Probabilistic Programming with CuPPL

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Abstract
Probabilistic Programming Languages (PPLs) are a powerful tool in machine learning, allowing highly expressive generative models to be expressed succinctly. They couple complex inference algorithms, implemented by the language, with an expressive modelling language that allows a user to implement any computable function as the generative model.

Such languages are usually implemented on top of existing high level programming languages and do not make use of hardware accelerators. PPLs that do make use of accelerators exist, but restrict the expressivity of the language in order to do so.

In this paper, we present a language and toolchain that generates highly efficient code for both CPUs and GPUs. The language is functional in style, and the toolchain is built on top of LLVM. Our implementation uses delimited continuations on CPU to perform inference, and custom CUDA codes on GPU.

We obtain significant speed ups across a suite of PPL workloads, compared to other state of the art approaches on CPU. Furthermore, our compiler can also generate efficient code that runs on CUDA GPUs.

1 Introduction
Probabilistic Programming Languages (PPLs) are a powerful machine learning tool, allowing highly expressive generative models to be expressed succinctly, and complex inference to be applied to them. They typically provide a range of built-in distributions from which samples can be drawn and scored, along with a range of inference algorithms.

CuPPL is a functional programming language, with all of the standard control flow constructs including let expressions, conditional expressions, recursive functions, algebraic datatypes and case statements. It also includes a vector data type and a suite of built-in vector operators such as map, reduce and repeat. CuPPL provides two basic probabilistic primitives: sample and factor. These can be used within a generative model to sample from and score a suite of built-in distributions from which samples can be drawn and scored, along with a range of inference algorithms.

1.1 PPL Example
An example of a generative model is given in Figure 1, which demonstrates the diverse control flow that CuPPL allows within the model function, and which gives PPLs their expressive power.

This model finds the \( n \)-degree polynomial that best fits some given data. The degree of the polynomial is sampled from a uniform prior, and its coefficients from gaussian priors. The polynomial is then conditioned on a measure of its “distance” from the data. The model returns the polynomial, as a vector of coefficients. Running inference on this model produces an empirical distribution over polynomials, and the mode of this distribution is the “line of best fit” for the data.

1.2 Delimited Continuations
Whenever the model function calls sample or factor, or returns a value, the inference algorithm needs to make decisions about its execution – more specifically the probability of a trace of execution through the model needs to be tracked and samples need to be generated.

We use delimited continuations (the shift and reset operators) to allow the inference algorithm to manipulate the execution of the model function and generate samples from its posterior distribution.

\( \text{shift}(k, e) \) captures the current state of the program up to the last enclosing \( \text{reset}() \), creates a function from this that can be called via \( k \), and evaluates \( e \). \( e \) may call \( k \) as few or as many times as it likes.

Using \( \text{shift} \) whenever sample or factor are called captures the current state of execution of the model function (up to the start of the execution of the model function) and allows the inference algorithm to decide what to execute next.

Section 3 describes our implementation of sample and factor in more detail.

Figure 1. An example program that demonstrates the use of universal language features in a model function. The implementation of distance is omitted for brevity.
1.3 Contributions
In this paper, we make the following contributions:

- We describe a probabilistic programming language that is functional in nature, and supports delimited continuations using the shift and reset operators described in [4]. The language uses answer typ polymorphism in its type system to statically type check the code enabling statically typed LLVM IR to be generated from it.
- A novel implementation strategy for delimited continuations in LLVM IR that enables inference to be implemented in LLVM IR in a similar style to that described in [11].
- The code generated by our compiler performs significantly better than both Anglican [19] and webppl [13] over a range of benchmark programs.
- Moreover, the code generated by our compiler also scales well to large numbers of samples.

1.4 Structure
The rest of the paper is structured as follows. In Section 2 we discuss related work, in Section 3 we give an overview of the features and type system CuPPL, and in Section 4 we discuss the design and implementation of the code generator. This is followed in Section 5 by a performance analysis of our language across a range of benchmarks, comparing against both webppl [13] and Anglican [19]. Section 6 concludes the paper.

