Gen: A General-Purpose Probabilistic Programming System with Programmable Inference

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Abstract
Probabilistic modeling and inference are central to many fields. A key challenge for wider adoption of probabilistic programming languages is designing systems that are both flexible and performant. This paper introduces Gen, a new probabilistic programming system with novel language constructs for modeling and for end-user customization and optimization of inference. Gen makes it practical to write probabilistic programs that solve problems from multiple fields. Gen programs can combine generative models written in Julia, neural networks written in TensorFlow, and custom inference algorithms based on an extensible library of Monte Carlo and numerical optimization techniques. This paper also presents techniques that enable Gen’s combination of flexibility and performance: (i) the generative function interface, an abstraction for encapsulating probabilistic and/or differentiable computations; (ii) domain-specific languages with custom compilers that strike different flexibility/performance tradeoffs; (iii) combinators that encode common patterns of conditional independence and repeated computation, enabling speedups from caching; and (iv) a standard inference library that supports custom proposal distributions also written as programs in Gen. This paper shows that Gen outperforms state-of-the-art probabilistic programming systems, sometimes by multiple orders of magnitude, on problems such as nonlinear state-space modeling, structure learning for real-world time series data, robust regression, and 3D body pose estimation from depth images.

1 Introduction
Probabilistic modeling and inference are central to diverse fields, such as computer vision, robotics, statistics, and artificial intelligence. Probabilistic programming languages aim to make it easier to apply probabilistic modeling and inference, by providing language constructs for specifying models and inference algorithms. Most languages provide automatic “black box” inference mechanisms based on Monte Carlo, gradient-based optimization, or neural networks. However, applied inference practitioners routinely customize an algorithm to the problem at hand to obtain acceptable performance. Recognizing this fact, some recently introduced languages offer “programmable inference” [29], which permits the user to tailor the inference algorithm based on the characteristics of the problem.

However, existing languages have limitations in flexibility and/or performance that inhibit their adoption across multiple applications domains. Some languages are designed to be well-suited for a specific domain, such as hierarchical Bayesian statistics (Stan [6]), deep generative modeling (Pyro [5]), or uncertainty quantification for scientific simulations (LibBi [33]). Each of these languages can solve problems in some domains, but cannot express models and inference algorithms needed to solve problems in other domains. For example, Stan cannot be applied to open-universe models, structure learning problems, or inverting software simulators for computer vision applications. Pyro and Turing [13] can represent these kinds of models, but exclude many important classes of inference algorithms. Venture [29] expresses a broader class of models and inference algorithms, but incurs high runtime overhead due to dynamic dependency tracking.

Key Challenges
Two key challenges in designing a practical general-purpose probabilistic programming system are: (i) achieving good performance for heterogeneous probabilistic models that combine black box simulators, deep neural networks, and recursion; and (ii) providing users with abstractions that simplify the implementation of inference algorithms while being minimally restrictive.

This Work
We introduce Gen, a probabilistic programming system that uses a novel approach in which (i) users define probabilistic models in one or more embedded probabilistic DSLs and (ii) users implement custom inference algorithms in the host language by writing inference programs that manipulate the execution traces of models. This architecture affords users with modeling and inference flexibility that is important in practice. The Gen system, embedded in Julia [4], makes it practical to build models that combine structured probabilistic code with neural networks written in platforms such as TensorFlow. Gen also makes it practical to write inference programs that combine built-in operators for Monte Carlo inference and gradient-based optimization with custom algorithmic proposals and deep inference networks.
A Flexible Architecture for Modeling and Inference  
In existing probabilistic programming systems [13, 15, 48], inference algorithm implementations are intertwined with the implementation of compilers or interpreters for specific probabilistic DSLs that are used for modeling (Figure 1b). These inference algorithm implementations lack dimensions of flexibility that are routinely used by practitioners of probabilistic inference. In contrast, Gen’s architecture (Figure 1a) abstracts away probabilistic DSLs and their implementation from inference algorithm implementation using the generative function interface (GFI). The GFI is a black box abstraction for probabilistic and/or differentiable computations that exposes several low-level operations on execution traces. Generative functions, which are produced by compiling probabilistic DSL code or by applying generative function combinators to other generative functions, implement the GFI. The GFI enables several types of domain-specific and problem-specific optimizations that are key for performance:

- Users can choose appropriate probabilistic DSLs for their domain and can combine different DSLs within the same model. This paper outlines two examples: a TensorFlow DSL that supports differentiable array computations resident on the GPU and interoperates with automatic differentiation in Julia, and a Static DSL that enables fast operations on execution traces via static analysis.
- Users can implement custom inference algorithms in the host language using the GFI and optionally draw upon a higher-level standard inference library that is also built on top of the GFI. User inference programs are not restricted by rigid algorithm implementations as in other systems.
- Users can express problem-specific knowledge by defining custom proposal distributions, which are essential for good performance, in probabilistic DSLs. Proposals can also be trained or tuned automatically.
- Users can easily extend the language by adding new probabilistic DSLs, combinators, and inference abstractions implemented in the host language.

Evaluation  
This paper includes an evaluation that shows that Gen can solve inference problems including 3D body pose estimation from a single depth image; robust regression; inferring the probable destination of a person or robot traversing its environment; and structure learning for real-world time series data. In each case, Gen outperforms existing probabilistic programming languages that support customizable inference (Venture and Turing), typically by one or more orders of magnitude. These performance gains are enabled by Gen’s more flexible inference programming capabilities and high-performance probabilistic DSLs.

