Daphne: Multi-Pass Compilation of Probabilistic Programs into Graphical Models and Neural Networks

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Abstract

Daphne is a probabilistic programming system that provides an expressive syntax to denote a large, but restricted, class of probabilistic models. Programs written in the Daphne language can be compiled into a general graph data structure of a corresponding probabilistic graphical model with simple link functions that can easily be implemented in a wide range of programming environments. Alternatively Daphne can also further compile such a graphical model into understandable and vectorized PyTorch code that can be used to train neural networks for inference. The Daphne compiler is structured in a layered multi-pass compiler framework that allows independent and easy extension of the syntax by adding additional passes, while leveraging extensive partial evaluation to reduce all syntax extensions to the graphical model at compile time.

1 Introduction

Probabilistic modeling is integral for modern machine learning and statistics. The recent advent of generative AI has situated a large part of deep learning applications in an approximate Bayesian modeling framework (Brown et al., 2020; Rombach et al., 2022) and the statistics communities around structured probabilistic programming systems equally are expanding quickly (Štrumbelj et al., 2023). Such probabilistic programming systems allow to specify models and inference problems in programming languages with different expressivity and tractability trade-offs. Turing-complete languages are universal and can be very expressive at the expense of rendering inference harder. But systems with restricted languages still can cover large classes of problems while rendering inference more tractable.

An interesting position in the language design space are languages that can be readily translated into a representation for which efficient inference algorithms exist, e.g. Stan (Carpenter et al., 2017). Such systems compile an **expressive input syntax** into a lower-level model that can be **efficiently evaluated** with the numerical primitives of the inference engine. Furthermore it should be possible for users to **extend the language** with new syntax if needed. Finally the host environment in which the compiler and runtime operates ideally should be built in a **rich programming environment** with probabilistic primitives and access to modern machine learning primitives. This combination of properties renders a probabilistic programming system also particularly well suited for teaching and research. Following these design principles we introduce Daphne. Compared to other probabilistic programming systems we are aware of, Daphne is set apart by its expressive higher-order syntax and the extensive use of partial evaluation inside of its compiler (Section 3).

2 Graphical Probabilistic Programming Language

A *graphical* probabilistic programming language (GPPL) is a language in which all random variables can be identified without evaluating the stochastic expressions in the program, a prominent example being Stan (Carpenter et al., 2017). Such a language allows to unroll all loops and control flow a priori at compile time and represents all random variables explicitly in a traditional probabilistic graphical model (PGM) (Koller & Friedman, 2009). This is in contrast to probabilistic programming languages (PPLs) which support loop and recursion constructs that cannot be simplified before evaluating the stochastic expressions

of the program, e.g. because some loop or recursion termination condition depends on a sample of a random variable. This distinction is described in slightly different terms in van de Meent et al. (2018) as first-order (FOPPL) vs. higher-order (HOPPL) languages.

2.1 Syntax

The core language syntax supported by the compiler is defined by the following grammar in Backus-Naur form (BNF),

s ::= symbol (indicating variables)
c ::= constant value or primitive operation (syntactic atoms)
f ::= procedure
e ::= c | s | `(let [`s_1 e_1 ... s_n e_n`]` e_b`)` | `(if` e_1 e_2 e_3`)` | `(`e_f e_1 ... e_n`)`
| `(sample` e`)` | `(observe` e_1 e_2`)`
q ::= e | `(defn` f `[`s_1 ... s_n`]` e`)` q

Language 1: Daphne GPPL.

The basic syntax is derived from the Clojure programming language (Hickey, 2008; 2020). For the reader unfamiliar with Lisp syntax it can be thought of as an extended form of JSON where "code is data". Lisp expressions are denoted with a list based meta-syntax, i.e. explicitly grouped in lists starting with "(" and ending with ")". As can be seen in the grammar composition rule for e, expressions can contain symbols. For this reason such expressions are also referred to as symbolic expressions (sexps). The language supports lexical binding with the `let` form and control flow through conditional expressions with `if`. Function applications are denoted in prefix notation, i.e. the function is positioned in the first element in the list and all the arguments follow, e.g. `(+ 1 2)`, and e_f needs to evaluate either to a previously defined procedure or a primitive operation. `defn` provides a means to define reusable functions that can be referred to by name f. The last expression is the global entry point into the program having access to all defined functions. Like in Anglican (Tolpin et al., 2016), the probabilistic programming primitives for this language are denoted as `sample` for drawing samples from a random variable and `observe` to condition it on data.

