Data-Driven Invariant Learning for Probabilistic Programs

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Abstract. Morgan and McIver's *weakest pre-expectation* framework is one of the most well-established methods for deductive verification of probabilistic programs. Roughly, the idea is to generalize binary state assertions to real-valued *expectations*, which can measure expected values of probabilistic program quantities. While loop-free programs can be analyzed by mechanically transforming expectations, verifying loops usually requires finding an *invariant expectation*, a difficult task.

We propose a new view of invariant expectation synthesis as a *regression* problem: given an input state, predict the *average* value of the post-expectation in the output distribution. Guided by this perspective, we develop the first *data-driven* invariant synthesis method for probabilistic programs. Unlike prior work on probabilistic invariant inference, our approach can learn piecewise continuous invariants without relying on template expectations. We also develop a data-driven approach to learn *sub-invariants* from data, which can be used to upper- or lower-bound expected values. We implement our approaches and demonstrate their effectiveness on a variety of benchmarks from the probabilistic programming literature.

Keywords: Probabilistic programs · Data-driven invariant learning · Weakest pre-expectations

1 Introduction

Probabilistic programs—standard imperative programs augmented with a sampling command—are a common way to express randomized computations. While the mathematical semantics of such programs is fairly well-understood [25], verification methods remain an active area of research. Existing automated techniques are either limited to specific properties (e.g., [3,9,35,37]), or target simpler computational models [4,15,28].

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Reasoning About Expectations. One of the earliest methods for reasoning about probabilistic programs is through *expectations*. Originally proposed by Kozen [26], expectations generalize standard, binary assertions to quantitative, real-valued functions on program states. Morgan and McIver further developed this idea into a powerful framework for reasoning about probabilistic imperative programs, called the *weakest pre-expectation calculus* [30,33].

Concretely, Morgan and McIver defined an operator called the *weakest pre-expectation* (wpe), which takes an expectation E and a program P and produces an expectation E' such that $E'(\sigma)$ is the expected value of E in the output distribution $[\![P]\!]_\sigma$. In this way, the wpe operator can be viewed as a generalization of Dijkstra's weakest pre-conditions calculus [16] to probabilistic programs. For verification purposes, the wpe operator has two key strengths. First, it enables reasoning about probabilities and expected values. Second, when P is a loop-free program, it is possible to transform $\mathsf{wpe}(P, E)$ into a form that does not mention the program P via simple, mechanical manipulations, essentially analyzing the effect of the program on the expectation through syntactically transforming E.

However, there is a caveat: the wpe of a loop is defined as a least fixed point, and it is generally difficult to simplify this quantity into a more tractable form. Fortunately, the wpe operator satisfies a *loop rule* that simplifies reasoning about loops: if we can find an expectation I satisfying an *invariant* condition, then we can easily bound the wpe of a loop. Checking the invariant condition involves analyzing just the body of the loop, rather than the entire loop. Thus, finding invariants is a primary bottleneck towards automated reasoning about probabilistic programs.

Discovering Invariants. Two recent works have considered how to automatically infer invariant expectations for probabilistic loops. The first is Prinsys [21]. Using a template with one hole, Prinsys produces a first-order logical formula describing possible substitutions satisfying the invariant condition. While effective for their benchmark programs, the method's reliance on templates is limiting; furthermore, the user must manually solve a system of logical formulas to find the invariant.

The second work, by Chen et al. [14], focuses on inferring polynomial invariants. By restricting to this class, their method can avoid templates and can apply the Lagrange interpolation theorem to find a polynomial invariant. However, many invariants are not polynomials: for instance, an invariant may combine two polynomials piecewise by branching on a Boolean condition.

Our Approach: Invariant Learning. We take a different approach inspired by data-driven invariant learning [17,19]. In these methods, the program is executed with a variety of inputs to produce a set of execution traces. This data is viewed as a training set, and a machine learning algorithm is used to find a classifier describing the invariant. Data-driven techniques reduce the reliance on templates, and can treat the program as a black box—the precise implementation of the program need not be known, as long as the learner can execute the

program to gather input and output data. But to extend the data-driven method to the probabilistic setting, there are a few key challenges:

- **Quantitative invariants.** While the logic of expectations resembles the logic of standard assertions, an important difference is that expectations are *quantitative*: they map program states to real numbers, not a binary yes/no. While standard invariant learning is a *classification* task (i.e., predicting a binary label given a program state), our probabilistic invariant learning is closer to a *regression* task (i.e., predicting a number given a program state).
- **Stochastic data.** Standard invariant learning assumes the program behaves like a *function*: a given input state always leads to the same output state. In contrast, a probabilistic program takes an input state to a distribution over outputs. Since we are only able to observe a single draw from the output distribution each time we run the program, execution traces in our setting are inherently *noisy*. Accordingly, we cannot hope to learn an invariant that fits the observed data perfectly, even if the program has an invariant—our learner must be robust to noisy training data.
- **Complex learning objective.** To fit a probabilistic invariant to data, the logical constraints defining an invariant must be converted into a regression problem with a loss function suitable for standard machine learning algorithms and models. While typical regression problems relate the unknown quantity to be learned to known data, the conditions defining invariants are somehow self-referential: they describe how an unknown invariant must be related to itself. This feature makes casting invariant learning as machine learning a difficult task.

Outline. After covering preliminaries (Sect. 2), we present our contributions.

- A general method called Exist for learning invariants for probabilistic programs (Sect. 3). Exist executes the program multiple times on a set of input states, and then uses machine learning algorithms to learn models encoding possible invariants. A CEGIS-like loop is used to iteratively expand the dataset after encountering incorrect candidate invariants.
- Concrete instantiations of Exist tailored for handling two problems: learning *exact invariants* (Sect. 4), and learning *sub-invariants* (Sect. 5). Our method for exact invariants learns a *model tree* [34], a generalization of binary decision trees to regression. The constraints for sub-invariants are more difficult to encode as a regression problem, and our method learns a *neural model tree* [41] with a custom loss function. While the models differ, both algorithms leverage off-the-shelf learning algorithms.
- An implementation of Exist and a thorough evaluation on a large set of benchmarks (Sect. 6). Our tool can learn invariants and sub-invariants for examples considered in prior work and new, more difficult versions that are beyond the reach of prior work.

We discuss related work in Sect. 7.

2 Preliminaries

Probabilistic Programs. We will consider programs written in **pWhile**, a basic probabilistic imperative language with the following grammar:

$$P := \textbf{skip} \mid x \leftarrow e \mid x \xleftarrow{\$} d \mid P \,;\, P \mid \textbf{if } e \textbf{ then } P \textbf{ else } P \mid \textbf{while } e : P,$$

where e is a boolean or numerical expression. All commands P map memories to distributions over memories [25], and the semantics is entirely standard and can be found in the extended version. We write $[\![P]\!]_\sigma$ for the output distribution of program P from initial state σ. Since we will be interested in running programs on concrete inputs, *we will assume throughout that all loops are almost surely terminating*; this property can often be established by other methods (e.g., [12, 13, 31]).