Main Contributions  
The contributions of this paper are:

- A probabilistic programming approach where users (i) define models in embedded probabilistic DSLs; and (ii) implement probabilistic inference algorithms using inference programs (written in the host language) that manipulate execution traces of models (Section 2).
- The generative function interface, a novel black box abstraction for probabilistic and/or differentiable computations that separates probabilistic DSLs from the implementation of inference algorithms (Section 3).
- Generative function combinators, which produce generative functions that exploit common patterns of conditional independence to enable efficient operations on execution traces. We give three examples of combinators: map, unfold, and recurse (Section 4).
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- Gen, a system implementing this approach with three interoperable probabilistic DSLs (Section 5).
- An empirical evaluation of Gen’s expressiveness and efficiency relative to other probabilistic programming languages on five challenging inference problems (Section 6).

2 Overview

In this section, we walk through an example probabilistic model, demonstrate three probabilistic inference programs for the model, and highlight the main features of Gen’s architecture along the way. The example in Figure 2 is based on modeling a response variable $y$ as a linear function of a dependent variable $x$. Figure 2a presents the inference problem: given a data set of observed pairs $(x_i, y_i)$, the goal of probabilistic inference is to infer the relationship between $y$ and $x$, as well as identify any data points $i$ that do not conform to the inferred linear relationship (i.e. detect outliers). Figure 2b presents code in a probabilistic domain-specific language that defines the probabilistic model. The three inference programs, implemented in Julia, are shown in Figure 2f. Each of these inference programs implements a different algorithm for solving the inference task and, as a result, exhibits different performance characteristics, shown in Figure 2g.

2.1 Example Probabilistic Model

We now describe the ideas in Figure 2b in greater detail.

Models are Generative Functions Users define probabilistic models by writing generative functions in probabilistic DSLs. Generative functions generate realizations of (typically stochastic) processes. The probabilistic DSL used in this example is called the Dynamic DSL (syntax in Figure 3). The model in this example is defined by the generative function ‘model’ (Lines 14-29). Generative functions in the Dynamic DSL are identified by a @gen annotation in front of a regular Julia function definition. Dynamic DSL functions may use arbitrary Julia code, as long as they do not mutate any externally observable state. Dynamic DSL functions make random choices with functions like normal and bernoulli that sample from an extensible set of probability distributions (for instance, normal($\theta, 1$) draws a random value from the standard normal distribution) Each random choice represents either a latent (unknown) or observable quantity.

The generative function model takes as input a vector of dependent variables $x$s (containing the $x_i$) and returns a vector of response variables $y$s (containing the $y_i$). First, in Lines 15-18, the model makes random choices (shown in green) for the parameters (prob_outlier, noise, slope, intercept) that govern the linear relationship from their prior distributions. The parameters slope and intercept parameterize the assumed linear dependence of $y_i$ on $x_i$. The parameter noise determines, for data points that are not outliers, the variance of the response variable around the straight regression line.

Finally, the parameter prob_outlier is the probability that any given data point is an outlier.

Addresses of Random Choices Each random choice made when executing a generative function defined in the Dynamic DSL is given a unique address (shown in purple) using the @addr keyword. For example, the prob_outlier choice (Line 18) has address :prob_outlier. In general, the address of a choice is independent of any name to which its value may be assigned in the function body (note that random choices need not be bound to any identifier in the function body). Addresses are arbitrary Julia values that may be dynamically computed during function execution. The random choices seen so far have addresses that are Julia symbol values.

Generative Function Combinators Having generated the parameters, the generative function model next generates each $y_i$ from the corresponding $x_i$, for each data point $i$ (Lines 19-27). The @diff block (Lines 19-23, brown) is an optional performance optimization which we will discuss later. Lines 25-27 call the generative function ‘generate_datum’ (Lines 1-10) once for each data point, passing in the $x_i$ and each of the four parameters. To do this, we use MapCombinator, which is a generative function combinator (Section 4) that behaves similarly to the standard higher order function ‘map’. On Line 12, the MapCombinator Julia function takes the generative function generate_datum and returns a second generative function (generate_data) that applies the first function repeatedly to a vector of argument values, using independent randomness for each application. On Line 25, the model function calls generate_data, which in turns calls generate_datum once for each data point $i$ to generate the $y_i$ from the corresponding $x_i$ and the parameters. Within the $i$th application of generate_datum, a Bernoulli random choice (Line 4) determines whether data point $i$ will be an outlier or not. If the data point is not an outlier (Line 7), then the response variable $y_i$ has an expected value (mu) that is a linear function of $x_i$ and standard deviation (std) equal to noise. If the data point is an outlier (Line 5), then $y_i$ has an expected value of 0 and a large standard deviation (10). Finally, we sample the response variable $y_i$ from a normal distribution with the given expected value and standard deviation (Line 9).

Hierarchical Address Spaces When calling other generative functions, @addr is used to indicate the namespace relative to which all random choices made during the call are addressed. For example, model calls generate_data with namespace :data (Lines 25-27). Generative functions that are produced by generative function combinators also give a namespace to each call they make—generate_data calls generate_datum once for each data point with a unique integer namespace ranging from 1 to 100 (for 100 data points). Figure 2c presents the hierarchical address space of random choices made by model. Hierarchical addresses are constructed by chaining together address components using the
Figure 2. Example of the proposed programming model. Probabilistic DSLs are used to define (b) probabilistic models and (d) custom proposal distributions. (e)–(f) algorithms are implemented by users in the host language, using methods provided by the standard inference library (shown in bold). (g) shows the time-accuracy profiles of the three inference programs in (f).
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\[ D := \text{normal} | \text{gamma} | \text{categorical} | \ldots \]
\[ E := J | R | F \]
\[ R := @\text{addr} (D(E_2, E_3, ..), E_1) \]
\[ F := @\text{addr} (G(E_2, E_3, ..), E_1) \]

**Figure 3.** Syntax of the Dynamic DSL, which is embedded in Julia. \( J \) are Julia expressions, \( G \) are names of generative functions, \( D \) are probability distributions, \( E \) are expressions, \( R \) are random choices, and \( F \) are calls to generative functions.

