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Practical Probabilistic Programming with Monads

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Abstract

The machine learning community has recently shown a lot of interest in practical probabilistic programming systems that target the problem of Bayesian inference. Such systems come in different forms, but they all express probabilistic models as computational processes using syntax resembling programming languages. In the functional programming community monads are known to offer a convenient and elegant abstraction for programming with probability distributions, but their use is often limited to very simple inference problems. We show that it is possible to use the monad abstraction for constructing probabilistic models, while still offering good performance of inference in challenging models. We use a GADT as an underlying representation of a probability distribution and apply Sequential Monte Carlo-based methods to achieve efficient inference. We define a formal semantics via measure theory and check the monad laws. We demonstrate a clean and elegant implementation that achieves performance comparable with Anglican, a state-of-the-art probabilistic programming system.

1. Introduction

1.1 Bayesian Models for Machine Learning

The paradigm of Bayesian modelling is to express one's beliefs about the world as a probability distribution over some suitable space, and then to use observed data to update this distribution via Bayes' rule

$$P(\theta|D) = \frac{1}{Z} P(\theta) P(D|\theta)$$

where θ denotes the model parameters (the unobservable beliefs about the world), D is the observed data, $P(\theta)$ is the prior distribution over the parameters (beliefs before the data is observed), $P(\theta|D)$ is the posterior distribution (beliefs after data is observed), $P(D|\theta)$ is the likelihood (probability of generating observed data given particular values of parameters), and Z is a normalising constant that ensures the posterior is a proper probability distribution.

For example, in a model for linear regression, the data D consists of a set of points (x_i, y_i) , while the parameters $\theta = (A, B)$ are the slope A and intercept B of the best-fitting line y = Ax + B through the points.

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Bayesian inference is the question of computing the posterior $P(\theta|D)$, so as to make predictions or decisions. In the example of linear regression, inference consists of computing the posterior distribution of the slope and intercept, $P((A, B) | (x_i, y_i))$, which may be used to predict y' given an unseen x', for instance.

Although Bayesian modelling is a robust and flexible framework, inference is often intractable. This problem is usually addressed in several ways. First of all, the prior and the likelihood are often chosen to be simple distributions, computationally tractable if not having analytical closed forms. Sometimes this is enough to compute the posterior exactly. If not, a wide range of approximate inference methods can be used to approximately compute the posterior. We will not review here the vast field of approximate inference, but instead we refer to Barber (2012). We are primarily concerned with Monte Carlo methods for approximate inference.

1.2 Probabilistic Programming for Bayesian Inference

In traditional approaches to Bayesian models, the mechanics of inference is tightly coupled with the model description. Instead, in probabilistic programming (Goodman 2013; Gordon et al. 2014), the intent is to make models and inference algorithms more composeable and reusable by specifying the model as a piece of probabilistic code, and implementing Bayesian inference as an interpreter or compiler for the probabilistic code.

There are many probabilistic programming languages with different trade-offs. Many languages, such as BUGS (Gilks et al. 1994), Infer.NET (Minka et al. 2009), and Stan (Stan Development Team 2014), restrict the underlying deterministic language by disallowing recursion, to ensure that the model can be compiled to a finite graphical model. This approach simplifies writing inference algorithms, but at the price of reduced expressiveness. Others such as HANSEI (Kiselyov and Shan 2009) use sophisticated interpretation techniques, but are limited to discrete distributions.

Many different solutions were proposed to extend probabilistic programming systems to potentially infinite models, such as combining graphical models with first-order logic, as in BLOG (Milch et al. 2005), Markov Logic Networks (Domingos and Richardson 2004), and ProbLog (Kimmig et al. 2011).

