[ = \sup_{n \in \omega} \int (\text{Rew}_{C, n}^{\sigma})^k \, d\nu_{c_0, n} \]
\[ = \sup_{n \in \omega} M_{C,\sigma, n}^{\text{Rew},k}(c_0) \]

Definition C.16. For any \( c \) and \( \sigma \), we define a scheduler \( \sigma^c = (\sigma^c_t, \sigma^c_a) \) by \( \sigma^c_t(\rho) = \sigma_t(c \rho) \) and \( \sigma^c_a(\rho) = \sigma_a(c \rho) \).

The following lemma easily follows from the definition of \( \mu^\sigma_P \).

Lemma C.17. \( \mu^\sigma_{c_0} = \mu^\sigma_{c_0, c} \) \hfill \qed

The following lemma expresses the \( n + 1 \) step approximation \( M_{C,\sigma, n+1}^{\text{Rew},k} \) in terms of the \( n \) step approximations \( M_{C,\sigma_0, n}^{\text{Rew},1}, \ldots, M_{C,\sigma_0, n}^{\text{Rew},K} \), which plays a crucial role in the induction step in the proof of Theorem C.10 and Theorem C.11.

Lemma C.18. Assume \( c_0 \notin C \) and \( k \in \{1, \ldots, K\} \). For each \( n \in \omega \),

\[ M_{C,\sigma, n+1}^{\text{Rew},k}(c_0) = E_{\text{Rew}(c_0)}^{K,k} \left( \int_{S} M_{C,\sigma_0, n}^{\text{Rew},1}(c_1) \, d\mu_{c_0}(c_1), \ldots, \int_{S} M_{C,\sigma_0, n}^{\text{Rew},K}(c_1) \, d\mu_{c_0}(c_1) \right). \]
Proof.
\[ M_{C,\sigma,n+1}^{\text{Rew},k}(c_0) \]
\[ = \int_{S^{n+1}} (\text{Rew}^c_{C,n+1})^k d\mu_{c_0,n+1}^{\sigma} \]
\[ = \int_S \cdots \int_S \left( \text{Rew}^c_{C,n+1}(c_1, \ldots, c_{n+1}) \right)^k d\mu_{c_0}^{\sigma}(c_1) \]
\[ = \int_S \cdots \int_S \left( \text{Rew}(c_0) + \text{Rew}^c_{C,n}(c_2, \ldots, c_{n+1}) \right)^k d\mu_{c_0}^{\sigma}(c_1) \]
\[ = \int_S \cdots \int_S \left( \sum_{j=0}^{k} \binom{k}{j} (\text{Rew}(c_0))^{k-j} \left( \text{Rew}^c_{C,n}(c_2, \ldots, c_{n+1}) \right)^j \right) d\mu_{c_0}^{\sigma}(c_1) \]
\[ = (\text{Rew}(c_0))^k + \sum_{j=1}^{k} \binom{k}{j} (\text{Rew}(c_0))^{k-j} \int_S \cdots \int_S \left( \text{Rew}^c_{C,n}(c_2, \ldots, c_{n+1}) \right)^j d\mu_{c_0}^{\sigma}(c_1) \]
\[ = (\text{Rew}(c_0))^k + \sum_{j=1}^{k} \binom{k}{j} (\text{Rew}(c_0))^{k-j} \int_S \int_S \left( \text{Rew}^c_{C,n}(c_1, c_2, \ldots, c_{n+1}) \right)^j d\mu_{c_0}^{\sigma}(c_1) \]

Proof (Theorem C.10).
1. We prove
\[ (F_K)^n(\perp) \geq \left\langle M_{C,\sigma,n}^{\text{Rew},1}, \ldots, M_{C,\sigma,n}^{\text{Rew},K} \right\rangle \]

for each \( \sigma \) and \( n \) by induction on \( n \).
- If \( n = 0 \), the l.h.s. and the r.h.s. are equal to 0.
- If \( n > 0 \), it suffices to prove that for each \( c_0 \), there exists \( \sigma' \) such that

\[ F_K \left( \left\langle M_{C,\sigma',n}^{\text{Rew},1}, \ldots, M_{C,\sigma',n}^{\text{Rew},K} \right\rangle \right)(c_0) \geq \left\langle M_{C,\sigma,n+1}^{\text{Rew},1}, \ldots, M_{C,\sigma,n+1}^{\text{Rew},K} \right\rangle \]