\( \Rightarrow \) operator. For example, \( :\text{data} \Rightarrow 2 \Rightarrow \text{is\_outlier} \) refers to the \texttt{is\_outlier} random choice for the second data point.

**Argdiffs Enable Efficient Trace Updates** The @diff code block in \texttt{model} (Lines 19-23, brown) is optional, but important for good performance of Markov Chain Monte Carlo (MCMC) inference. MCMC inference often involves making small changes to an execution of a generative function. The @diff block is a feature of the Dynamic DSL that allows users to insert code that computes the change to the arguments to a call (the \texttt{argdiff}) from one execution to another execution, as well as the change to the return value of a function (the \texttt{retdiff}, not used in this example). The \texttt{argdiff} can indicate that the arguments to a call have not changed (\texttt{noargdiff}) or that they may have changed (\texttt{unknownargdiff}), or can provide detailed information about the change. In this case, the \texttt{argdiff} passed to the call to \texttt{generate\_data} indicates whether or not the parameters of the model have changed from the previous execution. If the parameters have changed, then the call to \texttt{generate\_data} must be visited for each data point to construct the new execution trace. If the parameters have not changed, then most calls to \texttt{generate\_data} can be avoided. This feature enables efficient asymptotic scaling of MCMC. Note that code in the @diff block and the \texttt{argdiff} variable (Line 27) are not part of the generative function body and are only used when updating an execution.

### 2.2 Example User Inference Programs

Figure 2f shows three user inference programs, which are Julia functions that implement different custom algorithms for inference in the example probabilistic model. These inference programs are implemented using high-level abstractions provided by our system (these methods e.g. \texttt{select} and \texttt{initialize} are shown bold-face in the code figures). Each inference program takes as input a data set containing many \((x_i, y_i)\) values; it returns inferred values for the parameters that govern the linear relationship and the outlier classifications.

**Execution Traces as Data Structures** The results of inference take the form of an execution trace (trace) of the generative function \texttt{model}. An execution trace of a generative function contains the values of random choices made during an execution of the function, and these values are accessed using indexing syntax (e.g. \texttt{trace[:slope], trace[:data => 5 => :is\_outlier]}). The inference programs return traces whose random choices represent the inferred values of latent variables in the model. In addition to the random choices, an execution trace (or just ‘trace’) also contains the arguments on which the function was executed, and the function’s return value. Traces are persistent data structures.

**Generative Function Interface** Each inference program in Figure 2f first obtains an initial trace by calling the \texttt{initialize} method on the generative function (\texttt{model}) and supplying (i) arguments (\( xs \)) to the generative function; and (ii) a mapping (constraints) from addresses of certain random choices to constrained values (Lines 65, 79, 89). The \texttt{initialize} method is part of the generative function interface (GFI, Section 3), which exposes low-level operations on execution traces. The constraints are an assignment (produced by Figure 2e, Line 41), which is a prefix tree that maps addresses to values. Users construct assignments that map addresses of observed random choices to their observed values. Each inference program constrains the \( y \)-coordinates to their observed values. Inference program 2 also constrains the slope and intercept (Lines 77-78) to values obtained from a heuristic procedure (\texttt{least\_squares}) implemented in Julia. The other two inference programs initialize the slope and intercept to values randomly sampled from the prior distribution.

**Standard Inference Library** After obtaining an initial trace, each program in Figure 2f then uses a Julia for loop (Lines 66, 80, 90) to repeatedly apply a cycle of different Markov Chain Monte Carlo (MCMC) updates to various random choices in the trace. These updates improve the random choices in the initial trace in accordance with the constrained observations. The MCMC updates use the methods \texttt{default\_mh} and \texttt{custom\_mh} from the standard inference library, which provides higher-level building blocks for inference algorithms that are built on top of the GFI. Inference program 1 uses \texttt{default\_mh}, which proposes new values for certain selected random choices according to a default proposal distribution and accepts or rejects according to the Metropolis-Hastings (MH, [19]) rule.

**Custom Proposals are Generative Functions** Each inference program in Figure 2f updates the outlier indicator variables using \texttt{is\_outlier\_update} (Figure 2e, Lines 57-62). This procedure loops over the data points and performs an MH update to each \texttt{is\_outlier} choice using the \texttt{custom\_mh} method from the standard inference library. The update uses a custom proposal distribution defined by \texttt{is\_outlier\_proposal} (Figure 2d, Lines 30-34) which reads the previous value of the variable and then proposes its negation by making a random choice at the same address :\texttt{data => 1 => :is\_outlier}. Custom proposal distributions are defined as generative functions using the same probabilistic DSLs used to define probabilistic models. Inference program 3 uses a different MH
update with a custom proposal (\texttt{ransac_proposal}, Figure 2d Lines 36-40) to propose new values for the slope and intercept by adding noise to values estimated by the RANSAC [12] robust estimation algorithm.

**Using Host Language Abstraction** Inference programs 2 and 3 in Figure 2d both invoke \texttt{parameter_update} (Figure 2e, Lines 49-55), which applies MH updates with default proposals to :\texttt{prob_outlier} and :\texttt{noise}, but uses a Metropolis-Adjusted Langevin Algorithm (MALA, [39]) update for the slope and intercept (\texttt{mala}, Line 53). The standard inference library method \texttt{mala} relies on automatic differentiation in the model function (@ad annotation, Lines 2-3) to compute gradients of the log probability density with respect to the selected random choices. Inference programs make use of familiar host language constructs, including procedural abstraction (e.g., reusable user-defined inference sub-routines like \texttt{parameter_update}) and loop constructs (to repeatedly invoke nested MCMC and optimization updates). These host language features obviate the need for new and potentially more restrictive 'inference DSL' constructs [13, 28]. Using familiar host language constructs, including procedural abstraction (e.g., reusable user-defined inference sub-routines like \texttt{parameter_update}) and loop constructs (to repeatedly invoke nested MCMC and optimization updates).

