Verifying Handcoded Probabilistic Inference Procedures

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Researchers have recently proposed several systems that ease the process of performing Bayesian probabilistic inference. These include systems for automatic inference algorithm synthesis as well as stronger abstractions for manual algorithm development. However, existing systems whose performance relies on the developer manually constructing a part of the inference algorithm have limited support for reasoning about the correctness of the resulting algorithm.

In this paper, we present Shuffle, a programming language for manually developing inference procedures that 1) enforces the basic rules of probability theory, 2) enforces the statistical dependencies of the algorithm’s corresponding probabilistic model, and 3) generates an optimized implementation. We have used Shuffle to develop inference algorithms for several standard probabilistic models. Our results demonstrate that Shuffle enables a developer to deliver correct and performant implementations of these algorithms.

1 INTRODUCTION

Bayesian Probabilistic Inference provides a well-studied formalism for modeling and reasoning about uncertain computations. As an example, Figure 1 presents a diagram of the classic Burglary model [Russell and Norvig 2011]. This model captures the probabilistic response of a house’s security alarm when it may be triggered by either an active burglary or an earthquake. Furthermore, if either event triggers an alarm, a number of people may call the authorities to report the alarm.

**Modeling.** The first step in developing a probabilistic model is to model the state of the world with random variables. Each node in the diagram corresponds to a boolean random variable. Each variable is random because it has a probability distribution associated with its values. For example, the classic presentation of this model assumes a priori that a burglary has a 0.1% chance of occurring and an earthquake has a 0.2% chance of occurring. Further, each edge in the graph specifies a conditional dependence. For example, if both a burglary and an earthquake occur, then the alarm has a 95% chance of triggering, and if neither occur, the alarm has a 0.1% chance of triggering. Given random variables and a complete specifications of their probability distributions, the techniques of Bayesian probabilistic inference enable one to query and compute the answer to the question, “what is the probability that a burglary happened given knowledge of who called the authorities?”

Although simply stated here, Bayesian probabilistic inference has been applied to domains such as perception, state estimation, target tracking, and data science, where the models capture rich properties of the physical world.

**Inference.** The inference task for a probabilistic model is to compute the probability distribution of a set of random variables in the model, potentially conditioned on the values of the model’s other random variables. For example, the aforementioned query regarding who called the authorities corresponds to computing the probability distribution $P(\text{burglary} \mid \text{calls})$. More formally, the inference task for this distribution is to produce an inference procedure $f : \mathbb{B}^n \rightarrow (\mathbb{B} \rightarrow \mathbb{R})$ where $f$
takes as input a tuple of values for the n call variables and produces a function that given a value of burglary, returns the probability of that value. Moreover, we can specify the inference problem, generally, as a traditional synthesis problem:

\[ M \models \exists f. \forall b_1, \hat{b}_2.f(\hat{b}_2)(b_1) = P(\text{burglary} = b_1 \mid \text{calls} = \hat{b}_2) \]

The task is therefore to perform quantifier elimination and produce an inference procedure \( f \) that satisfies the specification that it computes the distribution.

### 1.1 Approaches to and Systems for Probabilistic Inference

There is a rich space of systems that seek to tackle the inference problem. These systems range from synthesis approaches to direct, hand-coded implementations.

**Synthesis.** We deliberately pose the inference problem as an synthesis problem because many systems for probabilistic inference take a synthesis approach. Specifically, for a pre-specified class of models, systems such as PSI [Gehr et al. 2016a], Mathematica [Wolfram Research, Inc. 2018] and Maple [Maple Inc. 2018] will automatically generate an inference procedure for a given model.

Other systems with even looser restrictions on the models will automatically generate an inference procedure that uses approximate inference techniques based on the Monte Carlo method, such as Markov-Chain Monte Carlo or Sequential Monte Carlo. These techniques are approximate in that the resulting inference procedure approximates the distribution. While these techniques produce stochastic functions, if we were to view their resulting inference procedures as deterministic functions, then they solve the following modified problem:

\[ M \models \exists f. \forall b_1, \hat{b}_2. \lim_{n \to \infty} f(n, \hat{b}_2)(b_1) = P(\text{burglary} = b_1 \mid \text{calls} = \hat{b}_2) \]

In words, these techniques produce an inference procedure that, given a parameter \( n \) that controls the amount of work that the procedure performs, exactly computes the distribution – as that parameter goes to infinity (i.e., as the procedure does more work).

**Handcoded.** Libraries, such as scipy.stats [Jones et al. 01] and PyMC [Patil et al. 2010], support solving the inference problem by hand. A primary reason why a developer may choose to hand-code an inference algorithm over using a synthesis-based system is efficiency. Specifically, in the approximate inference procedure case, a developer may choose a different inference technique that produces a better estimate of the distribution with the same amount of – or even less – computation. For example, a developer could implement a Collapsed Monte Carlo technique [Liu 1994] – instead of a potentially less efficient general Monte Carlo technique – because the developer knows the dependencies between the random variables in the model, the exact distributions behind those dependencies, and can therefore, 1) apply analytical techniques to efficiently solve part of the inference problem exactly and 2) solve the remainder of the problem with an approximate technique.

To support this development approach, these libraries offer basic probabilistic primitives, such as computing the value of a Gaussian distribution at a point or producing a value from a Gaussian distribution. A developer can then use these primitives in their manual implementation of an inference procedure.

### 1.2 Probabilistic Inference Programming

Constructing efficient inference procedures by hand, alternatively probabilistic inference programming, requires tackling several programming idioms in the domain.

**Distributions.** The primitive objects in this programming model are probability distributions. For example, if implementing an analytical approach for Burglary, a developer will have – conceptually
for (i = 0; i < N; i++) {
    s = 0;
    for (j = 0; j < i; j++)
        s += A[j];
    B[i] = s;
}

(a) unoptimized prefix-sum

for (i = 0; i < N; i++) {
    i, s = 0, 0;
    for (j = 0; j < i; j++)
        s += A[j];
    B[i] = s;
}

(b) optimized prefix-sum

– a representation for the prior distribution for burglary and another for the prior distribution of earthquake. In a standard programming language one way to represent these is by two functions, burglaryPrior : B → R and earthquakePrior : B → R, respectively.

Distribution Operations. The next programming idiom is that developers will compose new distributions using the representations of other distributions. For example, if a developer would like to compute the joint prior probability of both a burglary and simultaneously an earthquake, then the developer can rely on the traditional rule from probability theory that \( P(A, B) = P(A) \times P(B) \) and multiply together each variable’s prior distributions.

\[
\text{def jointBE(b, e) : burglaryPrior(b) * earthquakePrior(e);}
\]

Sound Probability Theory. A proviso to the developer’s above application of probability theory is that this rule is sound only if \( A \) and \( B \) – alternatively, burglary and earthquake – are statistically independent. Namely, it must be the case that \( P(A|B) = P(A) \) (and vice-versa). In a standard programming language – with no explicit representation of the probabilistic model and its dependencies – such assertions about the model can only be informally documented as comments.

Code Generation and Optimization. To effectively program with the abstraction of probability distributions and their traditional operations, the developer must carefully translate their implementations of these operations to manage the realizability of the computation.

For example, developers would ideally like to specify integrations. In general, these integrations may not be tractable, but for certain models they are. In such cases, the developer must jointly transform multiple operations into its analytical solution. Such transformations result in algebraically simplified opaque blocks of code that have limited correspondence to the original high-level operations. Such blocks are akin to the code generated by optimizing compilers.

Another concern is the performance of the inference procedure’s implementation. Sample-based approximate inference techniques often generate code that needs to be incrementalized [Wu et al. 2016]. As a simplified example, an inference procedure might need to collect statistics about the input data and the natural specification of the algorithm results in prefix sum. The algebraic formulation of prefix sum is written as \( \forall i, B[i] = \sum_{j<i} A[j] \). Figure 2a shows this computation directly translated into imperative code. This code has complexity quadratic to input’s length. In contrast, Figure 2b presents an equivalent optimized prefix sum that has linear complexity. In general, these optimizations are challenging to implement manually and – like algebraic simplifications – they are hard to interpret and maintain.

While probabilistic inference programming presents an opportunity to craft a programming domain based on the well-developed theory of probability distributions, delivering practical implementations by hand presents multiple challenges.

1.3 Contributions: Shuffle

In this paper we present Shuffle, a programming language for probabilistic inference programming that gives developers the abstraction of probability distributions with also supplementary support to ensure that their inference procedures are sound, realizable, and optimized.
Modeling. In Shuffle, a developer first writes a probabilistic model in Shuffle’s modeling language. The model’s specification includes the model’s random variables, the dependencies between the random variables, and the probability distributions that characterize these dependencies.

Inference. The developer next writes their inference procedure using first-class abstractions of probability distributions and Shuffle-provided operations to compose probability distributions into new probability distributions. Shuffle provides the abstraction of probability distributions where their underlying implementation and corresponding interface is either 1) a probability density function – a function that computes the probability that a variable takes a value – 2) a Monte Carlo Sampler – a stochastic function that produces a value of the target variables of a probability distribution, according to their probability – or 3) a Monte-Carlo Markov Chain Transition Kernel – stochastic functions that if repeatedly iterated behave as Monte Carlo Samplers.

Shuffle also provides a set of strongly-typed operators that are inspired by the rules of probability theory that enable developers to compose distributions. An inference procedure written in Shuffle composes together distributions, with the resulting sequence of compositions corresponding to an implementation of an inference procedure for a distribution in the model. Shuffle’s distribution abstractions are expressive enough for a developer to write inference algorithms such as variable elimination [Zhang and Poole 1994], Gibbs sampling [Geman and Geman 1984], Metropolis-Hastings [Hastings 1970; Metropolis et al. 1953], and likelihood weighting [Fung and Chang 1989].

Type Checking. Given an inference procedure, Shuffle’s type system verifies that each distribution composition is sound with respect to the rules of probability theory as well as the dependencies expressed in the model. For example, if \( d_1 \) is a density for the distribution \( \Pr(A | B, C) \), where \( A, B, \) and \( C \) are sets of random variables, and \( d_2 \) is a density for the distribution \( \Pr(B|C) \), then Shuffle’s type system determines that the density \( d_1 \ast d_2 \) is a density for the distribution \( \Pr(A, B | C) \). This fact follows from probability theory.

Code Generation. Given a type-checked inference procedure, Shuffle then automatically generates code that implements the procedure. Shuffle’s code generator 1) automatically applies algebraic simplifications to eliminate integrals when possible, 2) automatically translates the developer’s inference procedure to compute with log probabilities, and 3) automatically applies incremental optimizations to improve performance.

Case Studies. We evaluate Shuffle by specifying several probabilistic models and implementing several inference procedures. Our evaluation demonstrates that Shuffle can express several inference procedures for several models and generates code that is more efficient than Venture [Mansinghka et al. 2014], another system for probabilistic inference programming. Specifically, we show speedups of at least 3.1x on these benchmarks.

Altogether, Shuffle enables a developer to build a rich set of inference procedures with strong guarantees as to the correctness, realizability, and efficiency of their implementation.

2 EXAMPLE: BURGLARY MODEL

To use Shuffle to create an inference procedure, a developer first specifies a probabilistic model. Figure 3 presents a Shuffle specification of the Burglary model presented in Section 1. The specification gives the model’s random variables, prior distributions, and conditional distributions.

Random Variables. Lines 2 and 3 declare the boolean random variables burglary and earthquake, the values of which denote whether or not burglary or earthquake as occurred, respectively. These variables are random in that they have a probability distribution associated with their values.
Distributions. Each def statement in the model specifies a name, type, and implementation for a distribution. For example, the def statement on Line 5 specifies the distribution for burglary with the name burglaryPrior and type density(burglary).

The type specification is similar to the traditional probability notation $P(\text{burglary})$ and therefore explicitly links this distribution’s name and its implementation to the burglary random variable. However, instead of the traditional $P(\cdot)$ notation, the type has the syntax density(·), which denotes that the distribution is implemented as a density function.

Probability densities functions are a common tool for specifying the distribution of random variables. If a random variable $X$ may take on a value $x : A$, then then a probability density $f : A \to R$ at $x$ (i.e., $f(x)$) returns a real-valued score for how likely it is that $X$ takes on the value $x$. If $A$ is continuous (such as the real numbers), then $f(x)$ is the probability that $X$ lies in an infinitesimal region around $x$, divided by the size of that region. If $A$ is a discrete type (such as the integers), then $f(x)$ is simply the probability that $X = x$ (and is frequently instead called a probability mass function; in this paper we will not make a distinction). The implementation on Line 5 makes use of the flip($v$, $p$) primitive, which is a Shuffle primitive that returns $p$ if its first argument $v$ evaluates to 1, and $1 - p$ otherwise. Line 7 similarly specifies the distribution for earthquake with name earthquakePrior and type density(earthquake).

Conditional Distributions. Line 9 declares the boolean random variable for the occurrence of an alarm Line 11 specifies its distribution. As seen in Section 1, the distribution of alarm depends on, or is conditioned on, the values of burglary and earthquake. The distribution declaration on Line 11 declares that the distribution of alarm is conditioned on the values of of earthquake and burglary. Similar to the traditional probability notation $P(\text{alarm} | \text{burglary, earthquake})$, the declaration specifies that implementation has the type density(alarm | burglary, earthquake), thereby noting both the conditional nature of the distribution, but also its implementation as a density function. Note that conditioning extends the capabilities of the density implementation in that the conditioned variables are made available to the implementation as values that can be
def alarmMarg() : density(alarm | burglary) =
    int alarmDens() * ((ind burglary) earthquakePrior())
    by earthquake;

def independent callDensI(p in People) :
    density(calls[p] | calls{i in People: i < p}, alarm, burglary) =
    callDens(p);

def rec callDensAll(p in People) :
    density(calls{i in People: i <= p} | alarm, burglary) =
    callDensI(p) * callDensAll(p-1);

def callsMarg() : density(calls | burglary) =
    int callDensAll(max(People)) * alarmMarg()
    by alarm;

def macro bayes_rule(v,d) = d / (int d by v);

def burglaryPost() : density(burglary | calls) =
    bayes_rule(burglary, callsMarg() * burglaryPrior());

Fig. 4. Inference program for computing density(burglary | calls) for the Burglary model.

inspected. In this case, alarmDens uses if statements that test the values of these conditioned variables statements to implement its distribution specification.

Random Variable Sets. The final random variable declaration on Line 21 specifies a random variable set, calls, where each random variable in the set denotes whether an individual person calls the authorities. Variable sets enable Shuffle programs to specify first-order models where, in the model, no a priori bound on the number of people need to be specified. Variable sets map an index domain to a target set. For example the index domain of calls is People, and its target set is the domain Bool. Domains are, in general, named subsets of the natural numbers, and the target set may be either a domain or the real numbers. Enforcing a finite index domain enables Shuffle’s type system to reason about variable set membership, while allowing the target set to be the real numbers enables developers to construct models that have real-valued random variables.