by the induction hypothesis. If \( c_0 \in C \), the l.h.s. and the r.h.s. are equal to 0. If \( c_0 \notin C \), we prove

\[ \mathcal{X} \left( E_{\text{Rew}(c_0)}^{K,k} \circ \left\langle M_{C,\sigma_0,n}^{\text{Rew},1}, \ldots, M_{C,\sigma_0,n}^{\text{Rew},K} \right\rangle \right)(c_0) \geq M_{C,\sigma,n+1}^{\text{Rew},k}(c_0). \]

By Lemma C.18, it suffices to prove

\[ \mathcal{X} \eta(c_0) \geq \int_S \eta(c_1) d\mu_{c_0}^{\sigma}(c_1) \]

where

\[ \eta = E_{\text{Rew}(c_0)}^{K,k} \circ \left\langle M_{C,\sigma_0,n}^{\text{Rew},1}, \ldots, M_{C,\sigma_0,n}^{\text{Rew},K} \right\rangle. \]

This holds by Lemma C.3.
2. We take supremum of \( F_K \) with respect to \( n \), and then with respect to \( \sigma \).

\[
\mu F_K \geq \sup_{n \in \omega} ((F_K)^n(\perp)) \geq \langle M^{\text{Rew},1}_C, \ldots, M^{\text{Rew},K}_C \rangle
\]

Proof (Theorem C.11). Here, we prove \((F_K)^n(\perp) = \langle M^{\text{Rew},1}_C, \sigma, n, \ldots, M^{\text{Rew},K}_C, \sigma, n \rangle\) for each \( n \) by induction on \( n \) in the same way as Theorem C.10 except that we use Lemma C.4 instead of Lemma C.3.

By the Kleene fixed-point theorem and Lemma C.9, we have \( \sup_{n \in \omega} ((F_K)^n(\perp)) = \mu F_K \).

\[
\mu F_K = \sup_{n \in \omega} ((F_K)^n(\perp)) = \sup_{n \in \omega} \langle M^{\text{Rew},1}_C, \sigma, n, \ldots, M^{\text{Rew},K}_C, \sigma, n \rangle = \langle M^{\text{Rew},1}_C, \ldots, M^{\text{Rew},K}_C, \sigma \rangle
\]

Since there is only one scheduler if \( L_N = L_{AN} = \emptyset \), we conclude

\[
\mu F_K = \langle M^{\text{Rew},1}_C, \ldots, M^{\text{Rew},K}_C, \rangle = \langle M^{\text{Rew},1}_C, \ldots, M^{\text{Rew},K}_C \rangle.
\]

\( \square \)

### C.4 Ranking supermartingale for \( K \)-th moments

The following definition and theorem generalize Definition 3.12 and Theorem 3.13, respectively.

**Definition C.19 (ranking supermartingale for \( K \)-th moments of accumulated rewards).** A ranking supermartingale for \( K \)-th moments is a function \( \eta : S \to \mathbb{R}^K \) such that for each \( k \),

\[
\begin{align*}
\eta_k(c) &\geq (F_{\text{Rew},c}^k \circ \eta_k)(c) \quad \text{for each } c \in I \setminus C \\
\eta_k(c) &\geq 0 \quad \text{for each } c \in I
\end{align*}
\]

where \( \eta_k : S \to \mathbb{R} \) is defined by \( (\eta_1(c), \ldots, \eta_K(c)) = \eta(c) \) for each \( c \in S \).

**Theorem C.20.** If \( \eta \) is a supermartingale for \( K \)-th moments, then for any \( c \in I \), \( (M^{\text{Rew},1}_C(c), \ldots, M^{\text{Rew},K}_C(c)) \leq \eta(c) \).