**Performance Depends on the Inference Algorithm** As seen in Figure 2g, the three inference programs perform differently. The default proposal for the parameters used in inference program 1 causes slow convergence as compared to the combination of MALA updates and custom initialization used in inference program 2. The custom RANSAC proposal used in inference program 3 also improves convergence—it does not employ local random walk search strategy like the MALA update, but instead proposes approximate estimates from scratch with each application. The constructs in our system make it practical for the user to experiment with and compare various inference strategies for a fixed model.

## 3 Generative Function Interface

The generative function interface (GFI) is a black box abstraction for probabilistic and/or differentiable computations that provides an abstraction barrier between the implementation of probabilistic DSLs and implementations of inference algorithms. Generative functions are objects that implement the methods in the GFI and are typically produced from DSL code by a probabilistic DSL compiler. For example, the Dynamic DSL compiler takes a @gen function definition and produces a generative function that implements the GFI. Each method in the GFI performs an operation involving execution traces of the generative function on which it is called.

### 3.1 Formalizing Generative Functions

We now formally describe generative functions.

**Assignment** An assignment \( s \) is a map from a set of addresses \( A \) to a set of values \( V \), where \( s(a) \) denotes the value assigned to address \( a \in A \). The special value \( s(a) = \bot \) indicates that \( s \) does not assign a meaningful value to \( a \). We define \( \text{dom}[s] := \{ a \in A \mid s(a) \neq \bot \} \) of \( s \) as the set of non-vacuous addresses in \( s \). Let \( s|_B \) be the assignment obtained by restricting \( s \) to a subset of addresses \( B \subseteq \text{dom}[s] \), i.e., \( s|_B(a) = s(a) \) if \( a \in B \) and \( s|_B(a) = \bot \) otherwise. For two assignments \( s \) and \( t \), let \( s \equiv t \) mean \( s(a) = t(a) \) for all \( a \in \text{dom}[s] \cap \text{dom}[t] \). Finally, we let \( S := V^A \) be the set of all assignments from \( A \) to \( V \).

**Generative function** A generative function \( \mathcal{G} \) is a tuple \( \mathcal{G} = (X, Y, f, p, q) \). Here, \( X \) and \( Y \) are sets that denote the domain of the arguments and the domain of the return value of the function, respectively. Moreover, \( p : X \times S \to [0, 1] \) is a family of probability distributions on assignments \( s \in S \) indexed by argument \( x \in X \). In words, \( x \) is a fixed argument to the generative function and \( s \) is a realization of all the random choices made during the execution. Since \( p \) is a distribution, for each \( x \), the series \( \sum_{s \in S} p(x, s) = 1 \). We use the notation \( p(s; x) \) to separate the arguments \( x \) from the assignment \( s \). The output function \( f : X \times \{ s : p(s; x) > 0 \} \to Y \) maps an argument \( x \) and an assignment \( s \) of all random choices (whose probability under \( p \) is non-zero) to a return value \( f(x, s) \in Y \). Finally, \( q : X \times S \times S \to [0, 1] \) is an internal proposal distribution that assigns a probability \( q(s; x, u) \) to each assignment \( s \) for all \( x \in X \) and all \( u \in S \). The proposal distribution \( q \) satisfies (i) \( \sum_u q(s; x, u) = 1 \) for all \( x \in X \) and \( u \in S \); and (ii) \( q(s; x, u) > 0 \) if and only if \( s \equiv u \) and \( p(s; x) > 0 \).

### 3.2 Interface Methods

We now describe several methods in the GFI. Each method takes a generative function \( \mathcal{G} \) in addition to other method-specific arguments. We will denote an assignment by \( \mathbf{u}, \mathbf{v}, \mathbf{w} \), etc., where \( \mathbf{u} \) is a pair of a complete assignment \( u \) and a set of addresses \( B \). If \( \mathbf{u} \) is a tuple of a complete assignment \( u \) and a set of addresses \( B \) we let \( u \mathbf{B} \). We let \( \mathbf{u} = \emptyset \) (i.e. no addresses are provided) then the method sets \( u := t \).

**initialize** (sampling an initial trace) This method takes an assignment \( u \), arguments \( x \), and returns \( t \) (a trace of \( t \)) such that \( t \equiv u \), sampled using the internal proposal distribution (denoted \( t \sim q(\cdot; x, u) \)); as well as (ii) a weight \( w := p(t; x) / q(t; x, u) \). It is an error if no such assignment \( t \) exists.

**propose** (proposing an assignment) This method samples an assignment from a generative function \( \mathcal{G} \) that is used as a proposal distribution and computes (or estimates) the proposal probability. In particular, propose takes arguments \( x \) and a set of addresses \( B \), and returns an assignment \( u \) and a weight \( w \) by (i) sampling \( t \sim p(\cdot; x) \); then (ii) setting \( u := t|_B \) and \( w := p(t; x) / q(t; x, u) \). If \( B = \emptyset \) (i.e. no addresses are provided) then the method sets \( u := t \).
**assess (assessing the probability of an assignment)** This method computes (or estimates) the probability that a generative function \( G \) produces a given assignment \( u \). It is equivalent to initialize except that it only returns the weight \( w \), and not the trace. Note that \( w \) is either the exact probability that the assignment \( u \) is produced by \( G \) (on arguments \( x \)) or an unbiased estimate of this probability.

```
1 # Sample a random initial trace (tr1).
2 x = () # empty tuple, foo takes no args
3 u = Assignment((b, false), (d, true)) # empty assignment
4 (tr1, u, w) = initialize(foo, x, u) # 'tr1' is the trace
5
6 # Use 'update' to obtain a trace (tr2) with :b=false, :d=true.
7 u = Assignment(((b, false), (d, true)))
8 (tr2, w, v, retdiff) = update(foo, x, noargdiff, tr1, u)
```

\[
p(t; x) = 0.7 \times 0.4 \times 0.4 \times 0.7 = 0.0784
\]
\[
p(t'; x') = 0.7 \times 0.6 \times 0.1 \times 0.7 = 0.0294
\]
\[
w = p(t'; x')/p(t; x) = 0.0294/0.0784 = 0.375
\]

**Figure 4.** Illustration of update on a simple generative function foo. Shaded regions indicate sets of addresses.

**update (updating a trace)** The update method makes adjustments to random choices in an execution trace \((t, x)\) of \( G \), which is a common pattern in iterative inference algorithms such as MCMC and MAP optimization. In particular, the update method takes a trace \((t, x)\) of \( G \); new arguments \( x' \); and a partial assignment \( u \). It returns a new trace \((t', x')\) such that \( t' \equiv u \) and \( t'(a) = t(a) \) for \( a \in (\text{dom}[t] \cap \text{dom}[x']) \setminus \text{dom}[u] \).

