Abstract

As machine learning is increasingly used in essential systems, it is important to reduce or eliminate the incidence of serious bugs. A growing body of research has developed machine learning algorithms with formal guarantees about performance, robustness, or fairness. Yet, the analysis of these algorithms is often complex, and implementing such systems in practice introduces room for error. Proof assistants can be used to formally verify machine learning systems by constructing machine checked proofs of correctness that rule out such bugs. However, reasoning about probabilistic claims inside of a proof assistant remains challenging. We show how a probabilistic program can be automatically represented in a theorem prover using the concept of reparameterization, and how some of the tedious proofs of measurability can be generated automatically from the probabilistic program. To demonstrate that this approach is broad enough to handle rather different types of machine learning systems, we verify both a classic result from statistical learning theory (PAC-learnability of decision stumps) and prove that the null model used in a Bayesian hypothesis test satisfies a fairness criterion called demographic parity.

1 Introduction

A machine learning application can fail for many reasons: maybe the training data is insufficient, maybe there is a flaw in the design of the learning algorithm, or maybe there is an error in the implementation of the algorithm. Such errors can go unnoticed for long periods of time. This is particularly worrisome for machine learning applications that, for example, process loan requests or suggest hiring recommendations.

Thorough testing is one way to help catch such errors. But testing ML applications is challenging because of their random behavior. Many iterations may be needed to encounter a bug or detect a statistical irregularity in behavior. And when it comes to adversarial or safety critical scenarios, no amount of testing may be enough to make a system trustworthy. Moreover, while there has been much work on developing algorithms that are provably robust or fair, bugs in implementations of these algorithms may render these guarantees meaningless.

One way to eliminate these kinds of errors is to formally verify a machine learning system with a machine checked proof of correctness. A formal proof is one in which every step and logical inference is checked. The computer programs that help write and check such proofs are called proof assistants. Proof assistants provide a language to express programs and mathematical proofs in some logic. In recent years, it has become feasible to use proof assistants to verify large, realistic software systems, including compilers [24], cryptographic primitives [12], file systems [7], and microkernels [23].
In principle, proof assistants are expressive enough to represent the mathematics underlying ML systems and check proofs of their correctness. But in practice, formally verifying ML systems remains challenging. Prior work has begun to develop formal proofs of correctness for machine learning software. Although these early results are impressive, representing machine learning programs and their correctness statements inside a proof assistant remains a major challenge. Proof assistants only have built-in support for representing “pure” mathematical functions. The approach taken in the aforementioned works is to define, within the proof assistant, a small domain-specific programming language that has commands for drawing random samples from distributions. While this approach is feasible, it becomes challenging to use, particularly when reasoning about samples from continuous probability distributions. In particular, the way past work represents such programs in the proof assistant is rather different from the way ML researchers usually think about things in pencil-and-paper proofs.

We propose using an alternative representation that more closely matches the familiar style of paper proofs. Our approach is to automatically reparameterize parts of a probabilistic program so that it can be written as a pure, non-randomized, functional program operating over a pre-sampled list of random inputs. This simplifies reasoning about the resulting program and avoids the foregoing difficulties. We have implemented an automatic translation to perform this reparameterization, so that we can convert programs from a probabilistic programming language based on Pyro into input to the theorem prover.

A simple example of our translation is shown in Figure 1. On the left is a Python program that samples from two distributions and returns a pair as result. On the right is our reparameterized version of this program in the Lean proof assistant. Background on Lean follows, but for now, the important point is that in the translation, majority_fun takes as input an argument u that represents a pair of uniform [0, 1] samples. Then instead of sampling, it uses the inverse CDF transform to convert the input u into the distributions it needs. Finally, we define the distribution represented by this program by taking the pushforward of the input distribution through the function majority_fun.

To demonstrate our approach, we have verified two case studies. The first is a proof that the class of decision stumps is PAC-learnable, a classic introductory result that appears in many textbooks on computational learning theory. Formalizing this proof revealed errors and many omitted details found in several expository accounts of this result. Our second case-study is a proof that a null model used in a Bayesian hypothesis test, implemented in a probabilistic programming language, correctly satisfies a fairness criterion called demographic parity. The source code for our case studies and translator are publicly available.

[1] https://github.com/jtristan/FormalML
2 A Short Introduction to Lean

The Lean theorem prover can be viewed as both a functional programming language (like Haskell) and a foundation for mathematics, based on dependent type theory. Dependent type theories are an alternative to Zermelo-Frankel set theory where types are associated with mathematical expressions, in the same way that types can be used in programming languages, but with much stronger guarantees. Before we introduce the concept of dependent types, it is useful to consider a simple example of mathematical formalization in Lean.

