Extending Stan for Deep Probabilistic Programming

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Stan is a popular declarative probabilistic programming language with a high-level syntax for expressing graphical models and beyond. Stan differs by nature from generative probabilistic programming languages like Church, Anglican, or Pyro. This paper presents a comprehensive compilation scheme to compile any Stan model to a generative language and proves its correctness. This sheds a clearer light on the relative expressiveness of different kinds of probabilistic languages and opens the door to combining their mutual strengths. Specifically, we use our compilation scheme to build a compiler from Stan to Pyro and extend Stan with support for explicit variational inference guides and deep probabilistic models. That way, users familiar with Stan get access to new features without having to learn a fundamentally new language. Overall, our paper clarifies the relationship between declarative and generative probabilistic programming languages and is a step towards making deep probabilistic programming easier.

1 INTRODUCTION

Probabilistic Programming Languages (PPLs) are designed to describe probabilistic models and run inference on these models. There exists a variety of PPLs [Bingham et al. 2019; Carpenter et al. 2017; De Raedt and Kersting 2008; De Raedt et al. 2007; Goodman et al. 2008; Goodman and Stuhlmüller 2014; Lunn et al. 2009; Mansinghka et al. 2014; McCallum et al. 2009; Milch et al. 2005; Murray and Schön 2018; Pfeffer 2001, 2009; Plummer et al. 2003; Tolpin et al. 2016; Tran et al. 2017]. Declarative Languages like BUGS [Lunn et al. 2009], JAGS [Plummer et al. 2003], or Stan [Carpenter et al. 2017] focus on efficiency, constraining what can be expressed to a subset of models for which fast inference techniques can be applied. This family enjoys broad adoption by the statistics and social sciences communities [Carlin and Louis 2008; Gelman and Hill 2006; Gelman et al. 2013]. Generative languages like Church [Goodman et al. 2008], Anglican [Tolpin et al. 2016], WebPPL [Goodman and Stuhlmüller 2014], Pyro [Bingham et al. 2019], and Gen [Cusumano-Towner et al. 2019] focus on expressivity and allow the specification of intricate models with rich control structures and complex dependencies. Generative PPLs are particularly suited for describing generative models, i.e., stochastic procedures that simulate the data generation process. Generative PPLs are increasingly used in machine-learning research and are rapidly incorporating new ideas, such as Stochastic Gradient Variational Inference (SVI), in what is now called Deep Probabilistic Programming [Bingham et al. 2019; Tran et al. 2017].

While the semantics of probabilistic languages have been extensively studied [Gordon et al. 2014; Gorinova et al. 2019; Kozen 1981; Staton 2017], to the best of our knowledge little is known about the relation between the two families. Unfortunately, while one might think that there is a simple 1:1 translation from Stan to generative languages, it is not that easy. We show that such a translation would be incorrect or incomplete for a set of subtle but widely-used Stan features, such as left expressions or implicit priors. In contrast, this paper formalizes the relation between Stan and generative PPLs and introduces, with correctness proof, a comprehensive compilation scheme that can be used to compile any Stan program to a generative PPL. This makes it possible to leverage the rich set of existing Stan models for testing, benchmarking, or experimenting with new features or inference techniques.
In addition, recent probabilistic languages offer new features to program and reason about complex models. Our compilation scheme combined with conservative extensions of Stan can be used to make these benefits available to Stan users. As a proof of concept, this paper shows how to extend Stan with support for deep probabilistic models by compiling Stan to Pyro. Besides supporting neural networks, our Stan extension (dubbed DeepStan) also introduces a polymorphic type system for Stan. This type system together with a tensor shape analysis allows programmers to omit redundant tensor sizes of dimensions, leaving them to the compiler to deduce. DeepStan has the following advantages: (1) Pyro is built on top of PyTorch [Paszke et al. 2017]. Programmers can thus seamlessly import neural networks designed with the state-of-the-art API provided by PyTorch. (2) Variational inference was central in the design of Pyro. Programmers can easily craft their own inference guides to run variational inference on deep probabilistic models. (3) Pyro also offers alternative inference methods, such as NUTS [Homan and Gelman 2014] (No U-Turn Sampler), an optimized Hamiltonian Monte-Carlo (HMC) algorithm that is the preferred inference method for Stan. We can thus validate the results of our approach against the original Stan implementation on classic probabilistic models.

To summarize, this paper makes the following contributions:

1. A comprehensive compilation scheme from Stan to a generative PPL (Section 2).
2. A proof of correctness of the compilation scheme (Section 3).
3. A type system to deduce the size and shape of Stan vectorized constructs (Section 4).
4. A compiler from Stan extended with explicit variational inference guides and deep probabilistic models to Pyro (Section 5).

The fundamental new result of this paper is to prove that every Stan program can be expressed as a generative probabilistic program. Besides advancing the understanding of probabilistic programming languages at a fundamental level, this paper aims to provide concrete benefits to both the Stan community and the Pyro community. From the perspective of the Stan community, this paper presents a new compiler back-end that unlocks additional capabilities while retaining familiar syntax. From the perspective of the Pyro community, this paper presents a new compiler front-end that unlocks a large number of existing real-world models as examples and benchmarks.

The code of our experimental compiler from extended Stan to Pyro is available at https://github.com/deepppl/deepppl.

2 OVERVIEW

This section shows how to compile a declarative language that specifies a joint probability distribution like Stan [Carpenter et al. 2017] to a generative PPL like Church, Anglican, or Pyro. Translating Stan to a generative PPL also demonstrates that Stan’s expressive power is at most as large as that of generative languages, a fact that was not clear before our paper.

As a running example, consider the biased coin model shown in Figure 1. This model has observed variables $x_i$, $i \in [1 : N]$, which can be 0 for tails or 1 for heads, and a latent variable $z \in [0, 1]$ for the bias of the coin. Coin flips $x_i$ are independent and identically distributed (IID) and depend on $z$ via a Bernoulli distribution. The prior distribution of parameter $z$ is Beta(1, 1).

```stan
data { int N; int<lower=0,upper=1> x[N]; }
parameters { real<lower=0,upper=1> z; }
model { z ~ beta(1, 1);
  for (i in 1:N) x[i] ~ bernoulli(z); }
```

Fig. 1. Biased coin model in Stan.
2.1 Generative translation

Generative PPLs are general-purpose languages extended with two probabilistic constructs [Gordon et al. 2014; Staton 2017; van de Meent et al. 2018]: \( \text{sample}(D) \) generates a sample from a distribution \( D \) and \( \text{factor}(v) \) assigns a score \( v \) to the current execution trace. Typically, \( \text{factor} \) is used to condition the model on input data [Tolpin et al. 2016]. We also introduce \( \text{observe}(D, v) \) as a syntactic shortcut for \( \text{factor}(D \cdot \text{pdf}(v)) \) where \( D \cdot \text{pdf} \) denotes the density function of \( D \). This construct penalizes executions according to the score of \( v \) w.r.t. \( D \) which captures the assumption that the observed data \( v \) follows the distribution \( D \).

Compilation. Stan uses the same syntax \( v ~ D \) for both observed and latent variables. The distinction comes from the kind of the left-hand-side variable: observed variables are declared in the data block, latent variables are declared in the parameters block. A straightforward generative translation compiles a statement \( v ~ D \) into \( v = \text{sample}(D) \) if \( v \) is a parameter or \( \text{observe}(D, v) \) if \( v \) is data. For example, the compiled version of the Stan model of Figure 1 is shown in Figure 2a (using Python syntax).

2.2 Non-generative features

In Stan, a model represents the unnormalized density of the joint distribution of the parameters defined in the parameters block given the data defined in the data block [Carpenter et al. 2017; Gorinova et al. 2019]. A Stan program can thus be viewed as a function from parameters and data to the value of a special variable target that represents the log-density of the model. A Stan model can be described using classic imperative statements, plus two special statements that modify the value of target. The first one, target+= \( e \), increments the value of target by \( e \). The second one, \( e ~ D \), is equivalent to \( \text{target} += D \cdot \text{pdf}(e) \) [Gorinova et al. 2019].

Unfortunately, these constructs allow the definition of models that cannot be translated using the generative translation defined above. Specifically, Table 1 lists the Stan features that are not handled correctly. A left expression is a case where the left-hand-side of \( ~ \) is an arbitrary expression. The multiple updates feature occurs when the same parameter appears on the left-hand-side of multiple \( ~ \) statements. An implicit prior occurs when there is no explicit \( ~ \) statement in the model for a parameter. A target update is a direct update to the log-density of the model.