Weakest Pre-expectation Calculus. Morgan and McIver's *weakest pre-expectation calculus* reasons about probabilistic programs by manipulating *expectations*.

Definition 1. *Denote the set of program states by Σ. Define the set of expectations, $\mathcal{E}$, to be $\{E \mid E : \Sigma \to \mathbb{R}^{\infty}_{\geq 0}\}$. Define $E_1 \leq E_2$ iff $\forall \sigma \in \Sigma : E_1(\sigma) \leq E_2(\sigma)$. The set $\mathcal{E}$ is a complete lattice.*

While expectations are technically mathematical functions from Σ to the non-negative extended reals, for formal reasoning it is convenient to work with a more restricted syntax of expectations (see, e.g., [8]). We will often view numeric expressions as expectations. Boolean expressions b can also be converted to expectations; we let $[b]$ be the expectation that maps states where b holds to 1, and other states to 0. As an example of our notation, $[flip = 0] \cdot (x+1)$, $x+1$ are two expectations, and we have $[flip = 0] \cdot (x+1) \leq x+1$.

$$\begin{aligned}
\mathsf{wpe}(\textbf{skip}, E) &:= E \\
\mathsf{wpe}(x \leftarrow e, E) &:= E[e/x] \\
\mathsf{wpe}(x \xleftarrow{\$} d, E) &:= \lambda\sigma. \sum_{v \in \mathcal{V}} [\![d]\!]_\sigma(v) \cdot E[v/x] \\
\mathsf{wpe}(P \,;\, Q, E) &:= \mathsf{wpe}(P, \mathsf{wpe}(Q, E)) \\
\mathsf{wpe}(\textbf{if } e \textbf{ then } P \textbf{ else } Q, E) &:= [e] \cdot \mathsf{wpe}(P, E) + [\neg e] \cdot \mathsf{wpe}(Q, E) \\
\mathsf{wpe}(\textbf{while } e : P, E) &:= \mathsf{lfp}(\lambda X.\ [e] \cdot \mathsf{wpe}(P, X) + [\neg e] \cdot E)
\end{aligned}$$

Fig. 1. Morgan and McIver's weakest pre-expectation operator

Now, we are ready to introduce Morgan and McIver's *weakest pre-expectation transformer* wpe. In a nutshell, this operator takes a program P and an expectation E to another expectation E', sometimes called the *pre-expectation*. Formally, wpe is defined in Fig. 1. The case for loops involves the least fixed-point (lfp) of $\Phi_E^{\mathsf{wpe}} := \lambda X.([e] \cdot \mathsf{wpe}(P, X) + [\neg e] \cdot E)$, the *characteristic function* of the loop

with respect to wpe [23]. The characteristic function is monotone on the complete lattice $\mathcal{E}$, so the least fixed-point exists by the Kleene fixed-point theorem.

The key property of the wpe transformer is that for any program P, $\mathsf{wpe}(P, E)(\sigma)$ is the expected value of E over the output distribution $[\![P]\!]_\sigma$.

Theorem 1 (See, e.g., [23]). *For any program P and expectation $E \in \mathcal{E}$,* $\mathsf{wpe}(P, E) = \lambda\sigma. \sum_{\sigma' \in \Sigma} E(\sigma') \cdot [\![P]\!]_\sigma(\sigma')$

Intuitively, the weakest pre-expectation calculus provides a syntactic way to compute the expected value of an expression E after running a program P, except when the program is a loop. For a loop, the least fixed point definition of $\mathsf{wpe}(\textbf{while } e : P, E)$ is hard to compute.

3 Algorithm Overview

In this section, we introduce the two related problems we aim to solve, and a meta-algorithm to tackle both of them. We will see how to instantiate the meta-algorithm's subroutines in Sect. 4 and Sect. 5.

Problem Statement. Analogous to when analyzing the weakest pre-conditions of a loop, knowing a loop *invariant* or *sub-invariant* expectation enables one to easily bound the loop's weakest pre-expectations, but a (sub)invariant expectation can be difficult to find. Thus, we aim to develop an algorithm to automatically synthesize invariants and sub-invariants of probabilistic loops. More specifically, our algorithm tackles the following two problems:

1. **Finding exact invariants:** Given a loop **while** $G : P$ and an expectation postE as input, we want to find an expectation I such that

$$I = \Phi^{\mathsf{wpe}}_{\mathsf{postE}}(I) \coloneqq [G] \cdot \mathsf{wpe}(P, I) + [\neg G] \cdot \mathsf{postE}. \tag{1}$$

   Such an expectation I is an *exact invariant* of the loop with respect to postE. Since $\mathsf{wpe}(\textbf{while } G : P, \mathsf{postE})$ is a fixed point of $\Phi^{\mathsf{wpe}}_{\mathsf{postE}}$, $\mathsf{wpe}(\textbf{while } G : P, \mathsf{postE})$ has to be an exact invariant of the loop. Furthermore, when **while** $G : P$ is almost surely terminating and postE is upper-bounded, the existence of an exact invariant I implies $I = \mathsf{wpe}(\textbf{while } e : P, E)$. (We defer the proof to the extended version.)
2. **Finding sub-invariants:** Given a loop **while** $G : P$ and expectations $\mathsf{preE}, \mathsf{postE}$, we aim to learn an expectation I such that

$$I \leq \Phi^{\mathsf{wpe}}_{\mathsf{postE}}(I) \coloneqq [G] \cdot \mathsf{wpe}(P, I) + [\neg G] \cdot \mathsf{postE} \tag{2}$$

$$\mathsf{preE} \leq I. \tag{3}$$

   The first inequality says that I is a sub-invariant: on states that satisfy G, the value of I lower bounds the expected value of itself after running one loop iteration from initial state, and on states that violate G, the value of I lower bounds the value of postE. Any sub-invariant lower-bounds the weakest pre-expectation of the loop, i.e., $I \leq \mathsf{wpe}(\textbf{while } G : P, E)$ [22]. Together with the second inequality $\mathsf{preE} \leq I$, the existence of a sub-invariant I ensures that preE lower-bounds the weakest pre-expectation.