The most general approach, known as *universal* probabilistic programming, is to use a Turing-complete language. The pioneer is Church (Goodman et al. 2008), a functional subset of Scheme equipped with primitives for constructing standard probability distributions and a conditioning predicate. Other universal probabilistic programming languages include Venture (Mansinghka et al. 2014) and Anglican (Wood et al. 2014), both essentially dialects of Scheme. These universal languages are more expressive than those that compile to factor graphs. For example, they support nonparametric models such as the Dirichlet Process, useful for learning the best number of clusters from the data, but which do not compile to finite factor graphs. Inference for these more expressive models is harder, and research on improving inference is flourishing (Goodman and Stuhlmüller 2014).

1.3 Universal Probabilistic Programming in Haskell

The purpose of this paper is to provide evidence that the generalpurpose functional language Haskell is an excellent alternative to special-purpose languages like Church, for authoring Bayesian models and developing inference algorithms.

We embrace the idea of writing Bayesian models using the probability monad (Ramsey and Pfeffer 2002; Erwig and Kollmansberger 2006; Larsen 2011). We go beyond by developing a series of practical inference methods for monadic models, as opposed to relying on precise but unscalable methods of exhaustive enumeration of discrete distributions. We show Haskell code for a range of rich models, including the Dirichlet Process, of the sort otherwise written in Church and its relatives. We demonstrate that stateof-the-art Monte Carlo inference algorithms, including Sequential Monte Carlo (Doucet et al. 2000), Particle Independent Metropolis Hastings (Andrieu et al. 2010), and Particle Cascade (Paige et al. 2014), written in Haskell, have performance better than the specialpurpose Anglican implementation (Wood et al. 2014), and comparable to Probabilistic C (Paige and Wood 2014).

As a formal foundation for reasoning about models and inference, we present a formal semantics for our monad. The semantics is in two stages, inspired by recent work on the semantics of probabilistic while-programs (Hur et al. 2015). In the first stage, we interpret the monad as a deterministic function that consumes a stream of random samples to produce results. In the second stage, we define the distribution (a probability measure) given by closed expression of monadic type, by integrating its results over arbitrary random tapes.

To the best of our knowledge, this is the first rigorous semantics for a higher-order probabilistic programming language with conditioning (such as Church, Venture, or Anglican).

The main contributions of the paper are as follows.

- A practical library for probabilistic programming with monads. Previous approaches were elegant but inefficient. Here we implement state-of-the-art inference algorithms and performance is comparable with Anglican implementation.
- Randomised inference algorithms are viewed as deterministic transformations of a data structure representing a distribution. This makes inference clean, easy to implement, and sometimes even compositional.
- We demonstrate that a lazy probabilistic programming language allows for easy implementation of the Dirichlet Process model and the Particle Cascade algorithm.
- We present a formal semantics based on measure theory.

1.4 Structure of the Paper

We start in section 2 by showing on multiple examples how to build probabilistic models with monads. We specify what additional interface functions are required for a probabilistic programming system for Bayesian inference and we demonstrate how to use them. In section 3 we present an implementation of a GADT that satisfies those requirements and we explain how the inference problem manifests itself in this context. Then in section 4 we discuss implementation of several sampling-based methods for performing inference in probabilistic programs. In section 5 we present empirical evidence to correctness of our implementation and compare its performance with a state-of-the-art probabilistic programming system Anglican, which implements the same set of inference methods. We also define formal semantics of our approach to probabilistic programming in section 6 and we use it to prove the monad laws. Finally, in section 7 we discuss related work and in section 8 we conclude.

1.5 Intended audience

Even though this paper is mainly directed towards the functional programming audience, we hope that it will also be of interest to the machine learning community. For this reason we include in the paper some material that may be difficult to read for people without deep knowledge of Bayesian statistics. We took care to build up slowly from simple models and algorithms, where possible appealing to intuition. In particular sections 2 and 4 start with simple examples, but end with sophisticated models and algorithms which require substantial background in Bayesian methods to understand. It is our hope that even readers without such background will be able to understand the main points of this paper.

2. Modelling with monads

In this section we define and motivate the requirements we place on an implementation of probability distributions. Those requirements result in an interface, which we use to define probabilistic models. A large part of this section consists of examples that demonstrate how to use this interface.