Quantified Distributions. The distribution declaration on Line 23 declares that the distribution of calls[p], where p is a quantifier over People, is conditioned on alarm. Quantifiers enable quantification over domains and can appear in the type (as they do in this declaration) and also can be referred to in the distribution’s implementation. This distribution therefore defines the distribution for each variable in calls in turn.

Summary. After specifying the model, the developer next specifies an inference procedure that implements a distribution of interest. In the burglary example, the distribution of interest is P(burglary | calls). A Shuffle developer can compute this distribution using either an exact or approximate inference procedure. An exact inference procedure computes a density for these distributions therefore the resulting code that implements the distribution would have the type density(burglary | calls). An approximate inference procedure computes other representations of these distributions using Shuffle’s sampler and kernel distribution abstractions.

2.1 Exact Inference

Figure 4 presents an exact inference algorithm written in Shuffle that computes the distribution density(burglary | calls) using arithmetic operations on density functions.

Shuffle’s density arithmetic operations correspond to the rules of probability theory and the type system enforces that the operands satisfy the statistical properties required for the operation to be valid.
Independence. In the definition of alarmMarg in Figure 4, we use the syntax (ind burglary) on Line 2 to coerce the type of earthquakePrior() using an independence assumption. In this case, we coerce the type of earthquakePrior(), density(earthquake), to the type density(earthquake | burglary) using the independence assumption earthquake ⊥ burglary. While the independence assumption is necessary for Shuffle to soundly produce this judgment, Shuffle does not verify independence assumptions internally. Instead, Shuffle generates a log of assumptions for the developer to manually audit.

Density Multiplication. Shuffle enables a developer to multiply densities using the syntax $d_1 \ast d_2$, where $d_1$ and $d_2$ are densities. Line 2 multiplies the densities alarmDens() and (ind burglary) earthquakePrior(), producing a density of type density(alarm, earthquake | burglary). This type results from the rule of probability theory that $\Pr(A, B | C) = \Pr(A | B, C) \cdot \Pr(B | C)$. Given that the type of alarmDens() is density(alarm | earthquake, burglary) and the type of (ind burglary) earthquakePrior() is density(earthquake | burglary), this type follows given the equivalences $A = \text{alarm}$, $B = \text{earthquake}$, and $C = \text{burglary}$. Shuffle automatically computes and checks this type.

Integration. Shuffle also enables a developer to integrate a density. On Line 2, the developer leverages integration to eliminate the variable earthquake from the intermediate distribution he or she computed. Integration implements the rule of probability theory $\Pr(B) = \int_A \Pr(A, B)$ using the syntax int $d$ by $B$, where $d$ is a probability density and $B$ is a set of random variables. Line 2 integrates the distribution density(alarm, earthquake | burglary) with respect to the variable earthquake and therefore eliminates it from the resulting type of the integration. Because earthquake is a boolean random variable with finite possibilities, Shuffle implements this integral by summing the inner density over all possible values of earthquake, namely 0 and 1.

Constrained Variable Sets. Shuffle also enables a developer to specify types that include constrained relations between variables. The definition of callDensI on Line 5 is a quantified density that computes the density of call[p] conditioned, alarm, and burglary (as before), but also conditioned on all values call[i] where $i$ is less than $p$. Constrained sets enable developers to specify both structured and dynamically changing dependencies because constraints can depend on either quantifiers (as here) or even the value of random variables.

The developer provides an implementation here through an independence assumption. The independent annotation on the definition operates as an independence assumption where the set of independent variables is given by the difference between those in the specified type and that computed by the type system for the term.

Recursion. The definition of callDensAll on Line 9 demonstrates Shuffle’s recursive procedures. This definition computes the joint density of all random variables in the calls collection by computing the product of callDensI(p) with the recursively defined callDensAll(p-1). The effect on the type is an inductive proof. Specifically, assuming that invocations of callDensAll have the annotated type within the body of callDensAll, Shuffle verifies that the body also has this type. Shuffle specifies default base cases for all of its objects. In this case, Shuffle defines that callDensAll(i-1), where $i$ is the smallest value in the domain People, yields the value 1. This is because callDensAll’s type, density(calls{$i$ in People: $i < p$} | alarm, burglary), specifies uncertainty for an empty set of variables when $i$ falls below the minimum value in People. The constant function returning 1 is always a correct density for an empty set of random variables.

Result. In the last step of this inference program, the developer computes the posterior distribution density(burglary | calls). Given the intermediate density calculation steps outlined above, the developer accomplishes with an application of Bayes’ rule from probability theory. This rule
\begin{verbatim}
def independent earthquakeMarg():
    density(earthquake | alarm, burglary, calls) =
    bayes_rule(earthquake, alarmDens() * (ind burglary) earthquakePrior());

def independent burglaryMarg():
    density(burglary | earthquake, alarm, calls) =
    bayes_rule(burglary, alarmDens() * (ind earthquake) burglaryPrior());

def alarmMarg():
    density(alarm | burglary, earthquake, calls) =
    bayes_rule(alarm, (ind burglary, earthquake)
    callDensAll(max(People)) * alarmDens());

def abeKernel():
    kernel(alarm, burglary, earthquake | calls) =
    lift{
        alarm := sample alarmMarg();
        burglary := sample burglaryMarg();
        earthquake := sample earthquakeMarg();
    };

def abePost():
    sampler(alarm, burglary, earthquake | calls) =
    fix abeKernel;
\end{verbatim}

Fig. 5. Approximate Inference for the Burglary model.

states that \( \Pr(A|B) = \frac{\Pr(A,B)}{\int_B \Pr(A,B)} \). In Shuffle, a developer can represent this rule with a macro (Line 17) that takes as input a density \( d \) and a set of random variables \( v \). If \( d \) has the type \( \text{density}(A, v | B) \), where \( A \) and \( B \) are any sets of random variables, then the result of \( \text{bayes\_rule}(d, v) \) has the type \( \text{density}(A | v, B) \).

Given these set of definitions, Shuffle automatically translates these definitions to Python code. In this specific example, Shuffle translates integrals to summations (because the domains of these variables are discrete).

\subsection{Approximate Inference}

Distribution implementation methods that rely purely on computations of density functions are designed to compute the distribution exactly. An alternative implementation approach is to approximate the distribution. For example, while the integrals in Figure 4 are efficiently computable, other models may not admit tractable integrations and, therefore, may need to be approximated. Sample-based \textit{approximate inference} inference procedures, such as Gibbs Sampling [Geman and Geman 1984] and Metropolis-Hastings [Hastings 1970; Metropolis et al. 1953], have been designed to perform inference in such models. These inference procedures, called \textit{Monte Carlo samplers}, randomly produce samples from the desired distribution. The probability that an implementation produces a given value approximates the probability of that value according to the specified distribution. As a result, a client of such a distribution can use the \textit{Monte Carlo method} to ask questions about a distribution. Specifically, the developer can phrase a question as a function \( f(x) : X \to \mathbb{R} \) and then compute the expectation \( \int_X f(x) * P(x) \) approximately by \( \sum_i f(x_i) \), where each \( x_i \) is a sample from the distribution.

\textbf{Samplers.} In Shuffle, \textit{Monte Carlo Samplers}, or simply \textit{samplers}, are imperative procedures that take as input a concrete state that includes values for all of the model’s random variables and produces a modified state. The probability that a sampler produces a given state approximates the probability of that state – i.e., the values of modified variables – according to the specified distribution. Figure 5 presents a Gibbs Sampling implementation for the posterior distribution \( P(\text{alarm}, \text{burglary}, \text{earthquake} \mid \text{calls}) \) as a sampler. On Line 15, the developer assigns \texttt{alarm} to a random value drawn according to the distribution \texttt{alarmMarg()}. Because \texttt{alarmMarg()} has the
def bApprox(calls):
    sum = 0
    for i in range(num_samples):
        (alarm, burglary, earthquake) = abePost(calls)
        sum += (1 if (burglary == True) else 0)
    return sum / num_samples

Fig. 6. Python code for estimating the probability that a burglary occurs using extracted eabPost.

Fig. 7. approximate inference samples

type density(alarm | burglary, earthquake, calls), the sample statement on that line is a sampler with the type sampler(alarm | burglary, earthquake, calls). Specifically, the statement produces values of alarm conditioned on the values of burglary, earthquake, and calls. Because the type is conditioned, the sampler may read the values of burglary, earthquake, and calls while producing its value. Further, a sampler can only modify the target variables specified in its type. Therefore this sampler only modifies alarm. Shuffle’s typesystem verifies that a sampler’s imperative implementation is consistent with the specification in its type.

Markov-Chain Transition Kernels. The lift block between Lines 14-18 composes together multiple samplers on this inference procedure’s overall path towards producing a sampler. A key insight into understanding this procedure and its use of composition is the types of alarmMarg, burglaryMarg, and earthquakeMarg. Specifically, the sampler on Line 15 produces a sample of alarm conditioned on the value of burglary (and other variables of the model), the sampler on Line 16 produces a sample of burglary conditioned on the new value of alarm (as well as other variables of the model), and the sampler on Line 17 produces a sample of earthquake conditioned on the new values of alarm and burglary. Because the target variables and conditioned variables of these three samplers intersect, the values of these random variables after executing all three samplers can be correlated in a way that does not result in a sampler for the desired distribution: the joint distribution of $P(alarm, burglary, earthquake | calls)$.

However, if the developer were to repeatedly apply this block, then – in the limit – that iteration process does produce a correct sample-based implementation. A distribution implementation for which repeated iteration produces a sampler is called a Markov-Chain transition kernel. Therefore, the difference between a sampler and a kernel is that a sampler directly produces a sample from a distribution whereas a kernel converges to a sampler under repeated composition with itself.

Shuffle supports transition kernel implementations through its kernel type. Kernels have a weaker correctness condition which means they have more flexible composition rules. Shuffle developers construct kernels using the lift syntax, as on Line 14 and the checker computes that the block lift on Line 14 has the type kernel(alarm, burglary, earthquake | calls).

Fixpoints. The final step towards producing a sampler implementation of the posterior distribution is to follow the approach suggested by the previous paragraph: iterate the kernel implementation until it reaches a fixpoint. Line 21 uses the fix operator, which denotes the fixpoint of a distribution’s kernel implementation. The result this operator is a sampler for the distribution.

We have designed Shuffle’s type system such that all fixpoints can be computed by repeated iteration and therefore Shuffle generates code for fix that performs iteration. Shuffle’s guarantees hold in the limit and it is the responsibility of the developer to set the parameters of the generated implementation that control the number of iterations during execution. Automatically determining the number of iterations for a Markov-Chain Monte Carlo algorithm is an undecidable problem. However, developers can use a variety of profiling techniques to aid setting these parameters [Cowles and Carlin 1996].
Summary. Together, Shuffle’s abstractions for densities, samplers, and kernels enable developers to compose inference procedures with strongly-typed abstractions and generate efficient code. For example, Figure 6 presents an example of how a developer would use a sampler generated by Shuffle within a Python program. Specifically, by repeatedly calling a function like `abePost` to produce a stream of samples from the distribution of $P(\text{alarm, burglary, earthquake} \mid \text{calls})$, the function `bApprox` computes the expectation of the indicator function, `burglary == True`, which is therefore an approximation of the probability that a burglary occurs. Figure 7 shows a result of approximate inference when 3 out of 10 people call. The plot illustrates that out of 10k samples we obtained by calling `abePost`, 3725 samples had True for the value of `burglary`.

3 LANGUAGE

We next present the syntax of models, types, and inference procedures in Shuffle. For clarity of presentation, we elide a complete presentation of the syntax of Shuffle’s modelling language. However, the examples in Section 2 are representative in that a probabilistic model defines the model’s domain of values, the model’s set of random variables, and the probability densities that relate them. A domain declaration, specifies a domain $\delta \in \Delta$. A variable declaration, specifies a random variable $v \in V$. A random variable is an array and a domain $\delta$ specifies its index space.

3.1 Types

![Type Syntax](https://example.com/syntax.png)

Figure 8 presents the syntax Shuffle’s types. The language of types, $T_x$, denotes that an object is either a density, sampler, kernel, or estimator that computes the probability of a set of random variables conditioned on another set of random variables, while subject to a constraint on the conditioned random variables. The random variables within either set may be either a single random variable from an array of random variables, $v[A]$, or a constrained subset of the random variables within an array, $v(q \in \delta : \phi)$. The variable set $v$ is syntactic sugar for the set $v\{q_0 \in \delta : \text{true}\}$.

A constraint, $\phi$, that appears in either a type or a random variable subset notation is a boolean combination of (in)equalities over 1) integers, 2) quantifier variables from domains that are isomorphic to the integers, 3) a single random variable with a value from a domain that is isomorphic to the integers, and 4) the minimum or maximum elements of a domain.

3.2 Inference Procedures

Figure 9 presents the syntax of Shuffle’s inference procedures. As a simplification for presentation purposes, each definition admits one quantifier, but our implementation permits multiple quantifiers per definition.

Densities. A probability density, $D$, defines a probability distribution through density operators. An inference procedure may call an atomic density arguments $x(A)$, a multiply two densities, $D_m \ast D_m$, divide a density by another density, $D_m / D_m$, integrate a density using the syntax $\int D$ by $V_q$ or conditionally switch between densities. Each of these operators has a corresponding well-defined semantics in probability theory with respect to its operands.
We denote the minimum and maximum of a domain \( \delta \) by their definitions in the declaration:

\[
\Delta \rightarrow (\mathbb{N} \times \mathbb{N}) \times (V \rightarrow (\Delta \times (\Delta + (\mathbb{R})))) \times \mathbb{R}
\]

\[\max(\delta)(M) = \pi_3(\pi_1(M)(\delta))\]

\[\min(\delta)(M) = \pi_2(\pi_1(M)(\delta))\]

We denote the random variable declaration in the model to a function \( f : \Delta \rightarrow (\mathbb{N} \times \mathbb{N}) \times (V \rightarrow (\Delta \times (\Delta + (\mathbb{R})))) \times \mathbb{R} \) that consists of the syntax of the density function, a list of pairs of quantifier names and their associated domain names, a set of random variables denoting the density’s target variables, a set of random variables denoting the density’s conditioned variables, and a predicate \( \phi \) denoting the density function’s condition of application.

### 4.1 Preliminaries

**Errors.** A Shuffle inference procedure may produce one of two error values instead of a conventional value: 1) a procedure produces the error value \( \bot_\sigma \) if and only if it requires access to an element of the environment that is not within the environments domain and 2) a procedure produces the error value \( \bot_0 \) if and only if it contains a division by 0. In the semantics below we use \( \bot = \{ \bot_\sigma, \bot_0 \} \) to refer to the domain of errors and elide explicit failure propagation rules.