Note that an exact invariant is a sub-invariant, so one indirect way to solve the second problem is to solve the first problem, and then check $\mathsf{preE} \leq I$. However, we aim to find a more direct approach to solve the second problem because often exact invariants can be complicated and hard to find, while sub-invariants can be simpler and easier to find.

```
EXIST(geo, pexp, N_runs, N_states):
    feat ← getFeatures(geo, pexp)
    states ← sampleStates(feat, N_states)
    data ← sampleTraces(geo, pexp, feat, N_runs, states)
    while not timed out:
        models ← learnInv(feat, data)
        candidates ← extractInv(models)
        for inv in candidates:
            verified, cex ← verifyInv(inv, geo)
            if verified:
                return inv
            else:
                states ← states ∪ cex
                states ← states ∪ sampleStates(feat, N'_states)
        data ← data ∪ sampleTraces(geo, pexp, feat, nruns, states)
```

Fig. 2. Algorithm EXIST

Methods. We solve both problems with one algorithm, EXIST (short for EXpectation Invariant SynThesis). Our data-driven method resembles Counterexample Guided Inductive Synthesis (CEGIS), but differs in two ways. First, candidates are synthesized by fitting a machine learning model to data consisted of program traces starting from random input states. Our target programs are also probabilistic, introducing a second source of randomness to program traces. Second, our approach seeks high-quality counterexamples—violating the target constraints as much as possible—in order to improve synthesis. For synthesizing invariants and sub-invariants, such counterexamples can be generated by using a computer algebra system to solve an optimization problem.

We present the pseudocode in Fig. 2. EXIST takes a probabilistic program geo, a post-expectation or a pair of pre/post-expectation *pexp*, and hyper-parameters N_{runs} and N_{states}. EXIST starts by generating a list of features *feat*, which are numerical expressions formed by program variables used in geo. Next, EXIST samples N_{states} initialization *states* and runs geo from each of those states for N_{runs} trials, and records the value of *feat* on program traces as *data*. Then, EXIST enters a CEGIS loop. In each iteration of the loop, first the learner learnInv trains models to minimize their violation of the required inequalities (e.g., Eqs. (2)

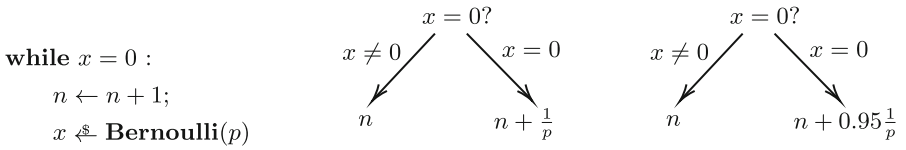
and (3) for learning sub-invariants) on *data*. Next, extractInv translates learned models into a set *candidates* of expectations. For each candidate *inv*, the verifier verifyInv looks for program states that *maximize* *inv*'s violation of required inequalities. If it cannot find any program state where *inv* violates the inequalities, the verifier returns *inv* as a valid invariant or sub-invariant. Otherwise, it produces a set *cex* of counter-example program states, which are added to the set of initial states. Finally, before entering the next iteration, the algorithm augments *states* with a new batch of N'_{states} initial states, generates trace data from running geo on each of these states for N_{runs} trials, and augments the dataset *data*. This data augmentation ensures that the synthesis algorithm collects more and more initial states, some randomly generated (sampleStates) and some from prior counterexamples (*cex*), guiding the learner towards better candidates. Like other CEGIS-based tools, our method is sound but not complete, i.e., if the algorithm returns an expectation then it is guaranteed to be an exact invariant or sub-invariant, but the algorithm might never return an answer; in practice, we set a timeout.

4 Learning Exact Invariants

In this section, we detail how we instantiate Exist's subroutines to learn an exact invariant I satisfying $I = \Phi^{\mathsf{wpe}}_{\mathsf{postE}}(I)$, given a loop geo and an expectation $pexp = \mathsf{postE}$.

At a high level, we first sample a set of program states *states* using sampleStates. From each program state $s \in states$, sampleTraces executes geo and estimates $\mathsf{wpe}(\mathsf{geo}, \mathsf{postE})(s)$. Next, learnInv trains regression models M to predict the estimated $\mathsf{wpe}(\mathsf{geo}, \mathsf{postE})(s)$ given the value of features evaluated on s. Then, extractInv translates the learned models M to an expectation I. In an ideal scenario, this I would be equal to $\mathsf{wpe}(\mathsf{geo}, \mathsf{postE})$, which is also always an exact invariant. But since I is learned from stochastic data, it may be noisy. So, we use verifyInv to check whether I satisfies the invariant condition $I = \Phi^{\mathsf{wpe}}_{\mathsf{postE}}(I)$.

The reader may wonder why we took this complicated approach, first estimating the weakest pre-expectation of the loop, and then computing the invariant: If we are able to learn an expression for $\mathsf{wpe}(\mathsf{geo}, \mathsf{postE})$ directly, then why are we interested in the invariant I? The answer is that with an invariant I, we can also *verify* that our computed value of $\mathsf{wpe}(prog, \mathsf{postE})$ is correct by checking the invariant condition and applying the loop rule. Since our learning process is inherently noisy, this verification step is crucial and motivates why we want to find an invariant.



(a) Program: geo (b) Model tree for $\mathsf{wpe}(\mathsf{geo}, n)$ (c) Another model tree

Fig. 3. Running example: program and model tree

A Running Example. We will illustrate our approach using Fig. 3. The simple program geo repeatedly loops: whenever x becomes non-zero we exit the loop; otherwise we increase n by 1 and draw x from a biased coin-flip distribution (x gets 1 with probability p, and 0 otherwise). We aim to learn $\mathsf{wpe}(\mathsf{geo}, n)$, which is $[x \neq 0] \cdot n + [x = 0] \cdot (n + \frac{1}{p})$.

Our Regression Model. Before getting into how Exist collects data and trains models, we introduce the class of regression models it uses – *model trees*, a generalization of decision trees to regression tasks [34]. Model trees are naturally suited to expressing piecewise functions of inputs, and are straightforward to train. While our method can in theory generalize to other regression models, our implementation focuses on model trees.

More formally, a model tree $T \in \mathcal{T}$ over features $\mathcal{F}$ is a full binary tree where each internal node is labeled with a predicate ϕ over variables from $\mathcal{F}$, and each leaf is labeled with a real-valued model $M \in \mathcal{M} : \mathbb{R}^{\mathcal{F}} \to \mathbb{R}$. Given a feature vector in $x \in \mathbb{R}^{\mathcal{F}}$, a model tree T over $\mathcal{F}$ produces a numerical output $T(x) \in \mathbb{R}$ as follows:

- If T is of the form $\mathsf{Leaf}(M)$, then $T(x) \coloneqq M(x)$.
- If T is of the form $\mathsf{Node}(\phi, T_L, T_R)$, then $T(x) \coloneqq T_R(x)$ if the predicate ϕ evaluates to true on x, and $T(x) \coloneqq T_L(x)$ otherwise.