2 Related Work
The probabilistic programming languages most similar to our own are Anglican [19] and webppl [13], however both of these languages are embedded in other programming languages. The semantics of our language also borrows heavily from [11] which describes many of the principles behind implementing probabilistic languages.

Anglican [19] is embedded in Clojure [1], a dialect of Lisp that works in the Java Virtual Machine. It is built on top of continuations and trampolines in order to capture control and pass it to the inference algorithm.

webppl [13] is written in Javascript, on top of the NodeJS ecosystem [2]. It uses coroutines to capture control and pass it to the inference algorithm.

Similarly to Anglican and webppl, Kiselyov et al [14] describe a domain specific probabilistic language that is embedded in OCaml. They also use the delimited continuation approach to explore programs as models.

Edward [20, 21] is a probabilistic modelling library for TensorFlow [3]. This is not a true PPL as it does not allow arbitrary control flow, and is limited by the graph structures that are representable in TensorFlow.

Compiler based techniques to producing PPL code include [22]. This approach translates a PPL problem into MCMC code, rather than compiling the model function in the language itself. TerpreT [10] is a domain specific probabilistic language for program induction, generating programs from a PPL model.

Earlier approaches to probabilistic programming and modelling include BUGS [16], which is restricted to Bayesian modelling and cannot handle the complex control structure that true PPLs can.

Stan [7], similarly to BUGS, is restricted to Bayesian modelling. Bindings exist for embedding Stan in either R or Python. Other early, and similar, approaches include Church [12].

Borgstrom et al [6] present a rigorous lambda calculus for probabilistic programming, in the style of CuPPL, Anglican, webppl and Church. They use this to prove that they perform MCMC inference on program traces correctly.

3 The Language
CuPPL is a statically-typed functional language, and its design is centered around vectors and data parallel operations. It is also designed to allow high-level language transformations such as deforestation of vector operations, closure conversion and other high level optimization passes.

The rest of this section is structured as follows. Section 3.1 describes the salient features of CuPPL. Section 3.3 describes how delimited continuations are expressed, Section 3.4 details how these are used to implement sample and factor, and finally Section 3.5 details how the polymorphic type system treats delimited continuations using answer types.

3.1 Language Features
CuPPL includes the usual control flow constructs you would expect from a functional language including lambda expressions, let-expressions, conditionals, case statements and recursion. The language also includes first class vector data types of arbitrary dimensions, and a suite of parallel operators that work over them, including:

- map applies a function to every element of the vector
- repeat generates a vector by running a function a given number of times
- reduce performs a parallel reduction over a vector
- filter constructs a new vector that includes only those elements from the input vector for which a given predicate returns true