The “%” column of Table 1 indicates the percentage of Stan models that exercise each of the non-generative features among the 502 files in https://github.com/stan-dev/example-models. The example column contains illustrative excerpts from such models. Since these are official and long-standing examples, we assume that they use the non-generative features on purpose. Comments in the source code further corroborate that the programmer knowingly used the features. While some features only occur in a minority of models, their prevalence is too high to ignore.
Table 1. Stan features: example, prevalence and compilation.

| Feature          | %  | Example                              | Compilation                                      |
|------------------|----|--------------------------------------|--------------------------------------------------|
| Left expression  | 7.7| `sum(phi) ~ normal(0, 0.001*N);`    | `observe(Normal(0., 0.001*N), sum(phi))`        |
| Multiple updates | 3.9| `phi_y ~ normal(0, sigma_py);`       | `observe(Normal(0., sigma_py), phi_y);`          |
| Implicit prior   | 60.7| `real alpha0;`                       | `alpha0 = sample(ImproperUniform())`            |
| Implicit prior   | 60.7| `/* missing 'alpha0 ~ ... */`        |                                                  |
| Target update    | 16.3| `target += -0.5 * dot_self(\phi[node1] - \phi[node2]);` | `factor(-0.5 * dot_self(\phi[node1] - \phi[node2]));` |

2.3 Comprehensive translation

The previous section illustrates that Stan is centered around the definition of `target`, not around generating samples for parameters, which is required by generative PPLs. The idea of the comprehensive translation is to add an initialization step to generate samples for all the parameters and compile all Stan `~` statements as observations. To initialize the parameters we draw from the uniform distribution in the definition domain of the parameters. For the biased coin example, the result of this translation is shown in Figure 2b: The parameter `z` is first sampled uniformly on its definition domain and then conditioned with an observation.

The compilation column of Table 1 illustrates the translation of non-generative features. Left expression and multiple updates are simply compiled into observations. Parameter initialization uses the uniform distribution over its definition domain. For unbounded domains, we introduce new distributions (e.g., `ImproperUniform`) with a constant density that can be normalized away during inference. The target update is compiled into a `factor` which increases the log-probability of the execution by the given number. The complete compilation scheme is detailed in Section 3.3.

Intuition of the correctness. The semantics of Stan as described in [Gorinova et al. 2019] is the semantics of a classical imperative language that defines an environment containing, in particular, the value of the special variable `target`: the unnormalized log-density of the model. On the other hand, the semantics of a generative PPL as described in [Staton 2017] defines a kernel mapping an environment to a measurable function. Our compilation scheme adds uniform initializations for all parameters which comes down to the Lebesgue measure on the parameters space, and translates all `~` statements to `observe` statements. We can then show that a succession of `observe` statements yields a distribution with the same log-density as the Stan semantics. The correctness proof is detailed in Section 3.4.

2.4 Implementation

The comprehensive compilation scheme can be used to compile any Stan program to a generative PPL leveraging the rich set of existing Stan models for testing and benchmarking. As a proof of concept, we implemented a compiler from Stan to Pyro [Bingham et al. 2019], a probabilistic programming language in the line of WebPPL.

Vectorization. Compiling Stan to Pyro also raises the problem of automatic vectorization. In Stan, expressions are automatically vectorized. For instance, the statement `z ~ normal(0, 1)` automatically lifts the scalars 0 and 1 to the shape of `z`. To generate correct Pyro code, we need to explicitly lift these constants: `z = sample(normal(zeros(s), ones(s)))` where `s` is the shape of `z`, and the functions `zeros` and `ones` return arrays of zeros and ones, respectively. We thus extend the Stan type system to infer dimensions and sizes (Section 4). Our type system allows the programmer to omit redundant dimensions, leaving them to the compiler to deduce.
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**Extensions.** Pyro is a *deep universal probabilistic programming language* with native support for variational inference, and we can thus can leverage the deep features of the language back to Stan (Section 5). Our Stan extension — DeepStan — thus support explicit variational guides (Section 5.1) and deep neural networks to capture complex relations between parameters (Section 5.2).

## 3 SEMANTICS AND COMPILATION

This section, building on previous work, first formally defines the semantics of Stan (Section 3.1) and the semantics of GProb, a small generative probabilistic language (Section 3.2). It then defines the compilation function from Stan to GProb (Section 3.3) and proves its correctness (Section 3.4).

### 3.1 Stan: a Declarative Probabilistic Language

The Stan language is informally described in [Carpenter et al. 2017]. A Stan program is a sequence of blocks in the following order, where the only mandatory block is `model`. Variables declared in one block are visible in subsequent blocks.

```
program ::= functions {fundecl*}? data {decl}? transformed data {decl stmt}? parameters {decl}? transformed parameters {decl stmt}? model {decl stmt} generated quantities {decl stmt}?
```

Variable declarations (`decl`) are lists of variables names with their types (e.g., `int N`) or arrays with their type and shape (e.g., `real x[N]`). Types can be constrained to specify the domain of a variable (e.g., `real <lower=0> x` for `x ∈ ℝ+`). Note that `vector` and `matrix` are primitive types that can be used in arrays (e.g., `vector[N] x[10]` is an array of 10 vectors of size N). Shapes and sizes of arrays, matrices, and vectors are explicit and can be arbitrary expressions.

```
decl ::= base_type constraint x ; | base_type constraint x [shape] ;
base_type ::= real | int | vector[size] | matrix[size, size]
constraint ::= ε | < lower = e , upper > | < lower = e > | < upper = e >
shape ::= size | shape, size
size ::= e
```

Inside a block, Stan is similar to a classic imperative language, with the addition of two specialized statements: `target += e` directly updates the log-density of the model (stored in the reserved variable `target`), and `x ~ D` indicates that a variable `x` follows a distribution `D`.

```
stmt ::= x = e variable assignment
       | x[e1, ..., en] = e array assignment
       | stmt1; stmt2 sequence
       | for (x in e1:e2) {stmt} loop over a range
       | for (x in e) {stmt} loop over the elements of a collection
       | while (e) {stmt} while loop
       | if (e) stmt1 else stmt2 conditional
       | skip no operation
       | target += e direct update of the log-density
       | e ~ f(e1, ..., en) probability distribution
```
Expressions comprise constants, variables, arrays, vectors, matrices, access to elements of an indexed structure, and function calls (also used to model binary operators):

\[ e ::= c \mid x \mid \{e_1, \ldots, e_n\} \mid [e_1, \ldots, e_n] \mid \{[e_1, \ldots, e_{1_m}], \ldots, [e_{n_1}, \ldots, e_{n_m}]\} \mid e_1 [e_2] \mid f(e_1, \ldots, e_n) \]

**Semantics.** The evaluation of a Stan program comprises three steps:

1. data preparation with data and transformed data
2. inference over the model defined by parameters, transformed parameters, and model
3. post-processing with generated quantities

Section 3.3 shows how to efficiently compile the pre- and post-processing blocks, but in terms of semantics, any Stan program can be rewritten into an equivalent program with only the three blocks data, parameters, and model.

Functions declared in functions have been inlined. To simplify the presentation of the semantics, we focus in the following on this simplified language.

**Notations.** To refer to the different parts of a program, we will use the following functions. For a Stan program \( p = \text{data} \{\text{decls}_d\} \text{parameters} \{\text{decls}_p\} \text{model} \{\text{decls}_m \text{stmt}_m\} \):

\[
\begin{align*}
\text{data}(p) & = \text{decls}_d \\
\text{params}(p) & = \text{decls}_p \\
\text{model}(p) & = \text{decls}_m \text{stmt}_m
\end{align*}
\]

In the following, an environment \( \gamma : \text{Var} \to \text{Val} \) is a mapping from variables to values, \( \gamma(x) \) returns the value of the variable \( x \) in an environment \( \gamma \), \( \gamma[x \leftarrow v] \) returns the environment \( \gamma \) where the value of \( x \) is set to \( v \), and \( \gamma_1, \gamma_2 \) denotes the union of two environments.

We note \( \int_X \mu(dx)f(x) \) the integral of \( f \) w.r.t. the measure \( \mu \) where \( x \in X \) is the integration variable. When \( \mu \) is the Lebesgue measure we also write \( \int_X f(x)dx \).

