



Lower Bounds for Possibly Divergent Probabilistic Programs

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We present a new proof rule for verifying lower bounds on quantities of probabilistic programs. Our proof rule is not confined to almost-surely terminating programs – as is the case for existing rules – and can be used to establish non-trivial lower bounds on, e.g., termination probabilities and expected values, for possibly *divergent* probabilistic loops, e.g., the well-known three-dimensional random walk on a lattice.

CCS Concepts: • **Theory of computation** → **Program reasoning**; • **Mathematics of computing** → **Probabilistic algorithms**; **Stochastic processes**.

Additional Key Words and Phrases: probabilistic programs, quantitative verification, weakest preexpectations, lower bounds, almost-sure termination, uniform integrability

ACM Reference Format:

Shenghua Feng, Mingshuai Chen, Han Su, Benjamin Lucien Kaminski, Joost-Pieter Katoen, and Naijun Zhan. 2023. Lower Bounds for Possibly Divergent Probabilistic Programs. *Proc. ACM Program. Lang.* 7, OOPSLA1, Article 99 (April 2023), 31 pages. <https://doi.org/10.1145/3586051>

1 INTRODUCTION

Probabilistic programs [Gordon et al. 2014; Kozen 1981; Saheb-Djahromi 1978; van de Meent et al. 2018] extend deterministic programs with stochastic behaviors, e.g., random sampling, probabilistic choice, and conditioning (via posterior observations). Probabilistic programs have witnessed numerous applications in various domains: They steer autonomous robots and self-driving cars [Evans et al. 2017; Shamsi et al. 2020], are key to describe security [Barthe et al. 2013] and quantum [Ying 2011] mechanisms, intrinsically code up randomized algorithms for solving NP-hard or even deterministically unsolvable problems (in, e.g., distributed computing [Aspnes and Herlihy 1990; Schneider 1993]), and are at the heart of modern machine learning and approximate computing [Carbin et al. 2016]. See [Barthe et al. 2020] for recent advancements in probabilistic programming.

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2475-1421/2023/4-ART99

<https://doi.org/10.1145/3586051>

Probabilistic programs, though typically relatively small in size, are hard to grasp: The crux of probabilistic programming is to treat normal-looking programs as if they were *probability distributions* [Hicks 2014; Saheb-Djahromi 1978]. Such a lift from deterministic program states to possibly infinite-support distributions (over states) renders the verification problem of probabilistic programs notoriously hard [Kaminski et al. 2019]. In particular, given a random variable f (mapping program states to numbers), a key verification task is to reason about the *expected value* of f after termination of a program C on input σ . If f is the indicator function of an event A , then this expected value is the *probability* that A occurs upon termination of C . In case of a potentially *unbounded loopy program* C , the expected value of f is often characterized as the *least fixed point* of some monotonic operator capturing the semantics of C w.r.t. f . Computing the exact expected value of f hence amounts to inferring the least fixed point which is in general highly intractable.

As a consequence, existing verification techniques for reasoning about probabilistic loops are mostly concerned with proving *upper* and/or *lower bounds* on expected values, i.e., on least fixed points. Verifying lower bounds is notably essential for establishing *total correctness* of probabilistic programs [Katoen et al. 2015; McIver and Morgan 2001] and for assessing the quality and tightness of upper bounds. For verifying a candidate upper bound u , the well-known principle of *Park induction* [Kozen 1985; Park 1969], or more generally, κ -*induction* [Batz et al. 2021a], suffices by “pushing u through the loop semantics” *once*. Whereas for lower bounds on least fixed point, a “dual” version of Park induction is *unsound* (see Sect. 4.3).

Existing (sound) lower induction rules for probabilistic programs are confined to either (i) *bounded* random variables with a priori knowledge on the *termination probability* of the program [McIver and Morgan 2005]; or (ii) (universally) *almost-surely terminating* (AST) programs (i.e., programs that terminate with probability 1 on all inputs) and *uniformly integrable* random variables – a notion from stochastic processes, which requires reasoning about looping times and/or bounds on random variables [Hark et al. 2020]. In contrast to Park induction for upper bounds, applying these lower induction rules requires heavy proof efforts in, e.g., looking for supermartingales [Chatterjee et al. 2020] witnessing AST, checking uniform integrability, and inferring termination probabilities. *In particular, none of these rules is capable of inferring lower bounds on termination probabilities strictly less than 1*, i.e., for non-AST (aka, *divergent*) programs. Consider, e.g., the following probabilistic loop $C_{3\text{dsrw}}$ modelling the well-known *three-dimensional (3-D) random walk* on the lattice over \mathbb{Z}^3 .¹

$$C_{3\text{dsrw}}: \text{ while } (x \neq 0 \vee y \neq 0 \vee z \neq 0) \{ \\ \quad x := x - 1 \oplus x := x + 1 \oplus y := y - 1 \oplus y := y + 1 \oplus z := z - 1 \oplus z := z + 1 \} .$$

The random nature underneath $C_{3\text{dsrw}}$ is fundamentally *different* from its 1- and 2-D counterparts: Pólya [1921] proved that the probability \mathcal{P} that such a random walk returns to the origin at $(0, 0, 0)$ is strictly less than 1, indicating that $C_{3\text{dsrw}}$ does *not* terminate almost-surely. More precisely, the termination probability of $C_{3\text{dsrw}}$ starting from any neighbor location of the origin is

$$\mathcal{P} = 1 - \left(\frac{3}{(2\pi)^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dx dy dz}{3 - \cos x - \cos y - \cos z} \right)^{-1} = 0.3405373296 \dots \quad (\dagger)$$

Existing verification techniques cannot tackle $C_{3\text{dsrw}}$ due to its complex nature of divergence.

In this paper, we present a new proof rule, termed the *guard-strengthening rule* for verifying lower bounds on the expected value of a potentially *unbounded* random variable f for a possibly *divergent* probabilistic loop $C_{\text{loop}} = \text{while } (\varphi) \{ C \}$. *Our proof rule employs reduction*: Suppose we aim to certify l as a lower bound on the expected value of f after termination of C_{loop} . We first forge a new loop $C'_{\text{loop}} = \text{while } (\varphi') \{ C \}$ out of C_{loop} by *strengthening* its loop guard φ to φ' , yielding a

¹The iterated symbol \oplus is shorthand for discrete uniform choice (in this case, with probability $1/6$ each).

reduced problem where (i) the modified loop C'_{loop} features a *stronger* termination property (e.g., provably AST), and (ii) both the uniform integrability of l and the boundedness conditions are *easier* to verify. Our proof rule then asserts – by exploiting the “difference” between C'_{loop} and C_{loop} w.r.t. f in terms of the *weakest preexpectation calculus* [Kozen 1985; McIver and Morgan 2005] – that a lower bound l for C'_{loop} (w.r.t. a restricted form of f) also suffices as a lower bound for C_{loop} (w.r.t. f). The former, due to (i) and (ii) by guard strengthening, can often be established by applying the aforementioned lower induction rules or – if C'_{loop} has a *finite* state space – probabilistic model checking [Baier and Katoen 2008; Katoen 2016; Kwiatkowska 2003]. In this case, our proof rule can be (partially) *automated* to derive *increasingly tighter* lower bounds – as φ' “approaches” φ – on, e.g., the termination probability \mathcal{P} of the 3-D random walk in (†), see details in Exmp. 24.

The main results of this paper are the following:

- (a) We present a new proof rule via *guard strengthening* for verifying lower bounds on expected values of probabilistic programs. To the best of our knowledge, this is the first lower bound rule that admits *divergent* probabilistic loops with *unbounded* expected values.
- (b) We show that the modified loops with strengthened guards feature *easily provable* almost-sure termination and uniform integrability. This eases and enlarges the use of existing proof rules for lower bounds; Moreover, we propose a novel sufficient criterion for proving uniform integrability which recognizes cases that are *out-of-reach* by existing sufficient conditions based on the optional stopping theorem [Hark et al. 2020].
- (c) We show that the approximation error incurred by our guard-strengthening technique can be *arbitrarily small* thereby yielding *tight* lower bounds.
- (d) We identify scenarios where our proof rule facilitates inferring quantitative properties of *infinite-state* probabilistic programs by model checking *finite-state* probabilistic models.

We demonstrate the effectiveness of our proof rule on a collection of examples, including the 3-D random walk and a real-world randomized networking protocol.

Additional background materials, elaborated proofs, and details on the examples can be found in the appendix of the full version of this paper [Feng et al. 2023].

2 OVERVIEW OF OUR APPROACH

In a nutshell, our idea is to transform a given potentially non-AST loop C_{loop} into a provably AST loop C'_{loop} and then certify lower bounds for C'_{loop} . Our transformation is performed in a way s.t. the expected outcome of C'_{loop} is guaranteed to be a lower bound on the expected outcome of C_{loop} . Thus, as encoded in our proof rule, a lower bound for C'_{loop} suffices as a lower bound for C_{loop} .

Let us demonstrate our approach by analyzing one of the most basic expected outcomes of a probabilistic loop: termination. Consider the 1-D random walk C_{1dbrw} on \mathbb{Z} (shown below on the left) with *biased* probability $1/3$ moving to the left and probability $2/3$ moving to the right. Due to its biased nature, this loop does not terminate almost-surely and *none of the existing proof rules*² suffices to establish non-trivial lower bounds on its termination probability; see details in Exmp. 16.

$$\begin{array}{ll}
 C_{\text{1dbrw}}: & \text{while } (0 < n) \{ \\
 & \quad n := n - 1 \ [1/3] \ n := n + 1 \\
 & \} \\
 C_{\text{1dbrw}}^M: & \text{while } (0 < n < M) \{ \\
 & \quad n := n - 1 \ [1/3] \ n := n + 1 \\
 & \}
 \end{array}$$

Above right, we see the modified version of this loop, C_{1dbrw}^M , which is obtained from C_{1dbrw} by introducing an artificial upper bound $M \in \mathbb{N}$ on n in the loop guard. This modified loop *does* terminate almost-surely and can moreover visit only finitely many different states.

²Referring to syntactic proof rules in the expectation-based program logic [Kozen 1985; McIver and Morgan 2005].

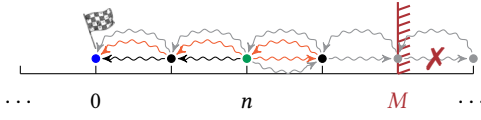


Fig. 1. Guard-strengthening effect: In $C_{1\text{dbrw}}$, all the three program traces (distinguished by colors) initiating from \bullet terminate at \bullet . In $C_{1\text{dbrw}}^M$, however, the gray trace crossing the “barrier” M is no longer possible.

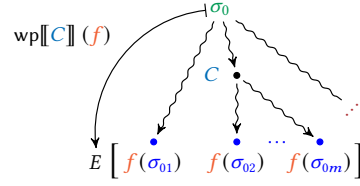


Fig. 2. Illustration of wp : $\text{wp}[[C]](f)(\sigma_0)$ determines the expected value of f evaluated in the final states \bullet reached after termination of C on input σ_0 ; \dots indicates nonterminating (aka, divergent) path of C .

$C_{1\text{dbrw}}^M$ terminates by “hitting” $n \leq 0$ or $n \geq M$. The key observation is that *the probability of $C_{1\text{dbrw}}^M$ terminating at $n \leq 0$ is smaller than the termination probability of $C_{1\text{dbrw}}$* , since some terminating program traces of $C_{1\text{dbrw}}$ – contributing to its termination probability – are no longer possible in $C_{1\text{dbrw}}^M$ due to the artificial “barrier” M ; see Fig. 1 for an illustration. Meanwhile, underapproximating the probability that $C_{1\text{dbrw}}^M$ terminates at $n \leq 0$ – thereby yielding a lower bound on the termination probability of $C_{1\text{dbrw}}$ – can be addressed by existing lower induction rules. In fact, since $C_{1\text{dbrw}}^M$ has a finite state space for any fixed $M \in \mathbb{N}$, its *exact* termination probability at $n \leq 0$ can be obtained by probabilistic model checking. Moreover, if we push the “barrier” further to the right by increasing M , then we obtain *increasingly tighter* lower bounds. See Exmp. 16 for a detailed analysis.

3 WEAKEST PREEEXPECTATION REASONING

3.1 The Probabilistic Guarded Command Language

We consider probabilistic programs described by the simple yet Turing-complete, imperative *probabilistic guarded command language* (pGCL) [McIver and Morgan 2005] which augments Dijkstra’s GCL [Dijkstra 1976] with probabilistic choices and random assignments.

Syntax. The syntax of a pGCL program C adheres to the grammar

$$C ::= \text{skip} \mid x := e \mid x \approx \mu \mid C \circ C \mid \{C\} [p] \{C\} \mid \\ \text{if}(\varphi) \{C\} \text{ else } \{C\} \mid \text{while}(\varphi) \{C\}$$

where x is a program variable taken from a countable set Vars , e is an arithmetic expression over program variables, φ is a quantifier-free first-order predicate over program variables, and μ denotes a discrete or continuous distribution. We do not specify the syntax of expressions e and predicates φ – they can be arbitrary as long as the corresponding evaluation functions are measurable, as is in [Szymczak and Katoen 2019]. The semantics of most program constructs – including skip , (deterministic) assignments, sequential composition, conditional, and (nested) loops – is standard. The *probabilistic choice* $\{C_1\} [p] \{C_2\}$ flips a coin with bias $p \in [0, 1]$ and executes C_1 in case the coin yields heads, and C_2 otherwise. The *random assignment* $x \approx \mu$ draws a sample from the distribution μ – either discrete or continuous – and assigns it to the program variable x .

Program States. A program state σ maps every variable in Vars to its value, i.e., a real number in \mathbb{R} . We denote the (possibly uncountable) set of program states by $\Sigma \triangleq \{\sigma \mid \sigma: \text{Vars} \rightarrow \mathbb{R}\}$. The evaluation of expressions e and guards φ under a state σ , denoted by $e(\sigma)$ and $\varphi(\sigma)$ respectively, is standard. For instance, the evaluation of arithmetic addition is

$$(e_1 + e_2)(\sigma) \triangleq e_1(\sigma) + e_2(\sigma) = e_1[x/\sigma(x)] + e_2[x/\sigma(x)] \quad \text{for all } x \in \text{Vars}$$

where $e[x/\sigma(x)]$ denotes the substitution of variable x by its value $\sigma(x)$ in e .

Predicates. We interpret guards in pGCL programs as predicates. A *predicate* φ represents a subset of program states Σ . We write $\sigma \models \varphi$, reading “ σ satisfies φ ”, to indicate that state σ is in the set represented by predicate φ , i.e., $\varphi(\sigma) = \text{true}$; and $\sigma \not\models \varphi$ otherwise. We write $\varphi_1 \implies \varphi_2$, reading “ φ_1 strengthens φ_2 ”, to indicate that under every state $\sigma \in \Sigma$, if $\varphi_1(\sigma) = \text{true}$ then $\varphi_2(\sigma) = \text{true}$.

3.2 The Weakest Preexpectation Calculus

To reason about quantitative properties of probabilistic programs, in particular, to lower-bound expected values of certain probabilistic quantities, we view pGCL programs as *expectation transformers* [Kaminski 2019; Kozen 1985; McIver and Morgan 2005] – a quantitative extension of the predicate-transformer calculus for non-probabilistic programs of Dijkstra [1975, 1976].

An expectation transformer acts on real-valued functions called *expectations*, which map program states to non-negative reals (extended by infinity)³. Note the distinction between expectations and expected values: instead of an expected value, one can think of an expectation as a *random variable*.