Using Lean as a programming language, we can define a function `double` that takes a natural number as input and multiplies it by 2.

```lean
def double(n: nat): nat := 2 * n
```

This definition is similar to what one would find in any modern functional programming language. However, there is one significant difference between programming in Lean and those languages: in order to ensure that Lean is a consistent foundation for mathematics, functions cannot have side effects (printing on the screen, reading a file) and they must be proven to always terminate. Next, we can define a predicate that formalizes the concept of an even number.

```lean
def isEven(n: nat): Prop := exists k: nat, n = 2 * k
```

This example clearly shows how Lean differs from a programming language. The function we define does not return simple data like a number or string, but instead a logical proposition that states that a natural number `n` is even if there exists a natural number `k` such that `n = 2 * k`.

**Proofs with tactics:** Finally, Lean lets us specify mathematical properties and prove them. For example, the following states and proves a lemma called `doubleIsEven` that says that the result of `double` is always even:

```lean
lemma doubleIsEven: forall n: nat, isEven (double (n)) :=
begin
  intros, unfold isEven, unfold double, existsi n, trivial,
end
```

The first line is the mathematical statement we wish to prove. What follows the ":=" and enclosed by the keywords “begin” and “end” is a set of commands, called tactics, that describes the proof in a manner that Lean can check. The programmer constructs this tactic proof interactively: their IDE displays a list of current assumptions and what remains to be proved. This is represented by a sequent, which is a tuple of the form `Γ ⊢ φ`, where `Γ` is the list of hypotheses and variables (called the context) and `φ` is a proposition (called the target). When the proof starts, the sequent is `∅ ⊢ ∀n : N, isEven(double(n))`. Executing the tactic “intros” transforms the sequent into `n : N ⊢ isEven(double(n))` where `n` is now a fixed but arbitrary natural number. Executing the tactic “unfold” applied to `isEven` unfolds the definition of `isEven` to give the sequent `n : N ⊢ ∃k : N, double(n) = 2 * k`. Likewise, by unfolding `double`, we obtain the sequent `n : N ⊢ ∃k : N, 2 * n = 2 * k`. Now we must exhibit a choice for `k` that satisfies the property, for which we can use the tactic “existsi” applied to `n`, which appears in the context. This gives the sequent `n : N ⊢ 2 * n = 2 * n` to which we can apply the “trivial” tactic that ensures that a basic axiom (namely, that equality is reflexive) has been reached.

**mathlib library:** The mathlib library is a large library of mathematical results formalized in Lean [31]. In particular, it contains a formalization of measure theory, based on Hölzl and Heller [16]’s library from the Isabelle theorem prover. Unfortunately, mathlib does not have a probability theory library, and in order to formalize our results, we had to develop one, as a special case of measure theory. This development accounts for about 2,500 lines of Lean formalization.

**Proof by reduction:** An important feature of Lean that makes proofs easier is that the proof checker can automatically execute or reduce parts of programs. For example, suppose at some point we need to show that the boolean expression `(a and false)` or `(false and b)` is always `false`. Instead of using lemmas for the basic rules of boolean algebra, we can instruct Lean to case split on all the possible values for `a` and `b`, evaluate the expression, and then check that all cases reduce to `false`. Of course, not all definitions can be executed or simplified this way. For example, if we have a proof involving the Lesbesgue integral from mathlib, we cannot expect Lean to symbolically compute the solution to an arbitrary definite integral. Definitions like the integral are marked noncomputable in Lean, which means they will not be executed.
3 Denotational Semantics of Programs

With the probability theory library defined, we next need a way to write down learning algorithms and probabilistic programs in Lean, so that we can state and prove theorems about them, much as we did with double above. However, by default, all functions in Lean have to be purely functional (that is, they have to behave like mathematical functions, with deterministic output and no side-effects).