**Environments.** An environment, \( \sigma \in \Sigma = (V \times \mathbb{N}) + Q + X \rightarrow (\mathbb{R}^+ + \mathbb{N} + (Q, \Lambda, \beta)) \) is a finite map from random variables, quantifier variables, and bound distributions to their respective values. The notation \( \sigma(a) \) denotes the value to which \( a \) is mapped by \( \sigma \), which can either be 1) a random

\[
P \rightarrow \left( \text{def } K_d x \langle q \text{ in } \delta \rangle : T_k = \beta \right) +
\]

\[
K_d \rightarrow (\text{independent } | \text{rec})
\]

\[
\beta \rightarrow D \mid S \mid K \mid E
\]

\[
D \rightarrow x(A) \mid D \times D \mid D / D
\]

\[
| \text{ int } D \text{ by } V_g \mid \text{ if } \phi \{ D \} \{ D \} \mid 1.0
\]

\[
S \rightarrow x(A) \mid v[A] := \text{ sample } D
\]

\[
| \text{ return } | S ; S | \text{ if } \phi \{ S \} \{ S \} | \text{ fix } K
\]

\[
K \rightarrow x(A) \mid \text{ lift } \{ S \}
\]

| if \( \phi \{ K \} \{ K \} \mid K ; K | \text{ return }
\]

**Samplers.** A sampler, \( S \), defines a probability distribution through sampler operators. Sampler operators include sampling a value from a density, \( v[A] := \text{ sample } D \), sequentially composing two samplers together, \( S ; S \), and computing the fixed point of a kernel, \( \text{ fix } K \).

**Kernels.** A kernel, \( K \), defines a probability distribution in terms of kernel operators. Kernel operators include lifting a sampler, \( \text{ lift } \{ S \} \), and composing two kernels together with the syntax \( K \cdot K \).

Fig. 9. The Syntax of Shuffle Inference Procedures

\( H \) consists of its domain declarations, random variable declarations, and density definitions, respectively.

**Domain Declaration.** We map the set of domain definitions in the syntactic specification of the model to a function \( f : \Delta \rightarrow (\mathbb{N} \times \mathbb{N}) \) that maps domain names to a pair, consisting of the domain’s minimum and maximum elements, respectively. We denote the semantics of a domain \( \delta \) by the set of integers between (inclusive) its minimum and maximum values.

\[
[\delta](M) = \{ n | \pi_1(\pi_1(M)(\delta)) \leq n \leq \pi_2(\pi_1(M)(\delta)) \}
\]

We denote the minimum and maximum of a domain \( \delta \) by their definitions in the declaration:

\[
\min(\delta)(M) = \pi_1(\pi_1(M)(\delta)) \quad \max(\delta)(M) = \pi_2(\pi_1(M)(\delta))
\]

**Random Variable Declaration.** We map the set of random variable declarations in the model to a function \( f : V \rightarrow (\Delta \times (\Delta \cup R)) \) that maps random variable names to a pair consisting of the name of the random variable’s index domain and the name of its target set, respectively.

**Density Definition.** We map a density definition in the syntactic specification of the model to a tuple \( \eta \in H = (X \times D_m \times (Q \times \Delta) \times V_g \times V_g \times \Phi) \) that consists of the syntax of the density function, a list of pairs of quantifier names and their associated domain names, a set of random variables denoting the density’s target variables, a set of random variables denoting the density’s conditioned variables, and a predicate \( \phi \) denoting the density function’s condition of application.
variable \((v, n)\) where \(n\) is a natural number 2) a quantifier variable \(q\) or 3) a named distribution \(x\).

We use the notation \(\sigma[a \mapsto b]\) to mean \(a\) with \(a\), which could be any of the above, remapped to \(b\).

**Variables.** Our formalization relies on several disjoint variable spaces. A quantifier variable \(q \in Q\) is drawn from the space \(Q\); a named distribution \(x \in X\) drawn from \(X\), the space of distribution names; a random variable \(v \in V\) is drawn from \(V\), the space of variable names; and a domain \(\delta \in \Delta\) is drawn from \(\Delta\), the space of domain names.

**Variable Sets.** A variable set is a comma delimited list of random variables \((V_q^+ \text{ in Figure } 8)\) that we denote by the symbols \(A\), \(B\), and \(C\). We specify the semantics of a variable set by the semantic function \([A] : \mathbb{M} \times \Sigma \rightarrow \mathcal{P}(V)\) where \(V = V \times N\). The denotation of a variable set is therefore a set of pairs that each consist of a random variable name and the corresponding index within that variable.

For each syntactic form, we give variable sets the following denotation:

- **Set Comprehensions.** For variable sets of the form \(A = v(q_0 \text{ in } \delta_1 : \phi)\), let \([A](M, \sigma) = \{(v, n) \mid n \in [\delta_1](M) \land [\phi](M, \sigma[q_0 \mapsto n])\}\).

- **Indexed Variables.** The single variable \(v[a]\), in the context of a variable set is syntactic sugar for the set \(v(q_0 \text{ in } \delta : q_0 == a)\), with the corresponding denotation given by that for set comprehensions.

- **Union.** The comma operator \(A, B\) unions two disjoint variable sets. Namely, the denotation of this operator is \([A, B](M, \sigma) = \begin{cases} [A](M, \sigma) \cup [B](M, \sigma) & [A](M, \sigma) \cap [B](M, \sigma) = \emptyset \\ \bot_{\sigma} \end{cases} \)

**Source of Randomness.** A source of randomness, denoted by "sr \in SR = [0, 1]^+" is a sequence of uniform distributed values on the interval \([0, 1] \subset \mathbb{R}^+\). Let the notation \(\int_{\text{sr}} f(\text{sr})\) denote an integral over each element of this sequence. We assume the existence of a function \(\text{split} \in SR \rightarrow SR \times SR\) that produces two identical sources of randomness from one, such that \(\int_{\pi_1(\text{split}(sr))} f(\pi_1(\text{split}(sr))) = \int_{\pi_1(\text{split}(sr))} f(\pi_2(\text{split}(sr)))\) for any positive measurable function \(f\).

### 4.2 Definitions

The semantics of the syntax \(\text{def } x \ (q \text{ in } \delta) : t_x = \beta_1\) is a new environment with \(x\) bound to the procedure \(\beta_1\) with the quantifier \(q\).

**Recursive Definitions.** A recursive definition denoted \(\text{def rec } x \ (q \text{ in } \delta) : t_x = \beta_1\) is the same as that of an ordinary definition, except that recursive invocations refer to a modified \(\beta_1\) that define default base cases when the argument of the procedure \(q\) is out of its domain. The default base case for densities returns the constant 1; the default base case for samplers and kernels leaves the environment unchanged. Default base cases enable developers to write programs that type check, as Shuffle’s type system cannot reason about arbitrary base cases.

### 4.3 Densities

Figure 11 presents the denotation of a density. The denotation of a density \(d\), denoted by \([d] \in (\mathbb{M} \times \Sigma) \rightarrow (\mathbb{R}^+ + \bot)\), is a function from an environment to a positive real number or an error value. Multiplication, division, and conditionals have standard semantics.

| \[\text{def } x \ (q \text{ in } \delta) : t_x = \beta_1\](M, \sigma) = | \[\sigma[x \mapsto (q, \beta_1)]\] |
| \[\text{def rec } x \ (q \text{ in } \delta) : t_x = \beta_1\](M, \sigma) = | \[\sigma[x \mapsto (q, \text{default}(\beta_1))]\] |
| \[p_1 ; p_2\](M, \sigma) = | \[p_2\](M, [p_1](M, \sigma)) |}

**Fig. 10.** Semantics of definitions

![Diagram](image-url)
Integration. An expression $\int d$ by $V_0$ computes the integral of a probability density, $d$. It computes the integral of its density parameter over all possible values of the random variables, $V_0$.

Invocation. An expression $x(a)$ invokes a density the $x$. The invocation evaluates the density in an environment where the quantifier variable is rebound to its parameter $a$.

4.4 Samplers

Figure 12 presents the denotation of a sampler. The denotation of a sampler $s$, denoted by the semantic function $[s] \in (\mathcal{M} \times \Sigma \times SR) \rightarrow (\Sigma + \bot)$, is a function that takes an environment and a source of randomness, and produces a new environment or an error value. The new environment will have one to new values for its target variables that are randomly chosen according to the sampler’s distribution and the value of the source of randomness.

Sampling. A statement of the form $v[a] := \text{sample } d$ samples from the density $d$. The sampler updates $\sigma$ so that the mapped value of $(v, [a](\sigma))$ is overwritten with the newly sampled value. We specify the denotation of the sample command via inverse transform sampling. Inverse transform sampling chooses a value $r$ such that the integral of $d$ on the region $(-\infty, r]$ is equal to a uniform random value from the source of randomness. In cases where $r$ is discrete, an inverse transform sampler rounds up so that the uniform random value is smaller than this integral:

$$\text{InverseTransform}(\mathcal{M}, v, a, d, \sigma, sr, r) = \arg \min_r \left( \int_{x \in (-\infty, r]} [d](\sigma(v, [a](\sigma)) \mapsto x) \right) > \pi_1(sr)$$

Invocation. An expression $x(a)$ invokes the sampler $x$. The invocation evaluates the sampler in an environment where the quantifier variable is rebound to its parameter $a$.

4.5 Kernels

Figure 13 presents the denotation of a kernel. The denotation of a kernel $k$, written $[k] \in (\mathcal{M} \times \Sigma \times SR) \rightarrow (\Sigma + \bot)$, is a function that takes an environment and a source of randomness, and
produces a new environment or an error value. The semantics of kernel composition, invocation, and conditionals are the same as that for samplers.

**Lift.** A developer can lift a sampler to a kernel. The resulting kernel has exactly the same behavior as the original sampler, and is used to represent the same distribution.

\[
\text{lift } \{ s \}(M, \sigma) = [s](M, \sigma, sr) \\
\forall f. \int_{sr} f(\fix k)(M, \sigma, sr) = \int_{sr} f(k; \fix k)(M, \sigma, sr)
\]

Fig. 13. Semantics of kernels (abbreviated)

**Fixed Point.** For a given kernel for a distribution, a developer can produce a sampler for the same kernel via the \( \fix \) operator. The denotational semantics of \( \fix \) are declarative, as Figure 13 specifies that the operator must have the property that the sampled distribution is invariant under composition with the kernel. Shuffle type checks its code assuming an exact implementation of \( \fix \), but generates code that approximately implements it by running the kernel repeatedly in an iterative process. As the number of iterations grows large, the approximate distribution approaches the true distribution.

5 TYPE SYSTEM

A typing judgment in Shuffle is a logical proposition of the form \( M, \Gamma, L \vdash \beta : t \) where \( M \) is a model, \( \Gamma \) is a type environment, \( L \) is an assumption log, \( \beta \) is a Shuffle inference program, and \( t \) is a type. For example, the type judgment \( M, \Gamma, L \vdash \beta : \text{density}(A \mid B, \phi) \) states that the term \( \beta \) is a density for the conditional distribution \( \Pr(A \mid B) \), provided that \( \phi \) is true. In this section we present Shuffle’s type system, including the semantics of the model, assumption log, and type environment.

5.1 Model

We next give the model a semantics. Specifically, we define the semantics of the model by the joint density of the model’s variables. The joint density computes the probability that the model’s variables all together take on a set of prescribed values. We define the model’s joint probability density, \( J \), via the model’s density function definitions as follows:

\[
J(M, \sigma) = \prod_{(x,d,(q,\delta),A,B,\phi) \in \pi_3(M)} [d](M, q, \phi, \sigma)
\]

where the notation \([d](M, q, \phi, \sigma)\) denotes the quantified semantics of a density function. The quantified semantics of a density function denotes the joint density of all the possible target variables that the density defines. We therefore define the quantified semantics of a density function as the product over all instantiations of the density’s quantifier variables, which, therefore determine the set of target variables. We define the quantified semantics as follows:

\[
[d](M, q, \phi, \sigma) = \prod_{n \in [q](M)} \begin{cases} 
[d](M, \sigma[q \mapsto n]) & \text{if } \phi(M, \sigma[q \mapsto n]) \\
1 & \text{else}
\end{cases}
\]

This representation of the model demonstrates that the joint probability density of the model can be factored into a product of its constituent density definitions. Building on the definition of the joint density as well as Bayes’ Rule, we define the conditional density of a set of variables, \( A \), conditioned on the values of a set of variables \( B \), \( J(A \mid B)(M, \sigma) = \frac{\int_{V \subseteq \{A\}(M, \sigma) \cap \{B\}(M, \sigma)}{\int_{V \subseteq \{B\}(M, \sigma)}} J(M, \sigma) \)

**Model Type Environment.** A model type environment \( \Gamma_m \) is a finite map from quantified variables to domain names: \( \Gamma_m \in Q \rightarrow \Delta \).
Model Validity. We next define what it means for an environment to satisfy a model.

- **Random Variable Satisfaction.** The value of a random variable in an environment satisfies its domain if the value of the variable at each index in its domain has a value that is within the variable’s codomain.

  \[ \sigma, M \models v : (\delta_1, \delta_2) \Rightarrow \forall n_1 \in [\delta_1](M). \exists n_2 \in [\delta_2](M). \sigma((v, n_1)) = n_2 \]

- **Satisfaction.** An environment satisfies a model if its random variables satisfy their domains.

  \[ \sigma \models M \Rightarrow (\forall v \in \text{dom}(\sigma), \delta_1, \delta_2. (\pi_2(M)(v) = (\delta_1, \delta_2)) \Rightarrow \sigma, M \models v : (\delta_1, \delta_2)) \]

- **Quantifier Variable Satisfaction.** The value of quantifier variable in an environment satisfies its domain if it is an element of the domain.

  \[ \sigma, M \models q : \delta \Rightarrow \sigma(q) \in [\delta](M) \]

- **Environment Satisfaction.** An environment satisfies a model and model type environment if 1) it satisfies the model and 2) every quantifier variable in the environment is a member of the domain prescribed by the type environment.

  \[ \sigma \models M, \Gamma_m \Rightarrow \sigma \models M \land \forall q \in \text{dom}(\sigma). \sigma, M \models q : \Gamma_m(q) \]

**Model Validity.** For a Shuffle inference program to be sound with respect to a model \( M \), the model must be valid. Shuffle assumes that each density implementation defined in the model is equal to its conditional density as defined above in terms of \( J \). A valid model satisfies a sequence of properties that ensure this is the case. Appendix A defines these conditions in more detail.

**Theorem 1 (Model Validity).** If \( M \in \mathcal{M} \) is valid, then for any \( \eta = (x, d, (q, \delta), A, B, \phi) \in \pi_2(M) \) it must be true that \( \forall \sigma. (\sigma \models M, \Gamma_m | q \mapsto \delta \land [\phi](M, \sigma)) \Rightarrow [d](M, \sigma) = J(A | B)(M, \sigma) \)

### 5.2 Assumption Log

Figure 14 presents the structure of an assumption log. An assumption log, \( L \), is a record of the set of model and inference program assumptions made by the developer during the construction of their inference program. Figure 14 presents the structure of an assumption log. An assumption log, \( L \), is a record of the set of model and inference program assumptions made by the developer during the construction of their inference program. An entry in an assumption log, \( \alpha \), is a logical proposition the asserts either statistical independence or a reachability. We denote the semantics of an assumption log by the semantic function \( [L] : (\mathcal{M} \times \Sigma) \rightarrow \mathbb{B} \) with the semantics of a full log given by \([L : \alpha](M, \sigma) = [L](M, \sigma) \land [\alpha](M, \sigma) \) and the semantics of individual entries as follows.