Throughout this paper, we consider model trees of the following form as our regression model. First, node predicates ϕ are of the form $f \bowtie c$, where $f \in \mathcal{F}$ is a feature, $\bowtie \in \{<, \leq, =, >, \geq\}$ is a comparison, and c is a numeric constant. Second, leaf models on a model tree are either all *linear models* or all products of constant powers of features, which we call *multiplication models*. For example, assuming $n, \frac{1}{p}$ are both features, Fig. 3b and c are two model trees with linear leaf models, and Fig. 3b expresses the weakest pre-expectation $\mathsf{wpe}(\mathsf{geo}, n)$. Formally, the leaf model M on a feature vector f is either

$$M_l(f) = \sum_{i=1}^{|\mathcal{F}|} \alpha_i \cdot f_i \qquad \text{or} \qquad M_m(f) = \prod_{i=1}^{|\mathcal{F}|} f_i^{\alpha_i}$$

with constants $\{\alpha_i\}_i$. Note that multiplication models can also be viewed as linear models on logarithmic values of features because $\log M_m(f) = \sum_{i=1}^{|\mathcal{F}|} \alpha_i \cdot$

$\log(f_i)$. While it is also straightforward to adapt our method to other leaf models, we focus on linear models and multiplication models because of their simplicity and expressiveness. Linear models and multiplication models also complement each other in their expressiveness: encoding expressions like $x + y$ uses simpler features with linear models (it suffices if $\mathcal{F} \ni x, y$, as opposed to needing $\mathcal{F} \ni x+y$ if using multiplicative models), while encoding $\frac{p}{1-p}$ uses simpler features with multiplicative models (it suffices if $\mathcal{F} \ni p, 1-p$, as opposed to needing $\mathcal{F} \ni \frac{p}{1-p}$ if using linear models).

4.1 Generate Features (getFeatures)

Given a program, the algorithm first generates a set of features $\mathcal{F}$ that model trees can use to express unknown invariants of the given loop. For example, for geo, $I = [x \neq 0] \cdot n + [x = 0] \cdot (n + \frac{1}{p})$ is an invariant, and to have a model tree (with linear/multiplication leaf models) express I, we want $\mathcal{F}$ to include both n and $\frac{1}{p}$, or $n + \frac{1}{p}$ as one feature. $\mathcal{F}$ should include the program variables at a minimum, but it is often useful to have more complex features too. While generating more features increases the expressivity of the models, and richness of the invariants, there is a cost: the more features in $\mathcal{F}$, the more data is needed to train a model.

Starting from the program variables, getFeatures generates two lists of features, $\mathcal{F}_l$ for linear leaf models and $\mathcal{F}_m$ for multiplication leaf models. Intuitively, linear models are more expressive if the feature set $\mathcal{F}$ includes some products of terms, e.g., $n \cdot p^{-1}$, and multiplication models are more expressive if $\mathcal{F}$ includes some sums of terms, e.g., $n + 1$.

4.2 Sample Initial States (sampleStates)

Recall that Exist aims to learn an expectation I that is equal to the weakest pre-expectation wpe(**while** $G : P$, postE). A natural idea for sampleTraces is to run the program from all possible initializations multiple times, and record the average value of postE from each initialization. This would give a map close to wpe(**while** $G : P$, postE) if we run enough trials so that the empirical mean is approximately the actual mean. However, this strategy is clearly impractical—many of the programs we consider have infinitely many possible initial states (e.g., programs with integer variables). Thus, sampleStates needs to choose a manageable number of initial states for sampleTraces to use.

In principle, a good choice of initializations should exercise as many parts of the program as possible. For instance, for geo in Fig. 3, if we only try initial states satisfying $x \neq 0$, then it is impossible to learn the term $[x = 0] \cdot (n + \frac{1}{p})$ in wpe(geo, n) from data. However, covering the control flow graph may not be enough. Ideally, to learn how the expected value of postE depends on the initial state, we also want data from multiple initial states along each path.

While it is unclear how to choose initializations to ensure optimal coverage, our implementation uses a simpler strategy: sampleStates generates N_{states} states

in total, each by sampling the value of every program variable uniformly at random from a space. We assume program variables are typed as booleans, integers, probabilities, or floating point numbers and sample variables of some type from the corresponding space. For boolean variables, the sampling space is simply $\{0, 1\}$; for probability variables, the space includes reals in some interval bounded away from 0 and 1, because probabilities too close to 0 or 1 tend to increase the variance of programs (e.g., making some loops iterate for a very long time); for floating point number and integer variables, the spaces are respectively reals and integers in some bounded range. This strategy, while simple, is already very effective in nearly all of our benchmarks (see Sect. 6), though other strategies are certainly possible (e.g., performing a grid search of initial states from some space).

4.3 Sample Training Data (sampleTraces)

We gather training data by running the given program geo on the set of initializations generated by sampleStates. From each program state $s \in \mathit{states}$, the subroutine sampleTraces runs geo for N_{runs} times to get output states $\{s_1, \ldots, s_{N_{runs}}\}$ and produces the following training example:

$$(s_i, v_i) = \left(s_i, \frac{1}{N_{runs}} \sum_{i=1}^{N_{runs}} \mathsf{postE}(s_i) \right).$$

Above, the value v_i is the empirical mean of postE in the output state of running geo from initial state s_i; as N_{runs} grows large, this average value approaches the true expected value $\mathsf{wpe}(\mathsf{geo}, \mathsf{postE})(s)$.

4.4 Learning a Model Tree (learnInv)

Now that we have the training set $\mathit{data} = \{(s_1, v_1), \ldots, (s_K, v_K)\}$ (where $K = N_{states}$), we want to fit a model tree T to the data. We aim to apply off-the-shelf tools that can learn model trees with customizable leaf models and loss. For each data entry, v_i approximates $\mathsf{wpe}(\mathsf{geo}, \mathsf{postE})(s_i)$, so a natural idea is to train a model tree T that takes the value of features on s_i as input and predicts v_i. To achieve that, we want to define the loss to measure the error between predicted values $T(\mathcal{F}_l(s_i))$ (or $T(\mathcal{F}_m(s_i))$) and the target value v_i. Without loss of generality, we can assume our invariant I is of the form

$$I = \mathsf{postE} + [G] \cdot I' \tag{4}$$

because I being an invariant means

$$I = [\neg G] \cdot \mathsf{postE} + [G] \cdot \mathsf{wpe}(P, I) = \mathsf{postE} + [G] \cdot (\mathsf{wpe}(P, I) - \mathsf{postE}).$$

In many cases, the expectation $I' = \mathsf{wpe}(P, I) - \mathsf{postE}$ is simpler than I: for example, the weakest pre-expectation of geo can be expressed as $n + [x = 0] \cdot (\frac{1}{p})$;

while I is represented by a tree that splits on the predicate $[x = 0]$ and needs both $n, \frac{1}{p}$ as features, the expectation $I' = \frac{1}{p}$ is represented by a single leaf model tree that only needs p as a feature.