2.1 Requirements

We introduce a type Prob to represent probabilities and probability densities. It is implemented as a Double, but sometimes it is useful to distinguish between the two. Another advantage is that we could easily replace Double with LogFloat to improve numerical stability.

<pre>newtype Prob = Prob {toDouble :: Double}</pre>				
deriving (Show, Eq, Ord,	Num, Fractional, Real,			
RealFrac, Floating,	Random, Ext.Distribution Ext			
.StdUniform)				
prob :: Double -> Prob				

We represent probability distributions over type a using a datatype Dist a. We place the following requirements on Dist:

1. availability of standard distributions to be used as building blocks, such as

	:: [a] -> Dist a :: [(a,Prob)] -> Dist a
normal	:: Double -> Double -> Dist Double
beta	:: Double -> Double -> Dist Double
gamma	:: Double -> Double -> Dist Double

Monad instance to combine distributions into sophisticated models

instance Monad Dist where

3. conditioning function, which takes a likelihood and a prior, and can be used to observe some data generated by the model

condition :: (a -> Prob) -> Dist a -> Dist a

4. a way to sample from a Dist

sample :: StdGen -> Dist a -> a

where StdGen is a random number generator.

Together those four requirements form an interface for working with Dist. In the remainder of this section we show how to use this interface to build probabilistic models of increasing complexity.

2.2 Dice rolling

We start with a very simple example. Suppose we roll n six-sided dice and look at the sum of the values in top faces. A distribution over such outcomes can be written in the following way:

```
die :: Int -> Dist Int
die 0 = return 0
die 1 = uniform [1..6]
die n = liftM2 (+) (die 1) (die (n-1))
```

We can simulate one roll using the sample function and we can use standard functions replicate and sequence to generate a distribution over a number of independent rolls.

```
result = sample g (die n)
results = sample g $ sequence $ replicate k $ die n
```

An example run would be

```
> let (n,k) = (3,5)
> let g = mkStdGen 0
> sample g $ die n
14
> sample g $ sequence $ replicate k $ die n
[10,8,16,12,10]
```

This style of constructing a list of independent samples from a distribution turns out to be very useful and we use it extensively in this paper. It is worth noting here that our implementation of Dist is lazy, so it is equivalent to write

```
results = take k $ sample g $ sequence $ repeat $ die n
```

It would be natural to attempt different operations on the distribution, for example we could ask what is the probability of a specific outcome or outcomes that satisfy a certain condition. However, in this paper we are only concerned with sampling. The reason for that is we are primarily concerned with solving difficult problems where exact answers are intractable and we need to resort to approximate sampling. With a collection of samples we can approximately answer any query about a distribution.

2.3 Coin tossing

We now turn to another toy problem which demonstrates how to use conditioning. We are given a coin, which may be fair or biased, and we toss it several times to determine which is the case. If the coin is biased, we also want to determine its weight. We start by putting a prior over the weight of the coin. The coin is fair with probability 0.8 and biased with probability 0.2. For a biased coin we put a prior on its weight according to a Beta distribution. This is a standard choice that makes it possible to compute the posterior analytically.

```
weight :: Dist Prob
weight = do
    isFair <- bernoulli 0.8
    if isFair then return 0.5 else beta 5 1</pre>
```

Now we define the likelihood model. We represent outcomes of a coin toss with Boolean values and we identify the weight of the coin with the probability of landing True in a single toss. For a coin with weight w the likelihood is equal to w for the coin landing True and 1 - w for the coin landing False. We define a toss function which conditions the distribution over the possible weights of the coin on an outcome of a single toss. Conditioning on a series of outcomes is just a fold over the outcomes.

```
toss :: Bool -> Dist Prob -> Dist Prob
toss b = condition (v -> if b then w else 1 - w)
```

tosses :: [Bool] -> Dist Prob -> Dist Prob
tosses bs d = foldl toss d bs

The posterior over the weight of the coin is:

posteriorWeight = tosses observations weight

In order to get any useful results from the posterior we actually need to perform inference. We delay the discussion of how to do it until section 4.