**Statistical Independence.** Shuffle’s independence assumptions assume the conditional statistical independence of two sets of variables in the model. We define the semantics of the independence notation \( \phi \Rightarrow A \perp B \mid C \), meaning that under the constraint \( \phi \) the set of variables \( A \) is \( B \) independent of \( C \) given the values of \( C \), using a standard definition of statistical independence in probability theory. Specifically, the joint density, \( J \), gives a natural specification:

\[
[J(\phi \Rightarrow A \perp B \mid C)](M, \sigma) = [\phi](M, \sigma) \Rightarrow \left( J(A, B \mid C)(M, \sigma) = J(A \mid C)(M, \sigma) \land J(B \mid C)(M, \sigma) \right)
\]
Reachability. The predicate ReachesAll(s) states that a given sampler s reaches every value in its output space with positive probability. In other words, for any variable \((v, n) \in V\), if s modifies \(v, n\), then there must be some positive probability of reaching every value of n in n’s domain.

\[
[\text{ReachesAll}(s)](M, \sigma) = \forall v, n. \left( \exists sr. r. s(\sigma[v \mapsto r], sr)(v, n) \neq r \implies \forall r. \exists sr. s(\sigma, sr)(v, n) = r \right)
\]

Entailment Relation. We define the entailment relation between two assumption logs by the notation and semantics, \(M, L_1 \vdash L_2 = \forall \sigma. \left( \sigma \models M \land [L_1](M, \sigma) \right) \implies [L_2](M, \sigma)\)

Satisfaction Relation. An environment and model satisfy an assumption log if the denotation of the assumption log evaluates to true for the environment. \(\sigma, M \models L = ([L](M, \sigma) = \text{true})\)

5.3 Type Environment and Typing Context

A type environment, \(\Gamma \in (Q \cup X) \rightarrow t\) is a finite map from quantifier variables and distribution variables to types. Note that a type environment differs from a model type environment in that a model type environment only contains bindings for quantifier variables.

Model Environment Entailment. We use the notation \(\Gamma \models \Gamma_m\) to mean the type environment \(\Gamma \in (Q \cup X) \rightarrow t\) entails the model type environment \(\Gamma_m \in Q \rightarrow \Delta\).

\[
\Gamma \models \Gamma_m = \forall q \in \text{dom}(\Gamma_m). \Gamma_m(q) = \Gamma(q)
\]

Environment Satisfaction. We use the notation \(\sigma \models \Gamma, M, L\) to denote when an environment \(\sigma\) satisfies a type context, which consists of an environment \(\Gamma\), a Shuffle model \(M\), and assumption log \(L\). We partition the definition of this relation for environment by first specifying the satisfaction relation for each type of variable that may be present in an environment.

Distribution Variable Satisfaction. The value of a distribution variable in an environment satisfies its type \(t\) when the code definition of the distribution (\(\beta\)) satisfies \(t\).

\[
\sigma, M, \Gamma, L \models x : t \implies \left( \exists q, \delta, \beta. \left( (\sigma(x) = ((q, \delta), \beta)) \land M, \Gamma, L \models \beta : t \right) \right)
\]

In the following section we give precise definitions of the satisfiation relation for each type of code definition (e.g., densities and samplers).

Satisfaction. Given the above definitions, an environment satisfies a model, type environment, and assumption log if the environment has positive joint density (according to its definition via \(f\)) and each of its quantifier variables, random variables, and distribution variables meet their respective satisfaction relations.

\[
\sigma \models \Gamma, M, L = \forall \Gamma_m. \Gamma \models \Gamma_m \land \sigma \models M, \Gamma_m \land \sigma, M \models L \land \\
\forall x \in \text{dom}(\sigma). \sigma, M, \Gamma, L \models x : (\Gamma(x) \land f(M, \sigma) > 0)
\]

5.4 Type Semantics

A type \(t\) in Shuffle is an element of the grammar: \(T \rightarrow \delta \mid (\delta, \delta) \mid \text{Bool} \mid T_x \mid (q, \delta, T_x)\). In this grammar, \(\delta\) is a domain, \(q\) is a quantifier variable, \text{Bool} is the boolean type, and \(T_x\) is a distribution type. This language of types extends the developer-supplied types \(T_x\) as specified in Figure 8 with types Shuffle derives internally.

Definition 5.1 (Density). If \(M, \Gamma, L \models d : \text{density}(A \mid B, \phi)\), then \(\forall \sigma. \left( \sigma \models \Gamma, M, L \land [\phi](\sigma) \right) \implies \left( [d](\sigma) = f(A \mid B)(M, \sigma) \right)\)
A term with sampler type is a function with it is possible to compute the expectation of any positive variables. The function is function is correct if instantiations of the function body are correct. This in a typesafe manner. DMUL takes two densities and multiplies them together pointwise. It converts conditional probability, and give the developer the ability to multiply, divide, and integrate densities. Figure 15 shows the typing rules for probability densities. These follow the rules of Densities.

The Z3 theorem prover [Leonardo De Moura 2008]. details on the formal definition of validity and our implementation of the validity check that uses rules change z. Shuffle’s type rules make use of the predicate M, \( \Gamma \vdash \text{ValidInfer}(A|B, \phi) \). This predicate ensures that the type \( t_\phi(A|B, \phi) \) is valid. For an example of an invalid type, consider the variable set \( z\{i0 \in \text{Dom}: z[i0] == j} \). Integrating a density with respect this variable set would require changing a value of \( z \), but this would in and of itself change the set of integration variables. When type rules change A and B, they must check that the new type is still valid. Appendix A.2 provides more details on the formal definition of validity and our implementation of the validity check that uses the Z3 theorem prover [Leonardo De Moura 2008].

**Figure 15. Type rules for probability densities**

A term \( d \) with type density \( (A|B, \phi) \) is a function that computes the probability that the variables denoted by \( A \) taken on a given set of values when conditioned on \( B \). Given our definition of the semantics of the full model by its joint density, \( J(M, \sigma) \), and the subsequent definition of the conditional density, \( J(A|B) \) (Section 5.1), we directly use the definition of the conditional density to define the semantic judgment for density functions. Specifically, if a term \( d \) satisfies the semantic judgment for density types, then, for all environments that satisfy the type context as well as satisfy the type’s constraint, \( \phi \), then the term computes the conditional density of \( A \) given \( B \).

**Definition 5.2 (Sampler).** If \( M, \Gamma, \mathcal{L} \vdash s : \text{Sampler}(A|B, \phi) \), then
\[
\forall f \in \Sigma_{rv} \rightarrow \mathbb{R}^+, \sigma. \left( \sigma \equiv \Gamma, M, \mathcal{L} \wedge \left[ \phi \right](\sigma) \right) \Rightarrow \int_{sr} f([s]\sigma, sr) = \int_{[A]} f(\sigma) * J(A|B)(M, \sigma)
\]
A term with sampler type is a function with it is possible to compute the expectation of any positive function \( f \) under the distribution \( P(A|B) \).

**Definition 5.3 (Kernel).** If \( M, \Gamma, \mathcal{L} \vdash k : \text{Kernel}(A|B, \phi) \), then
\[
\forall s. M, \Gamma, \mathcal{L} \vdash s : \text{Sampler}(A|B, \phi) \Rightarrow M, \Gamma, \mathcal{L} \vdash s; k : \text{Sampler}(A|B, \phi)
\]
A kernel \( k \) is a function such that for any sampler \( s \) for a given distribution and any positive function \( f \), the expectation of \( f \) under \( s \) is the same as that under the composition of \( s \) with \( k \).

**5.4.1 Quantified Types.** Shuffle exports inference procedures that are functions of quantifier variables. The function is function is correct if instantiations of the function body are correct. This relationship is defined by the equality: \( M, \Gamma, \mathcal{L} \vdash \beta : (q, \delta, t) = M, \Gamma, \mathcal{L} \vdash \beta : t \)

**5.5 Type Rules**

Shuffle’s type rules make use of the predicate \( M, \Gamma \vdash \text{ValidInfer}(A|B, \phi) \). This predicate ensures that the type \( t_\phi(A|B, \phi) \) is valid. For an example of an invalid type, consider the variable set \( z\{i0 \in \text{Dom}: z[i0] == j} \). Integrating a density with respect this variable set would require changing a value of \( z \), but this would in and of itself change the set of integration variables. When type rules change A and B, they must check that the new type is still valid. Appendix A.2 provides more details on the formal definition of validity and our implementation of the validity check that uses the Z3 theorem prover [Leonardo De Moura 2008].

**Densities.** Figure 15 shows the typing rules for probability densities. These follow the rules of conditional probability, and give the developer the ability to multiply, divide, and integrate densities in a typesafe manner. DMUL takes two densities and multiplies them together pointwise. It converts one of the conditioned variables in the first density to a target variable. This assumes that the
The KCOMBINE rule requires a check that the type is valid because it might be the case that, for instance, the set of random variables $A$ depends on the values of random variables in $B$, which would render the type $\text{density}(A, B \mid C, \phi)$ invalid.DDIV divides the first density by the second. This has the effect of converting target variables in the first density to conditioned variables in the new density. The moved variables must be target variables in the second density. DDIV2 enables a developer to convert density over two target variable sets to density over only one of the variable sets. The developer does this by dividing the density by a density for the eliminated target variable, conditioned on the uneliminated target variables. The resulting density is valid because it might be the case that, for instance, the set of random variables $A$ depends on the values of random variables in $B$, which would render the type $\text{density}(A, B \mid C, \phi)$ invalid.  

Kernels. Figure 17 presents the typing rules for kernels. KLIFT constructs a kernel out of a sampler. The constructed kernel’s behavior is the same as the input sampler’s. However, for the sampler to be a valid kernel, two conditions must hold. First, the sampler’s output must be a finite random variable. Second, for each value in the target random variable’s domain, $s$ must have a positive probability of producing that value. Together these properties ensure that every kernel representable in Shuffle admits an approximate implementation of via repeated iteration $\text{fix}$ [David A. Levin 2008]. The type rule enforces the first constraint with the second premise of the rule and the second constraint with the third premise. The type system does not verify $\text{ReachesAll}$. Instead, $\text{ReachesAll}$ must be an implication of the provided assumption log.

KCOMBINE combines two kernels for conditional densities into a kernel for a joint density. Specifically, the two kernels must be conditioned on each other’s target variables. The resulting kernel represents the joint density of each kernel’s output conditioned on any global conditioned variables both kernels have. The KCOMBINE rule requires a check that the type is valid because it might be the case that, for instance, the set of random variables $A$ depends on the values of random variables in $B$, which would render the type $\text{kernel}(A, B \mid C, \phi)$ invalid. KFIX transforms a kernel for into a sampler for the same distribution using the $\text{fix}$ operator.
Definitions and Conditionals. The rules for definitions and conditionals have expected definitions. For clarity of presentation, we present these rules and the remaining rules in Appendix B.

5.6 Properties

Shuffle’s type system guarantees that densities, samplers, kernels, and estimators correctly implement the conditional probability distribution implied by their type. This means that for any type judgment produced by the type rules, the semantics of the type must be true.

Theorem 2 (Soundness). If $M$ is valid, and $M, \Gamma, L \vdash \beta : t$, then for all $D$, $(D, \pi_2(M), \pi_3(M)), \Gamma, L \vdash \beta : t$

We present a proof of this theorem in Appendix D.

6 THE SHUFFLE SYSTEM

Shuffle as a system performs type checking, assumption log generation, and inference program extraction. A developer therefore receives a concrete executable inference procedure that has been type checked against the program’s specified types as well as an auditable list of assumptions about the probabilistic model that must be true for the inference procedure to be correct.

6.1 Type Checking

The Shuffle system implements the type checking rules presented in Section 5. Shuffle uses the Z3 theorem prover [Leonardo De Moura 2008] to check assertions over sets of quantified and random variables. Shuffle models quantified variable values, random variable values, and domain bounds as 64-bit bitvectors, and constraints using a combination of bitvector comparisons and boolean operations. Shuffle checks equality and implication relations between constraints using quantifier-free bitvector theories, and checks type validity assertions through Z3’s quantified bit-vector formulas.

For example, the implementation of callDensAll on Line 9 in Figure 4 invokes the density callDensAll(p-1), which has the target random variable set calls{i in People: i <= (p-1)}. The developer wishes to multiply this density with callDensI, which has a conditioned random variable set that contains the set calls{i in People: i < p}. Shuffle uses Z3 to verify these variable sets are equivalent. Shuffle generates the following constraint to send to Z3:

1. $(\text{People_min} \geq 0 \land \text{People_max} \geq 0)$
2. $(\text{People_min} \leq p \land p \leq \text{People_max})$
3. $(\text{People_min} \leq i \land i \leq \text{People_max})$
4. $(i \leq p - 1) \neq (i < p)$

Z3 tries to find values for each of the bitvectors People_min, People_max, p, and i such that the values satisfy the constraint. If Z3 returned such an assignment, it would mean that there exist values for the variables that demonstrate that the two random variable sets are not equivalent, and Shuffle would terminate with a type error. However, in this case Z3 determines that this constraint is not satisfiable, and thus the variable sets are equivalent.

6.2 Inference Program Extraction.

Shuffle extracts a Python program for a given type-checked Shuffle program. Shuffle’s program extraction is by and large a straightforward, syntax-directed recursive procedure that produces a Python program that implements the denotational semantics presented in Section 4. Shuffle’s extraction procedure differs operationally from the denotational semantics in that it 1) simplifies integral expressions it can identify analytical solutions 2) reports an error when it cannot simplify intractable integral expressions or sample from a density 3) uses a representation for probabilities...
that ensures numerical stability, and 4) performs automatic incremental optimizations. Note that all of these code generation concerns are issues that – without Shuffle – a developer would otherwise have to perform by hand.

**Simplification.** Shuffle used standard algebraic simplification techniques to simplify integrals with known closed-form solutions. Shuffle currently simplifies conjugate and posterior-predictive distributions for Gaussian and Dirichlet distributions.

**Optimization.** Shuffle uses program transformation techniques for synthesizing efficient incremental inference procedures. Currently, Shuffle uses a variant of the algorithm presented in Liu et al. [2005] to incrementalize reduction operations. Generally, the algorithm first identifies two loops (generated by Shuffle’s simplification pass) where the inner loop contains an reduction. It then attempts to hoist the inner loop out, and incrementally updates the value of the hoisted loop when necessary. Shuffle supports a wider class of incremental optimization than Liu et al. [2005]. It identifies non-affine patterns in loop conditions and performs enabling program transformation for further potential incrementalization, which we found common among inference procedures. Note that incrementalization also generalizes Loop Invariant Code Motion, in which case the hoisted loop does not need incremental updates. We discuss an transformation example in Appendix E.

### 7 EVALUATION

Shuffle sits within a landscape of probabilistic programming tools and approaches that range from fully automated systems to systems that encourage handcoded implementations via a built-in library of primitives and – in the extreme – direct implementations in a standard programming language, such as C++. Here, we consider Venture as a reference point for the evaluation. We also include benchmarks compared with BLOG [Milch 2006] in Appendix G as complementary to showing Shuffle’s flexibility.