Following [Gorinova et al. 2018], we define the semantics of the model block as a deterministic function that takes an initial environment containing the input data and the parameters, and returns an updated environment where the value of the variable target is the un-normalized log-density of the model.

We can then define the semantics of a Stan program as a kernel [Kozen 1981; Staton 2017; Staton et al. 2016], that is, a function \( \{p\} : D \to \Sigma_X \to [0, \infty] \) where \( \Sigma_X \) denotes the \( \sigma \)-algebra of the parameter domain \( X \), that is, the set of measurable sets of the product space of parameter values. Given an environment \( D \) containing the input data, \( [p]_D \) is a measure that maps a measurable set of parameter values \( U \) to a score in \( [0, \infty] \) obtained by integrating the density of the model, \( \exp(\text{target}) \), over all the possible parameter values in \( U \).

\[
\{p\}_D = \lambda U \int_U \exp([\text{model}(p)]_{D, \theta}(\text{target})) \, d\theta
\]
target += e and updates the value of target in the environment produced by $s_1$. A for loop on ranges first evaluates the value of the bounds $n_1$ and $n_2$ and then repeats the execution of the body $n_2 - n_1$ times. Iterations over indexed structures depend on the underlying type. For vectors and arrays, iteration is limited to one dimension ($i$ is a fresh variable name):

$$\begin{align*}
\llbracket \text{for } (x \in e) \{ s \} \rrbracket_y &= \text{let } v = \llbracket e \rrbracket_y \text{ in } \\
&\quad \llbracket \text{for } (i \in 1: \text{length}(v)) \{ x = v[i] ; s \} \rrbracket_y
\end{align*}$$

For matrices, iteration is over the two dimensions ($i$ and $j$ are fresh variable names):

$$\llbracket \text{for } (x \in e) \{ s \} \rrbracket_y = \text{let } v = \llbracket e \rrbracket_y \text{ in } \\
\quad \llbracket \text{for } (i \in 1: \text{length}(v)) \text{ for } (j \in 1: \text{length}(v[i])) \{ x = v[i][j] ; s \} \rrbracket_y$$

A while loop repeats the execution of its body while the condition is not 0. A if statement executes one of the two branches depending on the value of the condition. A skip leaves the environment unchanged. A statement target += e adds the value of e to target in the environment. Finally, a statement $e_1 \sim e_2$ evaluates the expression $e_2$ into a probability distribution $D$ and updates the target with the value of the log-density of $D$ at $e_1$.  

Given the input data, the posterior distribution of a Stan program is then obtained by normalizing the measure $\llbracket p \rrbracket_D$. In practice, the integrals are often untractable, and the runtime relies on approximate inference schemes to compute the posterior distribution.

We now detail the semantics of statements and expressions that can be used in the model block. This formalization is similar to the semantics proposed in [Gorinova et al. 2018] but expressed in a denotational style.

**Statements.** The semantics of a statement $\llbracket s \rrbracket : (\text{Var } \rightarrow \text{Val}) \rightarrow (\text{Var } \rightarrow \text{Val})$ is a function from an environment $\gamma$ to an updated environment. Figure 3 gives the semantics of Stan statements. The initial environment always contains the the reserved variable target initialized to 0. An assignment updates the value of a variable or of a cell of an indexed structure in the environment. A sequence $s_1 ; s_2$ evaluates $s_2$ in the environment produced by $s_1$. A for loop on ranges first evaluates the value of the bounds $n_1$ and $n_2$ and then repeats the execution of the body $n_2 - n_1$ times. Iterations over indexed structures depend on the underlying type. For vectors and arrays, iteration is limited to one dimension ($i$ is a fresh variable name):
Expressions. The semantics of an expression \( [e] : (\text{Var} \rightarrow \text{Val}) \rightarrow \text{Val} \) is a function from an environment to values. Figure 4 gives the semantics of Stan expressions. The value of a constant is itself. The value of a variable is the corresponding value stored in the environment. The value of an array, a vector, or a matrix is obtained by evaluating all its components. Accessing a component of an indexed structure looks up the corresponding value in the associated data. A function call applies the function to the value of the arguments. Functions are limited to built-in operations like + or normal (user defined functions have been inlined).

### 3.2 GProb: a Simple Generative Probabilistic Language

To formalize the compilation, we first define the target language: GProb, a simple generative probabilistic language similar to the one defined in [Staton 2017]. GProb is an expression language with the following syntax:

\[
e ::= c \mid x \mid \{e_1, \ldots, e_n\} \mid [e_1, \ldots, e_n] \mid e_1[e_2] \mid f(e_1, \ldots, e_n)
\mid \text{let } x = e_1 \text{ in } e_2 \mid \text{let } x[e_1, \ldots, e_n] = e \text{ in } e'
\mid \text{if } (e) e_1 \text{ else } e_2 \mid \text{for}_X (x \text{ in } e_1 : e_2) \ e_3 \mid \text{while}_X (e_1) \ e_2
\mid \text{factor}(e) \mid \text{sample}(e) \mid \text{return}(e)
\]

An expression is either a Stan expression, a local binding (let), a conditional (if), or a loop (for or while). To simplify the presentation, loops are parameterized by the set \( X \) of variables that are updated in their body. GProb also contains the classic probabilistic expressions: \( \text{sample} \) draws a sample from a distribution, and \( \text{factor} \) assigns a score to the current execution trace to condition the model. The \text{return} expression is used to lift a deterministic expression to a probabilistic context.

We also introduce \text{observe}(D, v) as a syntactic shortcut for \( \text{factor}(D_{\text{pdf}}(v)) \) where \( D_{\text{pdf}} \) denotes the density function of \( D \). This construct penalizes the current execution with the likelihood of \( v \) w.r.t. \( D \) which captures the assumption that the observed data \( v \) follows the distribution \( D \).

Semantics. Following [Staton 2017] we give a measure-based semantics to GProb. The semantics of an expression is a kernel which, given an environments, returns a measure on the set of possible values. Again, given the input data, the posterior distribution of a GProb program is then obtained by normalizing the corresponding measure.

The semantics of GProb is given in Figure 5. A deterministic expression is lifted to a probabilistic expression with the Dirac delta measure (\( \delta_x(U) = 1 \) if \( x \in U \), 0 otherwise). A local definition \text{let } x = e_1 \text{ in } e_2 \text{ is interpreted by integrating the semantics of } e_2 \text{ over the set of all possible values for } x. \text{ In the following, we use the more concise union notation } \gamma, x \text{ to bind the value of } x \text{ in the environment } \gamma \text{ in the integrals. The semantics of a local definition can thus be rewritten:}

\[
\{ \text{let } x = e_1 \text{ in } e_2 \}_\gamma = \lambda U. \int_X [e_1]_\gamma (dx) \times [e_2]_{\gamma,x}(U)
\]

Compared to the language defined in [Staton 2017], we added Stan loops. Loops behave like a sequence of expressions and return the values of the variables updated by their body. Consider, for example, the \text{while}_X (e_1) \ e_2 \text{ expression. First, the condition is evaluated. If the loop terminates, we return the measure corresponding to the variables } X \text{ updated by the loop. Otherwise, similarly...
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\[
\begin{align*}
\text{\textbackslash{}return}(e) \rangle_Y &= \lambda U. \delta_{[e]}(U) \\
\text{\textbackslash{}let } x = e_1 \text{ in } e_2 \rangle_Y &= \lambda U. \int_X \langle e_1 \rangle_Y (d\nu) \times \langle e_2 \rangle_Y |x \leftarrow e_1|(U) \\
\text{\textbackslash{}let } x[e_1, \ldots, e_n] = e \text{ in } e' \rangle_Y &= \lambda U. \int_X \langle e \rangle_Y (d\nu) \times \langle e' \rangle_Y |x \leftarrow (x[e_1, \ldots, e_n]) \leftarrow e|(U) \\
\text{\textbackslash{}for}_X (x \in e_1 : e_2) e_3 \rangle_Y &= \lambda U. \text{let } n_1 = \langle e_1 \rangle_Y \text{ in let } n_2 = \langle e_2 \rangle_Y \text{ in } \\
& \quad \text{if } n_1 > n_2 \text{ then } \delta_{y} (X(U)) \\
& \quad \text{else } \int_X \langle e_3 \rangle_Y [x \leftarrow n_1] (dX) \times \langle \text{for}_X (x \in n_1 + 1 : n_2) e_3 \rangle_Y, X(U) \\
\text{\textbackslash{}while}_X (e_1) e_2 \rangle_Y &= \lambda U. \text{if } \langle e_1 \rangle_Y = 0 \text{ then } \delta_{y} (X(U)) \\
& \quad \text{else } \int_X \langle e_2 \rangle_Y (dX) \times \langle \text{while}_X (e_1) e_2 \rangle_Y, X(U) \\
\text{\textbackslash{}if } (e) e_1 \text{ else } e_2 \rangle_Y &= \lambda U. \text{if } \langle e \rangle \neq 0 \text{ then } \langle e_1 \rangle_Y (U) \text{ else } \langle e_2 \rangle_Y (U) \\
\text{\textbackslash{}sample}(e) \rangle_Y &= \lambda U. \langle e \rangle_Y (U) \\
\text{\textbackslash{}factor}(e) \rangle_Y &= \lambda U. \exp \langle e \rangle_Y \\
\end{align*}
\]

Fig. 5. Generative probabilistic language semantics

to the local binding, we integrates the next iteration of the loop over the set of all possible values for the set of variables \(X\).