3.1.1 Type Generalization and Specialization
CuPPL allows type generalization and specialization, in a similar manner to System F. Polymorphic types can be defined as follows:

```plaintext
type List 'a : (+ Nil : unit) (Cons : ('a, (List 'a)));```
This example demonstrates both type generalization and type specialization. List is the type constructor:

\[
\text{forall 'a . }
\]
\[
(+ (\text{Nil : unit})
\]
\[
(\text{Cons : ('a, (List 'a))))
\]

This type can be specialized to store a list of integers by using a type application:

\[
(\text{List int})
\]

This produces the concrete type:

\[
(+ (\text{Nil : unit})
\]
\[
(\text{Cons : (int, (List int))})
\]

We impose a few restrictions on the use of generalized types, forall types and type applications. Firstly, general types can only be constructed at the start of a module, as the type constructors need to be unique within a module. Secondly, after type checking a program, all types must be specialized, or turned into concrete types. This is because the LLVM IR target environment requires all types to be concrete. If an expression is discovered whose type is not specialized, or turned into concrete types. This is because the LLVM IR target environment requires all types to be concrete. If an expression is discovered whose type is not specialized to a concrete type (such as partial application of a parallel operator), the compiler complains that it could not statically determine the concrete type of the expression.

### 3.2 Distribution Values

The type system includes a distribution type, denoted $\sim t$ which is a distribution over values of type $t$. It also includes a suite of built-in distributions, including gaussian, bernoulli, poisson and many others. Built-in functions to perform operations on distribution values are also provided, such as $\text{sample*}$ which produces a sample from a distribution, $\text{dist-score}$ which scores a sample from a distribution and $\text{dist-var}$ which returns the variance of a distribution.

### 3.3 Delimited Continuations

CuPPL allows delimited continuations through the use of the $\text{shift}$ and $\text{reset}$ constructs [4, 8].

Informally, the meaning of $\text{shift}$ is to capture the current execution state up to the last $\text{reset}$, wrap it in a function, and bind a name to that function.

For example, consider the following:

\[
\text{reset}(1 + \text{shift}(k, k(2)))
\]

When $\text{shift}$ is encountered, it captures the current program as a function named $k$. In this case $k$ is:

\[
\text{function } (x) \{ 1 + x \}
\]

It then executes the body of the shift expression, which executes $k(2)$, so the program returns 3.

Reset limits the scope to which $\text{shift}$ will capture the state of the program. For example, consider the following:

\[
1 + \text{reset}(3 + \text{shift}(k, 1))
\]

When $\text{shift}$ is encountered, it captures the current program as a function $k$ up to the last reset. In this case $k$ is:

\[
\text{sample <- function } (\text{dist : } \sim a) : a \{
\text{shift } (k : a => b) (x <- \text{sample-impl}(\text{dist}, k);
(x[0])(x[1])
\})
\}
\]

\[
\text{factor = function } (\log-p : a) : \text{unit } \{
\text{shift } k (f <- \text{factor-impl}(\log-p, k);
\})
\}
\]

\[
\text{observe = function } (\text{dist}, x) : \text{unit } \{
\text{factor}(\text{dist-score}(\text{dist}, x))
\}
\]

Figure 2. Implementation of $\text{sample}$, $\text{factor}$ and $\text{observe}$ using delimited continuations

\[
\text{function } (x) \{ 3 + x \}
\]

It then executes the body of the shift expression, which simply returns 1 and does not execute $k$, so the program returns 2 as its result.

### 3.4 Inference, sample and Factor

The two basic PPL primitives $\text{sample}$ and $\text{factor}$ are expressed in terms of delimited continuations. Figure 2 gives the definition of $\text{sample}$ and $\text{factor}$ (and the $\text{observe}$ helper function) in terms of $\text{shift}$ and $\text{reset}$.

$\text{sample}$ uses the $\text{shift}$ operator to capture the current execution state of the model function as a function $k$. When inference starts, $\text{reset}$ is called to limit the scope of this capture up to the start of the execution of the model function. $\text{sample}$ then calls $\text{sample-impl}$ with the distribution object that was sampled from and $k$. The implementation of $\text{sample-impl}$ depends on the choice of inference algorithm, however it always returns a tuple of type $(a \Rightarrow b, a)$. This function represents what the program should do next: the first element of the tuple is a continuation, with the same type as $k$, and the second element of the tuple is a sample from the distribution, of type $a$.

$\text{factor}$ also uses $\text{shift}$ operator to capture the current execution state of the model function as a function $k$. It then calls $\text{factor-impl}$ with the log probability with which to update the program trace. The implementation of $\text{sample-impl}$ depends on the choice of inference algorithm, however it always returns a function of type $\text{unit} \Rightarrow \text{unit}$. This is a function denoting what the program should do next, and has the same type as $k$.