Aiming to learn weakest pre-expectations I in the form of Eq. (4), Exist trains model trees T to fit I'. More precisely, learnInv trains a model tree T_l with linear leaf models over features $\mathcal{F}_l$ by minimizing the loss

$$err_l(T_l, data) = \left(\sum_{i=1}^{K} \left(\mathsf{postE}(s_i) + G(s_i) \cdot T_l(\mathcal{F}_l(s_i)) - v_i \right)^2 \right)^{1/2}, \tag{5}$$

where $\mathsf{postE}(s_i)$ and $G(s_i)$ represents the value of expectation postE and G evaluated on the state s_i. This loss measures the sum error between the prediction $\mathsf{postE}(s_i) + G(s_i) \cdot T_l(\mathcal{F}_l(s_i))$ and target v_i. Note that when the guard G is false on an initial state s_i, the example contributes zero to the loss because $\mathsf{postE}(s_i) + G(s_i) \cdot T_l(\mathcal{F}_l(s_i)) = \mathsf{postE}(s_i) = v_i$; thus, we only need to generate and collect trace data for initial states where the guard G is true.

Analogously, learnInv trains a model tree T_m with multiplication leaf models over features $\mathcal{F}_m$ to minimize the loss $err_m(T_m, data)$, which is the same as $err_l(T_l, data)$ except $T_l(\mathcal{F}_l(s_i))$ is replaced by $T_m(\mathcal{F}_m(s_i))$ for each i.

4.5 Extracting Expectations from Models (extractInv)

Given the learned model trees T_l and T_m, we extract expectations that approximate $\mathsf{wpe}(\mathsf{geo}, \mathsf{postE})$ in three steps:

1. **Round T_l, T_m with different precisions.** Since we obtain the model trees T_l and T_m by learning and the training data is stochastic, the coefficients of features in T_l and T_m may be slightly off. We apply several rounding schemes to generate a list of rounded model trees.
2. **Translate into expectations.** Since we learn model trees, this step is straightforward: for example, $n + \frac{1}{p}$ can be seen as a model tree (with only a leaf) mapping the values of features $n, \frac{1}{p}$ to a number, or an expectation mapping program states where n, p are program variables to a number. We translate each model tree obtained from the previous step to an expectation.
3. **Form the candidate invariant.** Since we train the model trees to fit I' so that $\mathsf{postE} + [G] \cdot I'$ approximates $\mathsf{wpe}(\textbf{while } G : P, \mathsf{postE})$, we construct each candidate invariant $inv \in invs$ by replacing I' in the pattern $\mathsf{postE} + [G] \cdot I'$ by an expectation obtained in the second step.

4.6 Verify Extracted Expectations (verifyInv)

Recall that geo is a loop **while** $G : P$, and given a set of candidate invariants $invs$, we want to check if any $inv \in invs$ is a loop invariant, i.e., if inv satisfies

$$inv = [\neg G] \cdot \mathsf{postE} + [G] \cdot \mathsf{wpe}(P, inv). \tag{6}$$

Since the learned model might not predict the expected value for every data point exactly, we must verify whether *inv* satisfies this equality using verifyInv. If not, verifyInv looks for counterexamples that maximize the violation in order to drive the learning process forward in the next iteration. Formally, for every $inv \in invs$, verifyInv queries computer algebra systems to find a set of program states S such that S includes states maximizing the absolute difference of two sides in Eq. (6):

$$S \ni \mathbf{argmax}_s |inv(s) - ([\neg G] \cdot \mathsf{postE} + [G] \cdot wp(P, inv))\,(s)|.$$

If there are no program state where the absolute difference is non-zero, verifyInv returns *inv* as a true invariant. Otherwise, the maximizing states in S are added to the list of counterexamples *cex*; if no candidate in *invs* is verified, verifyInv returns False and the accumulated list of counterexamples *cex*. The next iteration of the CEGIS loop will sample program traces starting from these counterexample initial states, hopefully leading to a learned model with less error.

5 Learning Sub-invariants

Next, we instantiate Exist for our second problem: learning sub-invariants. Given a program $\mathsf{geo} = \mathbf{while}\ G : P$ and a pair of pre- and post- expectations $(\mathsf{preE}, \mathsf{postE})$, we want to find a expectation I such that $\mathsf{preE} \leq I$, and

$$I \leq \Phi^{\mathsf{wpe}}_{\mathsf{postE}}(I) := [\neg G] \cdot \mathsf{postE} + [G] \cdot \mathsf{wpe}(P, I)$$

Intuitively, $\Phi^{\mathsf{wpe}}_{\mathsf{postE}}(I)$ computes the expected value of the expectation I after one iteration of the loop. We want to train a model M such that M translates to an expectation I whose expected value decrease each iteration, and $\mathsf{preE} \leq I$.

The high-level plan is the same as for learning exact invariants: we train a model to minimize a loss defined to capture the sub-invariant requirements. We generate features $\mathcal{F}$ and sample initializations *states* as before. Then, from each $s \in states$, we repeatedly run just the loop body P and record the set of output states in *data*; this departs from our method for exact invariants, which repeatedly runs the entire loop to completion. Given this trace data, for any program state $s \in states$ and expectation I, we can compute the empirical mean of I's value after running the loop body P on state s. Thus, we can approximate $\mathsf{wpe}(P, I)(s)$ for $s \in states$ and use this estimate to approximate $\Phi^{\mathsf{wpe}}_{\mathsf{postE}}(I)(s)$. We then define a loss to sum up the violation of $I \leq \Phi^{\mathsf{wpe}}_{\mathsf{postE}}(I)$ and $\mathsf{preE} \leq I$ on state $s \in states$, estimated based on the collected data.

The main challenge for our approach is that existing model tree learning algorithms do not support our loss function. Roughly speaking, model tree learners typically assume a node's two child subtrees can be learned separately; this is the case when optimizing on the loss we used for exact invariants, but this is *not* the case for the loss for sub-invariants.

To solve this challenge, we first broaden the class of models to neural networks. To produce sub-invariants that can be verified, we still want to learn simple classes of models, such as piecewise functions of numerical expressions. Accordingly, we work with a class of neural architectures that can be translated into model trees, *neural model trees*, adapted from neural decision trees developed by Yang et al. [41]. We defer the technical details of neural model trees to the extended version, but for now, we can treat them as differentiable approximations of standard model trees; since they are differentiable they can be learned with gradient descent, which can support the sub-invariant loss function.