The semantics of probabilistic operators is the following. The semantics of \texttt{sample}(e) is the probability distribution \(\langle e \rangle_Y\) (e.g. \(N(0, 1)\)). A type system omitted here for conciseness ensures that we only sample from distributions. The semantics of \texttt{factor}(e) is the constant measure whose value is \(\exp(\langle e \rangle)\) (this operator corresponds to \texttt{score} in [Staton 2017] but in log-scale, which is common for numerical precision).

### 3.3 Comprehensive Translation

The key idea of the comprehensive translation is to first sample all parameters from priors with a constant density that can be normalized away during inference (e.g., Uniform on bounded domains), and then compile all \(\sim\) statements into \texttt{observe} statements.

The compilation functions for the parameters \(\mathcal{P}_k\) (\texttt{params}(p)) and the model \(\mathcal{S}_k\) (\texttt{model}(p)) are both parameterized by a continuation \(k\). The compilation of the entire program first compiles the parameters to introduce the priors, then compiles the model, and finally adds a return statement for all the parameters. In continuation passing style:

\[
C(p) = \mathcal{P}_{\text{return}(\text{params}, p)}(\text{model}(p)) (\text{params}(p))
\]

**Parameters.** In Stan, parameters can only be real, array of reals, vectors, or matrices, and are thus defined on \(\mathbb{R}^n\) with optional domain constraints (e.g. <lower=0>). For each parameter, the prior is either the Uniform distribution on a bounded domain, or an improper prior with a constant density w.r.t. the Lebesgue measure that we call ImproperUniform. The compilation function of the parameters, defined Figure 6, thus produces a succession of sample expressions:

\[
\mathcal{P}_k (\text{params}(p)) = \texttt{let } x_1 = D_1 \text{ in } \ldots \texttt{let } x_n = D_n \text{ in } k
\]

where for each parameter \(x_i, D_i\) is either Uniform or ImproperUniform.
variables that are assigned in their body (section and can be computed only once before the inference. We compile this section into a function

\[
P_k(t \ cstr \ x; \ k) = \text{let } x = \text{sample}(K(cstr)) \text{ in } k
\]

\[
P_k(t \ cstr \ x[\text{shape}]; \ k) = \text{let } x = \text{sample}(K(cstr), \text{shape}) \text{ in } k
\]

\[
P_k(\text{decl} \ decls) = P_{P_k(derrals)}(\text{decl})
\]

\[
K(<\text{lower}=e_1, \text{upper}=e_2>) = \text{Uniform}([e_1, e_2])
\]

\[
K(<\text{lower}=e_1>) = \text{ImproperUniform}([e_1, \infty])
\]

\[
K(<\text{upper}=e_2>) = \text{ImproperUniform}([\infty, e_2])
\]

\[
K(e) = \text{ImproperUniform}([\infty, \infty])
\]

Fig. 6. Comprehensive compilation of parameters

\[
S_k(x = e) = \text{let } x = \text{return}(e) \text{ in } k
\]

\[
S_k(x[e_1, \ldots, e_n] = e) = \text{let } x[e_1, \ldots, e_n] = e \text{ in } k
\]

\[
S_k(stmt_1; stmt_2) = S_{S_k(stmt_2)}(stmt_1)
\]

\[
S_k(\text{for } (x \in e_1:e_2) \{stmt\}) = \text{let } lhs(stmt) = \text{for}(lhs(stmt)) (x \in e_1:e_2) S_{return(lhs(stmt))}(stmt) \text{ in } k
\]

\[
S_k(\text{while } (e) \{stmt\}) = \text{let } lhs(stmt) = \text{while}(lhs(stmt)) (e) S_{return(lhs(stmt))}(stmt) \text{ in } k
\]

\[
S_k(\text{if } (e) stmt_1 \text{ else stmt}_2) = \text{if } (e) S_k(stmt_1) \text{ else } S_k(stmt_2)
\]

\[
S_k(\text{skip}) = k
\]

\[
S_k(\text{target } += e) = \text{let } () = \text{factor}(e) \text{ in } k
\]

\[
S_k(e \sim f(e_1, \ldots, e_n)) = \text{let } () = \text{observe}(f(e_1, \ldots, e_n), e) \text{ in } k
\]

Fig. 7. Comprehensive compilation of statements

**Statements.** Figure 7 defines the compilation function for statements \(S_k(stmt)\), which is also parameterized by a continuation \(k\). Stan imperative assignments are compiled into functional updates using local bindings. The compilation of the sequence chains the continuations. Updates to the target are compiled into \textit{factor} expressions and all \(~\) statement are compiled into observations (which can be desugared into \textit{factor} expressions).

The compilation of Stan loops raises an issue. In Stan, all the variables that appear on the left hand side of an assignment in the body of a loop are state variables that are incrementally updated at each iteration. Since GProb is a functional language, the state of the loops is made explicit. To propagate the environment updates at each iteration, loop expressions are annotated with all the variables that are assigned in their body (\(lhs(stmt)\)). These variables are returned at the end of the loop and can be used in the continuation.

**Pre- and post-processing blocks.** In Section 3.1, we showed that all Stan programs can be rewritten in a kernel using only the \textit{data}, \textit{parameters}, and \textit{model} sections. This approach has the drawback of making the model more complicated and thus the inference more expensive. In particular not all the pre- and post-processing steps need to be computed at each inference step.

In Stan, users can define functions in the \textit{functions} block. These functions can be compiled into functions in the target language using the comprehensive translation, i.e., the \(~\) statements are compiled into \textit{observe}.

The code in the \textit{transformed data} section only depends on variables declared in the \textit{data} section and can be computed only once before the inference. We compile this section into a function
that takes as argument the data and returns the transformed data. The variables declared in the `transformed data` section become new inputs for the model.

On the other hand, the code of the `transformed parameters` block must be part of the model since it depends on the model parameters. This section is thus inlined in the compiled model.

Finally, the `generated quantities` block can be executed only once on the result of the inference. We compile this section into a function of the data, transformed data, and parameters returned by the model. Since a generated quantity may depend on transformed parameters, the code of the `transformed parameters` block must also be inlined in this function to be usable.

**Compiling to Pyro.** In Pyro, the probabilistic operator are \( v = \text{sample}(\text{name}, D) \) (sample) and \( \text{sample}(\text{name}, D, \text{obs} = e) \) (observe). Note that, in both cases, the user must provide a unique name for the internal Pyro namespace.

Translating `target update` requires overcoming the obstacle that Pyro does not directly expose the log-density accumulator to the programmer. Instead, we use the exponential distribution with parameter \( \lambda = 1 \) whose density function is \( \text{Exp}\text{pdf}(1)(x) = e^{-x} \). Observing a value \(-v\) from this distribution multiplies the score by \( e^v \), which corresponds to the update \( \text{target} += v \). This approach is similar to the "zeros trick" from BUGS [Lunn et al. 2012].

Finally, in Stan, expressions can be automatically vectorized, but in Pyro, array dimensions must be explicit. Section 4 introduces a type system to deduce the size and shape of Stan vectorized constructs to enable the compiler to make them explicit.