For that reason, past work on verifying machine learning algorithms has used a denotational semantics in which programs are represented as distributions over the types of values they can return. Given a type $X$, we write $\text{Meas}(X)$ for this type of probability distributions on $X$. The first step is to define the primitive distributions that our programs will need to sample from. Next we need a way to sequence together multiple steps of sampling and running computations on sampled values. To do so, we can define a function called bind of type $\text{Meas}(X) \to (X \to \text{Meas}(Y)) \to \text{Meas}(Y)$. That is, bind takes a probability measure on $X$ and a function that transforms values from $X$ into probability measures over $Y$, and returns a probability measure on $Y$. Intuitively, we should read $\text{bind}(\mu, f)$ as representing a program which first samples from the distribution $\mu$ and then passes the result to $f$. It is common to use the notation $\text{do } x \leftarrow \mu; g(x)$ for $\text{bind}(\mu, g)$, which helps reinforce the intuition that bind samples from $\mu$ and then runs $g$. We also define a function ret of type $X \to \text{Meas}(X)$. It takes a value from $X$ and returns a probability measure on $X$.

Functions bind and ret construct probability measures, so their definitions say what probability they assign to an event. If $A$ is an event we define them as:

$$\text{bind}(\mu, f)(A) = \int_{x \in X} f(x)(A)d\mu$$  \hspace{1cm} (1)

$$\text{ret}(x)(A) = \chi_A(x)$$  \hspace{1cm} (2)

While the definitions use standard mathematical notation, our formalization uses the Lean definition of the Lebesgue integral, and so on. Here, $\text{ret}(x)$ is the $\delta$-Dirac distribution at $x$. To understand the definition of bind, consider the following example. Let $\mu$ be a distribution over $X$ and consider the random variables $U \sim \mu$ and $V \sim f(U)$. For example, $f$ could be the function that for an input $l$ returns the distribution $\mathcal{N}(l, 0.1)$. What is the distribution of $V$? By the sum rule of probability we have $\Pr(V = v) = \int_{u \in X} \Pr(V = v \mid U = u)d\mu$. Therefore, $\Pr(V)(A) = \int_{u \in X} f(u)(A)d\mu$. Hence, $\text{bind}(\mu, f)$ is simply computing the distribution that results from applying $f$ while marginalizing over $\mu$.

Example. Consider the Python function from the introduction in Figure 1a. The translation of this program into Lean as we have so far described is:

```lean
def majority1 :=
  do theta ← uniform(0, 1);
  do X ← bernoulli(theta);
  ret (theta, X)
```

The notation makes this look almost the same as the Python program that we started with. However, in the Lean code, the “function” actually evaluates to a nested integral representing the distribution that this procedure encodes. Similarly, in Lean, uniform and bernoulli are not random number generators, but definitions of those distributions in terms of their CDF. These bind and ret operations are an example of a monad. Monads are commonly used in functional languages like Haskell to represent programs that have side-effects. This probability monad was defined by Giry [13].

The Giry monad representation has some advantages. As we have seen, the denotation of a program has a structure that mimicks the original source code. However, there are drawbacks when we try to reason about programs expressed this way, particularly when we want to avoid using axioms or making restrictions to discrete spaces. First, recall from section 2 that proof by reduction is blocked when we work with noncomputable definitions like integrals. Because the Giry monad includes an integral every time we use bind, Lean cannot reduce such programs very much at all. Second, in our experience, this monadic semantics is unfamiliar to ML experts, and doesn’t correspond closely to the style used on paper proofs. In the next section, we describe our approach for alleviating these issues.
4 Reparameterizing to Simplify Semantics

How can we find a denotational semantics that would make it easier to reason formally about a learning or randomized algorithm and avoid the issues with the Giry monad described above? Recall that a classic result in probability theory is that any distribution on the reals with the Borel sigma algebra can be constructed as the pushforward of the uniform distribution on [0, 1], which we write as \( \mathcal{U} \). That is, for any distribution \( \mu \), there exists a (measurable) function \( f \) such that for any event \( E \)

\[
\mu(E) = \mathcal{L}(f^{-1}(E))
\]

(3)

Indeed, a more general version of this result is an important lemma in proving the Kolmogorov Extension Theorem, which is used to show the existence of many stochastic processes.

This fact hints at an alternate denotation for our programs: we could represent a program as some pure function \( f \), applied to samples from \( \mathcal{U} \). That is, we would take the pushforward measure of \( f \) applied to an appropriate input distribution. Because \( f \) will be pure, Lean will be able to evaluate it, enabling us to use proof by reduction. Moreover, once we prove that \( f \) is a measurable function, we can avoid most measure-theoretic issues in the proof. Of course, the theorem above suggests that \( f \) will exist in principle, but we still need a way to construct the function \( f \) in a useful form.