Proof. Let \( \eta' : S \to [0, \infty]^K \) be a function defined by

\[
\eta'(c) = \begin{cases} 
\eta(c) & c \in I \\
0 & \text{otherwise}
\end{cases}
\]

By Lemma C.1, \( F_K(\eta') \leq \eta' \) is easily proved. By the Knaster-Tarski theorem, we have \( \mu F_K \leq \eta' \). Therefore

\[
(M^{\text{Rew},1}_C(c), \ldots, M^{\text{Rew},K}_C(c)) \leq \mu F_K(c) \leq \eta'(c) = \eta(c)
\]

for each \( c \in I \). \( \square \)
D Details of Template-Based Synthesis Algorithm

In this section we describe the template-based synthesis algorithms in §5 in more detail. They are based on existing template-based algorithms for synthesizing a ranking supermartingale for first moments in [5, 7, 8]. Input to the algorithm is a pCFG $\Gamma$, an invariant $I$, a set $C \subseteq I$ of configurations, and a natural number $K$. Output is an upper bound of $K$-th moment.

D.1 Linear Template-based Algorithm

Synthesis of a ranking supermartingale via reduction to an LP problem is discussed in [5, 8]. We adapt this for our supermartingales.

We first define some notions.

Definition D.1. Let $V = \{x_1, \ldots, x_n\}$ be a set of variables. A linear expression over $V$ is a formula of a form $a_1x_{i_1} + \cdots + a_nx_{i_n} + b$ where $a_1, \ldots, a_n, b \in \mathbb{R}$ and $x_{i_1}, \ldots, x_{i_n} \in V$. We write $\mathbb{R}_{\text{lin}}[V]$ for the set of linear expressions. A linear inequality over $V$ is a formula of a form $\varphi \geq 0$ where $\varphi$ is a linear expression. A linear conjunctive predicate is a conjunction $\varphi_1 \geq 0 \land \cdots \land \varphi_p \geq 0$ of linear constraints, and a linear predicate is a disjunction $(\varphi_{1,1} \geq 0 \land \cdots \land \varphi_{1,p_1} \geq 0) \lor \cdots \lor (\varphi_{q,1} \geq 0 \land \cdots \land \varphi_{q,p_q} \geq 0)$ of linear conjunctive predicates. We define their semantics in the standard manner.

For a pCFG $\Gamma = (L, V, l_{\text{init}}, x_{\text{init}}, \rightarrow, \text{Up}, \text{Pr}, G)$, a linear expression map (resp. linear predicate map) over $\Gamma$ is a function that assigns a linear expression (resp. linear predicate) to each location of $\Gamma$. The semantics of the former is a function assigning a real number to each configuration, i.e. it has a type $L \times \mathbb{R}^V \rightarrow \mathbb{R}$, and that of the latter is a set of configurations, i.e. a subset of $L \times \mathbb{R}^V$. They are defined in the natural manners.

In the rest of this section, we describe a linear template-based synthesis algorithm for a pCFG $\Gamma$ an invariant $I$, a set $C \subseteq I$ of configurations, and a natural number $K$. We assume that the input satisfies the following conditions. Similar conditions were assumed in [5, 8].

Assumption D.2.

- For any $l \in L_A$ such that $\text{Up}(l) = (x_j, u)$,
  - if $u \in B(\mathbb{R}^V, \mathbb{R})$, then $u$ is represented by a linear expression over $V$;
  - if $u \in D(\mathbb{R})$, the expectation of $u$ is known; and
  - if $u \in B(\mathbb{R})$, then $u$ is represented by a linear predicate $\phi$ over $\{x_j\}$.
- For any $l \in L_D$ and $l' \in L$, $G(l, l') = [p]$ is represented by a linear predicate over $V$.
- the invariant $I$ is represented by a linear predicate map over $\Gamma$.
- the set $C$ of terminal configurations is represented by a linear conjunctive predicate map.
Let $V = \{x_1, \ldots, x_n\}$ be the set of variables appearing in $\Gamma$. We first fix a linear template to a supermartingale. It is a family of formulas indexed by $i \in \{1, \ldots, K\}$ and $l \in L$ that have the following form:

$$\eta_i(l, x) = a_{1,i}^l x_1 + \cdots + a_{n,i}^l x_n + b_i^l.$$ 

Here $a_{1,i}^l, \ldots, a_{n,i}^l, b_i^l$ are newly added variables called parameters. We write $U$ for the set of all parameters, i.e. $U := \{a_{1,i}^l, \ldots, a_{n,i}^l, b_i^l | i \in \{1, \ldots, K\}, l \in L\}$. Note that if we fix a valuation $U \rightarrow \mathbb{R}$ of parameters, then each $\eta_i(l, x)$ reduces to a linear expression over $V$, and therefore $\eta_i(l, x)$ can be regarded as a linear expression map $L \times \mathbb{R}^V \rightarrow \mathbb{R}_{\text{lin}}[V]$. Our goal is to find a valuation $U \rightarrow \mathbb{R}$ so that a $K$-tuple $(\eta_1(l, x), \ldots, \eta_K(l, x))$ of linear expression maps become a ranking supermartingale for $K$-th moment (Definition 3.12).