### 3.4 Correctness of the Compilation

We can now show that a Stan program and the corresponding compiled code yield the same un-normalized measure up to a constant factor (and thus the same posterior distribution). The proof comprises two steps: (1) we simplify the sequence of `sample` statements introduced by the compilation of the parameters, and (2) we show that the value of the Stan `target` corresponds to the score computed by the generated code.

**Priors.** First, we show that the nested integrals introduced by the sequence of `sample` statements for the parameters priors can be simplified into a single integral over the parameter domain.

**Lemma 3.1.** For all Stan program \( p \), and environment \( \gamma \):

\[
\langle C(p) \rangle_\gamma = \lambda U \cdot \int_U \langle S_{\text{return}}(\emptyset)(\text{model}(p)) \rangle_{\gamma, \theta(\emptyset)} \, \theta \, d \theta
\]

**Proof.** In the following \( \text{decls}_p = \text{params}(p) \) and \( \text{stmt} = \text{model}(p) \). By definition of the compilation function, \( C(p) \) has the following shape:

\[
\begin{align*}
\text{let } x_1 &= D_1 \text{ in } \ldots \text{let } x_n &= D_n \text{ in } S_{\text{return}}(\text{decls}_p)(\text{stmt})
\end{align*}
\]

where for each parameter \( x_i, D_i \) is either `Uniform` or `ImproperUniform`. In both cases the corresponding density is constant w.r.t. the Lebesgue measure on its domain. Since the kernels defined by GProb expressions are always s-finite [Staton 2017], from the semantics of GProb (Section 3.2) and the Fubini-Tonelli theorem, we have:

\[
\langle C(p) \rangle_\gamma = \lambda U \cdot \int_{X_1} \cdots \int_{X_n} D_1(dx_1) \cdots D_n(dx_n) \langle S_{\text{return}}(\text{decls}_p)(\text{stmt}) \rangle_{\gamma, \{x_1, \ldots, x_n\}(U)}
\]

\[
= \lambda U \cdot \int_{X_1} \cdots \int_{X_n} \langle S_{\text{return}}(\text{decls}_p)(\text{stmt}) \rangle_{\gamma, \{x_1, \ldots, x_n\}(U)} \, dx_1 \ldots dx_n
\]

\[
= \lambda U \cdot \int_{X = X_1 \times \cdots \times X_n} \langle S_{\text{return}}(\text{decls}_p)(\text{stmt}) \rangle_{\gamma, \theta(U)} \, d \theta
\]
In Stan, parameters declared in \( \text{decls}_p \) cannot appear in the left-hand side of an assignment, which means that the evaluation of the model statements \( \text{stmt} \) cannot update the value of the parameters. The evaluation of \( \text{let} \) thus leaves \( \theta \) unchanged and terminates with \( \text{return(decls_p)} \) which is equal to \( \text{return(decls_p)} \). We can thus decompose the evaluation of compiled code as follows:

\[
\text{let} \quad \text{return(decls_p)} = \int_X \text{return(decls_p)} \times \text{return(decls_p)} \, d\theta(U)
\]

Going back to the previous equation, we now have

\[
\text{let} \quad \text{return(decls_p)} = \lambda U. \int_X \text{return(decls_p)} \times \text{return(decls_p)} \, d\theta(U)
\]

**Score and target.** We now show that the value of the Stan target variable corresponds to the score computed by the generated code.

**Lemma 3.2.** For all Stan statements \( \text{stmt} \) compiled with a continuation \( k \), if \( \gamma(\text{target}) = 0 \), and \( \text{stmt} \) then, \( \gamma' \),

\[
\text{let} \quad \text{return(decls_p)} = \lambda U. \exp(\gamma'(\text{target})) \times \text{return(decls_p)}
\]

**Proof.** The proof is done by induction on the structure of \( \text{stmt} \) using the definition of the compilation function (Section 3.3) and the semantics of GProb. We now detail just a few key cases.

**Assignment.** The evaluation of \( x = e \) does not update the value of \( \text{target} \) and its initial value is 0. Therefore, we have \( \gamma' = [x = e] \), \( \gamma' = [x = e] \), and \( \exp(\gamma'(\text{target})) = 1 \). Then from the semantics of GProb we have:

\[
\text{let} \quad \text{return(decls_p)} = \lambda U. \int_X \text{return(decls_p)} \times \text{return(decls_p)} \, d\theta(U)
\]

**Target update.** Since the evaluation of \( \text{target} += e \) only updates the value of \( \text{target} \) and its initial value is 0, with \( \gamma' = [\text{target} += e] \), we have \( \gamma = \gamma'[\text{target} = 0] \), and \( \gamma'(\text{target}) = [e] \). Then from the semantics of GProb we have:

\[
\text{let} \quad \text{return(decls_p)} = \lambda U. \int_X \text{return(decls_p)} \times \text{return(decls_p)} \, d\theta(U)
\]
Sequence. From the induction hypothesis and the semantics of GProb we have with $\gamma_1 = \lbrack \text{stmt}_1 \rbrack_Y$ and $\gamma_2 = \lbrack \text{stmt}_2 \rbrack_{\gamma_1[\text{target} \leftarrow 0]}$:

$$
\{S_k (\text{stmt}_1 ; \text{stmt}_2)\}_Y = \{S_k (\text{stmt}_1)\}_Y \\
= \lambda U . \exp(\gamma_1(\text{target})) \times \{S_k (\text{stmt}_2)\}_Y[\text{target} \leftarrow 0](U) \\
= \lambda U . \exp(\gamma_1(\text{target})) \times \exp(\gamma_2(\text{target})) \times \{k\}_Y[\text{target} \leftarrow 0](U) \\
= \lambda U . \exp(\gamma_1(\text{target}) + \gamma_2(\text{target})) \times \{k\}_Y[\text{target} \leftarrow 0](U)
$$

On the other hand, from the semantics of Stan (Section 3.1), for any real value $t$ we have:

$$
[\text{stmt}]_Y[\text{target} \leftarrow t](\text{target}) = t + [\text{stmt}]_Y[\text{target} \leftarrow 0](\text{target})
$$

Therefore: $[\text{stmt}_1 ; \text{stmt}_2]_Y(\text{target}) = \gamma_1(\text{target}) + \gamma_2(\text{target})$ which conclude the proof. □

Correctness. We now have all the elements to prove that the comprehensive compilation is correct. That is, generated code yield the same un-normalized measure up to a constant factor that will be normalized away by the inference.

**Theorem 3.3.** For all Stan programs $p$, the semantics of the source program is equal to the semantics of the compiled program up to a constant:

$$
\{p\}_D \propto \{C(p)\}_D
$$

**Proof.** The proof is a direct consequence of Lemmas 3.1 and 3.2 and the definition of the two semantics.

$$
\{C(p)\}_D \propto \lambda U . \int_U \{S_{\text{return}(0)}(\text{model}(p))\}_{D,\theta(0)} ) \, d\theta \\
= \lambda U . \int_U \exp(\{\text{model}(p)\}_{D,\theta(\text{target})} ) \times \{\text{return}(0)\}_{0(0)} ) \, d\theta \\
= \lambda U . \int_U \exp(\{\text{model}(p)\}_{D,\theta(\text{target})} ) \, d\theta \\
= \{p\}_D \\
$$

□

4 VECTORIZATION

Vectorization is a style of programming where operations are applied to entire tensors (i.e, arrays, vectors, or matrices) instead of individual elements. For example, in Stan, $z \sim \text{normal}(0,1)$ lifts the scalars 0 and 1 to the shape of $z$. Vectorization is both convenient (briefer code) and efficient (faster on vector units). Unfortunately, while the Stan compiler gets away with keeping shapes and sizes implicit during compilation, our compiler to Pyro must make them explicit to generate correct code. Thus, it needs a tensor shape analysis, described in this section. Explicit knowledge of shapes and sizes also enables our compiler to check if types are correct and if not, report errors earlier than the Stan compiler would.

Sizes of tensor variables can depend on each other, as in the code

```stan
real encoded[2,nz] = encoder(x); real mu_z[nz] = encoded[1];
```

Due to the assignment, $mu_z$ must have the same size $nz$ as the second dimension of encoded. Given that it can be deduced, some users may prefer not to explicitly specify it by hand, as in

```stan
real encoded[2,nz] = encoder(x); real mu_z[_] = encoded[1];
```
This ability to keep some sizes implicit in the source code is another benefit of having a tensor shape analysis. While it is only a minor convenience in the above example, when used with our DeepStan extension to Stan, it becomes a major convenience. This is because neural network shapes are specified in PyTorch, and forcing users to redundantly specify them in DeepStan code would be brittle and cause clutter. Instead, DeepStan supports declarations such as `real mlp.11.weight[*];` where * leaves not only sizes but even the number of dimensions to be deduced by the compiler.