2.4 Linear regression

A very simple but very useful statistical model is that of linear regression, where we try to find a straight line that fits a set of observed data points best. The construction of this model is very similar to the coin tossing example above, so we only offer a brief explanation here. We put independent Gaussian priors over the slope and the intercept and we assume the noise is Gaussian too.

```
type Point = (Double, Double)
type Param = (Double, Double)
linear :: Dist Param
linear = do
    a <- normal 0 1
    b <- normal 0 1
    return (a,b)
point :: Point -> Dist Param -> Dist Param
point (x,y) =
    condition (\(a,b) -> pdf (Normal (a*x + b) 1) y)
points :: [Point] -> Dist Param -> Dist Param
points ps d = foldl point d ps
```

In the above Normal is a data constructor for a datatype representing a normal distribution. It is available in several libraries and we do not define it here, but we emphasise it is not the same as normal, which constructs a Dist. The pdf function computes the probability density function of a given distribution at a given point.

The above examples are very simple and do not demonstrate the power of the monadic approach to probabilistic modelling. We now demonstrate several standard probabilistic models expressed in a monadic form.

2.5 Hidden Markov Model

A Hidden Markov Model (HMM) is very popular for modelling sequential data. It consists of two sequences of random variables. The latent sequence is assumed to be Markovian and stationary, that is each of the latent variables only depends on the value of the previous one and the form of the dependency is the same for all elements. In the observed sequence each random variable only depends on the value of the associated latent variable, again in a stationary way. We aim to infer the values of the latent variables given the observed ones. In this particular model we assume that latent variables are discrete, while the observable ones are continuous.

```
hmm :: Dist [Int]
hmm = liftM reverse states where
states = foldl expand start values
expand :: Dist [Int] -> Double -> Dist [Int]
expand d y = condition (score y . head) $ do
rest <- d
x <- trans $ head rest
return (x:rest)
score y x = pdf (Normal x 1) y
trans 0 = categorical $ zip [-1..1] [0.1, 0.4, 0.5]
trans 1 = categorical $ zip [-1..1] [0.2, 0.6, 0.2]
trans 2 = categorical $ zip [-1..1] [0.15,0.7,0.15]
start = uniform [-1..1]
```

values = [0.9,0.8,0.7,0,-0.025,5,2,0.1,0, 0.13,0.45,6,0.2,0.3,-1,-1]

This particular way of implementing an HMM may be somewhat confusing. After all, we could simply expand the entire sequence of latent states and then use it to generate likelihoods of the observations. However, to make inference efficient, it is important to generate likelihoods as early as possible and to use them only on the left side of the monadic bind. We will discuss those points further in section 4.

2.6 Dirichlet Process mixture of Gaussians

A common task in machine learning is clustering. The problem is, given a set of data points, to separate it into disjoint clusters based on similarity. For continuous data points a common model choice is a mixture of Gaussians, where the likelihood of a point belonging to a particular cluster is given by a normal distribution. There are, however, many possible choices for deciding on the number of clusters. Sometimes it is possible to fix the number of clusters in advance, sometimes it is necessary to put a prior distribution over the number of clusters. We choose to use a Dirichlet Process (DP), where the number of clusters is not determined by a specific parameter, but rather can grow with the number of data points. The complete review of the DP is beyond the scope of this paper and we encourage interested readers to consult the specialised sources (Teh 2010). We merely note that we are using a stick-breaking representation here, where a DP is generated using an infinite sequence of random variables. As our implementation of Dist is lazy, we can code this representation directly.

```
pick :: [Prob] -> [a] -> Dist a
pick (b:breaks) (a:atoms) = do
  keep <- bernoulli b
  if keep then return a else pick breaks atoms</pre>
```

```
dpMixture :: Dist [Int]
dpMixture =
   let
      --lazily generate clusters
     clusters = do
       let atoms = [1..]
       breaks <- sequence $ repeat $ fmap prob $ beta 1</pre>
            1
       let classgen = stick breaks atoms
       vars <- sequence $ repeat $ fmap (1/) $ gamma 1 1</pre>
       means <- mapM (normal 0) vars</pre>
       return (classgen, vars, means)
     obs = [1.0,1.1,1.2,-1.0,-1.5,-2.0,
            0.001, 0.01, 0.005, 0.0]
     n = length obs
     --start with no data points
     start = fmap (,[]) clusters
     --add points one by one
     points = foldl build start obs
     build d y = condition (score y . head . snd) $ do
       (clusters, rest) <- d
       let (classgen, vars, means) = clusters
       cluster <- classgen
       let point = (cluster, vars !! cluster,
                   means !! cluster)
       return (clusters, point : rest)
     --the likelihood in a cluster in Gaussian
```

```
score y (cluster, var, mean) =
    -- Normal mean stddev
    prob $ pdf (Normal mean (sqrt var)) y
```