Definition 1 (Expectations [Kaminski 2019]). *The set of expectations, denoted by \mathbb{E} , is defined as*

$$\mathbb{E} \triangleq \{ f \mid f: \Sigma \rightarrow \mathbb{R}_{\geq 0}^{\infty} \} .$$

An expectation $f \in \mathbb{E}$ is *finite*, written as $f \ll \infty$, if $f(\sigma) < \infty$ for all $\sigma \in \Sigma$; $f \in \mathbb{E}$ is *bounded*, if there exists $b \in \mathbb{R}_{\geq 0}$ such that $f(\sigma) \leq b$ for all $\sigma \in \Sigma$.

For simplicity, a constant expectation $\lambda\sigma. r$ which evaluates to $r \in \mathbb{R}_{\geq 0}^{\infty}$ for every state is denoted by r . Similarly, given an arithmetic expression e , we denote by e the expectation $\lambda\sigma. e(\sigma)$.

A partial order \leq on \mathbb{E} is obtained by point-wise lifting the canonical ordering \leq on $\mathbb{R}_{\geq 0}^{\infty}$, i.e.,

$$f_1 \leq f_2 \quad \text{iff} \quad \forall \sigma \in \Sigma: f_1(\sigma) \leq f_2(\sigma) .$$

(\mathbb{E}, \leq) forms a complete lattice with least element 0 and greatest element ∞ .

A pGCL program C is interpreted as an expectation transformer which pushes a *postexpectation* $f \in \mathbb{E}$ (evaluated in the final states) backward through C and gives a *preexpectation* $g \in \mathbb{E}$ (evaluated in the initial states). In particular, as illustrated in Fig. 2, the *weakest preexpectation* of C w.r.t. f is a *function* $g: \Sigma \rightarrow \mathbb{R}_{\geq 0}^{\infty}$ mapping each *initial state* σ_0 of C to the corresponding expected value of f evaluated in the final states reached after termination of C on input σ_0 :

Definition 2 (Weakest Preexpectations [Kaminski 2019; Kozen 1985; McIver and Morgan 2005]).

Given probabilistic program C and initial state $\sigma_0 \in \Sigma$. Let $\sigma_0\mu_C$ be the (sub)probability measure⁴ over final states reached after termination of C on input σ_0 . Given postexpectation $f \in \mathbb{E}$ which is measurable w.r.t. $\sigma_0\mu_C$, the weakest preexpectation of C w.r.t. f maps any initial state σ_0 to the expected value of f evaluated in the final states reached after termination of C on σ_0 , i.e.,⁵

$$\text{wp}[[C]](f)(\sigma_0) \triangleq \int_{\Sigma} f \, d(\sigma_0\mu_C) .$$

It is known that (i) for every measurable $f \in \mathbb{E}$, $\text{wp}[[C]](f)$ is measurable (cf. [Szymczak and Katoen 2019, Lem. 3.2]), and (ii) the set of measurable expectations also forms a complete lattice under the partial order \leq (cf. [Szymczak and Katoen 2019, Lem. 2]). Hence, for simplicity, we abuse the notation \mathbb{E} to stand for the set of *measurable* expectations throughout the rest of the paper.

³For simplicity, we consider the standard case of *non-negative* expectations. An arithmetic expression is thus a well-defined expectation if and only if it takes non-negative values over *all reachable* program states. See [Kaminski and Katoen 2017] for more involved techniques addressing *mixed-sign* expectations mapping to the *full* extended reals.

⁴ $\sigma_0\mu_C(\sigma) \in [0, 1]$ is the probability that, on input σ_0 , C terminates in the final state σ . Note that $\sigma_0\mu_C(\Sigma) \leq 1$, where the “missing” probability mass is the probability of *nontermination* of C on σ_0 . A formal definition of $\sigma_0\mu_C$ requires an (operational) semantic model of pGCL, which is out of our scope; we refer interested readers to [Dahlqvist et al. 2020].

⁵In case of a countable state space Σ , the integral can be written as a countable sum $\sum_{\sigma \in \Sigma} \sigma_0\mu_C(\sigma) \cdot f(\sigma)$.

Table 1. Rules for the wp-transformer. $[\varphi]$ denotes the Iverson-bracket of φ , i.e., $[\varphi](\sigma)$ evaluates to 1 if $\sigma \models \varphi$ and to 0 otherwise. For any variable $x \in \text{Vars}$ and any expression e , $f[x/e]$ denotes the expectation with $f[x/e](\sigma) = f(\sigma[x/e])$ for any $\sigma \in \Sigma$, where $\sigma[x/e](x) = e(\sigma)$ and $\sigma[x/e](y) = \sigma(y)$ for all $y \in \text{Vars} \setminus \{x\}$.

C	$\text{wp} \llbracket C \rrbracket (f)$
skip	f
$x := e$	$f[x/e]$
$x \approx \mu$	$\int_{\mathbb{R}} f[x/v] \, d\mu(v)$
$C_1 \circ C_2$	$\text{wp} \llbracket C_1 \rrbracket (\text{wp} \llbracket C_2 \rrbracket (f))$
$\{C_1\} [p] \{C_2\}$	$p \cdot \text{wp} \llbracket C_1 \rrbracket (f) + (1-p) \cdot \text{wp} \llbracket C_2 \rrbracket (f)$
if (φ) $\{C_1\}$ else $\{C_2\}$	$[\varphi] \cdot \text{wp} \llbracket C_1 \rrbracket (f) + [\neg\varphi] \cdot \text{wp} \llbracket C_2 \rrbracket (f)$
while (φ) $\{C'\}$	$\text{lfp}_{\langle \varphi, C' \rangle} \Phi_f^{\text{wp}}$
$\langle \varphi, C' \rangle \Phi_f^{\text{wp}}: \mathbb{E} \rightarrow \mathbb{E}, \quad h \mapsto [\neg\varphi] \cdot f + [\varphi] \cdot \text{wp} \llbracket C' \rrbracket (h)$	
	characteristic function

Weakest preexpectations can be determined in a *backward, compositional* manner; see [Feng et al. 2023, Appx. B]. In fact, the wp-transformer can be codified by structural induction:

Theorem 3 (wp-Transformer [McIver and Morgan 2005]). *Let pGCL be the set of programs in the probabilistic guarded command language. The weakest preexpectation transformer*

$$\text{wp}: \text{pGCL} \rightarrow \mathbb{E} \rightarrow \mathbb{E}$$

adhering to the rules in Table 1 is well-defined; in fact, Table 1 coincides with Def. 2.

A proof of Thm. 3 can be found in [Szymczak and Katoen 2019, Sect. 5], which extends the well-definedness for discrete probabilistic programs [Kaminski 2019, Thm. 4.11]. The function $\langle \varphi, C \rangle \Phi_f^{\text{wp}}$ in Table 1 is called the *characteristic function of while (φ) $\{C\}$ w.r.t. f* . For simplicity, we omit wp, φ , C , or f from Φ whenever they are clear from the context. Φ is in fact a (Scott-)continuous – and thus *monotonic* – operator, i.e., $\Phi(\sup\{g_1 \leq g_2 \leq \dots\}) = \sup\Phi(\{g_1 \leq g_2 \leq \dots\})$; see [Szymczak and Katoen 2019, Lem. 3.1]. Thus by the Kleene fixed point theorem [Lassez et al. 1982], its *least fixed point* $\text{lfp } \Phi = \sup_{n \in \mathbb{N}} \Phi^n(0) = \lim_{n \rightarrow \omega} \Phi^n(0)$ and *greatest fixed point* $\text{gfp } \Phi = \inf_{n \in \mathbb{N}} \Phi^n(\infty) = \lim_{n \rightarrow \omega} \Phi^n(\infty)$ exist over the partial order \leq on \mathbb{E} .

The rules for the wp-transformer in Table 1 are compositional and, mostly, purely *syntactic*, thus providing the machinery for automating the weakest preexpectation calculus; see [Feng et al. 2023, Appx. B] for an example. One exception, however, is the transformation rule for while-loops: It amounts to determining the quantitative least fixed point which is often difficult or even impossible to compute [Kaminski et al. 2019]; it is thus desirable to *bound* them from above and/or from below. There are in principle two challenges (cf. [Hark et al. 2020]): (i) finding a candidate bound, and (ii) verifying that the candidate is indeed an upper or lower bound. In this paper, we aim to *verify candidate lower bounds* on $\text{wp} \llbracket C \rrbracket (f)$ where C is a (possibly nested) while-loop that may not terminate almost-surely. The termination probability of C is captured by $\text{wp} \llbracket C \rrbracket (1)(\sigma_0)$:

Definition 4 (Almost-Sure Termination and Divergence). *Let C be a pGCL program and let $\sigma_0 \in \Sigma$ be an initial program state. Then C terminates almost-surely on input σ_0 iff*

$$\text{wp} \llbracket C \rrbracket (1)(\sigma_0) = 1.$$

C terminates almost-surely (AST) iff C terminates almost-surely on all inputs, i.e.,

$$\text{wp}\llbracket C \rrbracket (1) = 1.$$

C diverges on input σ_0 iff $\text{wp}\llbracket C \rrbracket (1) (\sigma_0) < 1$. C diverges iff C diverges on some input σ_0 .

4 REASONING ABOUT LOWER BOUNDS

This section formulates our problem of proving lower bounds on $\text{lfp}_{\langle \varphi, C \rangle}^{\text{wp}} \Phi_f$, i.e., on the wp of a (possibly divergent) while-loop $C_{\text{loop}} = \text{while}(\varphi) \{ C \}$ w.r.t. postexpectation f . We then give a high-level description of our approach in position to existing proof rules employing induction.

4.1 Problem Statement

The problem concerned in this paper can be formulated as follows.

Given a *possibly divergent* probabilistic loop $C_{\text{loop}} = \text{while}(\varphi) \{ C \}$, a *possibly unbounded* postexpectation $f \in \mathbb{E}$, and a *possibly unbounded* candidate lower bound $l \in \mathbb{E}$, verify that

$$l \leq \text{wp}\llbracket C_{\text{loop}} \rrbracket (f). \quad (1)$$

We present a new proof rule to address this problem: Our rule does not employ induction, rather, it *reduces* the verification of (1) with possibly divergent C_{loop} and possibly unbounded $f, l \in \mathbb{E}$ to

$$l \leq \text{wp}\llbracket \text{while}(\varphi') \{ C \} \rrbracket ([\neg\varphi] \cdot f) \quad \text{with} \quad \varphi' \implies \varphi. \quad (2)$$

Namely, we forge a new loop $C'_{\text{loop}} = \text{while}(\varphi') \{ C \}$ out of C_{loop} by *strengthening* its loop guard φ to φ' . Such guard strengthening restricts the (reachable) state space and, consequently, (i) the modified loop C'_{loop} features a *stronger* termination property (e.g., becoming AST), and (ii) both the uniform integrability of l and the boundedness of expectations are *easier* to verify.

Our proof rule asserts – by exploiting the difference between $\text{wp}\llbracket C'_{\text{loop}} \rrbracket (f)$ and $\text{wp}\llbracket C_{\text{loop}} \rrbracket (f)$ – that a lower bound l w.r.t. C'_{loop} satisfying (2) also suffices as a lower bound w.r.t. C_{loop} satisfying (1). The former, due to guard strengthening, can often be obtained by applying existing lower induction rules (see Sect. 4.3 below) or – in case C'_{loop} has a finite state space – probabilistic model checking.

4.2 Induction Rules for Upper Bounds

The *Park induction* principle [Park 1969] for least fixed points establishes an elegant mechanism for verifying upper bounds on weakest preexpectations:

Theorem 5 (Park Induction for Upper Bounds [Kaminski 2019; Kozen 1985]). *Let Φ_f be the characteristic function of $C_{\text{loop}} = \text{while}(\varphi) \{ C \}$ w.r.t. postexpectation $f \in \mathbb{E}$ and let $u \in \mathbb{E}$. Then*

$$\Phi_f(u) \leq u \quad \text{implies} \quad \text{wp}\llbracket C_{\text{loop}} \rrbracket (f) \leq u. \quad (3)$$

We call $u \in \mathbb{E}$ satisfying $\Phi_f(u) \leq u$ a *superinvariant*. As pointed out by Hark et al. [2020], the striking power of Park induction lies in its *simplicity*: Once an appropriate candidate u is found (which, however, is usually not an easy task), all we have to do is to push u through Φ_f *once* and check whether it becomes smaller in terms of \leq . If this is the case, we have verified that u is indeed an upper bound on $\text{lfp} \Phi_f$ and thus on the weakest preexpectation.

The *soundness* of Park induction is illustrated by the left (descending) chain in Fig. 3. We refer the readers to [Hark et al. 2020] for a formal soundness argument leveraging the Tarski-Kantorovitch principle (cf. [Jachymski et al. 2000]). See also [Batz et al. 2021a] for a strictly more general proof rule via (lattice) k -induction for establishing upper bounds on least fixed points.

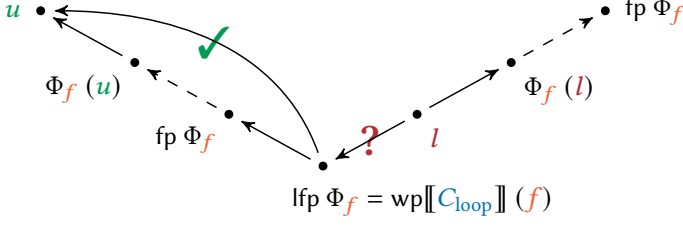


Fig. 3. Intuition of the soundness of Park induction (left branch) and the unsoundness of simple lower induction (right branch). An arrow from $g_1 \in \mathbb{E}$ to $g_2 \in \mathbb{E}$ indicates $g_1 \leq g_2$. For Park induction, the iteration of Φ_f on u converges downwards to a fixed point of Φ_f which is – by the Knaster-Tarski theorem [Knaster 1928; Lassez et al. 1982; Tarski 1955] – necessarily above $\text{lfp } \Phi_f$, thus proving $\text{wp}[[C_{\text{loop}}]](f) \leq u$. For simple lower induction, however, the ascending chain $l \leq \Phi_f(l) \leq \dots$ converges to a fixed point of Φ_f which is necessarily below the *greatest* fixed point $\text{gfp } \Phi_f$, but we do not know how l compares to $\text{lfp } \Phi_f$.

4.3 Induction Rules for Lower Bounds

A “dual” version of Park induction – by flipping \leq in (3) – works for verifying lower bounds on the *greatest* fixed point $\text{gfp } \Phi_f$, but not on $\text{lfp } \Phi_f$. More precisely, for $l \in \mathbb{E}$, the rule

$$l \leq \Phi_f(l) \quad \text{implies} \quad l \leq \text{wp}[[C_{\text{loop}}]](f), \quad \zeta$$

is *unsound* in general. We call $l \in \mathbb{E}$ satisfying $l \leq \Phi_f(l)$ a *subinvariant* and the above unsound rule *simple lower induction*. The *unsoundness* of simple lower induction is illustrated by the right (ascending) chain in Fig. 3, together with a counterexample below. We refer the readers to [Hark et al. 2020] for a formal argument again using the Tarski-Kantorovitch principle.

Example 6 (Unsoundness of Simple Lower Induction). Reconsider the loop $C_{1\text{dbrw}}$ in Sect. 2 with postexpectation $f = 1$; its characteristic function is $\Phi_f(h) = [n \leq 0] + [n > 0] \cdot (1/3 \cdot h(n-1) + 2/3 \cdot h(n+1))$. Observe that the constant expectation $g = 1$ is a superinvariant, since $\Phi_f(g) = 1 \leq g$. This implies that the termination probability of $C_{1\text{dbrw}}$ is (trivially) upper-bounded by 1 (cf. Thm. 5). Meanwhile, g is also a subinvariant as $g \leq 1 = \Phi_f(g)$, which however does *not* suffice to certify 1 as a lower bound on the termination probability (recall that $C_{1\text{dbrw}}$ is non-AST; cf. Sect. 2). \triangleleft

To retrieve soundness of lower induction, Hark et al. [2020] propose *side conditions* relying on notions of almost-sure termination (i.e., $\text{wp}[[C_{\text{loop}}]](1) = 1$, cf. Def. 4) and *uniform integrability* from the realm of stochastic processes. To formulate the latter, we denote by X_n the random variable representing the program state after the n -th iteration of the loop body C , by $T^{-\varphi} \triangleq \inf\{n \in \mathbb{N} \mid X_n \models \neg\varphi\}$ the stopping time (aka, *looping time*) indicating the first time that X_n hits $\neg\varphi$,⁶ and by $\{X_n^{T^{-\varphi}}\}_{n \in \mathbb{N}}$ the corresponding stopped stochastic process, i.e., $X_n^{T^{-\varphi}} = X_n$ if $n \leq T^{-\varphi}$ and $X_n^{T^{-\varphi}} = X_{T^{-\varphi}}$ otherwise; see [Feng et al. 2023, Appx. A] for formal definitions of stopping times and stopped processes.