To this end, we reduce the axioms of ranking supermartingale for $K$-th moments in Definition 3.12 to conditions over the parameters. We shall omit the detail, but it is not so hard to see that as a result of the reduction we obtain a conjunction of formulas of the following form:

$$\forall x \in \mathbb{R}^V. \varphi_1 \triangleright 0 \land \cdots \land \varphi_m \triangleright 0 \Rightarrow \psi \geq 0.$$ 

(7)

Here $\triangleright \in \{\geq, >\}$, each $\varphi_i$ is a linear expression without parameters, and $\psi$ is a linear formula over $V$ whose coefficients are linear expressions over $U$.

We next relax the strict inequalities as follows:

$$\forall x \in \mathbb{R}^V. \varphi_1 \geq 0 \land \cdots \land \varphi_m \geq 0 \Rightarrow \psi \geq 0.$$ 

(8)

It is easy to see that (8) implies (7). The same relaxation is also done in [5, 8].

Using matrices, we can represent a formula (8) as follows:

$$\forall x \in \mathbb{R}^V. Ax \leq b \Rightarrow c^T x \leq d.$$ 

(9)

Here $A$ is a matrix and $b$ is a vector all of whose components are real numbers, and $c$ is a vector and $d$ is a scalar all of whose components are linear expressions over $U$. In [5, 8], a formula (9) is reduced to the following formula:

$$\exists y \in \mathbb{R}^m. \exists y' \in \mathbb{R}. d - c^T x = y^T (b - Ax) + y'.$$ 

(10)

Here $m$ is the dimension of $b$. It is easy to see that (10) implies (9). By comparing the coefficients on both sides, we can see that (10) is equivalent to

$$\exists y \in \mathbb{R}^m. A^T y = c \land b^T y \leq d.$$ 

Note that the resulting (in)equalities are linear with respect to parameters in $U$ and $y$. Hence its feasibility can be efficiently checked using a linear programming (LP) solver.

Recall that our goal is to calculate an upper bound of $K$-th moment. Hence we naturally want to minimize the upper bound $\eta_K(l_{\text{init}}, x_{\text{init}})$ calculated by a supermartingale (see Thm. 3.13). We can achieve this goal by setting $\eta_K(l_{\text{init}}, x_{\text{init}})$,
a linear expression over \( U \), to the objective function of the linear programming problem and ask the LP solver to minimize it.

A natural question would about the converse of the implication (10) \( \Rightarrow \) (9). The following theorem answers the question to some extent.

**Theorem D.3** (affine form of Farkas’ lemma (see e.g. [29, Cor. 7.1h])).

Let \( A \in \mathbb{R}^{n \times m} \), \( b \in \mathbb{R}^m \), \( c \in \mathbb{R}^n \) and \( d \in \mathbb{R} \). If \( \{ x \mid Ax \leq b \} \) is not empty, the following two conditions are equivalent.

- \( \forall x \in \mathbb{R}^n, Ax \leq b \Rightarrow c^T x \leq d \)
- \( \exists y \in \mathbb{R}^m, A^T y = c \land b^T y \leq d \)

We note that if a pCFG \( \Gamma \) has no program variable \( (V = \emptyset) \) and all the transitions are probabilistic (that is, if \( \Gamma \) is a Markov chain), the above method gives the exact value of moments. It is because the LP problem has the obvious optimal solution: \( \eta_k(l) = (\text{the } k\text{-th moment of runtimes from location } l) \).

**D.2 Polynomial Template-based Algorithm**

We consider fixing a polynomial template for a supermartingale. The algorithm in this section is based on [7].

**Definition D.4.** Let \( V = \{x_1, \ldots, x_n\} \) be a set of variables. A *monomial* is a formula of a form \( x_1^{d_1} \cdots x_r^{d_r} \). We call \( d_1 + \cdots + d_r \) a *degree* of the monomial, and write \( M_{\leq d} \) for the set of monomials whose degrees are no greater than \( d \).