That is, values are copied from \( t \) for addresses that remain and that are not overwritten by \( u \). It is an error if no such \( t' \) exists. The method also returns a discard assignment \( v \) where \( v(a) = t(a) \) for \( a \in (\text{dom}[t] \setminus \text{dom}[t']) \cup (\text{dom}[t] \cap \text{dom}[u]) \).

In words, \( v \) contains the values from the previous trace for addresses that were either overwritten by values in \( u \) or removed altogether. The method additionally returns a weight \( w = p(t'; x')/p(t; x) \). Figure 4 illustrates the behavior of update in a simple setting.

Oftentimes, in an invocation of update the assignment \( u \) will contain values for only a small portion of the addresses in \( t \) and there will either be no change from \( x \) to \( x' \) or the change will be ‘small’. In these cases, information about the change from \( x \) to \( x' \) can be used to make the implementation of update more efficient. To exploit this invocation pattern for performance gains, update accepts an argdiff value \( \Delta(x, x') \) which contains information about the change in arguments (when available). To enable compositional implementations of update, it also returns a retdiff value \( \Delta(y, y') \) that contains information about the change in return value (when available). The types of argdiff and retdiff values depend on the generative function \( G \). Section 2 shows an example usage of argdiff.

**backprop (automatic differentiation)** This method computes gradients of the log probability of the execution trace with respect to the values of function arguments \( x \) and/or the values of random choices made by \( G \). In particular, backprop takes a trace \((t, x)\) and a selection of addresses \( B \) that identify the random choices whose weights are desired. It returns the gradient \( \nabla_B \log p(t; x) \) of \( \log p(t; x) \) with respect to the selected addresses as well as the gradient \( \nabla_x \log p(t; x) \) with respect to the arguments. backprop also accepts an optional return value gradient \( \nabla_y J \) (for some \( J \)) in which case it returns \( \nabla_B (\log p(t; x) + J) \) and \( \nabla_x (\log p(t; x) + J) \). Note that for \( \nabla_B \log p(t; x) \) to be defined, random choices in \( A \) must have differentiable density functions with respect to a base measure, in which case \( \log p(t; x) \) is a joint density with respect to the induced base measure on assignments which is derived from the base measures for each random choice.

### 3.3 Implementing a Metropolis-Hastings Update
A key contribution of the GFI is its ability to act as the building block for implementing many probabilistic inference algorithms. Next present an example showing how to use the GFI to implement the Metropolis-Hastings update (custom_mh) used in Figure 2e. We call propose on the proposal function (proposal) to generate the proposed assignment \( u \) and the forward proposal probability \( \text{fwd}\_\text{score} \). The update method takes the previous model trace \((t, x)\) and the proposed assignment, and returns (i) a new trace that is compatible with the proposed assignment; (ii) the model’s contribution \( w \) to the acceptance ratio; and (iii) the discard assignment \( v \), which would have to be proposed to reverse the move. Then, assess is used to compute the reverse proposal probability \( \text{rev}\_\text{score} \). Finally, \text{mh}\_\text{accept}\_\text{reject} stochastically accepts the move with probability alpha; if the move is accepted, the new trace is returned, otherwise the previous trace is returned. (Note that the weight \( w \) returned by the GFI is in log-space).
3.4 Compositional Implementation Strategy

Each GFI method is designed to be implemented compositionally by invoking the same GFI method for each generative function call within a generative function. In this implementation strategy, execution trace data structures are hierarchical and have a ‘sub-trace’ for each generative function call. Therefore, when a probabilistic DSL compiler produces a generative function \( G \) from probabilistic DSL code, it can treat any generative function that is called by \( G \) as a black box that implements the GFI. This compositional design enables (i) generative functions defined using independent probabilistic DSLs to invoke one another and (ii) powerful extensions with new types of generative functions, as we demonstrate in the next two sections.

4 Generative Function Combinators

Iterative inference algorithms like MCMC or MAP optimization often make small adjustments to the execution trace of a generative function. For example, consider a call to custom_mh with is_outlier_proposal in Figure 2e, Line 59. This call proposes a change to the :is_outlier choice for a single data point (i) and then invokes update on the model function. Because data points are conditionally independent given the parameters, an efficient implementation that exploits conditional independence can scale as \( O(1) \), whereas a naive implementation that always visits the entire trace would scale as \( O(n) \) where \( n \) is the number of data points.

To address this issue, we introduce generative function combinators, which provide efficient implementations of update (and other GFI methods) by exploiting common patterns of repeated computation and conditional independence that arise in probabilistic models. A generative function combinator takes as input a generative function \( G_i \), (called a “kernel”) and returns a new generative function \( G' \) that repeatedly applies the kernel according to a particular pattern of computation. The GFI implementation for \( G' \) automatically exploits the static pattern of conditional independence in the resulting computation, leveraging argdiff and retdiff to provide significant gains in scalability. We next describe three examples of generative function combinators.