Outline. We will discuss changes in sampleTraces, learnInv and verifyInv for learning sub-invariants but omit descriptions of getFeatures, sampleStates, extractInv because Exist generates features, samples initial states and extracts expectations in the same way as in Sect. 4. To simplify the exposition, we will assume getFeatures generates the same set of features $\mathcal{F} = \mathcal{F}_l = \mathcal{F}_m$ for model trees with linear models and model trees with multiplication models.

5.1 Sample Training Data (sampleTraces)

Unlike when sampling data for learning exact invariants, here, sampleTraces runs only one iteration of the given program $\mathsf{geo} = \textbf{while}\ G : P$, that is, just P, instead of running the whole loop. Intuitively, this difference in data collection is because we aim to directly handle the sub-invariant condition, which encodes a single iteration of the loop. For exact invariants, our approach proceeded indirectly by learning the expected value of postE after running the loop to termination.

From any initialization $s_i \in \mathit{states}$ such that G holds on s_i, sampleTraces runs the loop body P for N_{runs} trials, each time restarting from s_i, and records the set of output states reached. If executing P from s_i leads to output states $\{s_{i1}, \ldots, s_{iN_{runs}}\}$, then sampleTraces produces the training example:

$$(s_i, S_i) = (s_i, \{s_{i1}, \ldots, s_{iN_{runs}}\}),$$

For initialization $s_i \in \mathit{states}$ such that G is false on s_i, sampleTraces simply produces $(s_i, S_i) = (s_i, \emptyset)$ since the loop body is not executed.

5.2 Learning a Neural Model Tree (learnInv)

Given the dataset $\mathit{data} = \{(s_1, S_1), \ldots, (s_K, S_K)\}$ (with $K = N_{states}$), we want to learn an expectation I such that $\mathsf{preE} \leq I$ and $I \leq \Phi^{\mathsf{wpe}}_{\mathsf{postE}}(I)$. By case analysis on the guard G, the requirement $I \leq \Phi^{\mathsf{wpe}}_{\mathsf{postE}}(I)$ can be split into two constraints:

$$[G] \cdot I \leq [G] \cdot \mathsf{wpe}(P, I) \qquad \text{and} \qquad [\neg G] \cdot I \leq [\neg G] \cdot \mathsf{postE}.$$

If $I = \mathsf{postE} + [G] \cdot I'$, then the second requirement reduces to $[\neg G] \cdot \mathit{postE} \leq [\neg G] \cdot \mathit{postE}$ and is always satisfied. So to simplify the loss and training process, we again aim to learn an expectation I of the form of $\mathsf{postE} + [G] \cdot I'$. Thus, we want to train a model tree T such that T translates into an expectation I', and

$$\mathsf{preE} \leq \mathsf{postE} + [G] \cdot I' \tag{7}$$

$$[G] \cdot (\mathsf{postE} + [G] \cdot I') \leq [G] \cdot \mathsf{wpe}(P, \mathsf{postE} + [G] \cdot I') \tag{8}$$

Then, we define the loss of model tree T on *data* to be

$$err(T, data) \coloneqq err_1(T, data) + err_2(T, data),$$

where $err_1(T, data)$ captures Eq. (7) and $err_2(T, data)$ captures Eq. (8).

Defining err_1 is relatively simple: we sum up the one-sided difference between $\mathsf{preE}(s)$ and $\mathsf{postE}(s) + G(s) \cdot T(\mathcal{F}(s))$ across $s \in states$, where T is the model tree getting trained and $\mathcal{F}(s)$ is the feature vector $\mathcal{F}$ evaluated on s. That is,

$$err_1(T, data) := \sum_{i=1}^{K} \max\left(0, \mathsf{preE}(s_i) - \mathsf{postE}(s_i) - G(s_i) \cdot T(\mathcal{F}(s_i))\right). \tag{9}$$

Above, $\mathsf{preE}(s_i)$, $\mathsf{postE}(s_i)$, and $G(s_i)$ are the value of expectations preE, postE, and G evaluated on program state s_i.

The term err_2 is more involved. Similar to err_1, we aim to sum up the one-sided difference between two sides of Eq. (8) across state $s \in states$. On program state s that does not satisfy G, both sides are 0; for s that satisfies G, we want to evaluate $\mathsf{wpe}(P, \mathsf{postE} + [G] \cdot I')$ on s, but we do not have exact access to $\mathsf{wpe}(P, \mathsf{postE} + [G] \cdot I')$ and need to approximate its value on s based on sampled program traces. Recall that $\mathsf{wpe}(P, I)(s)$ is the expected value of I after running program P from s, and our dataset contains training examples (s_i, S_i) where S_i is a set of states reached after running P on an initial state s_i satisfying G. Thus, we can approximate $[G] \cdot \mathsf{wpe}(P, \mathsf{postE} + G \cdot I')(s_i)$ by

$$G(s_i) \cdot \frac{1}{|S_i|} \cdot \sum_{s \in S_i} \left(\mathsf{postE}(s) + G(s) \cdot I'(s)\right).$$

To avoid division by zero when s_i does not satisfy G and S_i is empty, we evaluate the expression in a short-circuit manner such that when $G(s_i) = 0$, the whole expression is immediately evaluated to zero.

Therefore, we define

$$err_2(T, data) = \sum_{i=1}^{K} \max\Bigg(0, G(s_i) \cdot \mathsf{postE}(s_i) + G(s_i) \cdot T(\mathcal{F}(s_i)) - G(s_i) \cdot \frac{1}{|S_i|} \cdot \sum_{s \in S_i} \left(\mathsf{postE}(s) + G(s) \cdot T(\mathcal{F}(s))\right)\Bigg).$$

Standard model tree learning algorithms do not support this kind of loss function, and since our overall loss $err(T, data)$ is the sum of $err_1(T, data)$ and $err_2(T, data)$, we cannot use standard model tree learning algorithm to optimize $err(T, data)$ either. Fortunately, gradient descent does support this loss function. While gradient descent cannot directly learn model trees, we can use gradient descent to train a *neural* model tree T to minimize $err(T, data)$. The learned neural networks can be converted to model trees, and then converted to expectations as before. (See discussion in the extended version.)

5.3 Verify Extracted Expectations (verifyInv)

The verifier verifyInv is very similar to the one in Sect. 4 except here it solves a different optimization problem. For each candidate inv in the given list $invs$, it looks for a set S of program states such that S includes

$$\mathbf{argmax}_s \mathsf{preE}(s) - inv(s) \qquad \text{and} \qquad \mathbf{argmax}_s G(s) \cdot I(s) - [G] \cdot \mathsf{wpe}(P, I)(s).$$

As in our approach for exact invariant learning, the verifier aims to find counterexample states s that violate at least one of these constraints by as large of a margin as possible; these high-quality counterexamples guide data collection in the following iteration of the CEGIS loop. Concretely, the verifier accepts inv if it cannot find any program state s where $\mathsf{preE}(s) - inv(s)$ or $G(s) \cdot I(s) - [G] \cdot \mathsf{wpe}(P, I)(s)$ is positive. Otherwise, it adds all states $s \in S$ with strictly positive margin to the set of counterexamples cex.