Definition 7 (Uniform Integrability). A stochastic process $\{X_n\}_{n \in \mathbb{N}}$ on a probability space (Ω, \mathcal{F}, P) is uniformly integrable (u.i., for short), if

$$\lim_{R \rightarrow \infty} \sup_{n \in \mathbb{N}} E[|X_n| \cdot \mathbb{1}_{|X_n| \geq R}] = 0 \quad (4)$$

where $\mathbb{1}_{|X_n| \geq R}$ is the indicator function, i.e., $\mathbb{1}_{|X_n| \geq R}(\omega) = 1$ if $\omega \in \{\omega \in \Omega \mid |X_n(\omega)| \geq R\}$ and 0 otherwise. Given $C_{\text{loop}} = \text{while}(\varphi)\{C\}$, an expectation $h \in \mathbb{E}$ is uniformly integrable for C_{loop} if $\{h(X_n^{T^{-\varphi}})\}_{n \in \mathbb{N}}$ is uniformly integrable on the probability space induced by C_{loop} (cf. Sect. 5).

⁶The looping time $T^{-\varphi}$ does not take into account the runtime of the loop body C .

Intuitively, (4) asserts that the tail expected values of X_n are *uniformly* (indicated by the supremum) small in terms of the L^1 -norm. A u.i. process X_n thus satisfies $E(\lim_{n \rightarrow \infty} X_n) = \lim_{n \rightarrow \infty} E(X_n)$ if $\lim_{n \rightarrow \infty} X_n$ exists almost-surely. Now, the sound induction rule for lower bounds reads as follows.

Theorem 8 (Hark et al.'s Induction for Lower Bounds [Hark et al. 2020]). *Let Φ_f be the characteristic function of $C_{\text{loop}} = \text{while}(\varphi)\{C\}$ w.r.t. postexpectation $f \in \mathbb{E}$ and let $l \in \mathbb{E}$. Then*

$$\underbrace{l \leq \Phi_f(l)}_{\text{subinvariance}} \quad \text{and} \quad \underbrace{\text{wp}\llbracket C_{\text{loop}} \rrbracket(1) = 1 \text{ and } l \text{ is u.i. for } C_{\text{loop}}}_{\text{side conditions}} \quad \text{implies} \quad l \leq \text{wp}\llbracket C_{\text{loop}} \rrbracket(f). \quad (5)$$

Unlike Park induction for upper bounds, the side conditions in (5) for establishing lower bounds require extra efforts in proving almost-sure termination and uniform integrability, both of which are computationally *intractable* in general, see, e.g., [Kaminski et al. 2019]. Various techniques and tools have been developed in the literature, e.g., [Chatterjee et al. 2020; McIver et al. 2018; Moosbrugger et al. 2021], to prove almost-sure termination of (*subclasses of*) probabilistic programs. For showing uniform integrability, Hark et al. [2020] propose *sufficient* conditions based on the well-known optional stopping time theorem [Williams 1991, Chap. 10]:

Theorem 9 (Sufficient Criteria for Uniform Integrability [Hark et al. 2020]). *Given $C_{\text{loop}} = \text{while}(\varphi)\{C\}$, let $\sigma_0 \mathbb{P}$ be the (sub)probability measure induced by C_{loop} on initial state $\sigma_0 \in \Sigma$.⁷ Then, an expectation $h \ll \infty$ is uniformly integrable for C_{loop} if one of the following conditions holds:*

- (a) *The looping time $T^{\neg\varphi}$ is almost-surely bounded, i.e., for any initial state $\sigma_0 \in \Sigma$, there exists $N \in \mathbb{N}$ such that $\sigma_0 \mathbb{P}(T^{\neg\varphi} \leq N) = 1$, and $\text{wp}\llbracket C \rrbracket^n(h) \ll \infty$ for any $n \in \mathbb{N}$.*
- (b) *The expected looping time is finite and h is conditionally difference bounded, i.e., $\sigma_0 E[T^{\neg\varphi}] < \infty$ for any $\sigma_0 \in \Sigma$, and there exists $c \in \mathbb{R}_{\geq 0}$ such that $\text{wp}\llbracket C \rrbracket(|h - h(\sigma)|) \leq c$ for any $\sigma \models \varphi$.*
- (c) *h is bounded, i.e., there exists $c \in \mathbb{R}_{\geq 0}$ such that $h(\sigma) \leq c$ for any $\sigma \in \Sigma$.*

In summary, Hark et al.'s sound lower induction rule in Thm. 8 does not apply to *divergent* programs, and even for AST ones, it requires extra proof efforts in, e.g., looking for supermartingales [Chatterjee et al. 2020] witnessing AST and reasoning about the looping time ((a) and (b) in Thm. 9) or establishing bounds on expectations ((b) and (c) in Thm. 9) to achieve u.i..

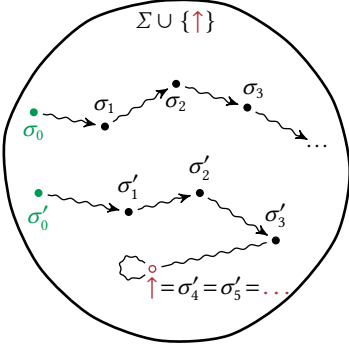
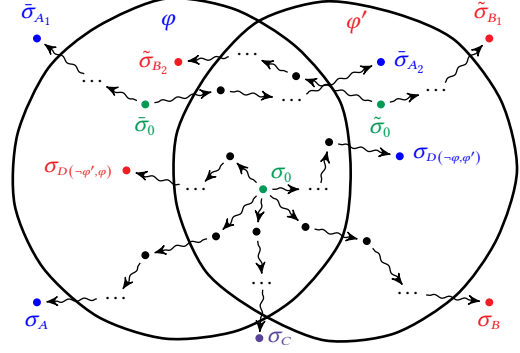
There is an orthogonal induction rule by McIver and Morgan [2005] for *bounded* expectations:

Theorem 10 (McIver & Morgan's Induction for Lower Bounds [McIver and Morgan 2005]). *Let Φ_f be the characteristic function of $C_{\text{loop}} = \text{while}(\varphi)\{C\}$ w.r.t. a bounded postexpectation $f \in \mathbb{E}$, $l \in \mathbb{E}$ be a bounded expectation such that $l \leq \Phi_f(l)$ and $[\neg\varphi] \cdot l = [\neg\varphi] \cdot f$, and $p = \text{wp}\llbracket C_{\text{loop}} \rrbracket(1)$ be the termination probability of C_{loop} . Then*

- (a) *If $l = [G]$ for some predicate G , then $p \cdot l \leq \text{wp}\llbracket C_{\text{loop}} \rrbracket(f)$.*
- (b) *If $[G] \leq p$ for some predicate G , then $[G] \cdot l \leq \text{wp}\llbracket C_{\text{loop}} \rrbracket(f)$.*
- (c) *If $\varepsilon \cdot l \leq p$ for some $\varepsilon \in \mathbb{R}_{>0}$, then $l \leq \text{wp}\llbracket C_{\text{loop}} \rrbracket(f)$.*

McIver and Morgan's lower induction rule applies to divergent programs (with termination probability < 1); however, it is confined to *bounded* expectations and requires a priori knowledge on the *termination probability* p of a while-loop which is difficult to infer in general (which may in turn ask for lower bounds on p). In fact, Hark et al.'s induction rule generalizes McIver and Morgan's in case C_{loop} is AST [Hark et al. 2020, Thm. 41]. These two proof rules, to the best of our knowledge, are the only existing (induction) rules for verifying lower bounds on weakest preexpectations.

⁷The measure $\sigma_0 \mathbb{P}$ will be formally defined in Sect. 5. Note that $\sigma_0 \mathbb{P}(T^{\neg\varphi} < \infty) = 1$ iff $\text{wp}\llbracket C_{\text{loop}} \rrbracket(1)(\sigma_0) = 1$.

Fig. 4. Infinite traces in \mathbb{S} .Fig. 5. Illustration of **Thm. 11** (cf. (10)).

5 DIFFERENCES OF WEAKEST PREEXPECTATIONS

Our lower-bound proof rule reduces the verification of a probabilistic loop to that of its strengthened counterpart. To justify such a reduction, we need to *quantitatively* relate two probabilistic loops in terms of weakest preexpectations. In this section, we show how to quantify the difference of the weakest preexpectations of two while-loops, which differ *only* in loop guards, with respect to the same postexpectation $f \in \mathbb{E}$, namely,

$$\underbrace{\text{wp}[\text{while}(\varphi)\{C\}]}_{C_{\text{loop}}} (f) - \underbrace{\text{wp}[\text{while}(\varphi')\{C\}]}_{C'_{\text{loop}}} (f) \quad (6)$$

where φ and φ' are arbitrary predicates representing subsets of Σ (here, φ' does *not* necessarily strengthen φ)⁸ and the shared loop body C itself can contain further nested while-loops. Such a quantification on the wp-difference forms the basis of our new proof rule (cf. **Sect. 6**).

Recall that the weakest preexpectation of a loop w.r.t. $f \in \mathbb{E}$ is defined (cf. **Def. 2**) as the integral of f over the (sub)probability measure over final states reached after termination of the loop, where the termination behavior is determined by the loop guard and the loop body. Thus, to connect the two weakest preexpectations in (6), we first abstract away the loop guards φ and φ' and thereby obtain a certainly divergent loop $C_{\text{loop}}^{\uparrow} = \text{while}(\text{true})\{C\}$. We then construct a probability space over the set \mathbb{S} of *infinite traces* (i.e., sequences of program states) of $C_{\text{loop}}^{\uparrow}$, formally,

$$\mathbb{S} \triangleq \{ \sigma_0 \sigma_1 \cdots \sigma_i \cdots \mid \sigma_0 \in \Sigma, \forall i \geq 1: \sigma_i \in \Sigma \cup \{\uparrow\} \wedge (\sigma_i = \uparrow \implies \sigma_{i+1} = \uparrow) \}$$

where $\sigma_i \neq \uparrow$ denotes the state in which the loop body C *terminates* after its i -th iteration and \uparrow denotes the *sink* state where C diverges. See **Fig. 4** for an illustration of two types of infinite traces (with or without sink states). Given a finite prefix π of an infinite trace, the *cylinder set* of π is $\text{cyl}(\pi) \triangleq \{ s \in \mathbb{S} \mid \exists t \in (\Sigma \cup \{\uparrow\})^{\omega}: s = \pi t \}$, i.e., the set of infinite traces that have π as a prefix.

The operational semantics [**Dahlqvist et al. 2020**] of $C_{\text{loop}}^{\uparrow}$ induces a family of (sub)probability measures – denoted by $\sigma\mathbb{P}$ for any $\sigma \in \Sigma$ – over \mathbb{S} with the smallest σ -algebra containing all cylinder

⁸Assuming $\varphi' \implies \varphi$ suffices to justify our proof rule. However, we are interested in a more general result on wp-difference with *unrelated* φ and φ' due to (i) symmetry in φ and φ' ; and (ii) the potential of such a general result for addressing problems beyond verifying lower bounds, e.g., sensitivity analysis [**Aguirre et al. 2021; Barthe et al. 2018; Wang et al. 2020**] and model repair [**Bartocci et al. 2011**] for probabilistic programs, as one of the interesting future directions.

sets. That is, for any finite prefix $\pi = \sigma_0\sigma_1 \cdots \sigma_n$,

$$\sigma\mathbb{P}(\text{cyl}(\pi)) = \begin{cases} [\sigma = \sigma_0] \cdot \sigma^0\mu_C(\sigma_1) \cdots \sigma^{i-1}\mu_C(\sigma_i) \cdots \sigma^{n-1}\mu_C(\sigma_n) & \text{if } \forall i \leq n: \sigma_i \neq \uparrow, \\ [\sigma = \sigma_0] \cdot \sigma^0\mu_C(\sigma_1) \cdots \sigma^{i-1}\mu_C(\sigma_i) \cdot (1 - \sigma^i\mu_C(\Sigma)) & \text{if } \exists i < n: \sigma_i \neq \uparrow \wedge \sigma_{i+1} = \uparrow, \end{cases}$$

where $\sigma\mu_C$ represents the (sub)probability measure over final states reached after termination of the loop body C on input σ . The random variable $X_n: \mathbb{S} \rightarrow \Sigma$ representing the program state after the n -th iteration of the loop body C is $X_n(\sigma_0\sigma_1 \cdots) = \sigma_n$. Given $C_{\text{loop}} = \text{while}(\varphi)\{C\}$, the looping time $T^{-\varphi}: \mathbb{S} \rightarrow \mathbb{N}$ of C_{loop} is defined as $T^{-\varphi}(s) = \inf\{n \mid X_n(s) \models \neg\varphi\}$. For any random variable X over \mathbb{S} and any predicate ϕ over X , we abbreviate $\sigma\mathbb{P}(\{s \in \mathbb{S} \mid \phi(X(s))\})$ as $\sigma\mathbb{P}(\phi(X))$, e.g., $\sigma\mathbb{P}(T^{-\varphi} \geq n)$ is a shorthand for $\sigma\mathbb{P}(\{s \in \mathbb{S} \mid T^{-\varphi}(s) \geq n\})$. Based on the measure $\sigma\mathbb{P}$ defined above, the difference between $\text{wp}\llbracket C_{\text{loop}} \rrbracket(f)$ and $\text{wp}\llbracket C'_{\text{loop}} \rrbracket(f)$ as in (6) can be quantified as follows.

Theorem 11 (wp-Difference). *Given loops $C_{\text{loop}} = \text{while}(\varphi)\{C\}$ and $C'_{\text{loop}} = \text{while}(\varphi')\{C\}$, then, for any postexpectation $f \in \mathbb{E}$,⁹*

$$\begin{aligned} \text{wp}\llbracket C_{\text{loop}} \rrbracket(f) - \text{wp}\llbracket C'_{\text{loop}} \rrbracket(f) = & \\ & \text{wp}\llbracket \text{while}(\varphi \wedge \varphi')\{C\} \rrbracket([\neg\varphi \wedge \varphi'] \cdot f) + \lambda\sigma. \int_A f_{C_{\text{loop}}} d(\sigma\mathbb{P}) - \\ & \text{wp}\llbracket \text{while}(\varphi \wedge \varphi')\{C\} \rrbracket([\varphi \wedge \neg\varphi'] \cdot f) - \lambda\sigma. \int_B f_{C'_{\text{loop}}} d(\sigma\mathbb{P}), \end{aligned} \quad (7)$$

where $A \subseteq \mathbb{S}$ is the set of infinite traces that hit $\neg\varphi'$ before hitting $\neg\varphi$, and $f_{C_{\text{loop}}}$ is a partial function mapping a trace $s \in \mathbb{S}$ to $f(\sigma_n)$ if s hits $\neg\varphi$ for the first time at σ_n , namely,

$$\begin{aligned} A \triangleq \{ \sigma_0\sigma_1 \cdots \sigma_i \cdots \in \mathbb{S} \mid \exists n \in \mathbb{N}: (\sigma_n \models \neg\varphi) \wedge (\forall i < n: \sigma_i \models \varphi) \wedge (\exists k < n: \sigma_k \models \neg\varphi') \}, \\ f_{C_{\text{loop}}}: \mathbb{S} \rightarrow \mathbb{R}_{\geq 0}^\infty \quad \sigma_0\sigma_1 \cdots \sigma_i \cdots \mapsto f(\sigma_n) \quad \text{if } (\sigma_n \models \neg\varphi) \wedge (\forall i < n: \sigma_i \models \varphi); \end{aligned} \quad (8)$$

dually, $B \subseteq \mathbb{S}$ is the set of infinite traces that hit $\neg\varphi$ before hitting $\neg\varphi'$, and $f_{C'_{\text{loop}}}$ maps a trace $s \in \mathbb{S}$ to $f(\sigma_n)$ if s hits $\neg\varphi'$ for the first time at σ_n (the definitions of B and $f_{C'_{\text{loop}}}$ are analogous to (8)).