**Map** The map combinator (Figure 5a) constructs a generative function \( G^* \) that independently applies a kernel \( G_k \) from \( X \) to \( Y \) to each element of a vector of inputs \( (x_1, \ldots, x_n) \) and returns a vector of outputs \( (y_1, \ldots, y_n) \). Each application of \( G_k \) is assigned an address namespace \( i \in \{1 \ldots n\} \). The implementation of update for map only makes recursive GFI calls for the kernel on those applications \( i \) for which the assignment \( u \) contains addresses under namespace \( i \), or for which \( x_i \neq x_i' \). The update method accepts an argdiff value \( \Delta(x, x') \) that indicates which applications \( i \) have \( x_i \neq x_i' \), and a nested argdiff value \( \Delta(x_i, x'_i) \) for each such application.

**Unfold** The unfold combinator (Figure 5b) constructs a generative function \( G' \) that applies a kernel \( G_k \) repeatedly in sequence. Unfold is used to represent a Markov chain, a common building block of probabilistic models, with state-space \( Y \) and transition kernel \( G_k \) from \( Y \times Z \) to \( Y \). The kernel \( G_k \) maps \( (y, z) \in Y \times Z \) to a new state \( y' \in Y \). The generative function produced by this combinator takes as input the initial state \( y_0 \in Y \), the parameters \( z \in Z \) of \( G_k \), and the number of Markov chain steps \( n \) to apply. Each kernel application is given an address namespace \( i \in \{1 \ldots n\} \). Starting with initial state \( y_0 \), unfold repeatedly applies \( G_k \) to each state and returns the vector of states \( (y_1, \ldots, y_n) \). The custom GFI implementation in unfold exploits the conditional independence of applications \( i \) and \( j \) given the return value of an intermediate application \( l \), where \( i < l < j \). The retdiff values returned by the kernel applications are used to determine which applications require a recursive call to the GFI.

**Recurse** The recurse combinator (Figure 5c) takes two kernels, a production kernel \( G^*_k \) and a reduction kernel \( G_k \), and returns a generative function \( G' \) that (i) recursively applies \( G^*_k \) to produce a tree of values, then (ii) recursively applies the \( G_k \) to reduce this tree to a single return value. Recurse is used to implement recursive computation patterns including probabilistic context free grammars, which are a common building block of probabilistic models [11, 18, 22, 46]. Letting \( b \) be the maximum branching factor of the tree, \( G^*_k \) maps \( X \) to \( V \times (X \cup \{\perp\})^b \) and \( G_k \) maps \( V \times (Y \cup \{\perp\})^b \) to \( Y \), where \( \perp \) indicates no child. Therefore, \( G' \) has input type \( X \) and return type \( Y \). The update implementation uses retdiff values from the kernels to determine which subset of production and reduction applications require a recursive call to update.

5 Implementation

This section describes an implementation of the above design, called Gen, that uses Julia as the host language, and includes three interoperable probabilistic DSLs embedded in Julia.

**Dynamic DSL** The compiler for the Dynamic DSL in Figure 3 produces generative functions whose traces are hash tables that contain one entry for each generative function call and random choice, keyed by the address relative to the caller’s namespace (Figure 2c). Each GFI method is implemented by applying a different transformational compiler to the body of the generative function, to generate a Julia function that implements the GFI method. Different GFI methods replace @addr expressions with different Julia code...
that implements the method’s behavior. This is closely related to the architecture of other probabilistic programming systems [13, 15, 47, 48] except that in existing systems, transformational compilers produce implementations of inference algorithms and not primitives for composing many inference algorithms. In the Dynamic DSL, reverse-mode automatic differentiation uses a dynamic tape of boxed values constructed using operator overloading. Default proposal distributions use ancestral sampling [23].

**Static DSL** The Static DSL is a subset of the Dynamic DSL in which function bodies are restricted to be static single assignment basic blocks, and addresses must be literal symbols (see Figure 6 for examples, identified by the @static keyword). These restrictions enable static inference of the address space of random choices, which enables specialized fast trace implementations; as well as static information flow analysis that enables efficient implementations of update. The compiler generates an information flow intermediate representation based on a directed acyclic graph with nodes for generative function calls, Julia expressions, and random choices. Traces are Julia struct types, which are generated statically for each function, and are more efficient than the generic trace data structures used by the Dynamic DSL. A custom JIT compiler, implemented using Julia’s generated function multi-stage programming feature, generates Julia code for each GFI method that is specialized to the generative function. The JIT compiler for update uses the intermediate representation and the address schema (the set of top-level addresses) of the assignment to identify statements that do not require re-evaluation. For JIT compilation based on assignment schemata, the Julia type of an assignment includes its address schema. This avoids the runtime overhead of dynamic dependency tracking [28], while still exploiting fine-grained conditional independencies in basic blocks.

**TensorFlow DSL** The TensorFlow DSL is expresses functional TensorFlow (TF, [1]) computations (see Figure 6 for an example, identified by the @tensorflow_function keyword). This DSL allows for scalable use of deep neural networks within probabilistic models and proposal distributions. The DSL includes declarations for function inputs (@input, corresponding to TF ‘placeholders’), trainable parameters (@param, corresponding to TF ‘variables’), and return values (@output); and statements that define the TF computation graph. Functions written in this DSL do not make random choices, but they do exercise the automatic differentiation (AD) methods in the GFI, which enable AD to compose across the boundary between TensorFlow computations and code written in other probabilistic DSLs. Trainable parameters of TensorFlow functions are managed by the TensorFlow runtime. We use a Julia wrapper [27] around the TensorFlow C API.
Marco F. Cusumano-Towner, Feras A. Saad, Alexander Lew, and Vikash K. Mansinghka

Figure 6. Modeling and inference code, and evaluation results for body pose inference task. The model, which is written in the Static DSL, invokes a graphics engine to render a depth image from pose parameters. The custom proposal combines the Static DSL and the TensorFlow DSL to pass an observed depth image through a deep neural network and propose pose parameters.