**Venture.** Venture is a probabilistic programming system that, like Shuffle, supports programmable inference. Venture’s approach makes use of stochastic procedures, which are Python objects that encapsulate complicated density arithmetic. Venture enables developers to manipulate stochastic procedures with modeling commands and inference commands. Modeling commands compose stochastic procedures together to form a probabilistic model, and inference commands use invoke a stochastic procedure’s methods to implement inference procedures. Venture developers hand-write the modeling commands, inference commands, and the contents of stochastic procedures. This is similar to Shuffle, in which developers hand-write the models and inference procedures. However, Venture provides no support for either verifying the correctness of an inference procedure nor automatically generating the code of an implementation. Specifically, in Venture, if a developer seeks to augment Venture with their own inference procedure, they must do so manually in Python.

**Research Questions.** We compare against Venture to evaluate the following research questions:

- **Verification Burden.** What is the annotation overhead for the developer to deliver a typesafe inference procedure, relative to an untyped procedure?
- **Performance.** Do Shuffle’s abstractions increase or decrease performance relative to implementations of the same algorithms within a comparable system?

**Benchmark Models.** To evaluate the first research question, we implement several different inference procedures for several different models. Each of these models has the property that portions of the model can be solved analytically, but practical algorithms rely on combining exact analytical methods with approximate, sampling-based methods.

- **GMM.** A Gaussian mixture model [Murphy 2012]. A GMM models a sequence of samples where each sample has a Gaussian distribution centered around a cluster center. Based on a
dataset size used in prior work [Daniel Huang 2017], this model contains 10000 samples and 10 cluster centers.

- **LDA.** A Latent Dirichlet Allocation model [Blei et al. 2003]. LDA models a sequence of documents by randomly selecting a topic for each word based on a document-specific topic distribution. It then randomly selects each word from a topic-specific word distribution. Based on dataset sizes used in prior work [Newman 2008], this model uses approximately 466k words, 50 topics, 3430 documents and a vocabulary size of 6.9k.

- **DMM.** A Dirichlet Multinomial Mixture model [Holmes et al. 2012]. A DMM models a sequence of documents by randomly selecting a topic for each document, and thereafter selecting each word from a topic-specific word distribution. Based on dataset sizes used in prior work [Turnbaugh et al. 2008], this model contains approximately 570k words, 4 topics, 278 documents and a vocabulary size of 129.

### Benchmark Inference Algorithms

For each benchmark model, we implemented several inference algorithms in Shuffle. We compare Shuffle’s support for these algorithms against Venture’s for Gibbs sampling [Geman and Geman 1984] (a Markov-chain Monte Carlo inference algorithm), Metropolis-Hastings [Hastings 1970; Metropolis et al. 1953] (a Markov-chain Monte Carlo algorithm) and Likelihood weighting [Fung and Chang 1989] (a sequential Monte Carlo algorithm).

#### 7.1 Verification Burden

To quantify Shuffle’s verification burden, we compare the length of Shuffle’s inference procedure against the length of Venture’s stochastic procedure implementation. We also report the number of assertions Shuffle generates in its assumption log for each benchmark.

**Methodology.** We compared the total number of lines of code – model plus inference – in the Venture and Shuffle implementations of each benchmark model and inference algorithm. For GMM in Venture, we included the lines of code for all model definition commands, inference commands, and stochastic procedures we wrote ourselves. For LDA and DMM, our implementations take advantage of pre-built stochastic procedures included in Venture. We report two numbers for these benchmarks: the lines of code we wrote ourselves and the lines of code the Venture developers used to construct the built-in stochastic procedures.

**Results.** Table 1 presents the size in lines of code for both Shuffle and Venture implementations of the benchmarks. The GMM implementations in Shuffle and Venture require similar amounts of code, but LDA and DMM require significantly more code in Shuffle than in Venture, even accounting for the code required to implement the stochastic procedure in Venture. This is primarily due to the fact that Venture enables a developer to reuse a stochastic procedure in multiple places, where as Shuffle does not support reuse and therefore a Shuffle developers need

| Model | Gibbs | Metropolis-Hastings | Likelihood Weighting |
|-------|-------|----------------------|----------------------|
|       | LOC   | Assump.   | LOC   | Assump. | LOC  | Assump. |
| GMM   | 112   | 6/1       | 118   | 7/1       | 86   | 6/0       |
| LDA   | 179   | 13/1      | 196   | 14/1      | 169  | 12/0      |
| DMM   | 180   | 11/1      | 190   | 12/1      | 190  | 11/0      |

**Table 1.** Evaluation of Shuffle’s verification burden. We use the notation $a/b$ in the Venture line count to mean that $a$ is the number of lines of code written by the inference developer and $b$ is the number of lines of code in the stochastic procedures that are built in to Venture. We use the notation $a/b$ in the “Assump.” column to mean that $a$ is the number of independence assertions and $b$ is the number of reachability assertions.
Table 2. Performance of Shuffle compared to Venture. Speedups are speedup of Shuffle over Venture.

| Model   | Gibbs       | Metropolis-Hastings | Likelihood Weighting |
|---------|-------------|----------------------|----------------------|
|         | Unoptimized | Speedup | Unoptimized | Speedup | Unoptimized | Speedup |
| GMM     | 1.3 ms      | 33 ms   | 25x        | 1.7 × 10^{-7} ms | 5.3 ms | 31x        | 7.5 × 10^{-1} s | 16.2 s | 21x |
| LDA     | 6.1 × 10^{-3} s | 10.4 s  | 1700x      | 1.1 × 10^{-2} ms | 270 ms | 2400x      | 45.3 s      | 800 s | 17x |
| DMM     | 1.1 s       | 72 s    | 65x        | 6.8 × 10^{-1} s | 2.1 s  | 3.1x       | 30 s        | 580 s | 19x |

Table 3. Performance of Shuffle without optimization. Speedups are speedup of optimized over unoptimized

to perform density arithmetic from scratch for each density with a unique type. This motivates a future direction for Shuffle that supports polymorphism or higher-order features that enable reuse.

7.2 Performance

To evaluate Shuffle’s performance, we compare the performance of Shuffle’s generated code versus the runtime of the Venture-implemented inference procedures for our benchmarks. A key aim of this evaluation is to demonstrate that our abstractions, which more closely model standard abstractions in probability than standard Python code, do not introduce performance overhead.

7.2.1 Methodology. For each benchmark, we measured wall clock time over 20 runs. We time out benchmarks that did not finish in 30 hours. The Gibbs and Metropolis-Hastings tests measure the time for one Gibbs update to a single random variable. The Likelihood Weighting test measures the time to perform inference on 1 particle. We also measure each benchmark’s peak memory consumption, as reported by `time -v` command. All benchmarks are performed on m5.12xlarge Amazon EC2 instance, which has 192 GB memory. All inference procedures are single threaded, and use only 1 CPU core.

Each benchmark uses synthetically generated observed data from the prior distribution of the statistical model. Because the comparison is between computational efficiencies of identical algorithms, we do not anticipate that changes in the data values alone will have an impact on performance. The size of the datasets are similar in scale to real-world examples of GMM [Daniel Huang 2017], LDA [Newman 2008], DMM [Turnbaugh et al. 2008] models.

7.2.2 Results. Figure 2 present the results of our performance evaluation. The results show that Shuffle’s abstractions do not introduce overhead and that the resulting inference procedures are at least as fast as Venture. In fact, Shuffle’s inference procedures are significantly faster than Venture on all of our benchmarks, with a minimum speedup of 3.1x. We note that this significant speedup is due to Venture’s overhead on manipulating its internal data structures for tracking the incremental updates, which in some cases leads to asymptotic degrade in performance; for DMM-MH, the current implementation of Shuffle fails to perform one potential incremental update, which explains the relatively smaller speedup of 3.1x.

We also measure Shuffle’s performance without incremental optimization. The results in Figure 3 demonstrate incremental optimizations are critical to performance, resulting in at least a 30x speedup over an unoptimized Shuffle program.

Appendix F presents more results on Shuffle’s performance, including standard deviations for performance experiments, peak memory consumption comparisons, and a more detailed discussion of Shuffle’s performance improvement over Venture.
8 RELATED WORK

Automated Inference. Church [Goodman et al. 2008] and WebPPL [Goodman and Stuhlmüller 2014] enable a user to specify Turing-complete stochastic programs as models, but restrict inference algorithms to all-purpose algorithms such as Metropolis-Hastings [Hastings 1970; Metropolis et al. 1953]. JAGS [Plummer 2015] provides a notation for expressing graphical models and automatically performs sampling for a fixed set of distributions. JAGS therefore provides automated support for a subset of Shuffle’s rules. For example, JAGS can automatically generate a collapsed sampler for GMM. However, it can do so only if the model is specified with a monolithic GMM primitive. This stands in contrast to Shuffle, which, via its compositional nature, enables a user to prove the correctness of collapsed sampling for a wide class of models.

Manual Unverified Inference. Other systems, such as Venture [Mansinghka et al. 2014] and PyMC [Patil et al. 2010] enable a user to augment the system’s inference procedure with arbitrary code. However, when the user augments the inference algorithm with arbitrary code, there is no guarantee that the resulting inference algorithm is correct. In contrast, the code that a user generates with Shuffle is in accordance with the Shuffle’s proof rules and therefore enjoys Shuffle’s correctness guarantees. Park et al. developed a language that includes samplers and other objects as first-class primitives [Park et al. 2005]. The type of a term in their language communicates the base type of the object (e.g., a sampler). While, Shuffle shares its base operations with their language, Shuffle’s novel contribution is to extend the types to describe the conditional distribution that the object represents.

Compiled Inference. AugurV2 [Daniel Huang 2017] provides a language of coarse-grained operators to build inference procedures out of, like Shuffle. AugurV2 supports a richer set of kernels than Shuffle. AugurV2 also provides more support for parallelism and alternative compilation targets. However, AugurV2 does not provide correctness guarantees as strong as Shuffle’s. In particular, AugurV2’s kernels are not guaranteed to converge iteratively to the target distribution. AugurV2 also does not have density operations to support collapsed Gibbs samplers. Thus AugurV2 does not support any of the benchmarks from Section 7, although it does support other inference procedures for the GMM and LDA models. Atkinson and Carbin [2016] motivate the need for correct-by-construction probabilistic inference. Shuffle is the first complete system that provides a programming language that moves probabilistic inference towards that goal.

Program Transformation. Hakaru [Narayanan et al. 2016] and related systems [Ścibior et al. 2018] enable developers to perform probabilistic inference by applying transformations to a program that specifies the underlying probabilistic model. The resulting transformed program implements an executable inference procedure for the query of interest. Shuffle’s approach is complementary in that it advocates ground-up composition of inference algorithms from base primitives. In addition, Shuffle’s type system enables developers to explicitly specify the behavior of an inference procedure, as opposed to transformation systems that implicitly specify this behavior outside of the language.

The PSI solver [Gehr et al. 2016b] transforms probabilistic models into densities representing inference procedures. PSI can find densities for a larger class of models than Shuffle, but doesn’t support samplers or kernels.

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A VALIDITY CONDITIONS FOR MODELS AND TYPES

A.1 Model Validity

Variable Set Validity. The variable sets A and B and constraint \( \phi \) in a type \( t_b(A \mid B, \phi) \) can freely depend on the values of random variables and therefore some specifications of A, B, or \( \phi \) may be undefined. A quantified triple of A, B, and \( \phi \) are valid, written \( M, \Gamma_m \models \text{Valid}(A|B, \phi) \) if the following properties hold.

- **Error Free.** Evaluations of \( \phi, B, \) and A must not error.

\[
\forall \sigma. \left( \sigma \models M, \Gamma_m \right) \Rightarrow \left( \llbracket \phi \rrbracket(M, \sigma) \neq \bot_\sigma \land \llbracket A \rrbracket(M, \sigma) \neq \bot_\sigma \land \llbracket B \rrbracket(M, \sigma) \neq \bot_\sigma \right)
\]

- **Stratified Conditioned Variables.** The conditioned set of random variables B in a type must have a total order < on the set of variable names V such that if \( v_i < v_j \), then the subset of \( v_j \) contained in B does not depend on the subset of \( v_j \) contained in B. This ensures that the integral over B in \( \mathcal{J}(A|B) \) is well-defined. For example, consider the variable set \( z[10 \in \text{Dom}: z[10] = j] \). Integrating a function over this variable set would require changing a value of \( z \), but this would change the set of integration variables. By contrast if a total order exists as defined above where \( v_i < v_j \), integrating over B requires integrating over \( v_j \) for every possible value of \( v_i \), and then integrating the resulting function by \( v_i \).

\[
\exists i \in \mathbb{N} \land \forall \sigma, v_1, v_2. \left( i(v_1) < i(v_2) \land \sigma \models M, \Gamma_m \right) \Rightarrow \\
\left( \forall(v_\ast, n_\ast), n_{\text{new}}, \sigma' \right. \\
\left( (v_\ast, n_\ast) \notin [B \cap v_j](M, \sigma) \land \sigma' = \sigma[(v_\ast, n_\ast) \mapsto n_{\text{new}}] \land \sigma' \models M \right) \Rightarrow \\
\llbracket B \cap v_j \rrbracket(M, \sigma) = [B \cap v_j](M, \sigma')
\]

where \( [B \cap v_j](M, \sigma) = \{(v_i, n)(v_i, n) \in [B](M, \sigma)\} \) is the variable set B projected onto the variable name \( v_i \).

- **Computable Constraint.** The constraint \( \phi \) must be computable given the only the values of the conditioned variables B. Therefore any variable that the value of \( \phi \) depends on must be contained in B. This is necessary to ensure integration within an inference procedure is correct. For example, the constraint \( z[i] = \max(\text{Dom}) \) would make Shuffle’s DINT type rule invalid for the program int \( \text{Dens()} \) by \( z[i] \), assuming \( z[i] \) is a target variable of \( \text{Dens()} \).

\[
\forall \sigma, \sigma', v_\ast, n_\ast, n_{\text{new}}. \left( (v_\ast, n_\ast) \notin [B](M, \sigma) \land \sigma' = \sigma[(v_\ast, n_\ast) \mapsto n_{\text{new}}] \land \sigma' \models M \right) \Rightarrow \\
\llbracket \phi \rrbracket(M, \sigma) = \llbracket \phi \rrbracket(M, \sigma')
\]

- **Computable Target Variables.** The random variable set A must be computable given only the values of the conditioned variables B. Therefore any variable that a type uses to constrain the members of A must be contained in B. This is necessary to ensure integration within an inference procedure is correct. For example, if the density \( \text{Dens()} \) has the target variable set \( z \), \( x\{i \in \text{Dom1}: z[i] = \max(\text{Dom2})\} \) would make Shuffle’s DINT type rule invalid for the program int \( \text{Dens()} \) by \( z \).

\[
\forall \sigma, \sigma', v_\ast, n_\ast, n_{\text{new}}. \left( (v_\ast, n_\ast) \notin [B](M, \sigma) \land \sigma' = \sigma[(v_\ast, n_\ast) \mapsto n_{\text{new}}] \land \sigma' \models M \right) \Rightarrow \\
\llbracket A \rrbracket(M, \sigma) = \llbracket A \rrbracket(M, \sigma')
\]
Density Validity. Another example of an invalid model is one where a density does not integrate to 1 over its target random variables, resulting in an invalid probability space. Given a definition of the form $(x, d, (q, \delta), A, B, \phi) \in \pi_3(M)$ we define several validity properties.