--exctract cluster assignments fmap (reverse . map (\($x, _, _$) -> x) . snd) points

3. Implementation

In the previous section we showed how to use the monadic interface to build probabilistic models. Here we discuss an implementation of the underlying data structure Dist, focusing in particular on the task of performing inference.

3.1 List of values

The simplest possible implementation would be a list of weighted values, such as suggested by Erwig and Kollmansberger (2006). This approach is very easy to understand, but it is also very limited. It can not be used with continuous distributions and it is tied to a particular, inefficient inference strategy. Nonetheless, we present this implementation below, in the hope that it makes the semantics of the interface easier to understand. We call this implementation Explicit, since it represents a distribution explicitly as a collection of weighted values.

```
newtype Explicit a = Explicit {toList :: [(a,Prob)]}
instance Functor Explicit where
   fmap f (Explicit xs) = Explicit $ map (first f) xs
instance Monad Explicit where
   return x = Explicit [(x, 1)]
    (Explicit xs) >>= f =
     Explicit [(y,p*q)| (x,p) <- xs, (y,q) <- toList (f</pre>
          x)]
condition (Explicit xs) c = Explicit $ normalize $
    reweight c xs
reweight c xs = map ((x,p) \rightarrow (x, p * c x)) xs
normalize xs = map (second (/ w)) xs where
 w = sum $ map snd xs
sample g (Explicit xs) =
   scan r xs where
       r = fst \ \ random R \ (0.0, 1.0) g
       scan v ((x,p):ps) = if v <= \tilde{p} then x else scan (v
            -p) ps
uniform
           = Explicit . normalize . map (,1)
categorical = Explicit . normalize
bernoulli p = categorical [(True,p), (False,1-p)]
```

3.2 GADT

There is no single best inference method to be used in all cases, so we decide on an implementation that provides as much flexibility as possible. Specifically, we implement Dist as a GADT which simply stores the applications of all the functions exposed by the interface.

```
data Dist a where
  Return :: a -> Dist a
  Bind :: Dist b -> (b -> Dist a) -> Dist a
  Primitive :: Dist Double
  Conditional :: (a -> Prob) -> Dist a -> Dist a
  condition = Conditional
instance Functor Dist where
  fmap = liftM
instance Monad Dist where
  return = Return
  (>>=) = Bind
```

4

```
sample g (Return x) = x
sample g (Bind d f) = sample g1 y where
y = f (sample g2 d)
(g1,g2) = split g
sample g Primitive = fst $ random g
sample g (Conditional c d) = undefined
```

Here we only use Primitive, a uniform distribution on the [0, 1] interval, as a basic building block. All other standard distributions can be built from one or more uniform random variables using monadic operations. We only do this for clarity and in practice we allow an arbitrary sampler to be used as a basic building block. In particular all the standard distributions can be pulled directly from existing libraries with very little effort.