A Bayesian linear regression example in Daphne can be seen in Program 2. A normal prior is defined for `slope` and `bias` and then the `reduce` iterates a normal likelihood `observe-data` over 6 xy data pairs before returning the posterior parameters. In contrast to van de Meent et al. (2018) Daphne does not rule out recursion or higher-order functions as can be seen in our simple implementation of `reduce`.

3 Compiler

The Daphne compiler runs ahead-of-time (AOT) before inference is conducted. It receives the full input syntax including input data and all needed function definitions as shown in Program 2 and translates it to a dictionary describing a probabilistic graphical model during standard compilation. Daphne provides JSON export for its compiler passes through its command line interface.

3.1 Compiler passes

The compilation process happens in multiple passes, where each pass defines the translation of some language features into a simpler syntax before finally only the graphical model remains (van de Meent et al., 2018). This approach allows to build extensible compilers with towers of languages that deal with single language features (Keep & Dybvig, 2013). The compiler has the following standard passes: `desugar`, `symbolic-simplify` and `partial-evaluation` (described in Section 3.2). The `desugar` pass factorizes one big `let` binding into nested single bindings and `symbolic-simplify` applies operations on syntactic objects if possible, e.g. `(first [sample1])` is translated to `sample1` since the argument to `first` is a syntactically represented vector and can be evaluated symbolically. The implementation of operational semantics in the compiler also uses an explicit substitution pass `substitute` that allows it to substitute symbols for values while respecting the binding structure of the language.

```
(defn reduce [f acc s]
  (if (> (count s) 0)
    (reduce f (f acc (first s)) (rest s))
    acc))

(defn observe-data [acc data]
  (let [slope (first acc)
        bias  (second acc)
        xn    (first data)
        yn    (second data)
        zn    (+ (* slope xn) bias)]
    (observe (normal zn 1.0) yn)
    [slope bias]))

(let [slope (sample (normal 0.0 10.0))
      bias  (sample (normal 0.0 10.0))
      data  [[1.0 2.1] [2.0 3.9] [3.0 5.3] [4.0 7.7] [5.0 10.2] [6.0 12.9]]]
  (reduce observe-data [slope bias] data)
  [slope bias])
```

Program 2: Daphne GPPL Example - Linear regression

3.2 Partial evaluation

Partial evaluation (Jones et al., 1993) is the process of interpreting parts of a program ahead of time. It is an effective method to implement compilation without the need of potentially inconsistent compilation semantics separate from the interpreter. Instead, the interpreter is able to take sub-expressions and evaluate them as soon as sufficient information is available. For example `(+ 1 2)` can be evaluated to `3` and replaced in the program code since all information to evaluate it is available. The Daphne language is, like Clojure (Hickey, 2020), a functional, stateless Lisp and hence naturally provides substitution semantics which is particularly well-suited for partial evaluation (Jones et al., 1993).

Daphne applies partial evaluation in a fixed point operator together with the other passes until no further simplification is possible. It does so by applying Clojure's `eval` with a properly scoped environment top-down on smaller and smaller sub-expressions of the input syntax until it is able to fully evaluate a sub-expression. Code without random variables can be fully evaluated by the partial evaluator, while expressions depending on random variables are simplified as much as possible (van de Meent et al., 2018) as can be seen in the resulting graph for linear regression in Program 3).

Note that these fixed point iterations entail that the compiler does not have a constant number of passes. Furthermore, it is not trivial to determine ahead of time how many fixed point iterations are needed. Note also that functions defined by `defn` naturally allow bounded recursion during partial evaluation as long as their inputs shrink in every recursion step.[1]

3.3 Graphical model

After iteratively substituting, expanding and reducing the input syntax a graph data structure with vertices `:V`, adjacency `:A`, link functions `:P` and observed nodes `:Y` remain,

The link functions of `:P` are expressed in a language that requires no binding or loop support, e.g. `(observe* (normal (+ (* sample1 1.0) sample2) 1.0) 2.1)`. Its evaluation can be readily implemented with numpy or PyTorch arithmetic and probability primitives in Python, e.g. to implement ancestral sampling in Appendix A.1. Many compilers simplify code to A-normal form (ANF) or single static assignment (SSA) form, which are very close to this graphical format, so the graphical model code could also be mapped