- **Self Contained.** A density must only depend on random variables that are in either its target random variable set or conditioned random variable set.

  $\forall \sigma, \sigma', u_*, n_*, n_{new}. \ (u_*, n_*) \notin [A, B](M, \sigma) \land \sigma' = \sigma[u_*, n_*] \mapsto n_{new} \land \sigma' \in M \Rightarrow \left[ [d](M, \sigma) = [d](M, \sigma') \right]$

- **Normalized.** A density must integrate to 1 over its target variables.

  $\forall \sigma, \Gamma_m. \ (\sigma \models M, \Gamma_m[q \mapsto \delta]) \Rightarrow \left( \int_{[A]([\sigma](M))} [d](\sigma) = 1 \right)$

- **Unique.** The quantified semantics of a density defines the density of a random variable at most once for all instantiations of its quantifiers. Namely, given two instantiations of a density’s quantifiers, the sets of target variables corresponding to each instantiation do not intersect.

  $\forall \sigma, \sigma', \Gamma_m. \ (\sigma \models M, \Gamma_m[q \mapsto \delta] \land (\exists n \in [\delta](M). \ \sigma' = \sigma[q \mapsto n]) \land ([A](M, \sigma') \cap [A](M, \sigma) \neq \emptyset) \Rightarrow \sigma' = \sigma$

- **Disjoint.** The variable sets $A$ and $B$ must be disjoint. This enforces that $\int_A J(A|B) = 1$, and is sufficient for ensuring the model is valid.

  $\forall \sigma, \Gamma_m. \ (\sigma \models M, \Gamma_m[q \mapsto \delta]) \Rightarrow \left( [A](M, \sigma) \cap [B](M, \sigma) = \emptyset \right)$

Model Schedulability. For a model to be valid, it must be schedulable. This means there must be an ordering of density-integer pairs $((\eta_0, n_0), (\eta_1, n_1), \ldots, (\eta_n, n_k)) \in H \times N$ such that the conditioned variables in any density definition come before the target variables. If no such ordering exists, the model’s densities can fail to represent the conditional densities implied by their types. For example, if in the Burglary model from Figure 3, the developer had specified two densities $d_1$ and $d_2$ with type density(earthquake), then $J(\text{earthquake}) = J(\text{earthquake}|\emptyset)$ would be equal to $\int (d_1 \times d_2) / \int d_1 \times d_2$ by earthquake. This is not necessarily equal to either $d_1$ or $d_2$, which means Shuffle’s type judgments – which rely on the fact that the type of a density corresponds to its conditional density – would not hold. An ordering $((\eta_0, n_0), (\eta_1, n_1), \ldots, (\eta_n, n_k))$ is a valid schedule if, using the notation $\eta_i = (x_i, d_i, (q_i, \delta_i), A_i, B_i, \phi_i)$

- **Complete:** A schedule $S = ((\eta_0, n_0), (\eta_1, n_1), \ldots, (\eta_n, n_k))$ is complete if all densities in the model and all values of a density’s quantifier variable from the appropriate domain appear in the schedule.

  $\forall \eta_i, n_i. \ (\eta_i \in \pi_3(M) \land n \in [\delta_i](M)) \Rightarrow (\eta_i, n_i) \in S$

- **Serial:** A schedule is $((\eta_0, n_0), (\eta_1, n_1), \ldots, (\eta_n, n_k))$ serial if the conditioned variables for a density $\eta_j$ invoked with parameter $n_j$ are target variables in a previous density in the schedule. Namely, for each variable in $\eta_j$’s conditioned variable set, there exists $\eta_j, n_j$ such that $j < i$ and the variable is in $\eta_j$’s target variable set when $\eta_j$ is invoked with $n_j$.

  $\forall (u, n), \sigma. \ (\sigma \models M(u, n) \in [A_i](M, \sigma[q_i \mapsto n_i]) \Rightarrow (\exists j. j < i \land (u, n) \in [B_j](M, \sigma[q_j \mapsto n_j]))$
• **Linear:** A schedule \( ((\eta_0, n_0), (\eta_1, n_1), \ldots, (\eta_n, n_k)) \) is linear if any random variable appears as a target variable in a density at most once in the schedule. In other words, for every variable there is exactly one \( i \) such that the variable is in \( \eta_i \)'s target variables when invoked with \( n_i \).

\[
\forall (v, n), (\sigma \models M \land n \in \pi_1(\pi_2(M)(v))) \implies (\exists i. (v, n) \in [\mathcal{A}_i](M, \sigma[q_i \mapsto n_i]))
\]

Together these properties ensure that the model’s specification does not prescribe circular dependencies between the model’s random variables.

### A.2 Type Validity

**Inference Variable Set Validity.** Shuffle’s type rules use a variant of variable set validity. The notation for this predicate is \( M, \Gamma \models \text{ValidInfer}(A|B, \phi) \) and it checks the same conditions as the corresponding \( \text{Valid}(A|B, \phi) \), but under any possible instantiation of the domains.

\[
M, \Gamma \models \text{ValidInfer}(A|B, \phi) = \exists \Gamma_m \in (Q \rightarrow \Delta). \Gamma \models \Gamma_m \land \forall D. \pi_2(M), \pi_3(M), \Gamma_m \models \text{Valid}(A|B, \phi)
\]

**Implementation.** Shuffle checks type validity by translating the above condition to constraints and solving it with Z3.

### B ADDITIONAL TYPE RULES

| Rule | Description |
|------|-------------|
| INV  | \[
\frac{M, \Gamma, L \vdash x : q, \delta, t_b(A \mid B, \phi)}{M, \Gamma, L \vdash x(a) : t_b(A \mid B, \phi)[a/q]}
\] |
| IF   | \[
\frac{M, \Gamma, L \vdash \beta_t : t_b(A_t \mid B_t, \phi_t)}{M, \Gamma, L \vdash \beta_f : t_b(A_f \mid B_f, \phi_f)}
\] |

**Variable Set Choice.** We use the notation \( (\phi, A, B) \) to denote a variable set choice, which yields \( A \) when \( \phi \) is true and yields \( B \) when \( \phi \) is false. Variable set choice extends the grammar in Figure 8 with the production \( V_g \rightarrow (\phi, V_g, V_g) \). Its denotation is given by \( \llbracket (\phi, A, B) \rrbracket(\sigma) = \begin{cases} [A](M, \sigma) & \phi(M, \sigma) \\ [B](M, \sigma) & \neg \phi(M, \sigma) \end{cases} \)

| Rule | Description |
|------|-------------|
| DEF  | \[
\frac{M, \Gamma[q \mapsto \delta], L \vdash \beta : t_b(A \mid B, \phi)}{M, \Gamma, L \vdash \text{def } x \ (q \in \delta) : t = \beta : \Gamma[x \mapsto (q, \delta, t_b(A \mid B, \phi \& q \in \delta))]}
\] |
| DEF-REC | \[
\frac{M, \Gamma[q \mapsto \delta][x \mapsto (q', \delta, t_b(A[q'/q] \mid B[q'/q], (\phi[q'/q] \& q' < q))], L \vdash \beta : t_b(A \mid B, \phi)}{M, \Gamma, L \vdash \text{def-rec } x \ (q \in \delta) : t_b(A \mid B, \phi) = \beta : \Gamma[x \mapsto (q, \delta, t_b(A \mid B, \phi \& q \in \delta))]}
\] |
| DEF-IND | \[
\frac{M, \Gamma[q \mapsto \delta], L \vdash \beta : t_b(A \mid B, \phi)}{M, \Gamma, L \vdash \text{def } \text{independent } x \ (q \in \delta) : t = \beta : \Gamma[x \mapsto (q, \delta, t_b(A \mid B, \phi \& q \in \delta))]}
\] |

Fig. 18. Type rules for if statements and invocations.

Fig. 19. Type rules for definitions.
**Conditionals.** Figure 20 shows Shuffle’s IF rule for handling conditionals. This rule enables the developer to construct inference procedures whose behavior differs based on whether a constraint is true or false. The system must check that the resulting type is valid, because the constraint may introduce an illegal dependency in the random variables or the constraint in the resulting type.

We denote standard capture-avoiding substitution on the free quantifier variables of a type \( t \) by the notation \( t[a/q] \) where \( a \) is a term and \( q \) is a quantifier variable.

**Invocation.** Shuffle checks type validity on invocations because for two reasons: 1) A type written by the developer must be valid, and 2) the substitution in the invocation rule (INV Figure 20) may yield an invalid type if, for example, it results in \( A \) depending on the value of a random variable that is not in \( B \).

**Definition.** Figure 20 shows Shuffle’s rules for defining procedures. These give the developer the ability to encapsulate components of the inference procedure while ensuring these components are correctly defined and invoked. We use the notation \( q \in \delta \) as syntactic sugar for the constraint \( \min(\delta) \leq q \land q \leq \max(\delta) \).

**Recursion.** Shuffle’s type system imposes restrictions on recursive programs. The DEF-REC rule in Figure 20 enforces that procedures may only recurse on their first argument, and must pass all other arguments through unchanged. In the DEF-REC rule in Figure 20, we use the notation \( q' \) to mean a fresh quantifier variable.

**Base Case Analysis.** The DEF-REC rule makes use of the base-case predicate \( M, \Gamma \models \text{BaseCase}(q, \delta, A) \) This enforces that a recursive procedure’s base case always corresponds to the set of target random variables \( A \) being empty. This justifies the default base cases in Shuffle’s semantics.

Additional Structural Rules. Figure 20 shows additional structural rules that connect different pieces of Shuffle’s type system together. These include 1) ENV rules that instantiate types from the environment and determine whether Shuffle terms belong to a named domain 2) C, IND, and CIND rules which apply normal and independent coercions CONSTRAINT rules which ensure constraints have the boolean type, 4) the MODEL rule instantiating the types in the model \( M \), which serve as axioms for Shuffle’s type system, and 5) the PROG-COMPOSE rule for composing programs.

**B.1 Coercions**

Figure 21 shows Shuffle’s rules for type coercions.

**Normal Coercions.** Shuffle uses a normal coercion of the form \( t_1 \to t_2 \) to assert that a type judgment \( t_1 \) implies another type judgment \( t_2 \). These require additional predicates that encode logical formulae. Shuffle employs the Z3 theorem prover [Leonardo De Moura 2008] to verify that these predicates are true. These predicates are:

- \( M \models \phi \Rightarrow A \equiv B \). This predicate states that whenever, \( \phi \) is true, the variable sets \( A \) and \( B \) must be equivalent. Shuffle checks this by constructing, for each random variable \( v \) specified by the model \( M \), the formulas \( \phi_{vA} \) and \( \phi_{vB} \) which specify the set of indices \( n \) such that \( (v, n) \in [A](\sigma) \) or \( (v, n) \in [A](\sigma) \), respectively. Shuffle then checks whether \( \phi \Rightarrow (\phi_{vA} \iff \phi_{vB}) \).
- \( M \models \phi_1 \Rightarrow \phi_2 \). This predicate states that the constraints \( \phi_1 \) imply the constraints \( \phi_2 \).
The semantics of each predicate are defined as follows:

- \( M \models \phi \Rightarrow (A \cap B) = \emptyset \). This predicate determines that the variable groups \( A \) and \( B \) are disjoint.

The semantics of each predicate are defined as follows:

\[
\frac{M, \Gamma \vdash \beta : t_1 \quad M \vdash t_1 \rightarrow t_2}{M, \Gamma \vdash \beta : t_2}
\]

\[
\frac{M, \Gamma, \mathcal{L} \vdash p_1 : \Gamma_1 \quad \pi_2(M)(v) = (\delta_1, \delta_2)}{M, \Gamma_1, \mathcal{L} \vdash p_1 : \Gamma_2}
\]

\[
\frac{M, \Gamma, \mathcal{L} \vdash p_1 : \Gamma_2 \quad M, \Gamma \vdash a : \delta_1}{M, \Gamma, \mathcal{L} \vdash +[a] : \delta_2}
\]

\[
\frac{M, \Gamma_0, \mathcal{L} \vdash p_1 : \Gamma_1 \quad M, \Gamma_0, \mathcal{L} \vdash p_2 : \Gamma_2}{M, \Gamma_0, \mathcal{L} \vdash +[a] : \delta_2}
\]

\[
\frac{M, \Gamma, \mathcal{L} \vdash a < : \text{Bool}}{M, \Gamma, \mathcal{L} \vdash \neg \phi : \text{Bool}}
\]

\[
\frac{M, \Gamma, \mathcal{L} \vdash \phi_1 : \text{Bool} \quad M, \Gamma, \mathcal{L} \vdash \phi_2 : \text{Bool}}{M, \Gamma, \mathcal{L} \vdash \phi_1 \cup \phi_2 : \text{Bool}}
\]

\[
\frac{M, \Gamma, \mathcal{L} \vdash \phi_1 : \text{Bool} \quad M, \Gamma, \mathcal{L} \vdash \phi_2 : \text{Bool}}{M, \Gamma, \mathcal{L} \vdash \beta : t}
\]

\[
\frac{M, \Gamma, \mathcal{L} \vdash \phi : \text{Bool}}{M, \Gamma, \mathcal{L} \vdash \beta : t}
\]

\[
\frac{(x, d, (q, \delta), A, B, \phi) \in \pi_3(M)}{M, \Gamma, \mathcal{L} \vdash x : (q, \delta, \text{density}(A | B, \phi \& q \in \delta))}
\]

\[
\frac{M, \Gamma_0 \vdash \phi \Rightarrow A \equiv B \quad \forall \sigma. \sigma \vdash M, \Gamma_m \wedge \lfloor \phi \rfloor (M, \sigma) \Rightarrow (\lfloor A \rfloor (M, \sigma) \equiv \lfloor B \rfloor (M, \sigma))}{M, \Gamma_m \vdash \phi \Rightarrow A \equiv B}
\]

\[
\frac{M, \Gamma_0 \vdash \phi_1 \Rightarrow \phi_2 \quad \forall \sigma. \sigma \vdash M, \Gamma_m \wedge \lfloor \phi_1 \rfloor (M, \sigma) \Rightarrow \lfloor \phi_2 \rfloor (M, \sigma)}{M, \Gamma_m \vdash \phi \Rightarrow (A \cap B) = \emptyset \quad \forall \sigma. \sigma \vdash M, \Gamma_m \wedge \lfloor \phi \rfloor (M, \sigma) \Rightarrow \lfloor A \rfloor (M, \sigma) \cap \lfloor B \rfloor (M, \sigma) = \emptyset}
\]

Fig. 20. Type rules for if statements, definitions, and invocations.

\[
\frac{M, \Gamma, \mathcal{L} \vdash \phi \Rightarrow A \equiv C \quad \pi_2(M_1) \pi_3(M_1) \quad M', \Gamma_m \vdash \phi_2 \Rightarrow B \equiv D}{M', \Gamma_m \vdash \phi \Rightarrow A \equiv C \quad M', \Gamma_m \vdash \phi_1 \Rightarrow \phi_2 \Rightarrow \phi_1}
\]

\[
\frac{M \vdash t_b(A | B, \phi_1) \rightarrow t_b(C | D, \phi_2)}{M \vdash t_b(A | B, \phi) \rightarrow t_b(A | C \cap D, \phi_2)}
\]

\[
\frac{M', \Gamma_m \vdash \phi \Rightarrow A \equiv C \quad M', \Gamma_m \vdash \phi \Rightarrow (A \cap C = \emptyset)}{M \vdash t_b(A | B, \phi) \rightarrow t_b(A | B, \phi)}
\]

Fig. 21. Rules for coercion side predicates.
Independence Coercions. Shuffle uses a normal coercion of the form \( t_1 \rightarrow t_2 \) to assert that a type judgment \( t_1 \) implies another type judgment \( t_2 \). This requires the assumption \( \text{log} \mathcal{L} \) to entail independence amongst certain variables present in \( t_1 \) and \( t_2 \).