$\text{observe}$ is a wrapper function around $\text{factor}$ that makes altering the log probability of the execution trace based on observing data from a distribution simpler. It calls $\text{factor}$ with
CuPPL provides two inference methods that implement \texttt{sample-impl} and \texttt{factor-impl}. They are invoked via built-in functions called \texttt{importance} (for running importance sampling) and \texttt{mcmc} (for running Monte Carlo Markov Chain based inference). More details on the implementation of these functions can be found in Section 4.

### 3.5 Type System

CuPPL uses Hindley-Milner type inference, augmented with polymorphic answer types [4]. Figure 3 gives a subset of the type rules. Te following notation is used:

- Types are denoted $\tau$.
- Type schemes are denoted $\sigma$. They have the syntax $\sigma = \tau | \forall A. \tau$ where $A$ is a set of type variables.
- $\tau < \sigma$ denotes that type $\tau$ is an instance of type scheme $\sigma$.
- Answer types are denoted $\alpha, \beta, \gamma$. Answer types can be any type $\tau$ or the empty type, denoted $\bot$.
- Expressions are denoted $e$.
- Constant values are denoted $c$.
- Variable identifiers are denoted $x$.
- Type environments are denoted $\Gamma$. These map variable identifiers $x$ to type schemes $\sigma$. The notation $\Gamma \{ x : \sigma \}$ denotes mapping $\Gamma$ updated with identifier $x$ mapped to type scheme $\sigma$. $\Gamma_0$ denotes an empty type environment, that does not map any identifiers to type schemes.
- There are two forms of type judgements:
  - \textit{Pure} type judgments are written $\Gamma \vdash_{\rho} e : \tau$. This means that expression $e$ has type $\tau$, given type environment $\Gamma$.
  - \textit{Impure} type judgments are written $\Gamma, \alpha \vdash e : \tau. \beta$. This means that expression $e$ has type $\tau$, given type environment $\Gamma$ and the execution of $e$ changes the answer type from $\alpha$ to $\beta$.

![Figure 3. Subset of the type rules for CuPPL.](image)

The expr rule allows an expression with the same input and output answer types to be type checked as a pure expression.

### 3.6 Inference Methods

CuPPL supports three inference methods.

#### 3.6.1 Enumeration

Enumeration performs precise inference on the model function, by executing all possible paths through the function. The probabilistic branching points are when the model calls \texttt{sample}. Whenever \texttt{sample} is called, the inference algorithm executes the model function from that point for all values in the support of the distribution. This only works for distributions with finite support, and returns a runtime error if a continuous distribution is encountered. This performs a breadth first traversal through the model function, and the depth of this traversal can be limited to a maximum depth if desired.

#### 3.6.2 Importance Sampling

This performs importance sampling [18] on the model function. This is done by repeatedly running the model function. The calls to \texttt{sample} and \texttt{factor} made by each execution prescribe a log probability the value returned by the model function. The model function is repeated up to a chosen number of times, and the posterior distribution is computed by normalizing the log probabilities of the returned values.

#### 3.6.3 Lightweight Metropolis-Hastings

This inference method [22] uses the Metropolis-Hastings algorithm to generate samples from the posterior distribution of the model function. First, the model function is run once to memorize the return values of any calls to \texttt{sample}. To generate a new sample, One of the memorized return values is chosen uniformly randomly, re-sampled, and the model function is re-executed from this point. Subsequent calls to sample reuse memorized values where possible. This may not be possible if the modification affects the control flow of the program, in which case new values are sampled and memorized. When the model function completes, the Metropolis-hasting acceptance criteria is used to either accept or reject the sample.

### 4 Code Generation

Our compiler parses the code, performs language-specific optimization passes on the AST, and then generates code for either CPU or GPU using a code generator built on top of the LLVM toolchain [15].

The rest of this section is structured as follows. Section 4.1 describes how various language features are compiled to LLVM IR, including closures and distribution objects. Section 4.2 describes the implementation of the call stack and
how different language constructs interact with it. Section 4.3 describes how delimited continuations are implemented for CPU. Finally Section 4.4 describes the code generation for the inference methods on CPU, using delimited continuations, and GPU, using custom generated NVVM IR.

4.1 Language Features

4.2 Call Stack

The generated LLVM IR does not use the call operator. Instead it uses a combination of indirectbr and a custom "managed stack”. This allows for more complex stack operations necessary for implementing delimited continuations as discussed in Section 4.3.

The managed stack is stored in region of heap allocated memory, allocated when the program starts. A stack pointer is also stored. LLVM IR is generated for the operations that modify the stack:

- Push and pop work just like a conventional stack.
- The stack save operation copies a chosen number of bytes from the top of the stack into a newly allocated region on the heap, and returns a pointer to it, and then pops this region off of the stack. This operation is used by delimited continuations to capture the current state of the program up to the last reset, as part of the implementation of shift discussed in Section 4.3.
- The stack restore operation pushes a previously saved stack region onto the top of the stack. This operation is used to restore the state of the stack when calling a continuation that was captured by the shift operator, as detailed in Section 4.3.

4.2.1 Closures

The LLVM IR code for a closure begins with a labelled basic block. A closure is called using an indirectbr to the address of this block (obtained using blockaddress). This label is annotated with all possible predecessor blocks, as required by LLVM IR. These are statically known, but may be a superset of all possibly call sites at runtime.

A closure value is represented by an LLVM IR struct of type {i64, i64}, containing a pointer to its code and some memory storing its environment. The environment of a closure is represented by an LLVM IR struct containing the values of its captured variables. If the environment is empty, this struct has type (). The instructions in the entry block of the closure first unpack this environment into registers, before continuing with the execution of the closure.

When calling a closure, the LLVM IR call instruction is not used, so that more complex stack operations can be handled. This requires the code generator to generate code for entry and return from the call. The code generation strategy is summarised by the pseudocode in Figure 4.

4.2.2 Distribution Values

Built-in distributions are represented by a struct of type (int32, int64, int64). The first element is a tag determining the type of the distribution, and the subsequent elements contain distribution specific data. These three values provide sufficient space to store parameters for any of the built-in distributions. This fixed sized encoding of distribution values allows them to be treated as plain values in LLVM IR, avoiding the need for heap allocation. This makes them suitable for use on a GPU where heap allocations are expensive.

4.2.3 Built-in Functions and Runtime Library

CuPPL includes a runtime library which implements the built-in functions that are not directly available in the LLVM IR instruction set. For example, sampling and scoring distributions is implemented in the runtime library. Separate implementations of this library are provided for CPU and CUDA GPUs.

4.2.4 Garbage Collection

On CPU, where it is needed, the Boehm-Demers-Weiser Garbage Collector [5] is used. On GPU, garbage collection
is not feasible. Static shape analysis is used to determine a fixed upper bound for the size of any vectors used so that they can be stack allocated. If the size of a vector cannot be statically determined the code generator will fall back to making a heap allocation. Depending on the structure of the program, this heap allocation fallback may exhaust the heap space available on the GPU, in which case the program will have to be reworked.

4.3 Delimited Continuations

The reset operator marks the current state of the program. It does this by pushing the value of the stack pointer onto the top of a separate "reset stack". When the reset operator exits, the value is popped off of the reset stack.

The shift operator captures the current program state as closure value that can be called at some later point. It creates a closure value containing a pointer to the current instruction and the contents of the stack up to the last call to reset. The address of the current instruction is obtained by starting a new basic block before that instruction and obtaining its address using blockaddress. A copy of the stack is obtained using the stack copy operation, to save the region from the current stack pointer up to the stack pointer stored on the top of the reset stack.

The environment for the captured continuation differs from that of a regular closure. Instead of a struct containing the values of any captured variables, it is a struct containing the saved stack region. It has type {int32, int8*} - storing the size of the captured stack and a pointer to it.

When a captured continuation is called the same steps are taken as calling a regular closure. However, instead of unpacking the environment structure into local variables, the saved stack from the environment structure and is pushed onto the top of the call stack. This restores the stack (up to the last reset) to the same state it was in when the continuation was captured.

Pseudocode for the implementation of this code generation is shown in Figure 5. generateResetEntry generates code for the entry into a reset expression, and returns the exit block so that the caller can pass it to generateResetExit later. generateResetExit is called, with the exit block and the return value of the sub-expression, after code has been generated for the sub-expression in the reset. generateShiftEntry and generateShiftExit generate code for the entry and exit from a shift expression.