[1]This is not enforced currently and the compiler will not terminate on violations. Termination checks could be implemented similar to the ones in Agda (Abel, 1998).

```
{:V #{sample1 sample2 observe3 observe4 observe5 observe6 observe7 observe8},
 :A
 {sample2 #{observe3 observe4 observe5 observe6 observe7 observe8},
  sample1 #{observe3 observe4 observe5 observe6 observe7 observe8}},
 :P
 {sample1 (sample* (normal 0.0 10.0)),
  sample2 (sample* (normal 0.0 10.0)),
  observe3 (observe* (normal (+ (* sample1 1.0) sample2) 1.0) 2.1),
  observe4 (observe* (normal (+ (* sample1 2.0) sample2) 1.0) 3.9),
  observe5 (observe* (normal (+ (* sample1 3.0) sample2) 1.0) 5.3),
  observe6 (observe* (normal (+ (* sample1 4.0) sample2) 1.0) 7.7),
  observe7 (observe* (normal (+ (* sample1 5.0) sample2) 1.0) 10.2),
  observe8 (observe* (normal (+ (* sample1 6.0) sample2) 1.0) 12.9)},
 :Y
 {observe3 2.1, observe4 3.9,  observe5 5.3,
  observe6 7.7, observe7 10.2, observe8 12.9}}
```

Program 3: Compiled Graphical Model - Linear regression

to low-level languages without garbage collection such as C or CUDA. In correspondence with the syntax primitives in the GPPL language, `observe*` and `sample*` refer to low-level implementations of sampling and log-probability evaluations.

3.4 Inference runtime

Daphne also provides optional runtime support for inference. A differentiable subset of the language is supported with source to source reverse-mode automatic differentiation (Baydin et al., 2017) and can be plugged into a simple Hamiltonian Monte Carlo (HMC) implementation. There is also support for Metropolis within Gibbs sampling. Both of these implementations have been used for testing and teaching and provide a starting point for further exploration, but should not be expected to perform competitively with mature probabilistic programming systems. Daphne builds on well tested Anglican (Tolpin et al., 2016) primitives though and and can be extended to a wide range of MCMC methods if needed.[2]

Research with Daphne lead to exploration of variational inference methods for amortized inference (Weilbach et al., 2020). In this work the compiler furthermore provides a sparse inversion of the graphical model structure according to Webb et al. (2018) and a translation of the graphical model to Python code. This additional compilation step provides a human readable PyTorch implementation of sampling and log probability evaluation of prior and likelihood for a given graphical model. The code supports batching and can be used to sample a synthetic data set for training a continuous normalizing flow (Grathwohl et al., 2018) as described in (Weilbach et al., 2020). Follow-up work has extended this approach and leveraged the diffusion model framework to yield reliable and more scalable amortized inference artifacts (Weilbach et al., 2023b;a). Daphne can provide automatic derivation of the attention masks from the GPPL language for the sparse transformer in this line of work (Weilbach et al., 2023b).

4 Deep learning application

$$e ::= \ldots \mid (\texttt{foreach}\ e_c\ [s_1\ e_1\ \ldots\ s_n\ e_n]\ e'_1\ \ldots\ e'_m) \mid (\texttt{loop}\ e_c\ e_{init}\ f_{acc}\ e_1\ \ldots\ e_n)$$

Language 2: Loop extensions.

Daphne also optionally supports the two loop forms of van de Meent et al. (2018). These forms do not make the language more expressive, but have been originally used to implement a linear algebra library for Weilbach