In order to help explain how we find a simple representation of \( f \), we first observe that such a function \( f \) is a reparameterization of the original program. A reparameterization is a transformation of a probabilistic model that changes how a variable is sampled, often by sampling an alternate distribution and transforming the result. For example, if \( X \) is a random variable with distribution \( \mathcal{N}(3, 4) \), we can reparameterize \( X \) to define it as \( X = 2Z + 3 \) where \( Z \) is a draw from the standard normal distribution. Reparameterization has many other applications in ML. For example, it can improve the convergence of MCMC algorithms [14], and enable the use of stochastic gradient descent in Variational Auto Encoders [22].

We now describe the steps to compute the reparameterization of functions in our setting. We have implemented this translation for a small probabilistic programming language implemented on top of Pyro. However, to keep things self-contained, we will explain how the translation works using simple Python programs, without dynamic looping or recursion. Our majority function from Figure 1a will serve as a running example.

Transforming primitive distributions: First we extend the probability theory library in Lean to include reparameterized definitions of all the primitive distributions that our programs can sample from. For example, \( \text{gen_uniform}(a, b, u) \) generates a uniform random variate on the interval \( [a, b] \) by scaling the input \( u \), which is assumed to be a uniform sample from \( [0, 1] \). More generally, we can implement the inverse CDF transform to convert a sample from the uniform distribution on \( [0, 1] \) into the appropriate distribution.

These primitive translations are added to a dictionary that tracks their input and output types, which in particular records how many uniform inputs they need. As we translate a function, we replace sampling from primitive distributions with these translations, and record how many total uniform samples will be needed. Then, an argument \( u \) is added that is a vector of all of the uniform samples that will be needed. We write \( u_1, u_2, u_3 \) etc. for the components of this vector. These are defined using Lean’s primitive operations \( \text{fst} \) and \( \text{snd} \) for extracting the first and second element of a pair.

Slicing and Coupling: Next, for each return value of the function, we compute a slice, which is the subset of expressions in the function that determine that return value. For example, in the majority example from Figure 1a there are two return values, \( \theta \) and \( X \). The slice for \( \theta \) is \( \text{gen_uniform}(0, 1, u_1) \); and the slice for \( X \) is \( \text{gen_bernoulli}(\text{gen_uniform}(0, 1, u_1), u_2) \). Note that the re-use of \( u_1 \) in both the computation of \( \theta \) and \( X \) ensures that we properly capture the dependence between these two random variables. In general, all dependencies between the variable definitions are explicitly captured by which inputs are passed to which parameters, so that the right joint distribution is obtained. Essentially, the inputs are being used to construct an appropriate coupling [25] between the random variables encoded by the slices. We generate Lean definitions for each slice, and then call these to compute each return value in the function. Now, we can perform standard compiler optimization transforms, such as removing common sub-expressions, to simplify the function.

Nested functions: After we complete the translation of majority, we can add an entry to the dictionary of translations tracking its type. When translating a subsequent function \( g \), if a call to
def demographic_parity():
    [theta, X] = majority()
    phi = uniform(0.8 * theta, 1)
    Y = bernoulli(phi)
    return (theta, X, phi, Y)

def demographic_parity_fun u :=
    let theta := u.fst.fst in
    let X := u.fst.snd in
    let u3 := u.snd.fst in
    let u4 := u.snd.snd in
    let phi := gen_uniform(0.8 * theta, 1, u3) in
    let Y := gen_bernoulli(phi, u4) in
    ((theta, X), (phi, Y))

def demographic_parity :=
    pushforward demographic_parity_fun
    (prod_measure majority pair_uniform(0, 1))

(a) Python program
(b) Reparameterization in Lean

Figure 2: Lean translation with nested functions for a Bayesian hypothesis testing example.

majority is encountered in g, we can replace it with a call to the translation and add additional uniform samples to the vector of inputs to g. Since the pre-translated version of majority takes no arguments as input, it is also possible to hoist the call to majority out of the body of g, and instead pass in the pre-sampled results of majority as an argument to g. Figure 2a shows an example, where majority is called by demographic_parity. The transformed function takes as input both a sample from majority and a pair of uniform samples, which it uses to generate phi and Y.

Automatic proof generation: In the course of generating the function f, we can also generate proofs in Lean that the function f, and all the slices used to compute the return values, are measurable. To do so, we first manually wrote proofs of measurability for all primitive operations in the language, as well as the transformer functions for the primitive distributions, such as gen_uniform. Then, using the fact that the composition of two measurable functions is measurable, these proofs for primitive operations are composed to produce a proof that an entire function, such as majority_fun is measurable. This proof can then be re-used if majority is called in another function.