PROOF. We prove the theorem by exploring different types of traces in \mathbb{S} , as depicted in Fig. 5. Given a predicate, ϕ let $\diamond\phi$ be the set of all traces that eventually hit ϕ , i.e.,

$$\diamond\phi \triangleq \{ \sigma_0\sigma_1 \cdots \sigma_i \cdots \in \mathbb{S} \mid \exists n \in \mathbb{N}: \sigma_n \models \phi \}.$$

By definition of the (sub)probability measure $\sigma\mathbb{P}$, we have

$$\begin{aligned} \text{wp}\llbracket C_{\text{loop}} \rrbracket(f) &= \lambda\sigma. \int_{\Sigma} f d(\sigma\mu_{C_{\text{loop}}}) = \lambda\sigma. \int_{\diamond(\neg\varphi)} f_{C_{\text{loop}}} d(\sigma\mathbb{P}), \\ \text{wp}\llbracket C'_{\text{loop}} \rrbracket(f) &= \lambda\sigma. \int_{\Sigma} f d(\sigma\mu_{C'_{\text{loop}}}) = \lambda\sigma. \int_{\diamond(\neg\varphi')} f_{C'_{\text{loop}}} d(\sigma\mathbb{P}). \end{aligned} \quad (9)$$

To quantify the wp-difference, we first decompose the set of traces in $\diamond(\neg\varphi)$ and $\diamond(\neg\varphi')$ into disjoint parts, respectively. To this end, let

$$C \triangleq \{ \sigma_0\sigma_1 \cdots \sigma_i \cdots \in \mathbb{S} \mid \exists n \in \mathbb{N}: (\sigma_n \models \neg\varphi \wedge \neg\varphi') \wedge (\forall i < n: \sigma_i \models \varphi \wedge \varphi') \},$$

and for any predicates ϕ_1, ϕ_2 , let

$$D(\phi_1, \phi_2) \triangleq \{ \sigma_0\sigma_1 \cdots \sigma_i \cdots \in \mathbb{S} \mid \exists n \in \mathbb{N}: (\sigma_n \models \phi_1) \wedge (\forall i \leq n: \sigma_i \models \phi_2) \}.$$

⁹For better understandability, (7) is formulated in the form of *difference* between weakest expectations. This formulation may raise the issue of “ $\infty - \infty$ ”, however, one can avoid this issue by shifting all the negative terms in (7) to the other side of the equation. The same reformulation tactic applies to the proof of Thm. 11.

It follows that

$$\begin{aligned}
\Diamond(\neg\varphi) &= \underbrace{A}_{\substack{\text{hitting } \neg\varphi' \text{ before hitting } \neg\varphi \\ \text{e.g., } \sigma_0 \cdots \sigma_A \cdots, \tilde{\sigma}_0 \cdots \text{ in Fig. 5}}} \uplus \underbrace{C}_{\substack{\text{hitting } \neg\varphi', \neg\varphi \text{ simultaneously} \\ \text{e.g., } \sigma_0 \cdots \sigma_C \cdots \text{ in Fig. 5}}} \uplus \underbrace{D(\neg\varphi, \varphi')}_{\substack{\text{hitting } \neg\varphi \text{ while satisfying } \varphi' \\ \text{e.g., } \sigma_0 \cdots \sigma_{D(\neg\varphi, \varphi')} \cdots \text{ in Fig. 5}}}, \\
\Diamond(\neg\varphi') &= \underbrace{B}_{\substack{\text{hitting } \neg\varphi \text{ before hitting } \neg\varphi' \\ \text{e.g., } \sigma_0 \cdots \sigma_B \cdots, \tilde{\sigma}_0 \cdots \text{ in Fig. 5}}} \uplus \underbrace{C}_{\substack{\text{hitting } \neg\varphi, \neg\varphi' \text{ simultaneously} \\ \text{e.g., } \sigma_0 \cdots \sigma_C \cdots \text{ in Fig. 5}}} \uplus \underbrace{D(\neg\varphi', \varphi)}_{\substack{\text{hitting } \neg\varphi' \text{ while satisfying } \varphi \\ \text{e.g., } \sigma_0 \cdots \sigma_{D(\neg\varphi', \varphi)} \cdots \text{ in Fig. 5}}}.
\end{aligned} \tag{10}$$

It is evident that, by definition, $f_{C_{\text{loop}}}$ and $f_{C'_{\text{loop}}}$ coincide on $C \subseteq \mathbb{S}$, i.e.,

$$\forall s \in C: f_{C_{\text{loop}}}(s) = f_{C'_{\text{loop}}}(s). \tag{11}$$

For $D(\cdot, \cdot)$, we have (see [Feng et al. 2023, Lem. 32] for a more detailed proof of (12) below)

$$\begin{aligned}
\lambda\sigma. \int_{D(\neg\varphi, \varphi')} f_{C_{\text{loop}}} d(\sigma\mathbb{P}) &= \underbrace{\text{wp}[\text{while}(\varphi \wedge \varphi')\{C\}]}_{\substack{\text{evaluating } f \text{ over, e.g., } \sigma_{D(\neg\varphi, \varphi')} \text{ in Fig. 5}}}([\neg\varphi \wedge \varphi'] \cdot f), \\
\lambda\sigma. \int_{D(\neg\varphi', \varphi)} f_{C'_{\text{loop}}} d(\sigma\mathbb{P}) &= \underbrace{\text{wp}[\text{while}(\varphi \wedge \varphi')\{C\}]}_{\substack{\text{evaluating } f \text{ over, e.g., } \sigma_{D(\neg\varphi', \varphi)} \text{ in Fig. 5}}}([\varphi \wedge \neg\varphi'] \cdot f).
\end{aligned} \tag{12}$$

By combining the facts above, we have

$$\begin{aligned}
&\text{wp}[\![C_{\text{loop}}]\!](f) - \text{wp}[\![C'_{\text{loop}}]\!](f) = \lambda\sigma. \int_{\Diamond(\neg\varphi)} f_{C_{\text{loop}}} d(\sigma\mathbb{P}) - \lambda\sigma. \int_{\Diamond(\neg\varphi')} f_{C'_{\text{loop}}} d(\sigma\mathbb{P}) \quad [\text{by (9)}] \\
&= \lambda\sigma. \int_A f_{C_{\text{loop}}} d(\sigma\mathbb{P}) + \lambda\sigma. \int_C f_{C_{\text{loop}}} d(\sigma\mathbb{P}) + \lambda\sigma. \int_{D(\neg\varphi, \varphi')} f_{C_{\text{loop}}} d(\sigma\mathbb{P}) - \\
&\quad \lambda\sigma. \int_B f_{C'_{\text{loop}}} d(\sigma\mathbb{P}) - \lambda\sigma. \int_C f_{C'_{\text{loop}}} d(\sigma\mathbb{P}) - \lambda\sigma. \int_{D(\neg\varphi', \varphi)} f_{C'_{\text{loop}}} d(\sigma\mathbb{P}) \quad [\text{by linearity of } \int, (10)] \\
&= \text{wp}[\![\text{while}(\varphi \wedge \varphi')\{C\}]\!]([\neg\varphi \wedge \varphi'] \cdot f) + \lambda\sigma. \int_A f_{C_{\text{loop}}} d(\sigma\mathbb{P}) - \\
&\quad \text{wp}[\![\text{while}(\varphi \wedge \varphi')\{C\}]\!]([\varphi \wedge \neg\varphi'] \cdot f) - \lambda\sigma. \int_B f_{C'_{\text{loop}}} d(\sigma\mathbb{P}). \quad [\text{by (11) and (12)}]
\end{aligned}$$

This completes the proof. \square

Example 12 (wp-Difference). Consider two loops with postexpectation $f = [0 \leq n \leq 11]$:

$$\begin{aligned}
C_{\text{loop}}: & \text{ while } (0 < n < 10) \{ n := n - 1 [1/2] \ n := n + 1 \}, \\
C'_{\text{loop}}: & \text{ while } (1 < n < 11) \{ n := n - 1 [1/2] \ n := n + 1 \}.
\end{aligned}$$

Let C_\wedge be the loop $\text{while}(1 < n < 10)\{n := n - 1 [1/2] \ n := n + 1\}$. To illustrate Thm. 11, we show

$$\begin{aligned}
&\text{wp}[\![C_{\text{loop}}]\!]([0 \leq n \leq 11]) - \text{wp}[\![C'_{\text{loop}}]\!]([0 \leq n \leq 11]) = \\
&\quad \text{wp}[\![C_\wedge]\!]([n = 10]) + \lambda\sigma. \int_A f_{C_{\text{loop}}} d(\sigma\mathbb{P}) - \\
&\quad \text{wp}[\![C_\wedge]\!]([n = 1]) - \lambda\sigma. \int_B f_{C'_{\text{loop}}} d(\sigma\mathbb{P}). \tag{13}
\end{aligned}$$

Observe that

$$\text{wp}[\![C_{\text{loop}}]\!]([0 \leq n \leq 11]) = \text{wp}[\![C'_{\text{loop}}]\!]([0 \leq n \leq 11]) = [0 \leq n \leq 11],$$

due to the key fact that C_{loop} and C'_{loop} both terminate with probability 1. Thus, the left-hand side of (13) equals 0. For the right-hand side of (13), by applying Hark et al.'s induction for lower bounds and Park induction for upper bounds (details omitted), one can show that

$$\text{wp}\llbracket C_{\wedge} \rrbracket ([n = 10]) = [1 \leq n \leq 10] \cdot \frac{n-1}{9}, \quad \text{wp}\llbracket C_{\wedge} \rrbracket ([n = 1]) = [1 \leq n \leq 10] \cdot \frac{10-n}{9}.$$

Moreover, notice that $f_{C_{\text{loop}}} = 1$ over A and $f_{C'_{\text{loop}}} = 1$ over B , we have

$$\int_A f_{C_{\text{loop}}} d(\sigma_{\mathbb{P}}) = [1 \leq n < 10] \cdot \frac{10-n}{9}, \quad \int_B f_{C'_{\text{loop}}} d(\sigma_{\mathbb{P}}) = [1 < n \leq 10] \cdot \frac{n-1}{9}.$$

It follows that the right-hand side of (13) also equals 0. \triangleleft

The intuition behind **Thm. 11** is to decompose the weakest preexpectations into disjoint parts covering different types of traces in \mathbb{S} – the type of a trace is determined by its temporal behavior of hitting $\neg\varphi$ and/or hitting $\neg\varphi'$, see (10) and Fig. 5 – thus yielding the *exact* difference between $\text{wp}\llbracket C_{\text{loop}} \rrbracket (f)$ and $\text{wp}\llbracket C'_{\text{loop}} \rrbracket (f)$ by eliminating their common parts, cf. (11). The integrals in (7) for their exclusive parts remain hard to resolve, however, it suffices to obtain a lower bound on $\text{wp}\llbracket C_{\text{loop}} \rrbracket (f)$ if φ' strengthens φ (tightness of the so-obtained lower bound is shown in Sect. 6.3):

Corollary 13. *Given loops $C_{\text{loop}} = \text{while}(\varphi)\{C\}$ and $C'_{\text{loop}} = \text{while}(\varphi')\{C\}$, suppose $\varphi' \implies \varphi$, then, for any postexpectation $f \in \mathbb{E}$,*

$$\text{wp}\llbracket C_{\text{loop}} \rrbracket (f) \geq \text{wp}\llbracket C'_{\text{loop}} \rrbracket ([\neg\varphi] \cdot f).$$

The intuition of **Cor. 13** is as follows: Recall that $\text{wp}\llbracket C_{\text{loop}} \rrbracket (f)$ maps any initial state σ_0 to the expected value of f evaluated in the final states reached after termination of C_{loop} on σ_0 , i.e., upon violating the loop guard φ . In order to obtain a sound lower bound on $\text{wp}\llbracket C_{\text{loop}} \rrbracket (f)$ via the modified loop C'_{loop} , we have to restrict the postexpectation f to $[\neg\varphi] \cdot f$ such that f is evaluated only in states violating the original guard φ (and hence also violating the strengthened guard φ'). The proof of **Cor. 13** leverages the fact that, as $\varphi' \implies \varphi$, we have $\varphi \wedge \varphi' = \varphi'$, $[\neg\varphi \wedge \varphi'] = 0$, and $B = \emptyset$ (i.e., no trace can ever hit $\neg\varphi$ before hitting $\neg\varphi'$, cf. (10)).

6 PROOF RULE FOR LOWER BOUNDS

In this section, we present our new proof rule for verifying lower bounds on weakest preexpectations – termed the *guard-strengthening rule* – based on the wp-difference and the guard-strengthening technique in Sect. 5. We then showcase the usefulness of this proof rule in several aspects, in particular, for reasoning about possibly divergent probabilistic programs.

Theorem 14 (Guard Strengthening for Lower Bounds). *Given loops $C_{\text{loop}} = \text{while}(\varphi)\{C\}$, $C'_{\text{loop}} = \text{while}(\varphi')\{C\}$, and postexpectation $f \in \mathbb{E}$, let $l \in \mathbb{E}$, then the following inference rule holds:*

$$\frac{\varphi' \implies \varphi \quad l \leq \text{wp}\llbracket C'_{\text{loop}} \rrbracket ([\neg\varphi] \cdot f)}{l \leq \text{wp}\llbracket C_{\text{loop}} \rrbracket (f)} \quad \text{GUARD-STRENGTHENING} \quad (14)$$

PROOF. The (soundness of the) proof rule in (14) is an immediate consequence of **Cor. 13**. We provide in [Feng et al. 2023, Appx. C.3] an alternative proof which is *trace-agnostic* and thus simpler, yet does not contribute to our argument on the tightness of the proof rule in Sect. 6.3. \square

Our guard-strengthening rule asserts that a lower bound l on $\text{wp}\llbracket C'_{\text{loop}} \rrbracket ([\neg\varphi] \cdot f)$ suffices as a lower bound on $\text{wp}\llbracket C_{\text{loop}} \rrbracket (f)$ provided that $\varphi' \implies \varphi$. Such guard strengthening restricts the (reachable) state space and, consequently, (i) the modified loop C'_{loop} features a *stronger* termination

property (e.g., becoming AST), and (ii) both the uniform integrability of l and the boundedness of expectations are *easier* to verify. We will show that, due to these effects, our proof rule is

- (a) *general* (Sect. 6.1 and 6.2): it is applicable to divergent C_{loop} and unbounded $f, l \in \mathbb{E}$ where existing rules, e.g., Thm. 8 and 10, do not apply; even when C_{loop} is AST, it is capable of certifying a lower bound l which is *not* uniformly integrable for C_{loop} (thus beyond the scope of Hark et al.’s lower induction rule [Hark et al. 2020]); moreover, it admits an orthogonal sufficient criterion for proving uniform integrability.
- (b) *tight* (Sect. 6.3): the error incurred by underapproximating $\text{wp}\llbracket C_{\text{loop}} \rrbracket (f)$ with $\text{wp}\llbracket C'_{\text{loop}} \rrbracket ([\neg\varphi] \cdot f)$ approaches zero when φ' approaches φ appropriately; and
- (c) *automatable* (Sect. 6.4): it is amenable to automation – modulo an appropriate strengthening – via probabilistic model checking in case C'_{loop} has a finite state space.