A Dist can only be sampled from if it is not conditioned. This design choice is motivated by the fact that conditioning is a declarative description of the posterior, which does not specify how to sample from it. Before a conditional distribution can be sampled from, we need to apply an inference algorithm that specifies a way of sampling from the posterior, either exactly or approximately. For this reason we choose to view inference as a deterministic Dist to Dist transformation. An inference method, several of which are discussed in section 4. converts a Dist into an equivalent Dist, but one without conditionals. The notion of equivalence of distributions is formally defined in section 6. In practice we can often get better results by trying to approximate a Dist with a collection of samples. For this reason we also consider inference methods that transform a Dist a into Dist [a] or Dist ([(a,Prob)]). In principle we could recover the relevant Dist a by sampling from such a collection at the end. We show some examples of this later on.

4. Inference

The central question in probabilistic modelling is how to do inference efficiently. In the previous section we explained that we interpret inference as a Dist to Dist transformation that preserves semantics while removing conditionals. Ideally inference methods would just be functions Dist a -> Dist a, but in practice this would often discard useful information. For this reason we provide two implementations of every inference algorithm. An inference function produces a distribution over collections of samples, while inference' produces a distribution over single values.

We present implementations of several inference methods, in particular of the Particle Markov Chain Monte Carlo (PMCMC) (Andrieu et al. 2010) methods that were first used for probabilistic programming in Anglican (Wood et al. 2014). Some of them require the presence of Conditionals to be independent of any random choices in the model. In modelling terms this is a reasonable assumption, since the observed data is fixed. To enforce this constraint we require that all the Conditionals should be placed on the left of the monadic Bind. We could use the type system to enforce this constraint, but then we could no longer make Dist an instance of the Monad class.

4.1 Sampling from the prior

The very first thing we show is how to draw samples from the prior. The prior can be regarded as the simplest approximation to the posterior, but not one relevant in practice. We still discuss it here for completeness. Algorithmically sampling from the prior amounts to discarding Conditionals in a Dist. As discussed above, the Conditionals should only be placed on the left of Bind, so we do not need to worry about what is right of Bind.

prior' :: Dist a -> Dist a
prior' (Conditional c d) = prior' d
prior' (Bind d f) = Bind (prior' d) f

prior'd

The subsequent inference methods rely on sampling from the prior, but rather than discarding the likelihood score they retain it and use it to reweight the samples. For this purpose we define a function that accumulates the scores rather than discarding them.

= d

```
prior :: Dist a -> Dist (a,Prob)
prior (Conditional c d) = do
  (x,s) <- prior d
  return (x, s * c x)
prior (Bind d f) = do
  (x,s) <- prior d
  y  <- f x
  return (y,s)
prior d = do
  x   <- d
  return (x,1)</pre>
```

4.2 Importance sampling

The subsequent methods will often use collections of weighted samples, so we define some helper functions to deal with them.

```
type Samples a = [(a,Prob)]
normalize :: Samples a -> Samples a
normalize xs = map (second (/ norm)) xs where
norm = sum $ map snd xs
resample :: Samples a -> Dist (Samples a)
resample xs = sequence $ replicate n $ fmap (,1) $
categorical xs where
n = length xs
flatten :: Samples (Samples a) -> Samples a
flatten xss = [(x,p*q) | (xs,p) <- xss, (x,q) <- xs]</pre>
```

A simple but useful inference method is that of importance sampling. In essence importance sampling amounts to drawing samples from a tractable proposal distribution (here the prior) and reweighting them in a suitable way (here by the likelihoods). As discussed above, we can either retain all the samples to approximate the posterior or just draw one of them at the end.

```
importance :: Int -> Dist a -> Dist (Samples a)
importance n d = sequence $ replicate n $ prior d
importance' :: Int -> Dist a -> Dist a
importance' n d = importance n d >>= categorical
```

4.3 Metropolis-Hastings

Another way to obtain the correct posterior by drawing samples from a different proposal distribution is Markov Chain Monte Carlo (MCMC) (Neal 1993). Perhaps the most popular MCMC method used for Bayesian inference is the Metropolis-Hastings (MH) algorithm. The MH algorithm generates an infinite sequence of samples, called a Markov Chain, by proposing a new sample from a proposal distribution and accepting or rejecting it with probability proportional to the ratio of scores between the current sample and the proposed one. In case of rejection the current sample is retained as the next sample. It can be proven that under certain mild conditions the marginal distributions of subsequent samples converge to the true posterior, regardless of the starting point. In practice, however, we often take the whole sequence of samples to approximate the posterior.