A *polynomial expression* (or simply a *polynomial*) over \( V \) is a formula of a form \( a_1 m_1 + \cdots + a_q m_q + b \) where \( a_1, \ldots, a_q, b \in \mathbb{R} \) and \( m_1, \ldots, m_q \) are monomials. We write \( \mathbb{R}[V] \) for the set of polynomial expressions over \( V \). The notions of *polynomial inequality*, *polynomial conjunctive predicate*, *polynomial predicate*, *polynomial expression map* and *polynomial predicate map* are defined in a similar manner to Def. D.1.

In the polynomial case, we assume that a pCFG \( \Gamma \), an invariant \( I \), a set \( C \subseteq I \) of configurations and a natural number \( K \) satisfy the following conditions.

**Assumption D.5.**

- For any \( l \in L_A \), \( U_p(l) = (x_j, u) \),
  - if \( u \in B(\mathbb{R}^V, \mathbb{R}) \), then \( u \) is represented by a polynomial expression over \( V \)
  - if \( u \in D(\mathbb{R}) \), the \( K\)-th moment of \( u \) is known.
  - if \( u \in B(\mathbb{R}) \), then \( u \) is represented by a polynomial predicate \( \phi \) over \( \{x_j\} \).
- For any \( l \in L_D \), \( l', G(l, l') = [p] \) is represented by a polynomial predicate \( p \) over \( V \).
- the invariant \( I \) is represented by a polynomial predicate map over \( \Gamma \).
- the set \( C \) of terminal configurations is represented by a polynomial conjunctive predicate map.
The polynomial template-based synthesis algorithm is similar to the linear template-based one. In the polynomial case, the user has to fix the maximum degree $d$ of the polynomial template. The algorithm first fixes a $d$-degree polynomial template for a supermartingale. It is a family of formulas indexed by $i \in \{1, \ldots, K\}$ and $l \in L$ that have the following form:

$$
\eta_i(l, x) = \sum_{m \in M, m \leq d} a_{m,i}^l m + b_{i}^l.
$$

Each $a_{m,i}^l$ and $b_{i}^l$ are newly added variables called \textit{parameters}, and we write $U$ for the set of all parameters. Our goal is to find a valuation $U \rightarrow \mathbb{R}$ so that a $K$-tuple $(\eta_1(\_), \ldots, \eta_K(\_))$ of polynomial expression maps is a ranking supermartingale for $K$-th moment (Definition 3.12).

Similarly to the linear case, the algorithm collects conditions on the parameters. It results in a conjunction of formulas of the following form:

$$
\forall x \in \mathbb{R}^V. \varphi_1 \triangleright_1 0 \land \cdots \land \varphi_m \triangleright_m 0 \Rightarrow \psi \geq 0.
$$

Here $\triangleright_i \in \{\geq, >\}$, each $\varphi_i$ is a polynomial expression without parameters, and $\psi$ is a polynomial formula over $V$ whose coefficients are linear expressions over $U$. Relaxing the strict inequalities, we obtain the following:

$$
\forall x \in \mathbb{R}^V. \varphi_1 \geq 0 \land \cdots \land \varphi_m \geq 0 \Rightarrow \psi \geq 0.
$$

(12)

To reduce (12) to a form that is solvable by a numerical method, we can use the notion of \textit{sum-of-square polynomials} \cite{7}. A polynomial expression $f$ is said to be \textit{sum-of-square} (SOS) if there exist polynomial expressions $g_1, \ldots, g_l$ such that $f = g_1^2 + \cdots + g_l^2$.

Obviously, a sum-of-square polynomial is nonnegative. Therefore the following formula is a sufficient condition for (12):

$$
\exists (h_w \text{ sum-of-square})_{w \in \{0,1\}^m} \cdot \psi = \sum_{w \in \{0,1\}^m} h_w \cdot \varphi_1^{w_1} \cdot \cdots \cdot \varphi_m^{w_m}.
$$

Here $w_i$ denotes the $i$-th component of $w \in \{0,1\}^m$.

One of the reasons that sum-of-square is convenient is that it is characterized using the notion of \textit{positive semidefinite matrix}.