Remark. The *completeness* of the guard-strengthening rule in (14) is evident: If l is a lower bound on $\text{wp}\llbracket C_{\text{loop}} \rrbracket (f)$, then there always exists φ' strengthening φ such that l is a lower bound of $\text{wp}\llbracket C'_{\text{loop}} \rrbracket ([\neg\varphi] \cdot f)$, as one can always choose $\varphi' = \varphi$ yielding $\text{wp}\llbracket C'_{\text{loop}} \rrbracket ([\neg\varphi] \cdot f) = \text{wp}\llbracket C_{\text{loop}} \rrbracket (f)$. This completeness argument, however, shall not be viewed as a characterization of the generality of our proof rule in *absolute* terms, as choosing $\varphi' = \varphi$ does not turn a non-AST loop into an AST one. We remark that characterizing the absolute generality of our proof rule is non-trivial as it depends highly on the “quality” of guard strengthening which may in turn rely on expert knowledge. Nonetheless, we provide useful heuristics in Sect. 6.4 for finding a “good” strengthening. \triangleleft

Remark. Our guard-strengthening rule in (14) applies also to *non-probabilistic* loops C_{loop} . In this case, the weakest preexpectation transformer degenerates to the weakest precondition transformer of Dijkstra [1975, 1976], l and f become predicates partially ordered by \implies , and \cdot becomes \wedge . Our proof rule is then capable of verifying an underapproximation l of the *set of initial states* on which C_{loop} certainly terminates in states satisfying f .

6.1 Application to Possibly Divergent Programs

Our guard-strengthening rule reduces the verification of $l \leq \text{wp}\llbracket C_{\text{loop}} \rrbracket (f)$ – with possibly divergent C_{loop} and possibly unbounded $f, l \in \mathbb{E}$ – to that of $l \leq \text{wp}\llbracket C'_{\text{loop}} \rrbracket ([\neg\varphi] \cdot f)$. In order to apply existing lower induction rules to the latter, one has to prove almost-sure termination of the modified loop C'_{loop} and/or boundedness of expectations. To show AST, one may apply established techniques based on *supermartingales*, e.g., [Chatterjee et al. 2020; McIver et al. 2018; Moosbrugger et al. 2021]. However, due to our guard-strengthening technique, a novel, simpler argument that does not rely on the discovery of fine-tuned supermartingales often suffices to prove AST of C'_{loop} :

Lemma 15 (AST Witness). *Given $C'_{\text{loop}} = \text{while}(\varphi')\{C\}$, let $T^{-\varphi'}$ be the looping time of C'_{loop} . If there exist $N \in \mathbb{N}$ and $p \in (0, 1)$ such that, for any initial state $\sigma \in \Sigma$,*

$$\sigma\mathbb{P}(T^{-\varphi'} > N) \leq p, \quad (15)$$

then C'_{loop} terminates almost-surely.

PROOF (SKETCH). It suffices to show that the *tail probability* $\sigma\mathbb{P}(T^{-\varphi'} > n)$ (see, e.g., [Sankaranarayanan 2020]), i.e., the probability that C'_{loop} does not terminate within $n \in \mathbb{N}$ steps, decreases exponentially in n . Then, by pushing n ad infinitum, we have $\sigma\mathbb{P}(T^{-\varphi'} < \infty) = 1 - \lim_{n \rightarrow \infty} \sigma\mathbb{P}(T^{-\varphi'} > n) \geq 1 - 0 = 1$. Hence, C'_{loop} terminates almost-surely. See details in [Feng et al. 2023, Appx. C.4] \square

Remark. How to specify the class of loops C_{loop} for which there exist strengthened counterparts C'_{loop} fulfilling the AST criterion in [Lem. 15](#) is left as an interesting open question. This may also contribute to the characterization of the absolute generality of our proof rule as discussed above. \triangleleft

There are (semi-)automated approaches, e.g., [[Chatterjee et al. 2016a](#)], tailored for proving exponentially decreasing nontermination probabilities via *ranking-supermartingales*. In our setting, however, [Lem. 15](#) is arguably *simpler* to verify since after strengthening the guard (by, e.g., bounding the variables, cf. [Sect. 6.4](#)), one can usually *read off* the constants N and p in (15) directly from the modified program with (certain) bounded variables. In fact, [Lem. 15](#) suffices to witness AST of the modified loops in *all* the examples presented in this paper; moreover, it enables an additional sufficient condition for establishing uniform integrability which is orthogonal to [Thm. 9](#) (cf. [Sect. 6.2](#)).

Example 16 (1-D Biased Random Walk on \mathbb{Z} [[McIver et al. 2018](#)]). Recall the example in [Sect. 2](#):

$$C_{\text{1dbrw}} : \text{ while } (n > 0) \{ n := n - 1 \ [1/3] \ n := n + 1 \} .$$

This loop terminates as soon as it reaches a state σ with $\sigma(n) \leq 0$. We are interested in establishing non-trivial lower bounds on the termination probability of C_{1dbrw} , i.e., on $\text{wp}[\![C_{\text{1dbrw}}]\!] (f)$ with $f = 1$. However, *none of the existing proof rules applies*: (i) C_{1dbrw} is not AST due to its biased nature (see, e.g., [[McIver et al. 2018](#)]), and thus Hark et al.'s lower induction [[Hark et al. 2020](#)] does not apply; moreover, (ii) it makes no sense to apply McIver and Morgan's lower induction [[McIver and Morgan 2005](#)] as having (a lower bound on) the termination probability – the quantity we aim to infer – is in turn one of the prerequisites for applying the rule (cf. [Thm. 10](#)).

We now show how our guard-strengthening rule can be used to verify non-trivial lower bounds on $\text{wp}[\![C_{\text{1dbrw}}]\!] (1)$. To this end, we strengthen the guard $(n > 0)$ of C_{1dbrw} to $\varphi^M = (0 < n < M)$ for any fixed $M \in \mathbb{N}$, and hence obtain a modified loop which differs from C_{1dbrw} only in the guard:

$$C_{\text{1dbrw}}^M : \text{ while } (0 < n < M) \{ n := n - 1 \ [1/3] \ n := n + 1 \} .$$

Our proof rule asserts that, for any fixed $M \in \mathbb{N}$, a lower bound on $\text{wp}[\![C_{\text{1dbrw}}^M]\!] ([n \leq 0] \cdot 1)$ suffices as a lower bound on $\text{wp}[\![C_{\text{1dbrw}}]\!] (1)$. Since C_{1dbrw}^M terminates after at most $M - 1$ steps of consecutively moving to the right with probability $(2/3)^{M-1}$, we have $\sigma\mathbb{P}(T^{-\varphi^M} > M) < 1 - (2/3)^{M-1}$ for any initial state $\sigma(n) \in \mathbb{Z}$. Thus, by [Lem. 15](#), C_{1dbrw}^M terminates almost-surely. We can therefore try to apply Hark et al.'s lower induction for a lower bound on $\text{wp}[\![C_{\text{1dbrw}}^M]\!] ([n \leq 0] \cdot 1)$. Let

$$l_M = [n < 0] + [0 \leq n \leq M] \cdot \left((1/2)^n - (1/2)^M \right) .$$

It is straightforward to check (see [[Feng et al. 2023](#), Appx. D.1]) that, for any fixed $M \in \mathbb{N}$, l_M is a subinvariant, i.e.,

$$l_M \leq \Phi_g^M (l_M)$$

where $g = [n \leq 0] \cdot 1$ is the restricted postexpectation, and Φ_g^M is the characteristic function of C_{1dbrw}^M with respect to g . Furthermore, l_M is bounded from above by 1, and thus is uniformly integrable for C_{1dbrw}^M due to condition (c) in [Thm. 9](#). Consequently, we have

$$\begin{aligned} l_M &\leq \text{wp}[\![C_{\text{1dbrw}}^M]\!] ([n \leq 0] \cdot 1) && \text{[by Hark et al.'s induction, cf. Thm. 8]} \\ &\leq \text{wp}[\![C_{\text{1dbrw}}]\!] (1) . && \text{[by guard-strengthening rule, cf. Thm. 14]} \end{aligned}$$

We therefore conclude that, for any fixed $M \in \mathbb{N}$, l_M is a lower bound on $\text{wp}[\![C_{\text{1dbrw}}]\!] (1)$. In particular, by pushing M ad infinitum – to obtain the *tightest* possible bound; this step is however *not necessary* to establish a *valid* lower bound – we have

$$\text{wp}[\![C_{\text{1dbrw}}]\!] (1) \geq \lim_{M \rightarrow \infty} l_M = [n < 0] + [n \geq 0] \cdot (1/2)^n ,$$

namely, $l_\infty = [n < 0] + [n \geq 0] \cdot (1/2)^n$ is a lower bound on $\text{wp}\llbracket C_{1\text{dbrw}} \rrbracket (1)$. In fact, for this example, one can verify (cf. [Feng et al. 2023, Appx. D.1]) that l_∞ is a superinvariant, i.e., $\Phi_f(l_\infty) \leq l_\infty$, where Φ_f is the characteristic function of $C_{1\text{dbrw}}$ w.r.t. postexpectation $f = 1$. Thus, by Park induction (cf. Thm. 5), l_∞ is also an upper bound on $\text{wp}\llbracket C_{1\text{dbrw}} \rrbracket (1)$. We can thus claim that the *exact* least fixed point of Φ_f , i.e., the *exact termination probability* of $C_{1\text{dbrw}}$ starting from initial position n , is

$$\text{wp}\llbracket C_{1\text{dbrw}} \rrbracket (1) = l_\infty = [n < 0] + [n \geq 0] \cdot (1/2)^n .$$

Finally, we remark that the reasoning process in this example applies to a more general form of one-dimensional random walk with *parametrized* biased probability $p \in [0, 1/2)$, whose exact termination probability can be shown to be $[n < 0] + [n \geq 0] \cdot (p/1-p)^n$. \triangleleft

Next, we show via the following example that even when the targeted loop C_{loop} almost-surely terminates, a genuine lower bound on $\text{wp}\llbracket C_{\text{loop}} \rrbracket (f)$ may *not* be uniformly integrable for C_{loop} , thereby staying out-of-reach by Hark et al.'s lower induction rule; our guard-strengthening rule, however, is capable of certifying such a lower bound.

Example 17 (Bernoulli's St. Petersburg Paradox [Bernoulli 1954]). Consider the following loop C_{pd} modelling a lottery game via fair-coin tosses: The stake $b \in \mathbb{Z}_{>0}$ is doubled every time heads appears; the first time tails occurs, the game ends and the player wins all the stake in the pot:

$$C_{\text{pd}}: \quad \text{while} (a = 1) \{ a := 0 [1/2] \ b := 2 \cdot b \} .$$

We are interested in establishing non-trivial lower bounds on the expected payoff of the lottery, i.e., lower bounds on $\text{wp}\llbracket C_{\text{pd}} \rrbracket (f)$ with $f = b$. Since C_{pd} terminates by setting a to 0 with probability $1/2$, we have $\sigma\mathbb{P}(T^{a \neq 1} > 1) < 1/2$ for any initial state σ . Thus, by Lem. 15, C_{pd} terminates almost-surely. However, the genuine lower bound $l_\infty = ([a \neq 1] \cdot b + [a = 1] \cdot \infty) \prec \infty$ – which we ultimately aim to verify – is *not* uniformly integrable for C_{pd} , and thus cannot be addressed by Hark et al.'s lower induction rule (see a detailed argument in [Hark et al. 2019, Appx. A]).

To apply our new proof rule, we strengthen the guard $(a = 1)$ of C_{pd} to $\varphi^M = (a = 1 \wedge b < M)$ for any fixed $M \in \mathbb{Z}_{>0}$, and thereby obtain the modified loop:

$$C_{\text{pd}}^M: \quad \text{while} (a = 1 \wedge b < M) \{ a := 0 [1/2] \ b := 2 \cdot b \} .$$

Our proof rule asserts that, for any fixed $M \in \mathbb{Z}_{>0}$, a lower bound on $\text{wp}\llbracket C_{\text{pd}}^M \rrbracket ([a \neq 1] \cdot b)$ suffices as a lower bound on $\text{wp}\llbracket C_{\text{pd}} \rrbracket (b)$. Program C_{pd}^M is clearly AST (by the same argument as for C_{pd}); in fact, its looping time $T^{-\varphi^M}$ is certainly bounded by $\lceil \log_2 M \rceil$, and thus by condition (a) in Thm. 9, any expectation $h \ll \infty$ is uniformly integrable for C_{pd}^M (as $\text{wp}\llbracket C \rrbracket^n (h) \ll \infty$ for any $n \in \mathbb{N}$ is vacuously satisfied by $h \ll \infty$ and loop-free body C , which is the case for C_{pd}^M). Let

$$l_M = [a \neq 1] \cdot b + \sum_{i=1}^{\lceil \log_2 M \rceil} [a = 1 \wedge (M/2^i \leq b < M/2^{i-1})] \cdot i \cdot b/2 .$$

It is straightforward to check (see [Feng et al. 2023, Appx. D.2]) that, for any fixed $M \in \mathbb{Z}_{>0}$, l_M is a subinvariant, i.e.,

$$l_M \leq \Phi_g^M (l_M)$$

where $g = [a \neq 1] \cdot b$ is the restricted postexpectation, and Φ_g^M is the characteristic function of C_{pd}^M with respect to g . Since $l_M \ll \infty$ is uniformly integrable for C_{pd}^M , by Thm. 8 and 14, we have

$$l_M \leq \text{wp}\llbracket C_{\text{pd}}^M \rrbracket ([a \neq 1] \cdot b) \leq \text{wp}\llbracket C_{\text{pd}} \rrbracket (b)$$

for any fixed $M \in \mathbb{Z}_{>0}$. It follows that, when M tends to infinity,

$$\text{wp}\llbracket C_{\text{pd}} \rrbracket (b) \geq \lim_{M \rightarrow \infty} l_M = [a \neq 1] \cdot b + [a = 1] \cdot \infty = l_\infty .$$

In analogy to [Exmp. 16](#), one can further show that l_∞ suffices as a superinvariant and ultimately conclude that $\text{wp}[\![C_{\text{pd}}]\!](b) = l_\infty$, that is, the *exact* expected value of b upon termination. \triangleleft

6.2 Orthogonal Sufficient Condition for Uniform Integrability

[Exmp. 16](#) and [17](#) demonstrate how we can certify lower bounds on $\text{wp}[\![C_{\text{loop}}]\!](f)$ leveraging existing sufficient criteria for uniform integrability (cf. [Thm. 9](#)) for the modified loop C'_{loop} . The fact that C'_{loop} often features a strong and easily checkable termination property (cf. [Lem. 15](#)) enables an alternative sufficient condition for establishing uniform integrability:

Theorem 18 (Orthogonal Sufficient Criterion for Uniform Integrability). *Suppose $C'_{\text{loop}} = \text{while}(\varphi')\{C\}$ satisfies the AST condition in [Lem. 15](#). Then, an expectation $h \ll \infty$ is uniformly integrable for C'_{loop} if (i) C'_{loop} has the bounded update property¹⁰, i.e., there exists $c \in \mathbb{R}_{\geq 0}$ such that for any $\sigma \in \Sigma$, $\sigma\mathbb{P}(\forall n \in \mathbb{N}: |X_{n+1} - X_n| \leq c) = 1$, and (ii) h is bounded by a polynomial expectation¹¹.*

The sufficient criterion for uniform integrability in [Thm. 18](#) is orthogonal to those in [Thm. 9](#), in particular, to condition (b) thereof: Our new sufficient condition leverages the fact that C'_{loop} with a strengthened guard often features a strong and easily checkable termination property (cf. [Lem. 15](#)); it is confined to loops with the bounded update property, yet relaxes the conditional difference boundedness of h to the polynomial boundedness of h . Our new sufficient criterion is usually *easier* to check than condition (b) in [Thm. 9](#) in the sense that (i) in case C'_{loop} has a loop-free body, one can simply read off the bounded update property from the syntax of C'_{loop} , and (ii) any (piece-wise) polynomial expectation h fulfils the polynomial boundedness condition. The following example demonstrates a scenario where *none* of the conditions in [Thm. 9](#) suffices to show uniform integrability, but our (orthogonal) sufficient condition in [Thm. 18](#) does.