[2]There is also zero-copy access to all of Python through `https://github.com/clj-python/libpython-clj` or `https://github.com/oracle/graalpython`

et al. (2020), which includes matrix multiplication and 2d convolution. Both `foreach` and `loop` require a loop counter e_c expression evaluating to an integer to determine the number of loop iterations. `foreach` binds $s_1, \ldots, s_n$ with each element of the collection yielding expressions $e_1, \ldots, e_n$ in the body expressions $e'_1, \ldots, e'_m$. `loop` iterates an accumulating function f_{init} starting with e_{init} over $e_1, \ldots, e_n$. To illustrate the use of the language we provide an excerpt of the library together with an example 2d convolution invocation at the end.

```
(defn dot-helper [t state a b]
  (+ state
     (* (get a t)
        (get b t))))

(defn dot [a b]
  (loop (count a) 0 dot-helper a b))

(defn row-mul [t state m v]
  (conj state (dot (get m t) v)))

(defn mmul [m v]
  (loop (count m) [] row-mul m v))

(defn row-helper [i sum a b]
  (+ sum
     (dot (get a i)
          (get b i))))

(defn inner-square [a b]
  (loop (count a) 0 row-helper a b))

(defn inner-cubic [a b]
  (apply + (foreach (count a) [n (range (count a))]
                    (inner-square (get a n) (get b n)))))

(defn slice-square [input size stride i j]
  (foreach size [k (range (* i stride)
                          (+ size (* i stride)))]
           (subvec (get input k)
                   (* j stride)
                   (+ size (* j stride)))))

(defn slice-cubic [inputs size stride i j]
  (foreach (count inputs) [input inputs]
           (slice-square input size stride i j)))

(defn conv-kernel [inputs kernel bias stride]
  (let [ic (count (first inputs))
        size (count (first kernel))
        remainder (- size stride)
        to-cover (- ic remainder)
        iters (int (Math/floor (/ to-cover stride)))]
    (foreach iters [i (range iters)]
             (foreach iters [j (range iters)]
                      (inner-cubic (slice-cubic inputs size stride i j)
                                   kernel)))))

(defn conv2d [inputs kernels bias stride]
  (foreach (count kernels) [ksi (range (count kernels))]
           (conv-kernel inputs (get kernels ksi) (get bias ksi) stride)))
```

```
(let [w1 [[[[0.8, 0.9],
            [0.9, 0.6]],
           [[0.0, 0.0],
            [0.1, 0.5]]],
          [[[0.2, 0.4],
            [0.6, 0.1]],
           [[0.4, 0.5],
            [0.1, 0.1]]]]
      b1 [0.1, 0.2]
      x  [[[0.4, 0.5, 0.8, 0.8]
           [0.5, 0.8, 0.6, 0.1]
           [0.9, 0.4, 0.7, 0.2]
           [0.5, 0.0, 0.4, 0.2]],
          [[0.0, 0.8, 0.2, 0.3]
           [0.2, 0.2, 0.8, 0.7]
           [0.1, 0.6, 0.6, 0.3]
           [0.6, 0.7, 0.5, 0.2]]]]
  (conv2d x w1 b1 2))
```

In combination those primitives can be used to implement the deep learning applications in Weilbach et al. (2023b) including a stochastic deconvolution layer and a small convolutional network.

5 Related work

Compared to Turing-complete languages such as Anglican (Tolpin et al., 2016), Pyro (Bingham et al., 2019) or Gen (Cusumano-Towner et al., 2019), the Daphne language only supports programs without stochastic recursion. This restricts it from implementing certain non-parametric models and complex stochastic recursion schemes. Inference in such models is often very challenging and brittle though and this motivates our restriction to graphical models. Stan (Carpenter et al., 2017) has a successful GPPL with programs that are restricted to play well with its HMC inference runtime. Compared to Stan, Daphne provides a much more expressive functional programming language including recursion and higher-order functions. BUGS, which is similar to Stan in syntax, has been translated to the Daphne language in van de Meent et al. (2018). The Daphne graphical model output could equally be translated back to Stan to use its inference engine with the more expressive language.

6 Conclusion and future work

Daphne is a small, yet versatile, probabilistic programming environment that represents a new point in the design space of probabilistic programming languages and compilers. Its goal is to capture as much of higher-order functional programming as possible while being reducible to traditional probabilistic graphical models ahead of inference time. The representations of different compiler passes can be exported to provide fine-grained program information, such as dependencies between random variables, to downstream inference runtimes. These representations have been used in a line of research on structured neural networks for amortized inference and for teaching graduate courses in probabilistic programming.