\textbf{Proposition D.6 (see e.g. \cite{14}).} A polynomial expression $f$ over $V$ is sum-of-square if and only if there exist a vector $y$ whose components are monomials over $V$ and a positive semidefinite matrix $A$ such that $f = y^T A y$. \hfill \Box

By the proposition above, existence of a valuation $U \rightarrow \mathbb{R}$ of parameters and sum-of-square polynomials as in (13) can be reduced to a \textit{semidefinite programming} (SDP) problem. Likewise the linear case, by setting a linear expression $\eta_K(l_{\text{init}}, x_{\text{init}})$ to the objective function, we can minimize it.

In the linear case, completeness was partially ensured by Farkas’ lemma. In the polynomial case, the role is played by the following theorem.
Theorem D.7 (Schm"{u}dgen’s Positivstellensatz [28]). Let \( g, g_1, \ldots, g_m \) be polynomial expression over a set of variable \( V \). If \( \{ x \in \mathbb{R}^V \mid \bigwedge_{i=1}^m g_i \geq 0 \} \) is compact, then the following conditions are equivalent:

- \( \forall x \in \mathbb{R}^V. g_1 \geq 0 \wedge \cdots \wedge g_m \geq 0 \Rightarrow g > 0. \)
- There exists a family \( \{ h_w \}_{w \in \{0, 1\}^m} \) of sum-of-square polynomial expressions such that \( g = \sum_{w \in \{0, 1\}^m} h_w \cdot g_1^w \cdot \cdots \cdot g_m^w \).

E Test Programs

We have augmented the standard syntax of randomized program (see e.g. [9]) so that we can specify an invariant and a terminal configuration. To specify an invariant, we can use either of the following syntax.

- \$\ldots\$ specifies an invariant globally.
- \{\ldots\} specifies an invariant locally.

We can specify a terminal configuration by using \texttt{refute(...)}.

```
Listing 1.1: (1-1) coupon_collector
...
1 \$ 0 <= c0 and c0 <= 1 and 0 <= c1 and c1 <= 1
2 3 c0 := 0;
4 c1 := 0;
5 while true do
6    if prob(0.5) then
7      c0 := 1
8      else
9      c1 := 1
10     fi;
11    refute (c0 + c1 > 1)
12  od
```

```
Listing 1.2: (1-2) coupon_collector4
...
1 \$ 0 <= c0 and c0 <= 1 and 0 <= c1 and c1 <= 1 and 0 <= c2 and c2 <= 1 and 0 <= c3 and c3 <= 1
2 3 c0 := 0;
4 c1 := 0;
5 c2 := 0;
6 c3 := 0;
7 while true do
8    if prob(0.5) then
9      if prob(0.5) then
10        c0 := 1
11        else
12        c1 := 1
13      fi
14    else
15      if prob(0.5) then
16        c2 := 1
17        else
18        c3 := 1
19      fi
20     fi;
21    refute (c0 + c1 + c2 + c3 > 3)
22  od
```
Listing 1.3: (2-1) random_walk_1d_intvalued

1 \{(true)\} x := 1;
2
3 \{x >= 1\} while true do
4 \{x >= 1\} if prob(0.6) then
5 \{x >= 1\} x := x - 1
6 else
7 \{x >= 1\} x := x + 1
8 fi;
9 \{x >= 0\} refute (x < 1)
10 od

Listing 1.4: (2-2) random_walk_1d_realvalued

1 \{(true)\} x := 2;
2
3 \{x >= 0\} while true do
4 \{x >= 0\} if prob(0.7) then
5 \{x >= 0\} z := Unif(0,1);
6 \{x >= 0 and 0 <= z and z <= 1\} x := x - z
7 else
8 \{x >= 0\} z := Unif(0,1);
9 \{x >= 0 and 0 <= z and z <= 1\} x := x + z
10 fi;
11 \{x >= -1\} refute (x < 0)
12 od