Impact of reparameterization on proofs: Our motivation for defining a semantics based on reparameterization is to simplify formal proofs for learning and randomized algorithms. By embedding programs as pure functions of random inputs, we make it possible to use Equation (3) to turn a probabilistic statement on random variables into a statement on events, getting the heavy machinery of measure-theoretic probability theory out of the way. At that point, reasoning about the program boils down to reasoning about the set of inputs to the program that satisfy some properties, which is usually very basic, intuitive, and allows us to apply reduction to the function to simplify the reasoning. We will see an example of this in Section 5.

Generality: A natural question is whether this kind of reparameterization translation can be applied to more complex, general purpose programs. As we have mentioned, results from measure theory suggest that in principle this can be performed on a large class of programs. But, for large programs with complicated control flow and looping, a naive reparameterization translation may make the program harder to understand. However, even when reparameterization would be unnatural to apply to the entire program, we believe that it can be useful to apply to subcomponents. For example, consider a typical implementation of stochastic gradient descent, which is usually structured as a loop. Within each iteration of the loop, training examples are randomly selected or ordered, and then gradients and updates are computed. We can factor out and reparameterize the computation of gradients to be pure functions. Then, use of the Giry monad would be limited to only the remaining impure parts that glue together iterations of the loop. This way, we would obtain the advantages of reparameterization for the bulk of the proof.

5 Case Study 1: Decision Stumps

For our first case study, we prove in Lean that the concept class of decision stumps is PAC learnable. We focus here on how this algorithm is formulated in Lean. More complete details about the classic pencil-and-paper proof and our formalization are found in an earlier report [30]. Recall that a decision stump is a classifier that assigns binary labels to real valued points based on whether they are above or below some threshold value. Points above the threshold are labeled 0, and points \leq are
labeled 1. We assume that there is some unknown distribution \( \mu \) of examples that the classifier will have to label, and that the true labels of these examples are determined by some threshold \( t \), which is also unknown. Training such a classifier is straightforward: we take the maximum of all the training examples with label 1, and use that as our threshold.

To show that this decision class is PAC learnable, we must prove that for all \( \epsilon, \delta \in (0, 1) \), there is some number \( n \) such that with \( n \) labeled training examples drawn independently from \( \mu \), this training algorithm gives a stump that achieves error rate below \( \epsilon \) with probability at least \( 1 - \delta \). This is the one-dimensional version of the problem of learning an axis-aligned rectangle, which is used as a motivating example and exercise in many introductory texts on learning theory \([21, 29, 26]\).

We first express the learning algorithm as a pure Lean function `choose`, which takes the training data as a vector of examples, where each example is a pair consisting of the data point and its label. The algorithm filters out the non-positive examples, removes the remaining labels, and takes the maximum. The parameter \( n \) below tracks the number of examples in the vector `data`:

```lean
def filter n data := vec_map (λ p, if p.snd then p.fst else 0) n data
def choose n data := max n (filter n data)
```

The process of training on \( n \) can then be described as taking the \( n \)-ary product measure on the input distribution \( \mu \), and then first pushing-forward a function to assign the true labels, and then pushing-forward the result with `choose`.

```lean
def denot :=
  let η := vec.prob_measure n μ in
  let ν := pushforward (label_sample target n) η in
  pushforward (choose n) ν
```

Finally, to make claims about the error rate of this algorithm, we define an event `error_set` which captures whether the label assigned by a classifier \( h \) differs from the true label provided by the unknown `target`. Finally, the error rate of a classifier is the probability of this set under the unknown distribution \( \mu \) of test examples:

```lean
def error_set h := {x | label h x = label target x}
def error h := μ (error_set h target)
```

All of the randomization lies in the process of modeling the training examples as if they have been sampled from some arbitrary training distribution. Because the training algorithm here is entirely deterministic, we are able to write down this algorithm directly without using the automated reparameterization we have described. Nevertheless, the experience of working with this formulation of the algorithm convinced us of the benefits of working with a pure function as much as possible, which led us to automating reparameterization to handle examples such as the one we describe next.