C.2 Semantics

Lift. A developer can lift a sampler to an estimator. The resulting estimator always returns the value 1 as the weight of a sampler.

Factor. The factor \( e \) by \( d \) modifies the weight of the estimator \( e \).

Conditionals. The syntax \( \text{if} \ \phi \ \{ \ e_t \ \} \ \{ \ e_f \ \} \) returns the value of the estimator \( e_t \) if the constraint \( \phi \) is true, and that of \( e_f \) if the constraint is false.

Invocation. The syntax \( x(\hat{a}) \) invokes an estimator named \( x \) that exists in the environment. The call evaluates the estimator in an environment where the quantified variables are rebound to their parameters \( \hat{a} \).

C.3 Types

Statement. An estimator is a function that produces a sample and corresponding weight such that the expectation of a positive function \( f \) under the estimator is correct. An estimator must also preserve the model relation on the sample portion of its output.
Definition C.1 (Estimator). if \( M, \Gamma, L \vdash e : \text{estimator}(A | B, \phi) \) then for all \( \sigma \) such that \( \sigma \vdash \Gamma, M, L \), and any \( f \in \Sigma_{rv} \to \mathbb{R}^+ \),

\[
\begin{align*}
\llbracket \phi \rrbracket(M, \sigma) \Rightarrow & \int_{sr} \pi_1([e](M, \sigma, sr)) * f(\pi_2([e](M, \sigma, sr))) = \\
& \int_{[A](M, \sigma)} f(\sigma) * J(A|B)(M, \sigma)
\end{align*}
\]

and

\[
\llbracket \phi \rrbracket(\sigma) \Rightarrow \pi_1([e](M, \sigma, sr)) \vdash C, \Gamma, L
\]

Type Rules. Figure 23 shows the typing rules for estimators. These give the developer the ability to conduct likelihood weighting. The EFACT rule requires a check that the type is valid because it might be the case that, for instance, the set of random variables \( C \) depends on the values of random variables in \( A \), which would render the type \( \text{estimator}(A | B, C, \phi) \) invalid.

D PROOFS

This appendix is structured as follows: in Section D.1 we establish two lemmas we require to complete the proofs; in Section D.2 we establish the model validity theorem; in Sections D.3, D.4, D.5, D.6, and D.7 we prove the soundness of densities, samplers, kernels, estimators, and structural rules, respectively; and in Section D.8 we establish the preservation theorem.

D.1 Preliminaries

Integration by Substitution. The following proofs make use of a property of integrals known as the substitution rule. For measurable functions \( f \) and \( g \),

\[
\psi(r) = \int_{x \in [-\infty, r]} g(x) \Rightarrow \int_{x \in \psi[S]} f(x) = \int_{x \in S} f(\psi(x)) * g(x)
\]

where the notation \( \psi[S] \) means the set obtained by mapping the function \( \psi \) over \( S \). This is a standard property of integration.

Environment-Substitution Lemma. The following proofs make use of a lemma. Let \( A \) be a variable set and \( \phi \) be a constraint. We have the following equivalences, for any environment \( \sigma \):

\[
[A[a/q]](\sigma) = [A](\sigma[q \mapsto [a](\sigma))][\phi[a/q]](\sigma) = [\phi](\sigma[q \mapsto [a](\sigma))
\]

Proof. This lemma follows from structural induction on the syntax of constraints and variable sets.
D.2 Model Validity

From the definition of $\mathcal{J}$, it must be true that

$$\mathcal{J}(A|B) = \frac{\int_{V-(\{A\} \cup \{B\})} \prod_i \begin{cases} [d_i](\sigma) & \text{else} \\ [\phi_i](\sigma) & \text{else} \end{cases}}{\int_{V-\{B\}} \prod_i \begin{cases} [d_i](\sigma) & \text{else} \\ [\phi_i](\sigma) & \text{else} \end{cases}}$$

There exists some $i^*$ such that $d_{i^*} = d$ and $\phi_{i^*} = \phi$. We can partition the product in the above expression based on the schedule every valid model must have:

$$\mathcal{J}(A|B) = \frac{\int_{V(<i^*)-\{B\}} \prod_i \begin{cases} [d_i](\sigma) & \text{else} \\ [\phi_i](\sigma) & \text{else} \end{cases} * [d](M,\sigma) * \prod_{i > i^*} \begin{cases} [d_i](\sigma) & \text{else} \\ [\phi_i](\sigma) & \text{else} \end{cases}}{\int_{(V < k)-\{B\}} \prod_i \begin{cases} [d_i](\sigma) & \text{else} \\ [\phi_i](\sigma) & \text{else} \end{cases} * [d](M,\sigma) * \prod_{i \geq i^*} \begin{cases} [d_i](\sigma) & \text{else} \\ [\phi_i](\sigma) & \text{else} \end{cases}}$$

In the numerator, every element of the product over $i$ where $i > i^*$ integrates to one over its target variables, and in the denominator, every element of the product over $i$ where $i \geq i^*$ integrates to one over its target variables. Using the notation $V < k$ to mean the subset of $V = V \times \mathbb{N}$ whose requisite target set in $H$ (the existence of which mandated module schedule linearity), $A_i$, is such that $i < k$, the expression simplifies to

$$\mathcal{J}(A|B) = \frac{\int_{(V < i^*)-\{B\}} [d](M,\sigma) * \prod_{i < i^*} \begin{cases} [d_i](\sigma) & \text{else} \\ [\phi_i](\sigma) & \text{else} \end{cases}}{\int_{(V < k)-\{B\}} \prod_{i < i^*} \begin{cases} [d_i](\sigma) & \text{else} \\ [\phi_i](\sigma) & \text{else} \end{cases}}$$

The expression $[d](M)(\sigma)$ is independent of $(V < i^*) - \{B\}(M,\sigma)$, so we can pull it out of the integral and cancel the remaining factors.

D.3 Density Soundness

Recall the density soundness theorem:

if $M$, $\Gamma$, $L \vdash d : \text{density}(A \mid B, \phi)$, then $M$, $\Gamma$, $L \vDash d : \text{density}(A \mid B, \phi)$

**Proof.** The proof follows from induction on the derivations. Specific rules are outlined below:

**MODEL.** Because $[q \in \delta](M,\sigma) \Rightarrow [q](\sigma) \in [\delta](M)$, we can apply Theorem 1.

**DMUL.** The rule is sound due to the following property of $\mathcal{J}$ (we have elided the parameters $M,\sigma$ for clarity)

$$\mathcal{J}(A|B,C)\mathcal{J}(B|C) = \frac{\int_{V-(A \cup B \cup C)} \mathcal{J}}{\int_{V-(B \cup C)} \mathcal{J}} \left( \frac{\int_{V-(B \cup C)} \mathcal{J}}{\int_{V-C} \mathcal{J}} \right) = \frac{\int_{V-(A \cup B \cup C)} \mathcal{J}}{\int_{V-C} \mathcal{J}} = \mathcal{J}(A,B|C)$$

**DDIV.** Applying the identity from DMUL in reverse, it must be true that

$$\mathcal{J}(A|B,C)\mathcal{J}(B|C) = \mathcal{J}(A,B|C) \Rightarrow$$

$$\mathcal{J}(A|B,C) = \frac{\mathcal{J}(A,B|C)}{\mathcal{J}(B|C)}$$
which justifies the basic rule construct.

**DDIV2.** From the identity in DMUL, it must be true that

\[ J(A|B,C)J(B|C) = J(A|B|C) \Rightarrow \]

\[ J(B|C) = \frac{J(A,B|C)}{J(A|B,C)} \]

which justifies the basic rule construct.

**DINT.** This rule relies on the following simplification of \( J \):

\[ \int_A J(A,B|C) = \int_A \frac{\int_{V-(A\cup B\cup C)} J}{\int_{V-C} J} = \frac{\int_A \int_{V-(A\cup B\cup C)} J}{\int_{V-C} J} = \frac{\int_{V-(B\cup C)} J}{\int_{V-C} J} = J(B|C) \]

The second step above is justified by the fact that \( A \cap C = \emptyset \), so the denominator is a constant with respect to the outer integral.

### D.4 Sampler Soundness

**Theorem D.1 (Sampler Preservation).** If \( \mathcal{M}, \Gamma, \mathcal{L} \vdash s : \text{sample}(A \mid B, \phi) \), then \( \forall \sigma. (\sigma \vdash \Gamma, \mathcal{M}, \mathcal{L} \land \llbracket \phi \rrbracket(\sigma)) \Rightarrow (\forall sr. [s](\sigma, sr) \vdash \Gamma, \mathcal{M}, \mathcal{L}) \)

**Proof.** Proceed by induction on the structure of type derivations. In the case of SLIFT, note that since \( \int_{[A]}(\mathcal{M}, \sigma) J(A|B)(\mathcal{M}, \sigma) = 1 \), so the returned value \( r \) can never be larger than the maximum of the target set of the variable being sampled. In the case of SBIND, apply the inductive hypotheses.

Recall the sampler soundness theorem:

if \( \mathcal{M}, \Gamma, \mathcal{L} \vdash d : \text{sample}(A \mid B, \phi) \), then

\( \mathcal{M}, \Gamma, \mathcal{L} \vdash d : \text{sample}(A \mid B, \phi) \)

**Proof.** The proof follows from structural induction on the type rules which may produce samplers. Individual cases are outlined below.

**SLIFT.** In the discrete case, notice that the size of the set

\[ \{sr[[v[a]] := \text{sample } d](\mathcal{M}, \sigma[[v, [a](\mathcal{M}, \sigma)) \mapsto n])\} \]

is exactly \( [d](\mathcal{M}, (v, [a](\mathcal{M}, \sigma)) \mapsto n) \), and furthermore each such set is disjoint for different values of \( a \). Therefore, the integral over \( sr \) is a linear combination over these different cases:

\[ \int_{sr} f([s](\mathcal{M}, \sigma)) = \sum_n [d](\mathcal{M}, \sigma[[v, a](\mathcal{M}, \sigma) \mapsto n]) * f(n) \]

which is exactly \( \int_{[A]}(\sigma)f * J(A|B)(\mathcal{M}, \sigma) \) in this case.

In the continuous case, the sample returned must be a real value \( r \) such that

\[ sr = \int_{x \in [a]} [d](\mathcal{M}, \sigma[[v, a](\mathcal{M}, \sigma) \mapsto x]) = g(r) \Rightarrow \int_{sr} f([s](\sigma)) = \int_{sr} f(g^{-1}(sr)) \]

Substituting \( g \) for \( \psi \) and \( f \circ g^{-1} \) for \( f \) in the definition for the substitution rule, it holds that

\[ \int_{sr} f([s](\mathcal{M}, \sigma, sr)) = \int_{[A](\mathcal{M}, \sigma)} f(\sigma) * [d](\mathcal{M}, \sigma) = \int_{[A](\mathcal{M}, \sigma)} f(\sigma) * J(A|B)(\mathcal{M}, \sigma) \]

where the above step is due to the soundness theorem for densities.
SBIND.. First, apply the soundness assumption for \( s_1 \) to find the expectation of the function \( s_1 \circ f \). Then, use the assumption soundness assumption on \( s_2 \). This yields the equation

\[
\int_{s_0, s_1} f([s_1](M, [s_1](M, \sigma, s_0), s_1)) =
\]

\[
\int_{[A]} f(\sigma) \ast \mathcal{J}(A|B)(M, \sigma) \ast \mathcal{J}(B|C)(M, \sigma)
\]

Using the identity from DMUL, this simplifies to

\[
\int_{[A]} f(\sigma) \ast \mathcal{J}(A, B|C)(M, \sigma)
\]

D.5 Kernel Soundness

Recall the kernel soundness theorem:

if \( M, \Gamma, L \vdash k : \text{kernel}((A | B, \phi) \rightarrow A, \Gamma, \sigma \rightarrow (A | B, \phi) \rightarrow \text{kernel}(A | B, \phi) \)

Proof. The proof follows from structural induction on the rule derivations for kernels. We strengthen the inductive hypothesis with the proposition

\( M, \Gamma, L \vdash d : \text{kernel}((A | B, \phi) \rightarrow M, \Gamma, \sigma \vdash d : \text{kernel}(A | B, \phi) \)

The specific cases are outlined below.

KLIFT.. This is equivalent to the statement that if \( s \) is a sampler, then \( \text{fix} x s \equiv s \). In other words, for any measurable function \( f \) over the output space, the equation

\[
\int_{s} f(\text{fix}(\sigma, s)) = \int_{s, s'} f(\text{fix}(s(\sigma, s'), s))
\]

is satisfied for \( \text{fix} = s \). To see this, inline the definition for a sampler, which reduces the soundness property to the equation

\[
\int_{[A]} f(\sigma) \ast \mathcal{J}(A|B)(M, \sigma) = \int_{[A]} \mathcal{J}(A|B)(M, \sigma) \int_{[A]} f(\sigma) \mathcal{J}(A|B)(M, \sigma)
\]

which must hold because \( \int_{A} \mathcal{J}(A|B) = 1 \).