Here we use a very simple variant of MH where the proposal distribution is the prior and the score is the likelihood. For the readers familiar with the existing probabilistic programming literature, note that this is not a single-site MH as proposed by Wingate et al. (2011), but rather an MH that proposes the entire trace from the prior.

```
mh :: Dist a -> Dist [a]
mh d =
fmap (map fst) $ proposal >>= iterate where
proposal = prior d
iterate (x,s) = do
    (y,r) <- proposal
    accept <- bernoulli $ min 1 (r / s)
    let next = if accept then (y,r) else (x,s)
    rest <- iterate next
    return $ next:rest
mh' :: Int -> Dist a -> Dist a
mh' n d = fmap (!! n) (mh d)
```

4.4 Sequential Monte Carlo

There exists a more powerful inference method, somewhat similar to importance sampling, called Sequential Monte Carlo (SMC) (Doucet et al. 2000). Originally SMC was used only with sequential data, where latent variables can be arranged in a sequence with some data being observed at each step. SMC approximates the partial posterior at each step by a collection of weighted samples, called particles, which are reweighted according to the likelihood of the observed data at each step. In order to avoid accumulating excessive weight on a small number of particles, the particles are resampled at each step.

It was recently shown that SMC can be applied to probabilistic programs (Wood et al. 2014) and similarly we can apply it to do inference on a Dist. The essential feature that allows for it is that the presence Conditionals is not affected by any random choices, that is all Conditionals are to the left of Bind.

We emphasize the fact that SMC does not actually remove Conditionals, but rather replaces them with different ones. The new scores are weighted averages of likelihood scores across all the particles, which is sometimes called a pseudo-marginal likelihood. It is useful to retain the pseudo-marginal likelihood, since it can be used to correct for bias introduced by SMC. The reason we do it this way is that it allows us to compose two inference methods to obtain better results. In particular, it is possible to discard the extra information and recover the ordinary SMC algorithm by composing smc with prior'.

```
smcStandard :: Int -> Dist a -> Dist (Samples a)
smcStandard n = prior' . smc n
smcStandard' :: Int -> Dist a -> Dist a
smcStandard' n = prior' . smc' n
```

Another possibility is to combine results of several SMC runs by weighting the particles according to the pseudo-marginal likelihoods. We can accomplish it by composing smc with importance.

```
smcMultiple :: Int -> Int -> Dist a -> Dist (Samples a)
smcMultiple k n = fmap flatten . importance k . smc n
smcMultiple' :: Int -> Int -> Dist a -> Dist a
```

```
smcMultiple' k n = importance' k . smc' n
```

4.5 Particle Independent Metropolis Hastings

The idea that SMC can be used as a part of a more powerful inference algorithm in not new. In particular, there exist a family of MCMC algorithms, called Particle MCMC (PMCMC) (Andrieu et al. 2010), which use SMC to obtain a proposal distribution for the MH algorithm. Perhaps the simplest PMCMC algorithm is Particle Independent Metropolis-Hastings (PIMH), which is an MH with proposals generated by independent SMC runs and the scores equal to pseudo-marginal likelihoods. We can obtain PIMH simply by composing smc with mh.

```
pimh :: Int -> Dist a -> Dist [Samples a]
pimh n = mh . smc n
```