Limitations For very large sized input programs, such as deep learning models, partial evaluation can lead to expression swell that significantly slows down compilation as all linear algebra operations need to be syntactically expanded and reduced. Scaling better to such programs requires further research, in particular a more structured approach to expanding and reducing forms during partial evaluation. Note that many other probabilistic programming systems (Bingham et al., 2019; Tolpin et al., 2016) treat tensors as single objects and do not model the full computational graph with all scalars and intermediate computations in the same way Daphne does, avoiding the problem at the expense of not tracking fine-grained sparse structures. The Daphne language also does not yet support definitions of anonymous functions, which would also provide closures, rendering it closer to standard Clojure and more convenient for complex programs. Adding closures is left for a future iteration of the language.

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A Appendix

A.1 Python export

The following export is done with the help of hy-lang[3] which allows a direct translation between lisps and then into Python syntax. This is the compiled code for Program 2.

```
import hy
import torch
import math
from torch.distributions import Normal, Bernoulli, Laplace, Uniform

class Model:
    dim_latent = 2
    dim_condition = 6
    faithful_adjacency = [[0, 1], [0, 2], [0, 3], [0, 4], [0, 5], [0, 6], [0, 7], [1, 2], [1, 3], [1, 4], [1, 5], [1, 6], [1, 7], [0, 0], [1, 1]]
    src = '((defn\n  reduce\n  [f acc s]\n  (if (> (count s) 0) (reduce f (f acc (first s)) (rest s)) acc))\n (defn\n
observe~data\n  [acc data]\n  (let\n   [slope\n    (first acc)\n    bias\n    (second acc)\n    xn\n    (first data)\n
yn\n    (second data)\n    zn\n    (+ (* slope xn) bias)]\n   (observe (normal zn 1.0) yn)\n   [slope bias]))\n (let\n
[slope (sample (normal 0.0 10.0)) bias (sample (normal 0.0 10.0))]\n  (reduce\n   observe~data\n   [slope bias]\n
[[1.0 2.1] [2.0 3.9] [3.0 5.3] [4.0 7.7] [5.0 10.2] [6.0 12.9]])\n  [slope bias]))\n'

    def sample(self):
        sample_1 = Normal(0.0, 10.0).sample()
        sample_0 = Normal(0.0, 10.0).sample()
        observe_4 = Normal(sample_0 * 3.0 + sample_1, 1.0).sample()
        observe_6 = Normal(sample_0 * 5.0 + sample_1, 1.0).sample()
        observe_5 = Normal(sample_0 * 4.0 + sample_1, 1.0).sample()
        observe_7 = Normal(sample_0 * 6.0 + sample_1, 1.0).sample()
        observe_2 = Normal(sample_0 * 1.0 + sample_1, 1.0).sample()
        observe_3 = Normal(sample_0 * 2.0 + sample_1, 1.0).sample()
        return [torch.tensor([sample_0, sample_1]), torch.tensor([observe_2, observe_3, observe_4, observe_5, observe_6, observe_7])]
```

[3] https://hylang.org/

```
def log_likelihood(self, sample, observe):
    log_likeli = torch.zeros(sample.shape[0])
    log_likeli += Normal(sample[[slice(None), 0]] * 2.0 + sample[[slice(None), 1]], 1.0).log_prob(observe[[slice(None), 1]])
    log_likeli += Normal(sample[[slice(None), 0]] * 5.0 + sample[[slice(None), 1]], 1.0).log_prob(observe[[slice(None), 4]])
    log_likeli += Normal(sample[[slice(None), 0]] * 6.0 + sample[[slice(None), 1]], 1.0).log_prob(observe[[slice(None), 5]])
    log_likeli += Normal(sample[[slice(None), 0]] * 1.0 + sample[[slice(None), 1]], 1.0).log_prob(observe[[slice(None), 0]])
    log_likeli += Normal(sample[[slice(None), 0]] * 3.0 + sample[[slice(None), 1]], 1.0).log_prob(observe[[slice(None), 2]])
    log_likeli += Normal(sample[[slice(None), 0]] * 4.0 + sample[[slice(None), 1]], 1.0).log_prob(observe[[slice(None), 3]])
    return log_likeli

def log_prior(self, sample):
    log_prior = torch.zeros(sample.shape[0])
    log_prior += Normal(0.0, 10.0).log_prob(sample[[slice(None), 1]])
    log_prior += Normal(0.0, 10.0).log_prob(sample[[slice(None), 0]])
    return log_prior
```