KCOMBINE.. First, we will show that \( k_1 \) is invariant for the distribution \( A, B|C \). This is true because, for a sampler \( s \) such that

\[
\int_{s} f(s(M, \sigma, s)) = \int_{[A, B]} f(\sigma) \ast \mathcal{J}(A, B|C)(M, \sigma)
\]

because of the property from DMUL, it must be true that

\[
\int_{s} f(s(M, \sigma, s)) = \int_{[A, B]} (f(\sigma) \ast \mathcal{J}(B|C)(M, \sigma)) \ast \mathcal{J}(A|B, C)(M, \sigma)
\]

Substituting in \( f \ast \mathcal{J}(B|C) \) for \( f \) in the soundness assumption for \( k_1 \), it must hold that

\[
\int_{s_0, s_1} f(k_1(s(M, \sigma, s_0), s_1)) = \int_{[A, B]} (f(\sigma) \ast \mathcal{J}(B|C)(M, \sigma)) \ast \mathcal{J}(A|B, C)(M, \sigma)
\]

Using again the identity from DMUL, this means that

\[
\int_{s_0, s_1} f(k_1(s(\sigma, s_0), s_1)) = \int_{[A, B]} f(\sigma) \ast \mathcal{J}([A, B](\sigma) [C](\sigma))(\sigma)
\]
completing the proof of the invariance property of $k_1$. By a similar logic, $k_2$ is also invariant for the distribution $A, B|C$. This means that $k_1$ and $k_2$ is invariant for the distribution $A, B|C$.

D.6 Estimator Soundness
Recall the estimator soundness theorem:

$\mathcal{M}, \Gamma, \mathcal{L} \vdash e : \text{estimator}(A \mid B, \phi) \Rightarrow \mathcal{M}, \Gamma, \mathcal{L} \vdash e : \text{estimator}(A \mid B, \phi)$

**Proof.** The proof follows from structural induction on the rules which may produce estimators. Individual cases are outlined below.

**ELIFT.** Since the first element of $e$ is defined to be 1 in all cases the expression,

$$\mathbb{E} \phi(\mathcal{M}, \sigma) \Rightarrow \int_{sr} \frac{\pi_1([e](\mathcal{M}, \sigma, sr)) f(\pi_2([e](\mathcal{M}, \sigma, sr)))}{\int_{sr} \pi_2([e](\mathcal{M}, \sigma, sr))}$$

can be simplified to $\int_{sr} \frac{f([s](\mathcal{M}, \sigma, sr))}{\int_{sr} 1} = \int_{sr} f([s](\mathcal{M}, \sigma, sr))$ which, according to the correctness of the sampler, must equal the expression $\int_{[\mathcal{A}]} f(\sigma) = \mathcal{J}(\mathcal{A} B)(\mathcal{M}, \sigma)$ as required.

**EFACT.** We use the estimator $e$ to estimate two functions, $\mathbb{E} f$ and $\mathbb{E} d$, and take the ratio. This yields the equation

$$\frac{\int_{sr} [d]([e](\mathcal{M}, \sigma, sr)) f([e](\mathcal{M}, \sigma, sr)) + \pi_1([e](\mathcal{M}, \sigma, sr))}{\int_{sr} \pi_1([e](\mathcal{M}, \sigma, sr))} = \frac{\int_{[\mathcal{A}]} f(\sigma) = \mathcal{J}(\mathcal{A} B)(\mathcal{M}, \sigma) \mathcal{J}(\mathcal{A} B)(\mathcal{M}, \sigma)}{\int_{[\mathcal{A}]} \mathcal{J}(\mathcal{A} B)(\mathcal{M}, \sigma)}$$

We note that the left hand side of this equation simplifies to $\mathbb{E} f$ by $d([\mathcal{M}, \sigma, sr]$ and the right hand side simplifies to $\mathcal{J}(\mathcal{A} B, C)(\mathcal{M}, \sigma)$

D.7 Structural Rule Soundness

**IF.** The soundness of conditionals follows from the fact that, if $\sigma$ is such that $\mathbb{E} \phi_i(\mathcal{M}, \sigma)$ is true,

$$\mathcal{M}, \Gamma, \mathcal{L} \vdash \beta : T_b((\phi_i, A_t, A_e) \mid (\phi_i, A_t, B_t), (\phi_i \& \& \phi_t) \mid (\neg \phi_i \& \& \phi_e))$$

$$\iff \mathcal{M}, \Gamma, \mathcal{L} \vdash \beta : T_b(A_t \mid B_t, \phi_t)$$

Otherwise, if $\sigma$ is such that $\mathbb{E} \phi_i(\mathcal{M}, \sigma)$ is false, it must be true that

$$\mathcal{M}, \Gamma, \mathcal{L} \vdash \beta : T_b((\phi_i, A_t, A_e) \mid (\phi_i, A_t, B_t), (\phi_i \& \& \phi_t) \mid (\neg \phi_i \& \& \phi_e))$$

$$\iff \mathcal{M}, \Gamma, \mathcal{L} \vdash \beta : T_b(A_e \mid B_e, \phi_e)$$

**INV.** This follows directly from the assumption that $\sigma \not\models \mathcal{M}, \Gamma, \mathcal{L}$.

C. Writing the types $t_1$ and $t_2$ as $T_b(A_1 \mid B_1, \phi_1)$ and $T_b(A_2 \mid B_2, \phi_2)$, respectively, the added assumptions mean that, for any $\sigma$, $[A_1] = [A_2]$, $[B_1] = [B_2]$, and $[\phi_1](\mathcal{M}, \sigma) \Rightarrow [\phi_2](\mathcal{M}, \sigma)$. This means that the soundness of the judgment $\mathcal{M}, \mathcal{L} \vdash \beta : t_1$ implies the soundness of the judgment $\mathcal{M}, \mathcal{L} \vdash \beta : t_2$. 

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CIND.. Writing the types \( t_1 \) and \( t_2 \) as \( T_b(A \mid B, \phi) \) and \( T_b(A \mid B, C, \phi) \), respectively, the added assumptions mean that, for any \( \sigma \), \( \mathcal{J}(C,A|B)(M, \sigma) = \mathcal{J}(C|B)(M, \sigma) \ast \mathcal{J}(A|B)(M, \sigma) \) which, applying the identity from the DMUL case, means \( \mathcal{J}(A|B,C)(M, \sigma) = \mathcal{J}(A|B)(M, \sigma) \).

D.8 Preservation

In this section, we prove the following property, which states that definitions preserve the satisfaction relation for environments. Specifically, for any type rule that produces a new type environment, if the original environment satisfies type environment, then the environment prescribed by the semantics satisfies the new type environment.

**Theorem 3 (Preservation).** If \( M \) is valid, \( \sigma \vdash \Gamma, M, \mathcal{L} \) and \( M, \Gamma, \mathcal{L} \vdash p : \Gamma' \), then \( \langle p \rangle(M, \sigma) \vdash \Gamma', M, \mathcal{L} \).

**Proof.** Proceed by induction on the structure of derivations for types.

**DEF and DEF-IND.** Because \( \langle \phi \& q \in \delta \rangle(M, \sigma) \Rightarrow \langle q \rangle(\sigma) \in \langle \delta \rangle(M) \)

\[ \sigma \vdash \Gamma, M, \mathcal{L} \land M, \Gamma[q \mapsto \delta], \mathcal{L} \vdash \beta : t_b(A \mid B, \phi) \]

\[ \Rightarrow \sigma[x \mapsto (q, \delta, \beta)] \vdash M, \Gamma[x \mapsto (q, \delta, t_b(A \mid B, \phi) \& q \in \delta)]], \mathcal{L} \]

**DEF-REC.** First, we show that \( M, \Gamma[q \mapsto \delta], \mathcal{L} \vdash \beta : t_b(A \mid B, \phi) \). We proceed by strong induction on \( q \).

- **Base Case.** If \( \langle q \rangle(\sigma) < \langle \min(\delta) \rangle(M) \), then because \( \mathcal{J}(\emptyset|B)(M, \sigma) = 1 \), \( M, \Gamma, \mathcal{L} \vdash \beta : t_b(A \mid B, \phi) \).
- **Inductive step.** The inductive step derives directly from the rule assumption involving \( \beta \):

\[ M, \Gamma[q \mapsto \delta][x \mapsto (q', \delta, t_b(A[q'/q] \mid B[q'/q], (\phi[q'/q]) \& q' < q)], \mathcal{L} \vdash \beta : t_b(A \mid B, \phi) \]

The remainder of the proof follows from the same logic in the DEF case that \( \langle \phi \& q \in \delta \rangle(M, \sigma) \Rightarrow \langle q \rangle(\sigma) \in \langle \delta \rangle(M) \).

**E Optimization Example**

An simplified example transformation is shown in Figure 24. The original program in Figure 24a has asymptotic complexity \( O(N^2) \), while the program in Figure 24b has complexity \( O(N) \). Shuffle’s
optimization pass identifies loop pair patterns like the above and greedily performs this optimization. Therefore, an optimized inference algorithm generated by Shuffle can have significantly better asymptotic complexity. Table 3 illustrates such effect.

**F PERFORMANCE DISCUSSION**

The performance tradeoffs between Shuffle and Venture are primarily due to incremental optimization opportunities. For example, in the Gaussian mixture model, an efficient inference procedure would maintain statistics regarding the number and sum of samples attributed to a given cluster center. When the inference procedure modifies the cluster assignment, it incrementally updates these statistics instead of computing them from scratch.

Venture facilitates incremental optimizations through its stochastic procedure interface. When a developer defines a stochastic procedure, he or she must implement methods that add or remove observations of the procedure’s output. Venture’s runtime builds a computation graph of stochastic procedures, and traverses this graph to determine which stochastic procedures require updates. For example, in the Gaussian mixture model, each cluster forms a stochastic procedure, and when the cluster assignment of a sample changes – meaning a sample is moved from one cluster to another – the runtime calls the update methods on the appropriate clusters, which in turn update their internal statistics regarding the number and sum of the samples in a given cluster. We hypothesize Venture’s computation graph contributes to its slow performance on LDA with Gibbs and Metropolis-Hastings. LDA is a larger model than GMM, and Gibbs and Metropolis-Hastings require more graph manipulation operations than Likelihood Weighting. We have noticed that on these benchmarks, Shuffle’s performance remains constant when varying the corpus size. On the other hand, Venture manifests sublinear scaling on LDA-{Gibbs, MH} benchmarks, which causes magnitudes of performance ratio compared to Shuffle. We suspect that Venture’s complicated data structure operations cause the run time to depend on the size of the corpus, whereas Shuffle’s lean data structures do not have this dependence. Specifically, from profiling we observed that Venture deepcopies its internal datastructure every sampling step which accounts for approximately 90 percent of the run time on these two benchmarks. The high memory usage of Venture also justifies that the data structure manipulations Venture leverages for performing incremental updates bottleneck the inference procedure’s performance.

In contrast, Shuffle requires developers to express their inference procedures with density arithmetic. While the resulting procedure computes the same statistics as the corresponding Venture stochastic procedure, the natural way to compile a Shuffle procedure is to recompute the statistics

| Model  | Shuffle | Venture | Ratio | Shuffle | Venture | Ratio | Shuffle | Venture | Ratio |
|--------|---------|---------|-------|---------|---------|-------|---------|---------|-------|
| GMM    | 3.3 × 10^{-2} ms | 8.3 × 10^{-1} ms |       | 3.5 × 10^{-1} ms | 8.9 × 10^{-1} ms |       | 7.8 × 10^{-4} s | 1.8 s |
| LDA    | 5.2 × 10^{-5} s  | 4.1 × 10^{-2} s  |       | 3.5 × 10^{-2} ms | 5.3 ms            |       | 1.2 × 10^{-1} s | 2.3 × 10^{1} s |
| DMM    | 1.1 × 10^{-2} s  | 1.5 × 10^{1} s   |       | 4.7 × 10^{-2} s  | 5.4 × 10^{-1} s   |       | 1.1 s    | 1.3 × 10^{1} s |

Table 4. Standard deviation for measurements in Table 2

| Model  | Gibbs | Metropolis-Hastings | Likelihood Weighting |
|--------|-------|----------------------|----------------------|
| GMM    | 53x   | 53x                  | 56x                  |
| LDA    | 533x  | 516x                 | 551x                 |
| DMM    | 511x  | 511x                 | 649x                 |

Table 5. Peak memory consumption. Ratios are computed as Venture over Shuffle.
Table 6. Microbenchmarks we have implemented in Shuffle.

| Benchmark          | Shuffle | BLOG |
|--------------------|---------|------|
| Burglary           | 19      | 13   |
| Context-Specific Inference | 14  | 11   |
| Healthiness        | 48      | 31   |
| Hurricane          | 22      | 21   |
| Weather            | 31      | 17   |

(a) Microbenchmark models, measuring lines of code for both Shuffle and BLOG.

from scratch. For example, in the Gaussian mixture model, the developer uses multiplication, division, and integration to compute conditional probability distributions pertaining to an individual cluster. Shuffle recognizes subexpressions of this computation as having a closed-form solution, and replaces these with expressions that compute counts and sums of the samples. As an additional step, Shuffle optimizes the procedure, translating it to an equivalent form that maintains values for subexpressions and incrementally updates them. Shuffle currently cannot optimize all possible subexpressions in the DMM model, which is the reason for its sporadic performance on this model.

Lastly, Shuffle without optimization scales poorly, and suffers orders of magnitude slow down when compared to Shuffle with optimization. This behavior re-confirms our hypothesis on the importance of incremental optimization.

Other Considerations. Another factor contributing to Shuffle’s relative performance over Venture is the fact that Venture performs dynamic checks to ensure the values of the random variables belong to the proper domain, whereas Shuffle’s type system makes this unnecessary.

G MORE ON BENCHMARKS

BLOG. BLOG is a probabilistic programming language that is designed to handle identity uncertainty, wherein the probabilistic model admits uncertainty regarding the source of an observation. We compare BLOG models to Shuffle models, but do not compare BLOG’s inference to Shuffle’s inference. BLOG developers write models by hand but use BLOG’s inference compiler [Wu et al. 2016] to generate inference procedures. By contrast, Shuffle developers write both the model and inference procedure by hand.

Shuffle is less expressive than BLOG and Venture in that Shuffle only supports models with finite size, whereas BLOG and Venture models may be statically unbounded. We note that even though Shuffle models must be bounded in size, that bound need not be specified at type checking time. Type checking results hold for all runtime instantiations of the model’s domains.

Microbenchmarks. To demonstrate Shuffle’s ability to represent a variety of statistical models and inference procedures, we ported examples from the BLOG and Venture probabilistic programming systems [Mansinghka et al. 2014; Milch 2006].

Table 6 lists the microbenchmarks we have implemented. For the BLOG microbenchmarks in Table 6a, we reimplemented each BLOG model as a Shuffle model. For the Venture microbenchmarks in Table 6b, we implemented a Shuffle inference procedure that performs the sampling method of an equivalent Venture stochastic procedure. For the conjugate models we consider here, this corresponds to sampling a new observation conditioned on a set of previous observations from the model.
G.1 Verification Burden

G.1.1 Methodology. To quantify the verification burden for the microbenchmarks, we compared the length of Shuffle models against that of BLOG models and the length of Shuffle’s inference procedure against the length of Venture’s stochastic procedure implementation.

G.1.2 Results. Tables 6 and 6b present the size of the microbenchmarks as implemented in each system. Shuffle requires more lines of code to represent a probabilistic model than BLOG due to Shuffle’s additional type annotations. Shuffle requires fewer lines of code to implement these inference procedures than in Venture because Venture’s stochastic procedure interface requires the developer to implement methods that are unnecessary for these particular inference tasks. By contrast, Shuffle developers only have to implement the densities that are required.