6 Evaluation

We evaluated Gen on a benchmark set of five challenging inference problems: (i) robust regression; (ii) inferring the probable destination of a person or robot traversing its environment; (iii) filtering in a nonlinear state-space model; (iv) structure learning for real-world time series data; and (v) 3D body pose estimation from a single depth image. For each problem, we compared the performance of inference algorithms implemented in Gen with the performance of implementations in other probabilistic programming systems. In particular, we compare Gen with Venture [28] (which introduced programmable inference), Turing [13] (which like Gen is embedded in Julia), and Stan [6] (which uses a black-box inference algorithm). Our evaluations show that Gen significantly outperforms Venture and Turing on all inference problems—often by multiple orders of magnitude. Stan can solve only one of the five benchmark problems, and Gen performs competitively with Stan on that problem. The performance gains in Gen are due to a combination of greater inference programming flexibility and more performant system architecture. We now summarize the results.

6.1 Robust Bayesian Regression

We first consider a model for robust Bayesian regression. Inference in robust Bayesian models is an active research area [45]. We evaluated Gen, Venture, and Stan implementations of MCMC and optimization-based inference algorithms
in two variants of this model—a more difficult uncollapsed variant and an easier collapsed variant, in which a manual semantics-preserving program transformation removes certain random choices. Stan’s modeling language cannot express the uncollapsed variant. The results in Table 1 indicate that Gen’s performant implementation of the Static DSL gives 200x–700x speedup over Venture and comparable runtime to Stan. The optimizations enabled by the Static DSL give up to 10x speedup over the Dynamic DSL.

### Table 1. Evaluation results for robust regression.

<table>
<thead>
<tr>
<th>Inference Algorithm</th>
<th>Runtime (ms/step)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gen (Static) MH Sampling</td>
<td>55ms ± 1</td>
</tr>
<tr>
<td>Gen (Static) Gradient-Based Optimization</td>
<td>66ms ± 2</td>
</tr>
<tr>
<td>Gen (Dynamic) Gradient-Based Optimization</td>
<td>435ms ± 12</td>
</tr>
<tr>
<td>Gen (Dynamic) MH Sampling</td>
<td>510ms ± 19</td>
</tr>
<tr>
<td>Venture MH Sampling</td>
<td>15,910ms ± 500</td>
</tr>
<tr>
<td>Venture Gradient-Based Optimization</td>
<td>17,702ms ± 234</td>
</tr>
</tbody>
</table>

(a) Runtime measurements for inference in uncollapsed model

<table>
<thead>
<tr>
<th>Inference Algorithm</th>
<th>Runtime (ms/step)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gen (Static) MH Sampling</td>
<td>4.45ms ± 0.49</td>
</tr>
<tr>
<td>Stan Gradient-Based Sampling</td>
<td>5.26ms ± 0.38</td>
</tr>
<tr>
<td>Gen (Static) Gradient-Based Sampling</td>
<td>18.29ms ± 0.24</td>
</tr>
<tr>
<td>Gen (Dynamic) Gradient-Based Optimization</td>
<td>37.14ms ± 0.93</td>
</tr>
<tr>
<td>Venture MH Sampling</td>
<td>3.202ms ± 0.17</td>
</tr>
<tr>
<td>Venture Gradient-Based Optimization</td>
<td>8.159ms ± 0.284</td>
</tr>
</tbody>
</table>

(b) Runtime measurements for inference in collapsed model

### 6.2 Structure Learning for Gaussian Processes

We next consider inference in a state-of-the-art structure learning problem. The task is to infer the covariance function of a Gaussian process (GP) model of a time series data set, where the prior on covariance functions is defined using a probabilistic context free grammar (PCFG). The inferred covariance function can then be used to make forecast predictions, shown in Figure 7a. This task has been studied in machine learning [11] and probabilistic programming [29, 40, 42].

We evaluated Gen, Venture, and Julia implementations of an MCMC inference algorithm that uses a custom schedule of MCMC moves that includes proposals to change sub-trees of the PCFG parse tree. Turing does not support this algorithm. We also implemented a variant in Gen that uses the `recurse` combinator to cache intermediate computations when evaluating the covariance function. The results in Table 2 show that Gen gives a >10x speedup over Venture, even without caching, at a cost of 1.7x greater code size. The Gen implementation without caching gives comparable performance to the Julia implementation, with a >4x reduction in code size. Finally, `recurse` gives a 1.7x speedup at the cost of somewhat more code. These results indicate that Gen substantially reduces code size while remaining competitive with a raw Julia implementation.

### Table 2. Evaluation results for GP structure learning.

<table>
<thead>
<tr>
<th>Inference Algorithm</th>
<th>Runtime (ms/step)</th>
<th>LOC (approx.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gen (Dynamic + recurse)</td>
<td>4.96ms ± 0.15</td>
<td>230</td>
</tr>
<tr>
<td>Julia (handcoded, no caching)</td>
<td>6.17ms ± 0.45</td>
<td>440</td>
</tr>
<tr>
<td>Gen (Dynamic)</td>
<td>8.37ms ± 0.53</td>
<td>100</td>
</tr>
<tr>
<td>Venture (no caching)</td>
<td>107.01ms ± 6.57</td>
<td>60</td>
</tr>
</tbody>
</table>

Figure 7. Predictions and accuracy for GP structure learning.

### 6.3 Algorithmic Model of an Autonomous Agent

We next consider inference in model of an autonomous agent that uses a rapidly exploring random tree [25] path planning algorithm to model the agent’s goal-directed motion [8]. The task is to infer the destination of the agent from observations of its location over time. We evaluated two Gen implementations and one Turing implementation of the same MCMC inference algorithm. Gen and Turing, unlike Venture, use probabilistic DSLs that are embedded in a high-performance host language, which permits seamless application of MCMC to models that use fast simulations like path planners. The results in Figure 8 show that the Gen Static DSL outperformed the Dynamic DSL by roughly 4x, and Turing by 3.3x.