### 6 Case Study 2: Bayesian Hypothesis Tests

In our next example, we prove a property of a null model used for a Bayesian hypothesis test. Recall that in Bayesian hypothesis testing, we have models for how a data set may have been generated, along with prior probabilities for those models. We use Bayes rule to update our probabilities of the models and then select from among them \([20]\). In this case study, we consider the use of Bayesian hypothesis testing to judge whether the output of a selection procedure satisfies a fairness property called the four-fifths rule, which is used as a criterion for disparate impact testing by the U.S. Equal Employment Opportunity Commission \([11]\). In particular, the four-fifths rule says that if the selection rate for a protected class is less than \( 4/5 \) the rate for the majority group, then this can be construed as evidence of violating legal standards for adverse impact.

In order to formulate a Bayesian hypothesis test for this criterion, the first step is to write down a null model that is supposed to satisfy the \( 4/5 \) test: that is, the selection rate is meant to be at least \( 4/5 \) the majority rate. The demographic parity example from Figure 2a is this null model. The selection rate of the majority class is \( \theta \), and the selection rate of the minority class is \( \phi \). The model is constructed so that \( \phi \) is at least \( 4/5 \cdot \theta \). Then, \( X \) and \( Y \) give the results of the selection procedure on one member of the majority class and the minority class, respectively. A more general version of this model might draw different numbers of samples from the two classes. By expressing this model in a probabilistic programming language such as Pyro, and specifying a prior, we could then compare the posterior probability, given some example data, to an alternative model.
Because the null model is supposed to represent a selection procedure that satisfies the 4/5 test, it is important to prove that it in fact does. We use Lean to prove this. We want to show that \(0.8 \cdot \Pr[X = 1] \leq \Pr[Y = 1]\). This follows from conditioning on \(\theta\), so that it suffices to show that for all \(t \in [0, 1]\), we have \(0.8 \cdot \Pr[X = 1|\theta = t] \leq \Pr[Y = 1|\theta = t]\).

For the Lean version of the demographic parity model, this is formalized with the following events:

\[
\begin{align*}
B(t: [0,1]) &:= \{v | v.fst.fst = t\} \\
\text{majority_selected} &:= \{v | v.fst.snd = 1\} \\
\text{minority_selected} &:= \{v | v.snd.snd = 1\}
\end{align*}
\]

We can divide the proof into two steps. Consider a Bernoulli random variable \(Y\) with selection rate \(4/5 \cdot \theta\), generated using the same \(u_4\) that is used to generate \(Y\). First, we can show that \(0.8 \cdot \Pr[X = 1|\theta = t] \leq \Pr[Y = 1|\theta = t]\). This is simpler because having conditioned on \(t\), the selection rate of \(Y\) is deterministic.

Second, we show that \(\Pr[Y = 1|\theta = t] \leq \Pr[Y = 1|\theta = t]\). The key is that this part of the proof can be entirely reduced to proving a pure fact about \(\text{demographic_parity_fun}\). In particular, because probabilities are monotone with respect to subset ordering, we just have to show that the set of random inputs of the function \(\text{demographic_parity_fun}\) which cause \(Y = 1\) is a subset of the inputs that cause \(Y = 1\). This is captured by the following Lean statement, where we write \(\mathcal{f}\) as an abbreviation for \(\text{demographic_parity_fun}\):

\[
\forall t \geq 0, \text{set.prod} \{a: [0,1] \times \mathbb{N} | a.fst = t\} \\
\subseteq \{a: (0,1] \times \mathbb{N} \times [0,1] \times [0,1] | (f a).snd.snd = 1 \land (f a).fst.fst = t\}
\]

7 Related Work

Measure-theory in proof assistants: There have been formalizations of measure-theoretic probability theory in a few proof assistants. Hurd \cite{hurd2011} formalized basic measure theory in the HOL proof assistant, including a proof of Caratheodory’s extension theorem. Hurd uses a semantics that is closest to some of the ideas underlying our reparameterization approach, in that he models randomized programs as having access to an infinite “tape” of pre-sampled random bits. Hötzl and Heller \cite{hertz19} developed a more substantial library in the Isabelle theorem prover. Avigad et al. \cite{avigad2008} use this library to formalize a proof of the Central Limit Theorem.