Listing 1.5: (2-3) random_walk_1d_adversary

1 \{(true)\} x := 2;
2
3 \{0 <= x and x <= 13\} while true do
4 \{0 <= x and x <= 13\} if prob(0.8) then
5 \{0 <= x and x <= 13\} skip
6 else
7 \{0 <= x and x <= 13\} if prob(0.8) then
8 \{0 <= x and x <= 13\} if prob(0.5) then
9 \{0 <= x and x <= 13\} x := x + 1
10 else
11 \{0 <= x and x <= 13\} x := x + 2
12 fi;
13 \{0 <= x and x <= 13\} if * then
14 \{0 <= x and x <= 13\} if prob(0.875) then
15 \{0 <= x and x <= 13\} x := x - 1
16 else
17 \{0 <= x and x <= 13\} skip
18 fi;
19 else
20 \{0 <= x and x <= 13\} if prob(0.8) then
21 \{0 <= x and x <= 13\} skip
22 else
23 \{0 <= x and x <= 13\} if prob(0.5) then
24 \{0 <= x and x <= 13\} x := x + 1
25 else
26 \{0 <= x and x <= 13\} x := x + 2
27 fi;
28 \{0 <= x and x <= 13\} x := x - 1
29 \{0 <= x and x <= 13\} refute (x <= 0)
30 od

Listing 1.6: (2-4) random_walk_2d_demonic
Listing 1.7: (2-5) random_walk_2d_variant

```plaintext
1 { true } x := 2;
2 { x = 2 } y := 2;
3 { 0 <= x and 0 <= y } while true do
 4 { 0 <= x and 0 <= y } if * then
 5 { 0 <= x and 0 <= y } z := Unif (-2,1);
 6 { 0 <= x and 0 <= y and -2 <= z and z <= 1 } x := x + z
 7 { 0 <= x and 0 <= y } else
 8 { 0 <= x and 0 <= y } z := Unif (-2,1);
 9 { 0 <= x and 0 <= y and -2 <= z and z <= 1 } y := y + z
10 fi;
11 { -2 <= x and -2 <= y } refute (x <= 0);
12 { 0 <= x and -2 <= y } refute (y <= 0)
13 od
```

F Detailed Comparison with Existing Work

F.1 Comparison with [6]

In the literature on martingale-based methods, the one closest to this work is [6]. Among its contribution is the analysis of tail probabilities by either of the following two combinations:

- difference-bounded ranking supermartingales and the corresponding choice of concentration inequality (namely Azuma’s martingale concentration lemma);
- (not necessarily difference-bounded) ranking supermartingales and Markov’s concentration inequality.

While implementation and experiments are lacking in [6], we can make the following theoretical comparison between these two methods and ours.

- The first method (with difference-bounded supermartingales) requires trying many difference bounds c, synthesizing a martingale for each c, and picking
the best one. This “try many and pick the best” workflow is much like in [9]; it increases the computational cost, especially in the case a polynomial template is used (where a single synthesis procedure takes tens of seconds).

– The second method corresponds precisely to the special case of our method where we restrict to the first moment. We argued that using higher moments is crucial in obtaining tighter bounds as the deadline becomes large, theoretically (§4) and experimentally (§6).

F.2 Comparison with [19]

In the predicate-transformer approach, the work [19] is the closest to ours, in that it studies variance of runtimes of randomized programs. The main differences are as follows: 1) computing tail probabilities is not pursued; 2) their extension from mean to variance involves an additional variable \( \tau \), which poses a challenge in automated synthesis as well as in generalization to even higher moments; and 3) they do not pursue automated analysis.

Let us elaborate on the above point 2). In syntax-based static approaches to estimating variances or second moments, it is inevitable to simultaneously reason about both first and second moments. See Def. 3.3. In this work, we do so systematically by extending a notion of supermartingale into a vector-valued notion; this way our theory generalizes to moments higher than the second in a straightforward manner. In contrast, in [19], an additional variable \( \tau \)—which stands for the elapsed time—is used for mixing first and second moments.

Besides the problem of generalizing to higher moments, a main drawback of this approach in [19] is that the degrees of templates become bigger when it comes to automated synthesis. For example, due to the use of \( \tau^2 \) in the condition for \( \hat{X} \) in [19 Thm. 7], if the template for \( \tau \) is of degree \( k \), the template for \( \hat{X} \) is necessarily of degree \( 2k \) or higher. One consequence is that a fully LP-based implementation of the approach of [19] becomes hard, while it is possible in the current work (see §6).

Let us also note that the work [19] focuses on precondition calculi and does not discuss automated synthesis or analysis.