The tensor shape analysis must support polymorphism both over sizes of individual dimensions and over the number of dimensions. Furthermore, it must handle Stan’s standard library of size-polymorphic functions and distributions (conceptually, our compiler desugars infix operators such as + into binary function invocations). Another factor that complicates the analysis is target-typing: the vectorization of a function or distribution is determined not just by its actual arguments but also by how the result gets used. Finally, the tensor shape analysis must handle Stan’s assortment of tensor types including vectors, arrays, matrices, and row vectors.

Our solution is a Hindley-Milner style analysis that conceptually comprises the following steps:

1. Give a type to each variable and expression in the program, emitting type errors as needed, while also gathering constraints for types that are not fully determined yet.
2. Use unification on the constraints to determine more concrete types, again emitting type errors as needed when attempting to unify incompatible types.
3. If some types are still ambiguous (i.e., the information is not available at startup, as opposed to constants or information that can be read from data or neural networks), emit warnings.
4. Use the deduced sizes in code generation, for instance, to properly initialize tensors.

The tensor shape analysis internally uses a more expressive set of types than the surface types used by the programmer. They are defined as follows:

```
type ::= base_type | type[size] | type[dim]
base_type ::= real | int | vector[size] | matrix[size,size]
size ::= e | σ
dim ::= shape | δ | shape(e)
shape ::= size | shape, size
func ::= type* * ... * type* → type | type* * ... * type* → func
vect ::= true | false
schema ::= ∀σ₁, ..., σₖ, ∀δ₁, ..., δₘ.func
```

Non-terminal `base_type` is the same as in the surface grammar from Section 3.1. We introduce polymorphic size variables (σ) that have to be deduced by the compiler. For example, `matrix[42,_] x;` yields the type `matrix[42,σ]`. Also, there is a new type `t[dim]` representing an array of elements of type `t` with a dimension specified by `dim`. Dimensions can be specified by the size of each dimension, a polymorphic shape variable (δ), or they can have the same shape as the result of an expression evaluation. For example, `int x[*];` yields the type `int[*]δ`. There are two kinds of `func` type,
which arguments can or cannot be implicitly vectorized. Finally, schema imbues functions with size and shape polymorphism.

Figure 8 presents type equivalence rules. These represent type constraints gathered from typing rules to be resolved later during unification. Equivalence is reflexive and symmetric. For example, \( \text{vector}[N] \equiv \text{vector}[10] \) adds the constraint that \( N \) must be equal to 10 and \( \text{int}[]^\delta \equiv \text{int}[50][50] \) adds the constraint that \( \delta \) must be a two dimensional array of size 50.

Figure 9 presents type rules for expressions. A typing environment \( H \) is a map from names to internal types. Constants \( c \) type-check against their intrinsic type. Type \( \text{int} \) is a subtype of \( \text{real} \). A use of a name \( x \) type-checks against its declared type in \( H \). Arrays, vectors, and matrices that are constructed from literals have concrete sizes. Indexing requires integer subscripts and returns element types. Due to vectorization, the rule for function call expressions is the most intricate. The set \( \text{inst}(f) \) represents instantiations of the type of the function \( f \) with vectorization information \( v \) for each argument. Each \( v_i \) indicates whether the corresponding argument \( e_i \) can be lifted to an array. Vectorization must infer the sizes of arrays.

Figure 10 presents the vectorization relation \( t \uparrow^v t' \). If \( v \) is true, then \( t \) is a composite type derived by appropriate replication of values of \( t' \) to yield components of \( t \). If \( v \) is false, then only the trivial vectorization where \( t \) and \( t' \) are the same works, i.e., there is no broadcasting. For example, if \( x \) is of type \( \text{real}[10] \) in \( H \), then we have the following typing derivation:

\[
H \vdash \text{real}[10]^\text{true} * \text{real}[10]^\text{true} \rightarrow \text{real}[10] \in \text{inst}(\forall \sigma. \text{real}[\sigma]^\text{true} * \text{real}[\sigma]^\text{true} \rightarrow \text{real}[\sigma]) \\
H \vdash x : \text{real}[10] \\
H \vdash 1 : \text{real} \\
H \vdash \text{normal}(x, 1) : \text{real}[10]
\]
This section shows that our compilation scheme combined with conservative syntax extensions can be used to lift these benefits for Stan users. Building on Pyro, we propose DeepStan, an extension.

5 EXTENDING STAN: EXPLICIT VARIATIONAL GUIDES AND NEURAL NETWORKS

Probabilistic languages like Pyro offer new features to program and reason about complex models. This section shows that our compilation scheme combined with conservative syntax extensions can be used to lift these benefits for Stan users. Building on Pyro, we propose DeepStan, an extension.
which introduce learnable parameters. Unlike Stan parameters that define random variables for use without running the inference first, which prevents the use of non-generative features and updates. Variational Inference (VI) tries to find the member $q$ that is the closest to the true posterior $p$, i.e., it must sample all the parameters of the model; and its fitness is measured using the Kullback-Leibler (KL) divergence from the true posterior, which VI aims to minimize: $q_\theta(z) = \underset{\theta \in \Theta}{\text{argmin}} \text{KL}(q_\theta(z) || p(z | x))$.

Pyro natively support variational inference and lets users define the family $Q$ of simpler distributions that is the closest to the true posterior $p(z | x)$ [Blei et al. 2017]. Members of the family $Q$ are characterized by the values of the variational parameters $\theta$. The fitness of a candidate is measured using the Kullback-Leibler (KL) divergence from the true posterior, which VI aims to minimize: $q_\theta(z) = \underset{\theta \in \Theta}{\text{argmin}} \text{KL}(q_\theta(z) || p(z | x))$.

DeepStan inherits restrictions for the definition of the guide from Pyro: the guide must be defined on the same parameter space as the model, i.e., it must sample all the parameters of the model; and the guide should also describe a distribution from which we can directly generate valid samples without running the inference first, which prevents the use of non-generative features and updates of target. Our compiler checks these restrictions statically for early error reporting. Once these conditions are verified, the generative translation from Section 2.1 generates a Python function that can serve as a Pyro guide. The guide block defines a distribution parameterized by the guide parameters. Variational inference then optimizes the values of these parameters to approximate the true posterior.

DeepStan inherits restrictions for the definition of the guide from Pyro: the guide must be defined on the same parameter space as the model, i.e., it must sample all the parameters of the model; and the guide should also describe a distribution from which we can directly generate valid samples without running the inference first, which prevents the use of non-generative features and updates of target. Our compiler checks these restrictions statically for early error reporting. Once these conditions are verified, the generative translation from Section 2.1 generates a Python function that can serve as a Pyro guide. The guide block defines a distribution parameterized by the guide parameters. Variational inference then optimizes the values of these parameters to approximate the true posterior.

5.2 Adding neural networks

One of the main advantages of Pyro is its tight integration with PyTorch which allows the authoring of deep probabilistic models, that is, probabilistic models involving neural networks. In comparison, it is impractical to define neural networks directly in Stan. To make this feature available for Stan users, we extend Stan with an optional block networks to import neural network definitions.
Neural networks can be used to capture intricate dynamics between random variables. An example is the Variational Auto-Encoder (VAE) illustrated in Figure 13. A VAE learns a vector-space representation $z$ for each observed data point $x$ (e.g., the pixels of an image) [Kingma and Welling 2013; Rezende et al. 2014]. Each data point $x$ depends on the latent representation $z$ in a complex non-linear way, via a deep neural network: the decoder. The leftmost part of Figure 13 shows the corresponding graphical model. The output of the decoder is a vector $\mu$ that parameterizes a Bernoulli distribution over each dimension of $x$ (e.g., each pixel is associated to a probability of being present in the image).

The key idea of the VAE is to use variational inference to learn the latent representation. The guide maps each $x$ to a latent variable $z$ via another neural network: the encoder. The middle part of Figure 13 shows the graphical model of the guide. The encoder returns, for each input $x$, the parameters $\mu_z$ and $\sigma_z$ of a Gaussian distribution in the latent space. Then inference tries to learn good values for the parameters $\theta$ and $\phi$, simultaneously training the decoder and the encoder.