### 6.4 Nonlinear State-Space Model

We next consider marginal likelihood estimation in a nonlinear state-space model. We tested two particle filtering inference algorithms [9] implemented in Gen, one using a default ‘prior’ proposal distribution and one using a custom ‘optimal’ proposal derived by manual analysis of the model. Turing does not support using custom proposals with particle filtering. We implemented only the default proposal variant in Turing. The results in Figure 9 show that the custom proposal gives accurate results in an order of magnitude less time than the default proposal. Also, Table 3 shows that
the Gen Static DSL implementation using the default proposal outperforms the Turing implementation of the same algorithm by a factor of 23x. Finally, we see that the unfold combinator provides a speedup of 12x for the Dynamic DSL.

Figure 9. Comparing default and custom proposals for particle filtering. Accuracy is the log marginal likelihood estimate.

Table 3. Evaluation results for state-space model.

<table>
<thead>
<tr>
<th></th>
<th>Runtime (ms)</th>
<th>LOC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gen (Static + unfold + default proposal)</td>
<td>13ms (± 2)</td>
<td>33</td>
</tr>
<tr>
<td>Gen (Dynamic + unfold + default proposal)</td>
<td>78ms (± 7)</td>
<td>33</td>
</tr>
<tr>
<td>Turing (default proposal)</td>
<td>306ms (± 153)</td>
<td>20</td>
</tr>
<tr>
<td>Gen (Dynamic + default proposal)</td>
<td>926ms (± 66)</td>
<td>26</td>
</tr>
</tbody>
</table>

6.5 3D Body Pose Estimation from Depth Images

We next consider an inference task from computer vision [24, 52]. The model shown in Figure 6 posits a 3D articulated mesh model of a human body, parametrized by pose variables including joint rotations, and a rendering process by which the mesh projects onto a two-dimensional depth image. The task is to infer the underlying 3D pose parameters from a noisy depth image. We implemented two importance sampling algorithms, one with a default proposal and one with a custom proposal that employs a deep neural network trained on data generated from the model. Neither Turing nor Venture support custom importance sampling proposals. We compared a Turing implementation using the default proposal, with a Gen implementation using the custom proposal. The Gen proposal is a generative function written in the Static DSL that invokes a generative function written in the TensorFlow DSL. The results (Figure 6) show that the Gen implementation gives more accurate results in orders of magnitude less time than Turing. This shows that custom proposals trained using amortized inference can be essential for good performance in computer vision applications.

7 Related Work

We discuss work in probabilistic programming, differentiable programming/deep learning, and probabilistic inference.

Probabilistic Programming Researchers have introduced many probabilistic programming languages over the last 20 years [6, 13–15, 28, 30, 31, 35, 36, 41, 44, 48]. With the exception of Venture and Turing, these languages do not support user-programmable inference [29]. Users of Venture and Turing specify inference algorithms in restrictive inference DSLs. In contrast, Gen users define inference algorithms in ordinary Julia code that manipulates execution traces of probabilistic models. The examples in this paper show how Gen’s approach to programmable inference is more flexible and supports modular and reusable custom inference code.

Compilers have been developed for probabilistic programming languages to improve the performance of inference [6, 21, 50, 51]. Gen’s JIT compiler is currently less aggressive than these compilers, but Gen’s architecture is significantly more extensible, allowing end users to integrate custom proposal distributions, new inference algorithms, custom combinator that influence the control flow of modeling and inference, and custom compilers for new DSLs. No existing system with compiled inference supports these features.

The TensorFlow DSL in Gen provides high-performance support for deep generative models, including those written in the style favored by Pyro [5] and Edward [44]. However, unlike Pyro, Gen can also express efficient Markov chain and sequential Monte Carlo algorithms that rely on efficient mutation of large numbers of traces. Also, these systems lack Gen’s programmable inference support and hierarchical address spaces.

Deep Learning and Differentiable Programming Unlike deep learning platforms such as TensorFlow [1], PyTorch [34], Theano [3], and MXNet [7], Gen programs explicitly factorize modeling and inference. Gen is also more expressive. For example, Gen provides support for fast Monte Carlo and numerical optimization updates to model state. Gen allows for models and inference algorithms to be specified in flexible combinations of Julia, TensorFlow, and other DSLs added by Gen users. Gen also automates the process of calculating the proposal densities needed for a broad range of advanced Monte Carlo techniques, given user-specified custom proposals that can combine Julia and TensorFlow code.

Probabilistic Inference Gen provides language constructs, DSLs, and inference library routines for state-of-the-art techniques from probabilistic modeling and inference, including generative modeling [32], deep neural networks [1], Monte Carlo inference [2, 16, 38], and numerical optimization [17]. Recently, artificial intelligence and machine learning researchers have explored combinations of these techniques. For example, recent work in computer vision uses generative models based on graphics pipelines and performs inference by combining Monte Carlo, optimization, and machine learning [24, 49]. Gen’s language constructs support these kinds of sophisticated hybrid architectures. This is illustrated via the case studies in this paper, which show how Gen can implement state-of-the-art algorithms for (i) inferring 3D body pose by inverting a generative model based on a graphics engine; (ii) inferring the probable goals of an agent by inverting an algorithmic planner [8]; and (iii) learning the structure of Gaussian process covariance functions for modeling time series data [11, 29, 40, 42].
8 Conclusion

This paper has shown how to build a probabilistic programming system that solves challenging problems from multiple fields, with performance that is superior to other state-of-the-art probabilistic programming systems. Key challenges that were overcome include (i) achieving good performance for heterogeneous probabilistic models that combine different types of computations such as simulators, deep neural networks, and recursion; and (ii) providing users with abstractions that simplify the implementation of custom inference algorithms while being minimally restrictive.

Acknowledgments

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