6 Evaluations

We implemented our prototype in Python, using sklearn and tensorflow to fit model trees and neural model trees, and Wolfram Alpha to verify and perform counterexample generation. We have evaluated our tool on a set of 18 benchmarks drawn from different sources in prior work [14,21,24]. Our experiments were designed to address the following research questions:

R1. Can Exist synthesize exact invariants for a variety of programs?
R2. Can Exist synthesize sub-invariants for a variety of programs?

We summarize our findings as follows:

- Exist successfully synthesized and verified exact invariants for 14/18 benchmarks within a timeout of 300 s. Our tool was able to generate these 14 invariants in reasonable time, taking between 1 to 237 s. The sampling phase dominates the time in most cases. We also compare Exist with a tool from prior literature, Mora [7]. We found that Mora can only handle a restrictive set of programs and cannot handle many of our benchmarks. We also discuss how our work compares with a few others in (Sect. 7).
- To evaluate sub-invariant learning, we created multiple problem instances for each benchmark by supplying different pre-expectations. On a total of 34 such problem instances, Exist was able to infer correct invariants in 27 cases, taking between 7 to 102 s.

We present in the extended version the tables of complete experimental results. Because the training data we collect are inherently stochastic, the results produced by our tool are not deterministic.[1] As expected, sometimes different trials on the same benchmarks generate different sub-invariants; while the exact invariant for each benchmark is unique, Exist may also generate semantically equivalent but syntactically different expectations in different trials (e.g. it happens for BiasDir).

[1] The code and data sampled in the trial that produced the tables in this paper can be found at https://github.com/JialuJialu/Exist.

Table 1. Exact Invariants generated by Exist

Name	postE	Learned Invariant	ST	LT	VT	TT
Bin1	n	$x + [n < M] \cdot (M \cdot p - n \cdot p)$	25.67	12.03	0.22	37.91
Fair	$count$	$(count + [c1 + c2 == 0] \cdot (p1 + p2)/(p1 + p2 - p1 \cdot p2))$	5.78	1.62	0.30	7.69
Gambler	z	$z + [x > 0 \text{ and } y > x] \cdot x \cdot (y - x)$	112.02	3.52	9.97	125.51
Geo0	z	$z + [flip == 0] \cdot (1 - p_1)/p_1$	12.01	0.85	2.65	15.51
Sum0	x	$x + [n > 0] \cdot (0.5 \cdot p \cdot n^2 + 0.5 \cdot p \cdot n)$	102.12	34.61	26.74	163.48

Table 2. Sub-invariants generated by Exist

Name	postE	preE	Learned Sub-invariant	ST	LT	VT	TT
Gambler	z	$x \cdot (y - x)$	$z + [x > 0 \text{ and } y > x] \cdot x \cdot (y - x)$	7.31	28.87	8.29	44.46
Geo0	z	$[flip == 0] \cdot (1 - p_1))$	$z + [flip == 0] \cdot (1 - p_1)$	8.70	26.13	0.19	35.02
LinExp	z	$z + [n > 0] \cdot 2$	$[n > 0] \cdot (n + 1)$	53.72	30.01	0.35	84.98
		$z + [n > 0] \cdot 2 \cdot n$	$z + [n > 0] \cdot 2 \cdot n$	29.18	28.61	0.68	58.48
RevBin	z	$z + [x > 0] \cdot x$	$z + [x > 0] \cdot x/p$	18.17	71.15	2.17	91.55
		z	z	15.62	18.74	0.06	34.42

Implementation Details. For input parameters to Exist, we use $N_{runs} = 500$ and $N_{states} = 500$. Besides input parameters listed in Fig. 2, we allow the user to supply a list of features as an optional input. In feature generation, getFeatures enumerates expressions made up by program variables and user-supplied features according to a grammar. Also, when incorporating counterexamples *cex*, we make 30 copies of each counterexample to give them more weights in the training. All experiments were conducted on a MacBook Pro 2020 with M1 chip running macOS Monterey Version 12.1.

6.1 R1: Evaluation of the Exact Invariant Method

Efficacy of Invariant Inference. Exist was able to infer provably correct invariants in 14/18 benchmarks. Out of 14 successful benchmarks, only 2 of them need user-supplied features ($n \cdot p$ for Bin2 and Sum0). Table 1 shows the post-expectation (postE), the inferred invariant (Learned Invariant), sampling time (ST), learning time (LT), verification time (VT) and the total time (TT) for a few benchmarks. For generating exact invariants, the running time of Exist is dominated by the sampling time. However, this phase can be parallelized easily.

Failure Analysis. Exist failed to generate invariants for 4/18 benchmarks. For two of them, Exist was able to generate expectations that are very close to

an invariant (DepRV and LinExp); for the third failing benchmarks (Duel), the ground truth invariant is very complicated. For LinExp, while a correct invariant is $z + [n > 0] \cdot 2.625 \cdot n$, Exist generates expectations like $z + [n > 0] \cdot (2.63 \cdot n - 0.02)$ as candidates. For DepRV, a correct invariant is $x \cdot y + [n > 0] \cdot (0.25 \cdot n^2 + 0.5 \cdot n \cdot x + 0.5 \cdot n \cdot y - 0.25 \cdot n)$, and in our experiment Exist generates $0.25 \cdot n^2 + 0.5 \cdot n \cdot x + 0.5 \cdot n \cdot y - 0.27 \cdot n - 0.01 \cdot x + 0.12$. In both cases, the ground truth invariants use coefficients with several digits, and since learning from data is inherently stochastic, Exist cannot generate them consistently. In our experiments, we observe that our CEGIS loop does guide the learner to move closer to the correct invariant in general, but sometimes progress obtained in multiple iterations can be offset by noise in one iteration. For GeoAr, we observe the verifier incorrectly accepted the complicated candidate invariants generated by the learner because Wolfram Alpha was not able to find valid counterexamples for our queries.

Comparison with Previous Work. There are few existing tools that can automatically compute expected values after probabilistic loops. We experimented with one such tool, called Mora [7]. (See high-level comparison in Sect. 7.) We managed to encode our benchmarks Geo0, Bin0, Bin2, Geo1, GeoAr, and Mart in their syntax. Among them, Mora fails to infer an invariant for Geo1, GeoAr, and Mart. We also tried to encode our benchmarks Fair, Gambler, Bin1, and RevBin but found Mora's syntax was too restrictive to encode them.