4.4 Inference

Code is generated for the model function, which uses shift expressions to capture the model functions continuation and pass it to sample-impl and factor-impl, as described in Section 3.4, and in the previous section.

Code is generated for the inference methods importance and mcmc, first by converting them to calls to infer-impl, as described in Section 3.6, and then generating the code for the resulting abstract syntax tree.

Figure 5. Pseudocode for code generation of delimited continuation operators shift and reset.
importance sampling from a custom distribution (sum of two gaussians)

**logistic_regression**
Logistic regression using MCMC

**binomial**
Importance sampling to generate a binomial distribution

**sevenscientists**
Importance sampling for the seven scientists problem

**linefitting**
n-degree polynomial line fitting using importance sampling

**enumerate_geometric**
Exact inference to generate a geometric distribution

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## 5 Evaluation

This section explores the performance of CuPPL. In Section 5.1 we compare CuPPL against webppl [13] and Anglican [19] across a range of benchmarks, including probabilistic models and micro-benchmarks. In Section 5.3 we compare the performance of our implementation of delimited continuations against Racket [9].

### 5.1 Performance vs Other PPLs

The experiments were run on an i7-5820K CPU with 16 GB of main memory and an NVIDIA GTX 710. The wall clock execution time of the entire program is measured for 10 repeats. Error bars in the plots show the standard deviation of the measured data.

The benchmark programs are summarized in Table 6. Each benchmark was implemented in Anglican [19], webppl [13] and CuPPL. The CuPPL versions of the benchmark code were compiled for both CPU and GPU and run separately. Anglican does not support exact inference, therefore the enumerate_geometric benchmark is omitted for this language.

For models using importance sampling, each language is configured to generate 2 million samples, For MCMC inference, each language is configured to generate 100 thousand samples and for exact inference, 10 thousand maximum executions are used. These values were chosen to provide execution times of the order of a few seconds across most benchmarks.

The results are shown in Figure 7. This plot shows that CuPPL is significantly more performant that both webppl and Anglican across all but one of the benchmarks. webppl fails to run the line fitting benchmark – the program was terminated after 10 minutes without producing a result.

The GPU implementation of CuPPL improves performance compared to the CPU implementation, for most of the importance sampling benchmarks. GPU inference does not yet support MCMC or exact inference. The customdist benchmark performs similarly on CPU and GPU, most likely due to the branching nature of the benchmark. The more complex line fitting benchmark also shows less of a performance improvement on GPU compared to CPU. This is also likely due to the branching nature of the program, which is dependent on an integer sampled from the uniform discrete distribution.

The scalability for two of the benchmarks is shown in Figure 8. linefitting is the more complex of the importance sampling benchmarks, and linear_regression uses lightweight MH inference. These results show that each language scales similarly, however the slope for CuPPL is reduced.
5.2 Micro-benchmarks

Figure 9 compares the scalability of CuPPL, webppl, Anglican and Racket for two microbenchmarks. fibonacci implements the naive recursive fibonacci algorithm to test function call performance. vectorsum sums a vector of \( n \) ones, to test memory bound performance.

The results show that CuPPL, Anglican and Racket all perform similarly for function call performance, whereas webppl performance is initially similar but does not scale well. For memory bound performance, webppl performs poorly. The other languages all scale similarly, however CuPPL is significantly faster.

5.3 Delimited Continuation Performance

The prefix algorithm, shown in Figure 10 is used to compare our implementation against Racket [9]. The results are shown in Figure 11, and show that the performance of our implementation is competitive.

6 Conclusions and Future Work

In this paper, we have presented CuPPL, a probabilistic programming language that generates highly efficient code for both CPUs and CUDA GPUs. The language is functional in style, and the toolchain is built on top of LLVM. Our implementation uses delimited continuations on CPU to perform inference, and custom CUDA codes on GPU.

Compared to other state of the art PPLs Anglican [19] and webppl [13], CuPPL achieves significantly better performance across a range of benchmarks, and scales linearly to large numbers of samples. Our implementation of delimited continuations is also competitive with Racket [9].

In future, we plan to extend our language to support a greater variety of inference methods on both CPU and GPU. We are investigating parallelizable particle-based inference methods [17] for use on GPU.

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