Example 19 (1-D Symmetric Random Walk with Bounded Updates). Consider the following loop C_{bu} modelling a symmetrized 1-D random walk on \mathbb{Z} , where we additionally increase (resp. decrease) the value of $b \in \mathbb{R}_{\geq 0}$ by 2 along every left (resp. right) move with probability $1/2$:

$$C_{\text{bu}}: \quad \text{while}(n > 0) \{ \{n := n - 1 \ ; \ b := b + 2\} [1/2] \{n := n + 1 \ ; \ b := b - 2\} \} .$$

We are interested in certifying non-trivial lower bounds on the expected value of b upon termination, i.e., lower bounds on $\text{wp}[\![C_{\text{bu}}]\!](f)$ with $f = b$. Notice that C_{bu} exhibits exactly the same termination behavior as the standard 1-D symmetric random walk [[McIver et al. 2018](#)], namely, C_{bu} terminates almost-surely yet with an *infinite* expected looping time. Moreover, the candidate lower bound $l_\infty = [n < 0] \cdot b + [n \geq 0] \cdot (b + 2 \cdot n)$ – which we ultimately aim to verify – is *unbounded*, thereby out-of-reach by Hark et al.’s lower induction (as [Thm. 9](#) does not suffice to show u.i. of l_∞).

To apply our new proof rule, we strengthen the guard $(n > 0)$ of C_{bu} to $\varphi^M = (0 < n < M)$ for any fixed $M \in \mathbb{Z}_{>0}$, and thereby obtain the modified loop:

$$C_{\text{bu}}^M: \quad \text{while}(0 < n < M) \{ \{n := n - 1 \ ; \ b := b + 2\} [1/2] \{n := n + 1 \ ; \ b := b - 2\} \} .$$

Our proof rule asserts that, for any fixed $M \in \mathbb{Z}_{>0}$, a lower bound on $\text{wp}[\![C_{\text{bu}}^M]\!]([n \leq 0] \cdot b)$ suffices as a lower bound on $\text{wp}[\![C_{\text{bu}}]\!](b)$. Let

$$l_M = [n < 0] \cdot b + [0 \leq n \leq M] \cdot (b + 2 \cdot n) \cdot (1 - n/M) .$$

One can readily verify that, for any fixed $M \in \mathbb{Z}_{>0}$, l_M is a subinvariant (see [[Feng et al. 2023](#), Appx. D.3]). Since C_{bu}^M terminates after at most $M - 1$ steps of consecutively increasing n with

¹⁰The bounded update property has been used to analyze expected costs for nondeterministic probabilistic programs [[Wang et al. 2019](#)]; it subsumes the class of constant probability programs [[Giesl et al. 2019](#)].

¹¹One can replace (ii) with (ii') h is bounded by a *piece-wise* polynomial expectation, and the theorem still holds.

probability $(1/2)^{M-1}$, we have $\sigma\mathbb{P}(T^{-\varphi^M} > M) < 1 - (1/2)^{M-1}$ for any initial state $\sigma(n) \in \mathbb{Z}$. Thus, by [Lem. 15](#), C_{bu}^M terminates almost-surely. Nevertheless, still *none of the conditions in [Thm. 9](#) suffices to show that l_M is uniformly integrable for C_{bu}^M* : the looping time $T^{-\varphi^M}$ is not almost-surely bounded, l_M is not bounded due to unbounded variable b thereof, and l_M is not conditionally difference bounded (see [[Feng et al. 2023](#), Appx. D.3]).

However, it is evident that our (orthogonal) sufficient criterion in [Thm. 18](#) is fulfilled, thereby witnessing uniform integrability of l_M for C_{bu}^M : C_{bu}^M has the bounded update property, as it has a loop-free body with only bounded updates; moreover, l_M meets the polynomial boundedness condition as, for any fixed $M \in \mathbb{Z}_{>0}$, l_M is a piece-wise polynomial in n and b . Consequently, by [Thm. 8](#) and [14](#), we have, for any fixed $M \in \mathbb{Z}_{>0}$,

$$l_M \leq \text{wp}[[C_{\text{bu}}^M]]([n \leq 0] \cdot b) \leq \text{wp}[[C_{\text{bu}}]](b).$$

We can eventually certify the lower bound l_∞ by pushing M ad infinitum:

$$\text{wp}[[C_{\text{bu}}]](b) \geq \lim_{M \rightarrow \infty} l_M = [n < 0] \cdot b + [n \geq 0] \cdot (b + 2 \cdot n) = l_\infty. \quad \triangleleft$$

6.3 Tightness of the Guard-Strengthening Rule

Next, we discuss the error incurred by our guard-strengthening rule, i.e., the difference between $\text{wp}[[C_{\text{loop}}]](f)$ and the established lower bound l as per [Thm. 14](#). To this end, observe that

$$\text{wp}[[C_{\text{loop}}]](f) - l = \underbrace{\left(\text{wp}[[C_{\text{loop}}]](f) - \text{wp}[[C'_{\text{loop}}]]([\neg\varphi] \cdot f) \right)}_{\text{error incurred by guard strengthening, } \geq 0} + \underbrace{\left(\text{wp}[[C'_{\text{loop}}]]([\neg\varphi] \cdot f) - l \right)}_{\text{error incurred in the reduced problem, } \geq 0} \quad (16)$$

where, on the right-hand side, the first summand encodes the error inherently caused by our guard-strengthening technique, whereas the second summand accounts for the error in underapproximating $\text{wp}[[C'_{\text{loop}}]]([\neg\varphi] \cdot f)$ by l , which is independent of the proof rule itself. In what follows, we quantify the first summand, i.e., the error incurred by strengthening the guard.

Lemma 20. *Given loops $C_{\text{loop}} = \text{while}(\varphi)\{C\}$ and $C'_{\text{loop}} = \text{while}(\varphi')\{C\}$, suppose $\varphi' \implies \varphi$, then, for any postexpectation $f \in \mathbb{E}$,*

$$\text{wp}[[C_{\text{loop}}]](f) - \text{wp}[[C'_{\text{loop}}]]([\neg\varphi] \cdot f) \leq \text{wp}[[C'_{\text{loop}}]]([\varphi]) \cdot \sup_{\sigma \models \neg\varphi' \wedge \varphi} \text{wp}[[C_{\text{loop}}]](f)(\sigma).$$

PROOF (SKETCH). As shown in the proof of [Cor. 13](#) (cf. [[Feng et al. 2023](#), Appx. C.2]), we have

$$\text{wp}[[C_{\text{loop}}]](f) - \text{wp}[[C'_{\text{loop}}]]([\neg\varphi] \cdot f) = \lambda\sigma. \int_A f_{C_{\text{loop}}} \text{d}(\sigma\mathbb{P}).$$

It thus suffices to bound the integral above, which can be achieved by examining different fragments (witnessed by guard violations) of traces in A . See details in [[Feng et al. 2023](#), Appx. C.6]. \square

An immediate consequence of [Lem. 20](#) yields the *tightness* of our guard-strengthening rule, that is, the error incurred by underapproximating $\text{wp}[[C_{\text{loop}}]](f)$ by $\text{wp}[[C'_{\text{loop}}]]([\neg\varphi] \cdot f)$ approaches zero when φ' approaches φ in an appropriate manner:

Theorem 21 (Tightness of Guard Strengthening). *Given $C_{\text{loop}} = \text{while}(\varphi)\{C\}$, suppose there exists a sequence of guards $\{\varphi^m\}_{m \in \mathbb{N}}$ such that $\forall m \in \mathbb{N}: \varphi^m \implies \varphi$. Let $C_{\text{loop}}^m = \text{while}(\varphi^m)\{C\}$. If one of the following two conditions holds:*

- (a) $\lim_{m \rightarrow \infty} \sup_{\sigma \models \neg\varphi^m \wedge \varphi} \text{wp}[[C_{\text{loop}}]](f)(\sigma) < \infty$ and $\lim_{m \rightarrow \infty} \text{wp}[[C_{\text{loop}}^m]]([\varphi]) = 0$,
- (b) $\lim_{m \rightarrow \infty} \sup_{\sigma \models \neg\varphi^m \wedge \varphi} \text{wp}[[C_{\text{loop}}]](f)(\sigma) = 0$,¹²

¹²Note that $\text{wp}[[C_{\text{loop}}^m]]([\varphi])$ maps a state to a *probability*, and thus $\lim_{m \rightarrow \infty} \text{wp}[[C_{\text{loop}}^m]]([\varphi]) \leq 1 \ll \infty$.

then, the error incurred by strengthening φ with φ^m converges to zero as m tends to ∞ , i.e.,

$$\text{wp}[\llbracket C_{\text{loop}} \rrbracket](f) = \lim_{m \rightarrow \infty} \text{wp}[\llbracket C_{\text{loop}}^m \rrbracket](\llbracket \neg\varphi \rrbracket \cdot f).$$

Remark. There are cases where both conditions (a) and (b) in [Thm. 21](#) do not hold: Recall the 1-D random walk given in [Sect. 2](#) and consider, for instance, the sequence of guards $\{\varphi^m\}_{m \in \mathbb{N}}$ with $\varphi^m = (0 < n < 9 + (2^m - 1)/2^m)$. We have that $\lim_{m \rightarrow \infty} \varphi^m = (0 < n < 10)$ and $\forall m \in \mathbb{N}: \varphi^m \implies \varphi$. However, one can verify that neither (a) nor (b) holds (as $\{\varphi^m\}_{m \in \mathbb{N}}$ do not approach φ at all). \triangleleft

Conditions (a) and (b) in [Thm. 21](#) can be checked by certifying upper bounds on the weakest preexpectations therein via, e.g., Park induction, as demonstrated by the following example.

Example 22. Reconsider the probabilistic loops C_{1dbrw} and C_{1dbrw}^M with postexpectation $f = 1$ in [Exmp. 16](#). We have shown – with the aid of Park induction – that $l_\infty = [n < 0] + [n \geq 0] \cdot (1/2)^n$ coincides with the exact termination probability of C_{1dbrw} starting from initial position n , i.e., $\text{wp}[\llbracket C_{\text{1dbrw}} \rrbracket](1) = l_\infty \ll \infty$. Thus, by [\(16\)](#), one can already conclude the tightness, namely,

$$\text{wp}[\llbracket C_{\text{1dbrw}} \rrbracket](1) = \lim_{M \rightarrow \infty} \text{wp}[\llbracket C_{\text{1dbrw}}^M \rrbracket](\llbracket n \leq 0 \rrbracket \cdot 1).$$

We now show that the same conclusion can be drawn via condition (b) in [Thm. 21](#). Observe that

$$\begin{aligned} \lim_{M \rightarrow \infty} \sup_{\sigma \models \neg\varphi^M \wedge \varphi} \text{wp}[\llbracket C_{\text{1dbrw}} \rrbracket](1)(\sigma) &= \lim_{M \rightarrow \infty} \sup_{\sigma \models n \geq M} \text{wp}[\llbracket C_{\text{1dbrw}} \rrbracket](1)(\sigma) \\ &\leq \lim_{M \rightarrow \infty} \sup_{\sigma \models n \geq M} ([n < 0] + [n \geq 0] \cdot (1/2)^n)(\sigma) \\ &\hspace{15em} [\text{by } \text{wp}[\llbracket C_{\text{1dbrw}} \rrbracket](1) \leq l_\infty] \\ &= \lim_{M \rightarrow \infty} \sup_{\sigma \models n \geq M} ((1/2)^n)(\sigma) \\ &= \lim_{M \rightarrow \infty} (1/2)^M = 0. \end{aligned}$$

Thus, by condition (b) in [Thm. 21](#), the error incurred by strengthening φ with φ^M converges to zero as M tends to ∞ . \triangleleft

6.4 On Automation of the Guard-Strengthening Rule

We briefly discuss the potential to *automate* our guard-strengthening rule for *finding* – rather than just verifying – lower bounds on weakest preexpectations. Such automation needs to address two questions: (i) how to find a “good” guard strengthening, i.e., $\varphi' \implies \varphi$? (ii) how to generate a non-trivial lower bound for the modified loop C'_{loop} ?

How to Find a “Good” Strengthening? In terms of logical strength, a good modified guard φ' cannot be too strong, otherwise only trivial lower bound can be derived (think of $\varphi' = \text{false}$); it cannot be too weak either, otherwise the resulting loop C'_{loop} may not fulfil our conditions on termination (cf. [Lem. 15](#)) and uniform integrability (cf. [Thm. 9](#) and [18](#)). In general, it is hard to find – or even to characterize – the “best” strengthening $\varphi' \implies \varphi$, however, a naive strengthening pattern by simply bounding a subset $\mathcal{V} \subseteq \text{Vars}$ of program variables turns out to be rather effective, i.e.,

$$\varphi' = \varphi \wedge \bigwedge_{x \in \mathcal{V}} x \diamond c,$$

where c is a constant and $\diamond \in \{<, >, \leq, \geq, =\}$. The subset $\mathcal{V} \subseteq \text{Vars}$ shall be selected in a way such that C'_{loop} meets our conditions on termination and uniform integrability. Such a strengthening pattern is indeed heuristic, but it suffices to produce good strengthened guards φ' (in the sense discussed above) for *all* the examples presented in this paper – except for those in [Sect. 8](#) where we

address limitations of the naive strengthening pattern. Investigating a potentially more advanced and clever guard-strengthening strategy is subject to future work.

How to Generate a Non-trivial Lower Bound for C'_{loop} ? Due to the nice properties of C'_{loop} on, e.g., termination, the desired lower bounds on $\text{wp}\llbracket C'_{\text{loop}} \rrbracket ([\neg\varphi] \cdot f)$ can be discovered by leveraging various (semi-)automated techniques for synthesizing lower bounds on least fixed points. These include – in the probabilistic setting – techniques based on *constraint solving* [Chen et al. 2015; Feng et al. 2017; Katoen et al. 2010] and *invariant learning* [Bao et al. 2022] for generating lower bounds on weakest preexpectations of probabilistic programs, *recurrence solving* [Bartocci et al. 2019] for synthesizing moment-based invariants of (solvable) probabilistic loops, and various forms of *value iteration* [Baier et al. 2017; Hartmanns and Kaminski 2020; Quatmann and Katoen 2018] for determining reachability probabilities in Markov models. In particular, we identify a special case where computing the *exact* least fixed point can be done by *probabilistic model checking*:

Theorem 23 (Reduction to Probabilistic Model Checking [Baier and Katoen 2008, Chap. 10]).

Given $C'_{\text{loop}} = \text{while}(\varphi')\{C\}$ and postexpectation $g \in \mathbb{E}$, if C'_{loop} has a finite set of reachable states, then $\text{wp}\llbracket C'_{\text{loop}} \rrbracket(g)$ can be computed exactly by solving a system of linear equations.