The right part of Figure 13 shows the corresponding code in DeepStan. A network is introduced by the name of its class and an identifier. This identifier can then be used in subsequent blocks, in particular the model block and the guide block. The network class must be implemented in PyTorch and the associated variable must be a valid instance of the class.

**Deducing shapes.** Since model code spans both Stan and PyTorch, one challenge is to minimize redundancy while checking for errors and generating efficient code. As shown in Figure 13 we let users elide some of the concrete tensor dimensions by writing the wildcards “\_” and “\*” instead. The tensor shape analysis from Section 4 automatically fills in the size and number of dimensions.

The following example illustrates how our analysis uses unification to figure out the type of variable $z$ in the VAE in Figure 13. The parameters block declares real $z[\ast\ast]$, which our analysis represents with the generic type real[\*\*]δ. But code generation needs concrete dimensions for initializing $z$ correctly. The analysis needs to derive those concrete dimensions elsewhere. The statement $z \sim \text{normal}(\theta, 1)$ yields no new information about the dimensions because it is auto-vectorized. The declaration real encoded[2, nz] tells the analysis that variable encoded has type real[2][nz], a nested array of dimensions 2 and nz. The assignment mu_z = encoded[1] unifies the type of mu_z with real[nz]. Finally, the statement $z \sim \text{normal}(\text{mu}_z, \text{sigma}_z)$ unifies the type of $z$ with the type of $\text{mu}_z$, so now $z$ has type real[nz]. So, in Figure 13, the compiler computes the shape of parameters $z$ (nz), $\mu_z$ (28, 28), $\mu_z$ and $\sigma_z$ (nz).
Extending Stan for Deep Probabilistic Programming

networks { MLP mlp; }
data { int<lower=0, upper=1> img[28, 28];
  int<lower=0, upper=9> label; }
parameters { real mlp.l1.weight[*]; real mlp.l1.bias[*];
  real mlp.l2.weight[*]; real mlp.l2.bias[*]; }
model { real lambda_[10];
  mlp.l1.weight ~ normal(0, 1);
  mlp.l1.bias ~ normal(0, 1);
  mlp.l2.weight ~ normal(0, 1);
  mlp.l2.bias ~ normal(0, 1);
  lambda_ = mlp(img);
  label ~ categorical_logits(lambda_); }
guide parameters { real w1_mu[*]; real w1_sgma[*];
    real b1_mu[*]; real b1_sgma[*];
    real w2_mu[*]; real w2_sgma[*];
    real b2_mu[*]; real b2_sgma[*]; }
guide { mlp.l1.weight ~ normal(w1_mu, exp(w1_sgma));
  mlp.l1.bias ~ normal(b1_mu, exp(b1_sgma));
  mlp.l2.weight ~ normal(w2_mu, exp(w2_sgma));
  mlp.l2.bias ~ normal(b2_mu, exp(b2_sgma)); }

Fig. 14. Graphical models and DeepStan code of the Bayesian MLP.

The code generator then uses these deduced shapes to put the concrete dimension size into the generated Python. For example, the compilation of \( z \sim \text{normal}(0, 1) \) produces:

\[
\text{sample}(\text{dist.Normal(zeros(nz), ones(nz)), obs=z})
\]

5.3 Bayesian networks

Neural networks can also be treated as probabilistic models. A Bayesian neural network is a neural network whose learnable parameters (weights and biases) are random variables instead of concrete values [Neal 2012]. Building on Pyro features, we make it easy for users to lift neural networks, i.e., replace concrete neural network parameters by random variables.

The left side of Figure 14 shows a simple classifier for handwritten digits based on a multi-layer perceptron (MLP) where all the parameters are lifted to random variables. Unlike the networks used in the VAE, the parameters (regrouped under the variable \( \theta \)) are represented using a circle to indicate random variables. The inference starts from prior beliefs about the parameters and learns distributions that fit observed data. We can then generate samples of concrete weights and biases to obtain an ensemble of as many MLPs as we like. The ensemble can vote for predictions and can quantify agreement.

The right of Figure 14 shows the corresponding code in DeepStan. We let users declare lifted neural network parameters in Stan’s parameters block just like any other random variables. Network parameters are identified by the name of the network and a path, e.g., mlp.l1.weight, following PyTorch naming conventions. The model block defines normal(0,1) priors for the weights and biases of the two linear layers of the MLP. Then, for each image, the computed label follows a categorical distribution parameterized by the output of the network, which associates a probability to each of the ten possible values of the discrete random variable label. The guide parameters define \( \mu \) and \( \sigma \), and the guide block uses those parameters to propose normal distributions for the model parameters.

Compiling Bayesian neural networks. To lift neural networks, we use Pyro random_module, a primitive that takes a PyTorch network and a dictionary of distributions and turns the network into
### (a) Double normal

```abh
parameters {
  real theta;
}

model {
  theta ~ normal(1000, 1);
  theta ~ normal(1000, 1);
}
```

### (b) Linear Regression

```abh
data {
  int<lower=0> N;
  vector[N] x;
  vector[N] y;
}

parameters {
  real alpha;
  real beta;
  real<lower=0> sigma;
}

model {
  y ~ normal(alpha + beta * x, sigma);
}
```

### (c) Reparameterization

```abh
parameters {
  real y_std;
  real x_std;
}

transformed parameters {
  real y = 3.0 * y_std;
  real x = exp(y/2) * x_std;
}

model{
  y_std ~ normal(0, 1);
  x_std ~ normal(0, 1);
}
```

---

**Fig. 15. Basic examples for the comparison of Stan and DeepStan**

a distribution of networks where each parameter is sampled from the corresponding distribution. We treat network parameters as any other random variables, that is, we apply the comprehensive translation from Section 2.3. This translation initializes parameters with a uniform prior.

```abh
priors = {}
priors['l1.weight'] = ImproperUniform(shape=mlp.l1.weight.shape)
... # priors of the other parameters
lifted_mlp = pyro.random_module('mlp', mlp, priors)()
```

Then, the Stan `~` statements in the `model` block are compiled into Pyro `observe` statements.

```abh
mlp_params = dict(lifted_mlp.named_parameters())
sample('l1.weight', Normal(zeros(mlp.l1.weight.size()), ones(mlp.l1.weight.size())), obs=mlp_params['l1.weight'])
```

It is also possible to mix probabilistic parameters and non-probabilistic parameters. Our translation only lifts the parameters that are declared in the `parameters` block by only adding those to the priors dictionary.

### 6 EVALUATION

This section evaluates DeepStan on multiple examples. To test our compilation scheme, for a subset of examples, we run inference on the generated Pyro code using NUTS (No U-Turn Sampler [Homan and Gelman 2014], an optimized HMC which is the preferred inference method for Stan, and compare the results with Stan (Section 6.1). We show on a simple example that, sometimes, using explicit VI gives comparable or even more accurate results (Section 6.1). Finally, for deep probabilistic models, we compare the generated Pyro code against hand-written code and find comparable results (Section 6.2).

#### 6.1 Comparison of Stan and DeepStan

This section describes eight experiments comparing inference output from Stan and DeepStan. The first four examples exercise our translation techniques on simple models with no data or synthetic data. **Coin** is the example presented Figure 1. **Double normal** is doing multiple updates of the same
Table 2. Comparison of execution time and parameter distributions between Stan and DeepStan.

| Parameter     | Stan  | DeepStan/Pyro | DeepStan/NumPyro |
|---------------|-------|---------------|------------------|
|               | time(s) | time(s) | KS p-value | time(s) | KS p-value |
| coin          | 110 + 0.3 | 219     | 0.41 (z)   | 70       | 0.41 (z)   |
| double normal | 107 + 0.2 | 76      | 0.34 (theta) | 57       | 0.66 (theta) |
| reparameterization | 121 + 0.7 | 114     | 0.50 (x_std) | 117      | 0.40 (y)   |
| linear regression | 85 + 0.5  | 348     | 0.23 (beta) | 61       | 0.26 (sigma) |
| aspirin       | 70 + 0.8  | 635     | 0.32 (tau)  | 83       | 0.16 (theta_raw[4]) |
| roaches       | 73 + 6.8  | 551     | 0.30 (beta[2]) | 38       | 0.50 (beta[3]) |
| 8 schools     | 67 + 1.0  | 842     | 0.38 (theta[5]) | 58       | 0.12 (eta[6]) |
| seeds         | 66 + 3.4  | 1,081   | 0.29 (sigma) | 74       | 0.21 (b[3]) |

Parameter \( \theta \) (Figure 15a). Linear Regression is the simplest linear regression model (Figure 15b). Reparameterization is the reparameterized Neal’s funnel example that uses transformed parameters (Figure 15c). The last four examples, aspirin, roaches, 1 8 schools, and seeds, are popular hierarchical models with real data that are taken from the Stan examples git repository. 2 These examples are also used for comparing SlicStan to Stan in [Gorinova et al. 2019].