Machine-checked proofs for ML: We have already mentioned some more recent work that has formalized machine learning results. Selsam et al. \cite{selsam2017} use Lean to prove the correctness of an optimization procedure for stochastic computation graphs. They prove that the random gradients used in their stochastic backpropagation implementation are unbiased. In their proof, they add axioms to the system for various mathematical facts. They argue that even if there are errors in these axioms that could potentially lead to inconsistency, the process of constructing formal proofs for the rest of the algorithm still helps eliminate mistakes. Bagnall and Stewart \cite{bagnall2018} give machine-checked proofs of bounds on generalization errors. They use Hoeffding’s inequality to obtain bounds when the hypothesis space is finite or there is a separate test-set and apply this result to bound the generalization error of neural networks with quantized weights. Their proof is restricted to discrete distributions and adds some results as axioms (Pinsker’s inequality and Gibbs’ inequality). Bentkamp et al. \cite{bentkamp2019} formalize a result by Cohen et al. \cite{cohen2017} which shows that deep convolutional arithmetic circuits are more expressive than shallow ones. This result deals with what is deterministically representable by these structures, so their proof does not require probability theory.

Semantics of probabilistic programs: The representation of programs in Lean in the Giry monad is an example of denotational semantics \cite{felleisen2013}. Where the meaning of a program is given in terms of a mathematical object (here, the distribution on the type of values it can return). We have already alluded to some of the problems of using the Giry monad and our reparameterization transform on programs with complicated control flow or looping structure. Defining denotational semantics for probabilistic programs with arbitrary general recursion and higher-order functions is challenging, and the subject of much recent research \cite{felleisen2013}.

\footnote{We use conditional probability notation to explain the argument. More precisely, we are using a disintegrating measure \cite{vannella2016}. Because we are conditioning on the first projection of the product measure that we are pushing-forward, the existence of this disintegration is a result of Fubini’s theorem.}
ML for automated theorem proving: A related but distinct line of work applies machine learning techniques to automatically construct formal proofs of theorems. By using a pre-existing corpus of formal proofs, supervised learning algorithms can be trained to select hypotheses and construct proofs in a formal system [3, 17, 19, 27].

8 Conclusion

We present an approach to simplify reasoning about probabilistic programs in proof assistants. By reparameterizing these programs to be pure functions of pre-sampled randomized input, we can exploit more of the native automation and support for reasoning about pure functions found in many proof assistants. Our case studies show that our approach can be applied to verify programs from a diverse range of subfields of ML.

References

[1] J. Avigad, J. Hölzl, and L. Serafin. A formally verified proof of the Central Limit Theorem. CoRR, abs/1405.7012, 2014. URL http://arxiv.org/abs/1405.7012.

[2] A. Bagnall and G. Stewart. Certifying the true error: Machine learning in Coq with verified generalization guarantees. In AAAI’19: The Thirty-Third AAAI Conference on Artificial Intelligence, 2019.

[3] K. Bansal, S. Loos, M. Rabe, C. Szegedy, and S. J. Wilcox. HOList: An environment for machine learning of higher order logic theorem proving. In Thirty-sixth International Conference on Machine Learning (ICML), 2019.

[4] A. Bentkamp, J. C. Blanchette, and D. Kikaw. A formal proof of the expressiveness of deep learning. Journal of Automated Reasoning, 63(2):347–368, 2019.

[5] E. Bingham, J. P. Chen, M. Jankowiak, F. Obermeyer, N. Pradhan, T. Karaletsos, R. Singh, P. Szerlip, P. Horsfall, and N. D. Goodman. Pyro: Deep universal probabilistic programming. Journal of Machine Learning Research, 20(28):1–6, 2019. URL http://jmlr.org/papers/v20/18-403.html.

[6] A. Blumer, A. Ehrenfeucht, D. Haussler, and M. K. Warmuth. Learnability and the Vapnik-Chervonenkis dimension. Journal of the ACM (JACM), 36(4):929–965, 1989.

[7] T. Chajed, H. Chen, A. Chlipala, M. F. Kaashoek, N. Zeldovich, and D. Ziegler. Certifying a file system using crash hoare logic: correctness in the presence of crashes. Commun. ACM, 60(4):75–84, 2017. doi: 10.1145/3051092. URL https://doi.org/10.1145/3051092.

[8] J. T. Chang and D. Pollard. Conditioning as disintegration. Statistica Neerlandica, 51(3):287–317, 1997.

[9] N. Cohen, O. Sharir, and A. Shashua. On the expressive power of deep learning: A tensor analysis. In Proceedings of the 29th Conference on Learning Theory, COLT 2016, New York, USA, June 23-26, 2016, pages 698–728, 2016. URL http://proceedings.mlr.press/v49/cohen16.html.

[10] T. Ehrhard, M. Pagani, and C. Tasson. Measurable cones and stable, measurable functions: A model for probabilistic higher-order programming. Proc. ACM Program. Lang., 2(POPL), Dec. 2017. doi: 10.1145/3158147. URL https://doi.org/10.1145/3158147.