Thm. 23 holds since a finite-state loop C'_{loop} can be unrolled into a finite-state Markov chain \mathcal{M} , and $\text{wp}\llbracket C'_{\text{loop}} \rrbracket(g)$ coincides with the unique solution to a linear-equation system induced by \mathcal{M} with rewards modelling g [Baier and Katoen 2008, Chap. 10], which can be computed symbolically by probabilistic model checkers, e.g., STORM [Dehnert et al. 2017], PRISM [Kwiatkowska et al. 2002].

The combination of our guard-strengthening rule with Thm. 23 facilitates inferring quantitative properties of infinite-state probabilistic programs by model checking finite-state probabilistic models:

Example 24 (3-D Symmetric Random Walk on \mathbb{Z}^3 [McCrea and Whipple 1940; Montroll 1956]).

Consider the loop $C_{3\text{dsrw}}$ modelling a symmetric random walk on the 3-D lattice over \mathbb{Z}^3 :

$$C_{3\text{dsrw}}: \quad \text{while}(x \neq 0 \vee y \neq 0 \vee z \neq 0) \{ \\ \quad x := x - 1 \oplus x := x + 1 \oplus y := y - 1 \oplus y := y + 1 \oplus z := z - 1 \oplus z := z + 1 \}$$

where iterated \oplus is shorthand for discrete uniform choice (in this case, with probability $1/6$ each).

The random nature underneath $C_{3\text{dsrw}}$ is fundamentally *different* from its 1- and 2-D counterparts: Pólya [1921] proved that the probability \mathcal{P} that such a random walk returns to the origin at $(0, 0, 0)$ is strictly less than 1, indicating that $C_{3\text{dsrw}}$ does *not* terminate almost-surely. More precisely, the termination probability of $C_{3\text{dsrw}}$ starting from any neighbor location of the origin is

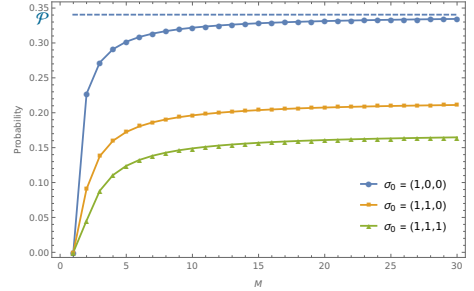
$$\mathcal{P} = 1 - \left(\frac{3}{(2\pi)^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dx dy dz}{3 - \cos x - \cos y - \cos z} \right)^{-1} = 0.3405373296 \dots$$

which is known as one of Pólya's random walk constants. To the best of our knowledge, existing techniques cannot cope with the verification of $C_{3\text{dsrw}}$ due to its complex nature of divergence.

We now show how our guard-strengthening rule can be used to *automatically* derive lower bounds on the termination probability \mathcal{P} of $C_{3\text{dsrw}}$ (i.e., with postexpectation $f = 1$) by leveraging probabilistic model checking. To this end, we first bound the possible positions (x, y, z) with a cube of side-length $2 \cdot M$ with fixed $M \in \mathbb{Z}_{>0}$, and thereby obtain the modified loop:

$$C_{3\text{dsrw}}^M: \quad \text{while}((x \neq 0 \vee y \neq 0 \vee z \neq 0) \wedge |x| < M \wedge |y| < M \wedge |z| < M) \{ \\ \quad x := x - 1 \oplus x := x + 1 \oplus y := y - 1 \oplus y := y + 1 \oplus z := z - 1 \oplus z := z + 1 \} .$$

Observe that, starting from any initial position in the lattice, the modified random walk $C_{3\text{dsrw}}^M$ can reach only a *finite* number of positions, i.e., it either (i) terminates by escaping the cube or returning to the origin, or (ii) keeps strolling within the cube. Thus, by the connection in [Thm. 23](#), the reduced weakest preexpectation $\text{wp}[[C_{3\text{dsrw}}^M]] \llbracket (x = 0 \wedge y = 0 \wedge z = 0) \cdot 1 \rrbracket$ – which underapproximates the termination probability \mathcal{P} of $C_{3\text{dsrw}}$ – can be computed symbolically by off-the-shelf probabilistic model checkers. For instance, [Fig. 6](#) depicts such underapproximations produced by PRISM [[Kwiatkowska et al. 2002](#)] under different choices of M (cf. the X-axis). In particular, [Fig. 6](#) confirms our previous claim on tightness (cf. [Thm. 21](#))¹³: as M gets larger, the strengthening gets weaker, thus yielding tighter lower bounds on the actual termination probability \mathcal{P} . [Fig. 6](#) also confirms our intuition that the further the walker is away from the origin, the lower probability returns the walker back to the origin. \triangleleft



[Fig. 6](#). Lower bounds obtained by PRISM on the termination probability of $C_{3\text{dsrw}}$ in [Exmp. 24](#) on initial position σ_0 . $\mathcal{P} \approx 0.34$ marks the true termination probability when starting from a neighbor location of the origin, e.g., $\sigma_0 = (1, 0, 0)$; the true termination probabilities on other initial positions are unknown.

Remark. In the aforementioned special case where our problem is reducible to model checking finite-state discrete-time Markov chains, our guard-strengthening rule acts analogously (yet on the source-code level) to the so-called *partial exploration* technique [[Brázdil et al. 2014](#)] established in probabilistic model checking. The latter constructs a sequence of increasingly precise approximations (lower and upper bounds on reachability probabilities) by (partially) exploring an incremental subset of the state space. This procedure yields a similar effect as we gradually weaken our strengthening to obtain tighter and tighter lower bounds. Since we always infer safe underapproximations, our technique may be used to generate *critical subsystems* [[Ábrahám et al. 2014](#)] serving as counterexamples to quantitative properties in probabilistic verification.

7 CASE STUDIES

In this section, we present a few non-trivial examples to demonstrate the effectiveness of our guard-strengthening rule in establishing lower bounds on weakest preexpectations. These examples include probabilistic programs with *continuous distributions*, *nested loops*, and *state-dependent probabilities*, as well as a real-world *randomized networking protocol*. These are all *infinite-state* programs, for some of which our proof rule can be used to prove almost-sure termination by certifying 1 as a lower bound on the termination probability.

Example 25 (Continuous Sampling). Consider the following loop C_{cs} modelling a 1-D random walk where the branching probability is drawn from a continuous uniform distribution over $(0, 1)$.

$$C_{\text{cs}}: \text{ while } (n > 0) \{ \\ \quad p := \text{uniform}(0, 1) ; \\ \quad \{ n := n - 1 ; b := b + \text{uniform}(0, 1) \} [p] \{ n := n + 1 ; b := b - \text{uniform}(0, 1) \} \} .$$

We aim to verify $l_\infty = [n < 0] \cdot b + [n \geq 0] \cdot (b + 1/2 \cdot n)$ as a lower bound on the expected value of b upon termination, i.e., $l_\infty \leq \text{wp}[[C_{\text{cs}}]](b)$. Observe that l_∞ is unbounded; moreover, C_{cs} behaves – in

¹³A rigorous proof of tightness in this example requires finding an appropriate superinvariant – like we did in [Exmp. 22](#), yet now for the 3-D random walk – which is extremely hard and beyond the scope of this paper.

expectation – as the standard 1-D symmetric random walk [McIver et al. 2018] and thus terminates almost-surely yet with an *infinite* expected looping time. Existing proof rules hence do not apply.

We now strengthen the guard ($n > 0$) of C_{cs} to $\varphi^M = (0 < n < M)$ for any fixed $M \in \mathbb{Z}_{>0}$, and denote the so-obtained loop by C_{cs}^M . It can be shown (cf. [Feng et al. 2023, Appx. D.4]) that

$$l_M = [n < 0] \cdot b + [0 \leq n \leq M] \cdot (b + 1/2 \cdot n) \cdot (1 - n/M)$$

is a subinvariant, i.e., $l_M \leq \Phi_g^M(l_M)$, where $g = [n \leq 0] \cdot b$ is the restricted postexpectation, and Φ_g^M is the characteristic function of C_{cs}^M with respect to g . Furthermore, C_{cs}^M terminates after at most $M - 1$ steps of consecutively increasing n with probability at least $(1/2 \cdot 1/2)^{M-1}$ (i.e., by first drawing $p \in (1/2, 1)$ and then picking the right branch), we have $\sigma_{\mathbb{P}}(T^{-\varphi^M} > M) < 1 - (1/4)^{M-1}$ for any initial state $\sigma(n) \in \mathbb{Z}$. Thus, by Lem. 15, C_{cs}^M terminates almost-surely. Moreover, C_{cs}^M is uniformly integrable for C_{cs}^M as witnessed by our new sufficient condition in Thm. 18. It follows that $l_M \leq \text{wp}[\![C_{cs}^M]\!]([n \leq 0] \cdot b) \leq \text{wp}[\![C_{cs}]\!](b)$ for any fixed $M \in \mathbb{Z}_{>0}$. We can eventually certify the lower bound l_∞ by pushing M ad infinitum:

$$\text{wp}[\![C_{cs}]\!](b) \geq \lim_{M \rightarrow \infty} l_M = [n < 0] \cdot b + [n \geq 0] \cdot (b + 1/2 \cdot n) = l_\infty. \quad \triangleleft$$

Example 26 (Nested Loops). Consider the program C_{nl} with two nested loops (the outer loop alters $n \in \mathbb{Z}$ based on the outcome of the inner loop; $a, b \in \mathbb{Z}_{>0}$ are parameters satisfying $a > b^{14}$):

```
Cnl:  while (n > 0) {
        k := n ;
        while (-a < k - n < b) { k := k - 1 [1/2] k := k + 1 } ;
        if (k < n) { n := n - 1 } else { n := n + 1 } } .
```

Suppose we are interested in proving a non-trivial lower bound on the termination probability $\text{wp}[\![C_{nl}]\!](1)$. This problem is out-of-reach by existing proof rules as C_{nl} is not AST. To apply our proof rule, we strengthen the guard of the outer loop to $\varphi^M = (0 < n < M)$ for any fixed $M \in \mathbb{Z}_{>0}$. The modified program C_{nl}^M is AST due to a similar argument per Lem. 15. Let

$$l_M = [n < 0] + [0 \leq n \leq M] \cdot \left((b/a)^n - (b/a)^M \right) .$$

Since l_M is bounded, we know by Thm. 8 and 14 that l_M underapproximates the termination probability of C_{nl} if l_M is a subinvariant of C_{nl}^M . In that case, we have proved the lower bound l_∞ :

$$\text{wp}[\![C_{nl}]\!](1) \geq \lim_{M \rightarrow \infty} l_M = [n < 0] + [n \geq 0] \cdot (b/a)^n \triangleq l_\infty .$$

We now show that l_M is indeed a subinvariant of C_{nl}^M , i.e., $l_M \leq \Phi_g^M(l_M)$, where $g = [n \leq 0] \cdot 1$ is the restricted postexpectation, and Φ_g^M is the characteristic function of C_{nl}^M w.r.t. g . Checking subinvariance in this case is more involved due to the nested feature of C_{nl}^M : one also has to reason about *lower bounds for the inner loop* w.r.t. a specific postexpectation depending on l_M . More precisely, let C_{body}^M and C_{inner}^M denote the loop body and the inner loop of C_{nl}^M , respectively. We have

$$\begin{aligned} \Phi_g^M(l_M) &= [n \leq 0 \vee n \geq M] \cdot [n \leq 0] + [0 < n < M] \cdot \text{wp}[\![C_{body}^M]\!](l_M) \\ &= [n \leq 0] + [0 < n < M] \cdot \\ &\quad \text{wp}[\![k := n]\!]\left(\text{wp}[\![C_{inner}^M]\!]\left([k < n] \cdot l_M[n/n - 1] + [k \geq n] \cdot l_M[n/n + 1]\right)\right) . \end{aligned}$$

¹⁴The restriction $a > b$ makes C_{nl} a non-AST program.

By combining the fact (see [Feng et al. 2023, Appx. D.5]) that, for any bounded postexpectation h ,

$$\text{wp}[\llbracket C_{\text{inner}}^M \rrbracket](h) \geq [(k-n < -a) \vee (k-n > b)] \cdot h + \\ [-a \leq k-n \leq b] \cdot \left(\frac{b-(k-n)}{b+a} \cdot h[k/n-a] + \frac{(k-n)+a}{b+a} \cdot h[k/n+b] \right),$$

we can conclude the subinvariance of l_M , i.e., $l_M \leq \Phi_g^M(l_M)$ (detailed in [Feng et al. 2023, Appx. D.5]). This completes our verification of the lower bound l_∞ . \triangleleft

Example 27 (Fair-in-the-Limit Random Walk [McIver et al. 2018]). Consider the following loop C_{flrw} modelling a biased random walk on \mathbb{Z} , where in particular, the probability of taking the next move depends on the current position of the walker:¹⁵

$$C_{\text{flrw}}: \quad \text{while } (n > 0) \{ n := n - 1 \ [^{n+1/2n+1}] \ n := n + 1 \} .$$

The further the walker moves to the right, the more fair becomes the random walk as $n+1/2 \cdot n+1$ approaches $1/2$ asymptotically. We show how our guard-strengthening rule can be used to prove almost-surely termination of C_{flrw} by certifying 1 as a lower bound on $\text{wp}[\llbracket C_{\text{flrw}} \rrbracket](1)$. Similarly, we strengthen the guard $(n > 0)$ to $\varphi^M = (0 < n < M)$ for any fixed $M \in \mathbb{Z}_{>0}$ and denote the so-obtained loop by C_{flrw}^M . Since C_{flrw}^M terminates after at most $M-1$ steps of consecutively moving to the left with probability at least $(1/2)^{M-1}$, C_{flrw}^M terminates almost-surely by Lem. 15. Let

$$l_M = [n < 0] + [0 \leq n \leq M] \cdot (1 - n/M) .$$

l_M is bounded from above by 1, thus is uniformly integrable for C_{flrw}^M by condition (c) in Thm. 9. Furthermore, l_M is a subinvariant since

$$\Phi_g(l_M) = [n \leq 0 \vee n \geq M] \cdot [n \leq 0] + [0 < n < M] \cdot \left(\frac{n+1}{2n+1} \cdot l_M[n/n-1] + \frac{n}{2n+1} \cdot l_M[n/n+1] \right) \\ = [n \leq 0 \vee n \geq M] \cdot [n \leq 0] + [0 < n < M] \cdot \left(\frac{n+1}{2n+1} \cdot \frac{M-n+1}{M} + \frac{n}{2n+1} \cdot \frac{M-n-1}{M} \right) \\ = [n \leq 0] + [0 < n < M] \cdot \left(1 - \frac{n}{M} + \frac{1}{(2n+1) \cdot M} \right) \geq l_M ,$$

where $g = [n \leq 0] \cdot 1$ is the restricted postexpectation, and Φ_g^M is the characteristic function of C_{flrw}^M with respect to g . This implies $l_M \leq \text{wp}[\llbracket C_{\text{flrw}} \rrbracket](1)$, i.e., l_M is a lower bound on the termination probability of C_{flrw} for any fixed $M \in \mathbb{Z}_{>0}$. In particular, when M approaches infinity, we have

$$\text{wp}[\llbracket C_{\text{flrw}} \rrbracket](1) \geq \lim_{M \rightarrow \infty} l_M = 1 .$$

We can thus conclude that C_{flrw} terminates almost-surely. \triangleleft

Example 28 (Zeroconf Protocol [Bohnenkamp et al. 2003]). Consider the loop C_{zc} encoding the randomized IPv4 Zeroconf protocol (parameterized in N) for self-configuring IP network interfaces:

$$C_{\text{zc}}: \quad \text{start} = 1 \ ; \ \text{established} = 0 \ ; \ \text{probe} = 0 \ ; \\ \text{while } (\text{start} \leq 1 \wedge \text{established} \leq 0 \wedge \text{probe} < N \wedge N \geq 4) \{ \\ \quad \text{if } (\text{start} = 1) \{ \\ \quad \quad \{ \text{start} := 0 \} [0.5] \ \{ \text{start} := 0 \ ; \ \text{established} := 1 \} \\ \quad \quad \text{else } \{ \{ \text{probe} := \text{probe} + 1 \} [0.001] \ \{ \text{start} := 1 \ ; \ \text{probe} := 0 \} \} \} .$$

¹⁵The loop remains AST if we replace the biased probability $n+1/2n+1$ by $n/2n+1$. However, in this case, one needs a more advanced subinvariant in order to certify AST of the loop. See, e.g., a proof using harmonic numbers in [McIver et al. 2018].