Experimental setup. Pyro offers two implementation of NUTS, one leveraging PyTorch (classic Pyro), and another one based on Numpy and JAX (NumPyro). We ran the experiments with these two runtimes and compared the computed distributions with the results of Stan.

Experiments were run in parallel on a Linux server with 32 cores (2GHz, 242 GB RAM) with the latest version of Pyro (1.3.1), NumPyro (0.2.4), and PyStan (2.19.1.1). The inference method is NUTS with 10,000 sampling steps, 1,000 warmup steps, and 1 Markov chain. To reduce the autocorrelation of the samples and increase the effective sample size, we then used a thinning factor of 10 (i.e., select one sample every 10 draws).

For each parameter, we compare the posterior marginal distributions generated by Stan and DeepStan using a two-sample Kolmogorov-Smirnov (KS) test on all the parameters. For multidimensional parameters we run the KS test for every component. If the p-value of the KS test is above the significance level (e.g., >0.05), we cannot reject the hypothesis that the distributions of the two samples are the same.

Results. Table 2 summarizes the results of our experiments. For each model, we report the compilation and execution time for Stan, the execution time of the two Pyro runtimes, and the parameter with the lowest p-value for the KS test. All the results are averaged over 10 runs (times and KS test results). Since none of the the KS p-values are below the significance level, these results empirically validate that our translation from DeepStan to Pyro preserves the Stan semantics.

Stan first compiles the model to C++ and compiles the C++ code, which takes significant time, but the inference is impressively fast. In comparison, the compilation from DeepStan to Pyro is quasi-instantaneous, but the Pyro version of NUTS is significantly slower. NumPyro was introduced to mitigate this issue by leveraging Numpy efficient vectorization and JAX just-in-time compilation (JIT). Table 2 shows that, while NumPyro is in average significantly faster than classic Pyro on our set of examples (with the notable exception of Reparameterization), it is still much slower than Stan.

1 We adapted the roaches model with priors found in https://avehtari.github.io/modelselection/roaches.html
2 https://github.com/stan-dev/example-models
Explicit variational guide. The multimodal example shown in Figure 16 is a mixture of two Gaussian distributions with different means but identical variances. The histograms in the left half of Figure 16 show that in both Stan and DeepStan, this example is particularly challenging for NUTS. Using multiple chains, NUTS finds the two modes, but the chains do not mix and the relative densities are incorrect.

This is a known limitation of HMC. As shown in the code of Figure 16 we can provide a custom variational guide that will correctly infer the two modes (DeepStanSVI). Note, however, that this approach requires a priori knowledge about the shape of the true posterior.

6.2 Deep probabilistic models

Since Stan lacks support for deep probabilistic models, we could not use it as a baseline. Instead, we compare the performance of the code generated by our compiler with hand-written Pyro code on the VAE described in Section 5.2 and a simple Bayesian neural network.

VAE. Variational autoencoders were not designed as a predictive model but as a generative model to reconstruct images. Evaluating the performance of a VAE is thus non-obvious. We use the following experimental setting. We trained two VAEs on the MNIST dataset using VI: one hand-written in Pyro, the other written in DeepStan. For each image in the test set, the trained VAEs compute a latent representation of dimension 5. We then cluster these representations using KMeans with 10 clusters. Then we measure the performance of a VAE with the pairwise F1 metric: true positives are the number of images of the same digit that appear in the same cluster. For Pyro F1=0.41 (precision=0.43, recall=0.40), and for DeepStan F1=0.43 (precision=0.44, recall=0.42). These numbers shows that compiling DeepStan to Pyro does not impact the performance of such deep probabilistic models.

Bayesian MLP. We trained two versions of a 2-levels Bayesian multi-layer perceptron (MLP) where all the parameters are lifted to random variables (see section 5.3): one hand-written in Pyro, the other written in DeepStan. We trained both models for 20 epochs on the training set. For each model we then generated 100 samples of concrete weights and biases to obtain an ensemble MLP.

\[ \text{parameters} \{ \]
\[ \text{real cluster;} \]
\[ \text{real theta;} \}
\[ \text{model} \{ \]
\[ \text{real mu;} \]
\[ \text{cluster} \sim \text{normal}(0, 1); \]
\[ \text{if} \ (\text{cluster} > 0) \ \text{mu} = 20; \]
\[ \text{else mu} = 0; \]
\[ \text{theta} \sim \text{normal}(\mu, 1); \}
\[ \text{guide parameters} \{ \]
\[ \text{real mc;} \]
\[ \text{real m1; real m2;} \]
\[ \text{real ls1; real ls2;} \}
\[ \text{guide} \{ \]
\[ \text{cluster} \sim \text{normal}(mc, 1); \]
\[ \text{if} \ (\text{cluster} > 0) \ \text{theta} \sim \text{normal}(m1, \text{exp(ls1)}); \]
\[ \text{else theta} \sim \text{normal}(m2, \text{exp(ls2)}); \}

Fig. 16. DeepStan code and histograms of the multimodal example using Stan, DeepStan with NUTS, and DeepStan with VI.

3https://mc-stan.org/users/documentation/case-studies/identifying_mixture_models.html
The log-likelihood of the test set is then computed for each MLP. We observe that the log-likelihood distribution is indistinguishable for the two models (KS p-value: 0.99) and the execution time is about the same. Again, these experiments show that compiling DeepStan models to Pyro has little impact on the model. Additionally, we observe that changing the priors on the network parameters from $\text{normal}(0,1)$ to $\text{normal}(0,10)$ (see section 5.3) increases the accuracy of the models from 0.92 to 0.96. This further validates our compilation scheme where priors on parameters are compiled to observe statements on deep probabilistic models.

7 RELATED WORK

To the best of our knowledge, we propose the first comprehensive translation of Stan to a generative PPL. The closest related work has been developed by the Pyro team [Chen et al. 2018]. Their work focuses on performance and our work on completeness. Their proposed compilation technique corresponds to the generative translation presented in Section 2.1 and thus only handles a subset of Stan. Compared to our approach, they are also looking into independence assumptions between loop iterations to generate parallel code. Combining these ideas with our approach, in particular leveraging our type system to add independence assumptions, is a promising future direction. They do not extend Stan with VI and neural networks. Appendix B.2 of [Gorinova et al. 2018] also outlines the generative translation of Section 2.1, but also mention the issue with multiple updates.

The goal of compiling Stan to Pyro is not to replace Stan’s highly optimized inference engine [Homan and Gelman 2014], but rather to create a platform for experimenting with new ideas. As an example, Section 5.1 showed how to extend Stan with explicit variational guides. In the same vein, Pyro now offers tools for automatic variational guide synthesis [Blei et al. 2017] that can now be tested on existing Stan models.

In recent years, taking advantage of the maturity of DL frameworks, multiple deep probabilistic programming languages have been proposed: Edward [Tran et al. 2017] and ZhuSuan [Shi et al. 2017] built on top of TensorFlow, Pyro [Bingham et al. 2019] and ProbTorch [Siddharth et al. 2017] built on top of PyTorch, and PyMC3 [Salvatier et al. 2015] built on top of Theano. All these languages are implemented as libraries. The users thus need to master the entire technology stack of the library, the underlying DL framework, and the host language. In comparison, DeepStan is a self-contained language and the compiler helps the programmer via dedicated static analyses (e.g., the tensor dimension analysis of Section 5.2).

Finally, Section 4 presents a type system for tensor shape analysis. Previous work on efficiently executing matlab performs a similar analysis using an algebraic approach [Joisha et al. 2003].

8 CONCLUSION

This paper proves a comprehensive compilation scheme from Stan to any generative probabilistic programming language. We thus show that Stan is at most as expressive as this family of languages. To validate our approach we implemented a compiler from Stan to Pyro. Additionally, we designed and implemented extensions for Stan with explicit variational guides and neural networks.

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