6.2 R2: Evaluation of the Sub-invariant Method

Efficacy of Invariant Inference. Exist is able to synthesize sub-invariants for 27/34 benchmarks. As before, Table 2 reports the results for a few benchmarks. Two out of 27 successful benchmarks use user-supplied features – Gambler with pre-expectation $x \cdot (y - x)$ uses $(y - x)$, and Sum0 with pre-expectation $x + [x > 0] \cdot (p \cdot n/2)$ uses $p \cdot n$. Contrary to the case for exact invariants, the learning time dominates. This is not surprising: the sampling time is shorter because we only run one iteration of the loop, but the learning time is longer as we are optimizing a more complicated loss function.

One interesting thing that we found when gathering benchmarks is that for many loops, pre-expectations used by prior work or natural choices of pre-expectations are themselves sub-invariants. Thus, for some instances, the sub-invariants generated by Exist is the same as the pre-expectation preE given to it as input. However, Exist is not checking whether the given preE is a sub-invariant: the learner in Exist does not know about preE besides the value of preE evaluated on program states. Also, we also designed benchmarks where pre-expectations are *not* sub-invariants (BiasDir with $\mathsf{preE} = [x \neq y] \cdot x$, DepRV with $\mathsf{preE} = x \cdot y + [n > 0] \cdot 1/4 \cdot n^2$, Gambler with $\mathsf{preE} = x \cdot (y - x)$, Geo0 with $\mathsf{preE} = [flip == 0] \cdot (1 - p1)$), and Exist is able to generate sub-invariants for 3/4 such benchmarks.

Failure Analysis. On program instances where EXIST fails to generate a sub-invariant, we observe two common causes. First, gradient descent seems to get stuck in local minima because the learner returns suboptimal models with relatively low loss. The loss we are training on is very complicated and likely to be highly non-convex, so this is not surprising. Second, we observed inconsistent behavior due to noise in data collection and learning. For instance, for GeoAr with $\mathsf{preE} = x + [z \neq 0] \cdot y \cdot (1-p)/p$, EXIST could sometimes find a sub-invariant with supplied feature $(1-p)$, but we could not achieve this result consistently.

Comparison with Learning Exact Invariants. The performance of EXIST on learning sub-invariants is less sensitive to the complexity of the ground truth invariants. For example, EXIST is not able to generate an exact invariant for LinExp as its exact invariant is complicated, but EXIST is able to generate sub-invariants for LinExp. However, we also observe that when learning sub-invariants, EXIST returns complicated expectations with high loss more often.

7 Related Work

Invariant Generation for Probabilistic Programs. There has been a steady line of work on probabilistic invariant generation over the last few years. The PRINSYS system [21] employs a template-based approach to guide the search for probabilistic invariants. PRINSYS is able encode invariants with guard expressions, but the system doesn't produce invariants directly—instead, PRINSYS produces logical formulas encoding the invariant conditions, which must be solved manually.

Chen et al. [14] proposed a counterexample-guided approach to find polynomial invariants, by applying Lagrange interpolation. Unlike PRINSYS, this approach doesn't need templates; however, invariants involving guard expressions—common in our examples—cannot be found, since they are not polynomials. Additionally, Chen et al. [14] uses a weaker notion of invariant, which only needs to be correct on certain initial states; our tool generates invariants that are correct on all initial states. Feng et al. [18] improves on Chen et al. [14] by using *Stengle's Positivstellensatz* to encode invariants constraints as a semidefinite programming problem. Their method can find polynomial sub-invariants that are correct on all initial states. However, their approach cannot synthesize piecewise linear invariants, and their implementation has additional limitations and could not be run on our benchmarks.

There is also a line of work on abstract interpretation for analyzing probabilistic programs; Chakarov and Sankaranarayanan [11] search for linear expectation invariants using a "pre-expectation closed cone domain", while recent work by Wang et al. [40] employs a sophisticated algebraic program analysis approach.

Another line of work applies *martingales* to derive insights of probabilistic programs. Chakarov and Sankaranarayanan [10] showed several applications of martingales in program analysis, and Barthe et al. [5] gave a procedure to generate candidate martingales for a probabilistic program; however, this tool gives no control over which expected value is analyzed—the user can only guess initial

expressions and the tool generates valid bounds, which may not be interesting. Our tool allows the user to pick which expected value they want to bound.

Another line of work for automated reasoning uses *moment-based analysis*. Bartocci et al. [6,7] develop the Mora tool, which can find the moments of variables as functions of the iteration for loops that run forever by using ideas from computational algebraic geometry and dynamical systems. This method is highly efficient and is guaranteed to compute moments exactly. However, there are two limitations. First, the moments can give useful insights about the distribution of variables' values after each iteration, but they are fundamentally different from our notion of invariants which allow us to compute the expected value of any given expression *after termination* of a loop. Second, there are important restrictions on the probabilistic programs. For instance, conditional statements are not allowed and the use of symbolic inputs is limited. As a result, most of our benchmarks cannot be handled by Mora.

In a similar vein, Kura et al. [27,39] bound higher *central moments* for running time and other monotonically increasing quantities. Like our work, these works consider probabilistic loops that terminate. However, unlike our work, they are limited to programs with constant size increments.

Data-Driven Invariant Synthesis. We are not aware of other data-driven methods for learning probabilistic invariants, but a recent work Abate et al. [1] proves probabilistic termination by learning ranking supermartingales from trace data. Our method for learning sub-invariants (Sect. 5) can be seen as a natural generalization of their approach. However, there are also important differences. First, we are able to learn general sub-invariants, not just ranking supermatingales for proving termination. Second, our approach aims to learn model trees, which lead to simpler and more interpretable sub-invariants. In contrast, Abate, et al. [1] learn ranking functions encoded as two-layer neural networks.

Data-driven inference of invariants for deterministic programs has drawn a lot of attention, starting from Daikon [17]. ICE learning with decision trees [20] modifies the decision tree learning algorithm to capture *implication counterexamples* to handle inductiveness. Hanoi [32] uses counterexample-based inductive synthesis (CEGIS) [38] to build a data-driven invariant inference engine that alternates between weakening and strengthening candidates for synthesis. Recent work uses neural networks to learn invariants [36]. These systems perform classification, while our work uses regression. Data from fuzzing has been used for *almost correct* inductive invariants [29] for programs with closed-box operations.

Probabilistic Reasoning with Pre-expectations. Following Morgan and McIver, there are now pre-expectation calculi for domain-specific properties, like expected runtime [23] and probabilistic sensitivity [2]. All of these systems define the pre-expectation for loops as a least fixed-point, and practical reasoning about loops requires finding an invariant of some kind.

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