This program is intended for providing a convenient way to analyze the probability that an unused IP address is successfully assigned to a host that is newly connected to a network of m existing devices: Once being connected, the host first randomly selects an IP address from a pool of n available addresses. With probability m/n (instantiated as 0.5), this address is already in use; with probability $1 - m/n$, the chosen address is unused and thus the IP connection can be established (signified by terminating with *established* = 1). For the former case, the host broadcasts a “probe” message to other devices in the network asking whether the chosen IP address is already taken; if the probe is received by a device that already uses the address, it replies with a message indicating so. After receiving this message, the host to be configured restarts.¹⁶ The probability 0.001 in the else-statement encodes the probability of message loss (for probe or reply). To increase reliability, the host is required to send multiple probes (upper-bounded by N). In fact, C_{zc} encodes an *infinite family* of Markov chains (cf. [Baier and Katoen 2008, Exmp. 10.5]) by parameterizing N , and thus cannot be handled by probabilistic model checking.

We are interested in verifying a non-trivial lower bound 0.9999999999 on the probability \mathcal{P} that, starting from a state satisfying the loop guard, C_{zc} terminates in a state with *established* = 1. We do so by trying to *synthesize* a subinvariant justifying this lower bound using the recently developed tool CEGISPRO2 [Batz et al. 2023] which automates Hark et al.’s sound lower induction rule [Hark et al. 2020]. Unfortunately, CEGISPRO2 failed in this case (timeout in 20 minutes). However, by strengthening the loop guard with upper bounds on N , e.g., $N \leq 10$, and applying our proof rule, CEGISPRO2 found a piece-wise linear subinvariant (in less than a second; omitted due to limited space) that suffices to certify 0.9999999999 as a lower bound on \mathcal{P} . Overall, this demonstrates the potential of our proof rule to enable verifying lower bounds via automated techniques for practical randomized algorithms that are otherwise out-of-reach. \triangleleft

Our proof rule applies further to a few extra case studies from the Quantitative Verification Benchmark Set [Hartmanns et al. 2019], including the (infinite family of) Bounded Retransmission protocol, the (parametrized) Rabin Mutual Exclusion algorithm, and the Coupon Collectors. These case studies are not included because they either do not bring extra insights over the Zeroconf protocol or can already be tackled by existing techniques. The main challenges of pursuing a wider range of real randomized algorithms are (i) to find good guard strengthening (cf. Sect. 8 below) and, in some cases, (ii) to find subinvariants certifying the given lower bounds. We plan to address these challenges by exploiting the potential for *automating* our proof rule as discussed in Sect. 6.4.

8 LIMITATIONS OF THE GUARD-STRENGTHENING RULE

There are interesting divergent programs for which the proposed guard-strengthening principle is insufficient or inadequate. We address such limitations by means of two examples.

The following example demonstrates the case where the naive strengthening heuristic is insufficient, yet a more advanced strengthening strategy suffices to establish non-trivial lower bounds.

Example 29 (2-D Discrete Spiral). Consider the probabilistic program

$$\begin{aligned} & x := 0 \ ; \ y := 0 \ ; \ flag := 0 \ ; \\ & \text{while } ((x - 1)^2 + (y - 1)^2 < 4) \{ \\ & \quad \{ x := -1 \ ; \ y := -1 \} \ [|x-1|/4] \{ \\ & \quad \quad \text{if } (flag) \{ y := (3-y)/2 \} \text{ else } \{ x := (3-x)/2 \} \ ; \ flag := 1 - flag \} \} . \end{aligned}$$

¹⁶The program C_{zc} is an abstract model of the actual protocol in the sense that C_{zc} abstracts away the need for broadcasting probe messages when the right branch of the if-statement is executed (in this case, no reply message will be sent anyway). Such an abstraction does not affect the analysis of the probability of terminating with *established* = 1.

This program terminates only if it visits the left branch of the probabilistic choice; otherwise, it diverges with (x, y) approaching $(1, 1)$ in the shape of a 2-D discrete spiral. Note that the program is non-AST and we aim to verify lower bounds on its termination probability. Observe that, in this case, the naive strengthening heuristic $\varphi' = \varphi \wedge x < c \wedge y < c$ by adding a constant bound c on program variables is *insufficient* for any $c > 3/2$ as the resulting program is still non-AST; whereas for any $c \leq 3/2$, the resulting program terminates after at most one loop iteration thus only yielding *trivial* lower bounds. In contrast, by applying the more advanced (yet intuitive) strengthening $\varphi' = \varphi \wedge (x - 1)^2 + (y - 1)^2 > \epsilon$ with a small constant $\epsilon > 0$ (i.e., to rule out the spiral center $(1, 1)$), we reduce the program to the case of a finite state space, which can then be tackled by probabilistic model checking for establishing *non-trivial* lower bounds. \triangleleft

As remarked in Sect. 6.4, it is an interesting future direction to investigate potentially more advanced, (semi-)automatable guard-strengthening strategies than the heuristic used in this paper.

The following example demonstrates a corner case where no useful strengthening exists.

Example 30 (Dummy Swapper). Consider the probabilistic program

$$\text{while}(x \neq y) \{ x := y \oplus \{ \text{temp} := x \ ; \ x := y \ ; \ y := \text{temp} \} \oplus \text{diverge} \}$$

where iterated \oplus is shorthand for discrete uniform choice (in this case, with probability $1/3$ each); *diverge* is syntactic sugar for $\text{while}(\text{true})\{\text{skip}\}$. This program is non-AST and it terminates only by visiting the leftmost branch of the uniform choice; otherwise, it diverges by either keeping swapping the values of x and y (i.e., pacing between two points) or diverges immediately by visiting the rightmost branch. It can be shown that *every* possible strengthening that can turn this program AST necessarily leads to $\varphi' = \text{false}$ – otherwise, at least one loop iteration is executed and the program diverges with probability at least $1/3$ – and therefore only yield *trivial* lower bounds. \triangleleft

9 RELATED WORK

Weakest Preexpectation Reasoning. As a probabilistic analog to Dijkstra’s predicate-transformer calculus [Dijkstra 1975, 1976], *expectation transformers* have been extensively used to reason about *quantitative* properties of probabilistic programs. wp-style reasoning goes back to the seminal work of Kozen [1983, 1985] on probabilistic propositional dynamic logic. Amongst others, Jones [1990], Morgan et al. [1996], McIver and Morgan [2005], and Hehner [2011] furthered this line of research by considering, e.g., nondeterminism and proof rules for bounding preexpectations in the presence of loops. The classical weakest preexpectation calculus has been significantly advanced in several directions to reason about, e.g., *expected runtimes* of (recursive) probabilistic programs [Kaminski et al. 2016, 2018; Olmedo et al. 2016], probabilistic programs with *conditioning* [Olmedo et al. 2018; Szymczak and Katoen 2019], *mixed-sign* postexpectations [Kaminski and Katoen 2017], *sensitivity* of probabilistic programs [Aguirre et al. 2021], probabilistic temporal logic [Morgan and McIver 1999], and quantitative separation logic [Batz et al. 2019]. A relative completeness result has been recently established by Batz et al. [2021b] for weakest preexpectation reasoning.

Bounds on Weakest Preexpectation and Fixed Points. There are a wide spectrum of results on establishing upper and/or lower bounds on loop semantics captured by (least) fixed points. These include (semi-)automated techniques based on *metering functions* [Frohn et al. 2020, 2016] for underapproximating runtimes of non-probabilistic programs, *constraint solving* [Chen et al. 2015; Feng et al. 2017; Katoen et al. 2010] and *invariant learning* [Bao et al. 2022] for generating lower bounds on weakest preexpectations of probabilistic programs, *recurrence solving* [Bartocci et al. 2019] for synthesizing moment-based invariants of the so-called prob-solvable probabilistic loops, *bounded model checking* [Jansen et al. 2016] for verifying probabilistic programs with nondeterminism and

conditioning, and various forms of *value iteration* [Baier et al. 2017; Hartmanns and Kaminski 2020; Quatmann and Katoen 2018] for determining reachability probabilities in Markov models.

Apart from the proof rules elaborated in this paper, Baldan et al. [2021] recently proposed lattice-theoretic proof rules for verifying lower bounds on least fixed points of *finite-state* stochastic systems. Batz et al. [2021a] invented *lattice k -induction* for establishing upper bounds on least fixed points of possibly infinite-state probabilistic programs. A closely related concept to our guard-strengthening rule is the notion of ω -*subinvariant* [Audebaud and Paulin-Mohring 2009; Jones 1990; Kaminski et al. 2016, 2018], which is a monotonically increasing sequence $\{I_n\}_{n \in \mathbb{N}}$ of expectations that are subinvariants relative to each other, i.e., $I_0 = 0$ and $I_{n+1} \leq \Phi(I_n)$. It is known that $\sup_{n \in \mathbb{N}} I_n$ suffices as a lower bound on the least fixed point of Φ , however, finding such a lower bound amounts to (i) learning a closed form of I_n in n by inspecting the “pattern” through fixed point iterations, and (ii) finding the supremum of the closed form. These two steps may barely save efforts compared to just inferring the supremum (limit) of the sequence $\sup_{n \in \mathbb{N}} \Phi^n(0)$ to obtain the exact least fixed point. In some of our examples, we also reason about limits of l_M w.r.t. M – the constant used to strengthen the guard – to get tight lower bounds. This step, however, is *not necessary* since $l_M \leq \Phi(l_M)$ suffices already as a lower bound for any fixed M , that is, we only need to “push l_M through the loop semantics” *once*. Moreover, for discrete-state programs with complex closed form solutions, e.g., the 3-D random walk in Exmp. 24, our rule is capable of inferring tight lower bounds (via probabilistic model checking) *without* the need for taking limits.

Space-Restricting in Analyzing Random Walks. There is an intellectual connection between our guard-strengthening technique and the *space-restricting* tactic in analyzing random walks over infinite, discrete lattices: Restricting an infinite-space random walk à la Feller [1950, Chap. XIV] and McCrea and Whipple [1940] by setting “barriers” and then taking the limit is analogous to our approach. Nonetheless, they both proceed, after the restriction, by *solving the recurrence equation* (aka, difference equation) to obtain a closed-form solution for the restricted random walk in order to take the limit. Although a similar methodology can be embedded in our approach – as solving recurrences is one (expensive) way to obtain subinvariants – it is *not necessary*: our proof rule *reduces* the problem and places it under the lens of probabilistic model checking. The rule is thus able to handle examples that are out-of-reach by existing verification techniques, e.g., the 3-D random walk, *without* the need for recurrence solving nor taking limits. Moreover, our proof rule codifies *ad-hoc* proof methods in probability theory as a *syntactic* rule of a program logic, and enables the use of existing proof rules on verification problems that are otherwise out-of-scope.

Martingale-Based Reasoning. Probabilistic program analysis via martingales was pioneered by Chakarov and Sankaranarayanan [2013, 2014] for finding upper bounds on expected runtimes and synthesizing expectation invariants. Chatterjee et al. [2016b] further extended the martingale-based approach to address nondeterminism. Barthe et al. [2016] focus on synthesizing exact martingale expressions. Fioriti and Hermanns [2015] develop a type system for uniform integrability in order to prove AST of probabilistic programs and provide upper bounds on *expected runtimes*. In contrast, Fu and Chatterjee [2019] give lower bounds on expected runtimes; Chatterjee et al. [2022] prove lower bounds on *termination probabilities*. Kobayashi et al. [2020] provide a semi-decision procedure for upper-bounding termination probabilities of probabilistic higher-order recursive programs. Chatterjee et al. [2017]; Wang et al. [2021b] focus on finding upper and lower bounds on *assertion-violation probabilities*. Ngo et al. [2018] perform automated template-driven *resource* analysis, yet infer upper bounds only. Wang et al. [2019] provide sufficient conditions for finding upper and lower bounds on *expected costs*. Wang et al. [2021a] present conditions to derive upper and lower bounds on higher moments of *expected accumulated costs*. In contrast to our proof rule, most of these martingale-based methods for inferring lower bounds address only AST probabilistic programs.

Probabilistic Bisimulation and Equivalence. Our result on wp-difference falls in the general scope of quantifying the “distance” between two programs. This gives rise to the notions of *probabilistic bisimulation* [Hong et al. 2019; Larsen and Skou 1991] and *probabilistic equivalence* (see [Murawski and Ouaknine 2005] over *finite* data types and [Barthe et al. 2009] for *straight-line* programs). Chen et al. [2022] recently proved a decidability result for checking the equivalence of an *infinite-state* discrete, loopy probabilistic program with a loop-free specification program (assuming AST). Barthe et al. [2009, 2012] developed a *relational Hoare logic* for probabilistic programs, which has been extensively used for proving program equivalence with applications in provable security and side-channel analysis. Our proof rule is dedicated to reasoning about lower bounds on expected values of possibly divergent probabilistic programs, nevertheless, it is interesting to explore its generalization in proving equivalence, bisimulation, and ϵ -closeness of possibly *infinite-state, non-AST* probabilistic programs by, e.g., embedding our proof rule in the probabilistic relational Hoare logic.

10 CONCLUSION

We have presented a new proof rule – based on wp-difference and the guard-strengthening technique – for verifying lower bounds on weakest preexpectations of probabilistic programs. This is the first lower bound rule that admits *divergent* probabilistic loops with possibly *unbounded* expectations. In particular, we unleash existing lower induction rules for general applicability to possibly divergent programs whose strengthened counterparts feature easily provable almost-sure termination and uniform integrability. Moreover, we have shown that the error incurred by our guard-strengthening technique can be arbitrarily small thereby yielding tight lower bounds, and in case the modified loop has a finite state space, our proof rule can be automated to generate lower bounds via probabilistic model checking. The effectiveness of our proof rule has been demonstrated on several examples. In particular, we managed to infer tight lower bounds on the termination probability of the well-known 3-D random walk on a lattice, which has not been addressed yet in the context of verification.

Future directions include (i) extending our proof rule to the expected runtime calculus for lower-bounding expected runtimes [Kaminski et al. 2016, 2018], to probabilistic programs with angelic/demonic nondeterminism [McIver and Morgan 2001, 2005] and/or with soft/hard conditioning [Olmedo et al. 2018; Szymczak and Katoen 2019]; (ii) exploring the applicability of our result on wp-difference in the context of sensitivity analysis [Aguirre et al. 2021; Barthe et al. 2018; Wang et al. 2020] and model repair [Bartocci et al. 2011] for probabilistic programs; and (iii) investigating (semi-)automated synthesis of (candidate) quantitative (sub)invariants used in our proof rule.

ACKNOWLEDGMENTS

This work has been partially funded by the National Key R&D Program of China under grant No. 2022YFA1005101, by the NSFC under grant No. 62192732 and 62032024, by the CAS Project for Young Scientists in Basic Research under grant No. YSBR-040, by the ZJU Education Foundation’s Qizhen Talent program, by the ERC Advanced Project FRAPPANT under grant No. 787914, and by the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 101008233. The authors would like to thank Kevin Batz, Tim Quatmann, and anonymous reviewers for the insightful discussions on the connection respectively to ω -invariants in weakest preexpectation reasoning, partial exploration in Markov models, and the space-restricting tactic in analyzing random walks.

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Received 2022-10-28; accepted 2023-02-25