[11] Equal Employment Opportunity Commission. Uniform Guidelines On Employee Selection Procedures.

[12] A. Erbsen, J. Philipoom, J. Gross, R. Sloan, and A. Chlipala. Simple high-level code for cryptographic arithmetic - with proofs, without compromises. In 2019 IEEE Symposium on Security and Privacy, SP 2019, San Francisco, CA, USA, May 19-23, 2019, pages 1202–1219, 2019. doi: 10.1109/SP.2019.00005. URL https://doi.org/10.1109/SP.2019.00005.

[13] M. Giry. A categorical approach to probability theory. In B. Banaschewski, editor, Categorical Aspects of Topology and Analysis, volume 915 of Lecture Notes in Mathematics, pages 68–85, 1982.

[14] M. I. Gorinova, D. Moore, and M. D. Hoffman. Automatic reparameterisation of probabilistic programs. CoRR, abs/1906.03028, 2019. URL http://arxiv.org/abs/1906.03028.
[15] C. Heunen, O. Kammar, S. Staton, and H. Yang. A convenient category for higher-order probability theory. In Proceedings of the 32nd Annual ACM/IEEE Symposium on Logic in Computer Science, LICS ’17. IEEE Press, 2017. ISBN 9781509030187.

[16] J. Hölzl and A. Heller. Three chapters of measure theory in Isabelle/HOL. In ITP, pages 135–151, 2011.

[17] D. Huang, P. Dhariwal, D. Song, and I. Sutskever. Gamepad: A learning environment for theorem proving. In 7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019, 2019.

[18] J. Hurd. Formal Verification of Probabilistic Algorithms. PhD thesis, Cambridge University, May 2003.

[19] C. Kaliszyk, F. Chollet, and C. Szegedy. HolStep: A machine learning dataset for higher-order logic theorem proving. In 5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings, 2017. URL https://openreview.net/forum?id=ryuxYmvel

[20] R. E. Kass and A. E. Raftery. Bayes factors. Journal of the American Statistical Association, 90(430):773–795, 1995.

[21] M. J. Kearns and U. V. Vazirani. An introduction to computational learning theory. MIT press, 1994.

[22] D. P. Kingma and M. Welling. Auto-encoding variational bayes. In 2nd International Conference on Learning Representations, ICLR 2014, Banff, AB, Canada, April 14-16, 2014, Conference Track Proceedings, 2014. URL http://arxiv.org/abs/1312.6114

[23] G. Klein, J. Andronick, K. Elphinstone, G. Heiser, D. Cock, P. Derrin, D. Elkaduwe, K. Engelhardt, R. Kolanski, M. Norrish, T. Sewell, H. Tuch, and S. Winwood. sel4: formal verification of an operating-system kernel. Commun. ACM, 53(6):107–115, 2010.

[24] X. Leroy. Formal verification of a realistic compiler. Communications of the ACM, 52(7):107–115, 2009.

[25] T. Lindvall. Lectures on the Coupling Method. Dover Books on Mathematics Series. Dover Publications, Incorporated, 2002. ISBN 9780486421452.

[26] M. Mohri, A. Rostamizadeh, and A. Talwalkar. Foundations of machine learning. MIT press, 2018.

[27] D. Selsam and N. Bjørner. Guiding high-performance SAT solvers with unsat-core predictions. In Theory and Applications of Satisfiability Testing - SAT 2019 - 22nd International Conference, SAT 2019, Lisbon, Portugal, July 9-12, 2019, Proceedings, pages 336–353, 2019.

[28] D. Selsam, P. Liang, and D. Dill. Developing bug-free machine learning systems with formal mathematics. In International Conference on Machine Learning (ICML), 2017.

[29] S. Shalev-Shwartz and S. Ben-David. Understanding machine learning: From theory to algorithms. Cambridge University Press, 2014.

[30] J. Tassarotti, J.-B. Tristan, and K. Vajjha. A Formal Proof of PAC Learnability for Decision Stumps. arXiv e-prints, art. arXiv:1911.00385, Nov. 2019.

[31] The mathlib Community. The lean mathematical library. In Proceedings of the 9th ACM SIGPLAN International Conference on Certified Programs and Proofs, CPP 2020, New Orleans, LA, USA, January 20-21, 2020, pages 367–381, 2020. doi: 10.1145/3372885.3373824. URL https://doi.org/10.1145/3372885.3373824