pimh' :: Int -> Int -> Dist a -> Dist a
pimh' k n = mh' k . smc' n

4.6 Particle Cascade

A final inference algorithm that we discuss here is the recently proposed Particle Cascade (PC) (Paige et al. 2014). PC is essentially SMC with an infinite number of particles, where resampling is done only based on previous particles and not on subsequent ones. The result of PC is an infinite sequence of samples that can be consumed lazily until desired accuracy is achieved. Within a lazy probabilistic programming language we can implement PC in almost the same way as SMC, changing only the resampling function.

```
cascade :: Dist a -> Dist (Samples a)
cascade (Conditional c d) = do
  ps <- cascade d
  let qs = map (\(x,w) -> (x, c x * w)) ps
  resamplePC qs
cascade (Bind d f) = do
  ps <- cascade d
  let (xs,ws) = unzip ps
  ys <- mapM f xs
  return (zip ys ws)
cascade d = sequence $ repeat $ fmap (,1) d
cascade' :: Int -> Dist a -> Dist a
  cascade' n d = cascade d >>= categorical . take n
```

We do not show the code for the resamplePC function here, as it implements a complicated mathematical formula that would be difficult to read. We refer the interested readers to (Paige et al. 2014).

5. Evaluation

We evaluate our implementation by running some of the inference algorithms from section 4 on selected models from section 2. Our purpose is to demonstrate correctness and efficiency of implementation, not to investigate relative performance of different inference methods. In order to establish correctness we compare the empirical posterior consisting of samples obtained from inference algorithms to an exact posterior. We carefully select models for which we can compute the exact posterior by a combination of analytical and computational methods. We use KL divergence, a standard metric of dissimilarity between distributions, to compare our results to the exact posteriors. For a correct sampler the KL divergence should decay approximately according to a power law, producing a straight line on a log-log scale. The results are given in figure 1.

We judge efficiency of our implementation by comparing execution times with Anglican and Probabilistic C. We run all the experiments using a single core of an Intel Core i7 CPU 920 @ 2.67GHz on a machine running Ubuntu 14.04. Although Anglican and Probabilistic C can run inference utilising multiple cores, we only used one to get a better comparison with our implementation, which is currently sequential. In section 8 we briefly discuss how it could be parallelised. Anglican was originally an interpreted language, but was recently reimplemented ¹ by compiling to Clojure code directly. We compare our implementation against the new, faster version (0.6.5).

We emphasise that the benchmarks are not meant to be definitive. We only present them to demonstrate that the performance of our implementation is comparable to state-of-the-art. The results of our tests are presented in table 1. We only report execution times for SMC, but PIMH is almost identical. Comparing speed of PC implementations is more difficult, since our version lets us control the final number of particles, while Anglican and Probabilistic C give control over the starting number of particles. We note that our implementation seems not to scale as well as Anglican with the number of particles. The probable cause for it is that we use an inefficient resampling algorithm, which could be fixed in a later version.

model	particles	Haskell	Anglican	Prob-C
	100	0.05s	0.2s	0.1s
HMM	1000	0.4s	1.0s	2.9s
	10000	10s	9s	-
	100	0.05s	0.1s	0.1s
DP	1000	0.4s	0.5s	3.2s
	10000	6.3s	3.9s	-

Table 1. Comparison of efficiency of Sequential Monte Carlobased inference engines in three different probabilistic programming systems: the one described in this paper (Haskell), Anglican, and Probabilistic C. We report the wall clock time taken to complete a single iteration of SMC with the given number of particles on a single core. We note that the results were largely consistent across different runs, but we do not attempt to rigorously analyse their variability. Those figures are not intended as a definitive evaluation, but rather as a rough indication of relative efficiencies. For Probabilistic C we were unable to run 10000 particles, which requires spawning 10000 processes simultaneously.

5.1 Dice rolling

As a first test we choose the very simple model of rolling dice from section 2.2. We turn it into an inference problem by conditioning it with likelihood inversely proportional to the result.

conditionalDie :: Int -> Dist int conditionalDie n = condition ((1 /) . fromIntegral) (die n)

We use 5 dice and obtain the exact posterior by exhaustively enumerating all possible outcomes. The results clearly show that all the inference methods converge to the exact posterior.

5.2 Hidden Markov Model

The next model is more challenging and practically relevant. We use the HMM, exactly in the form as defined in 2.5. We compute the

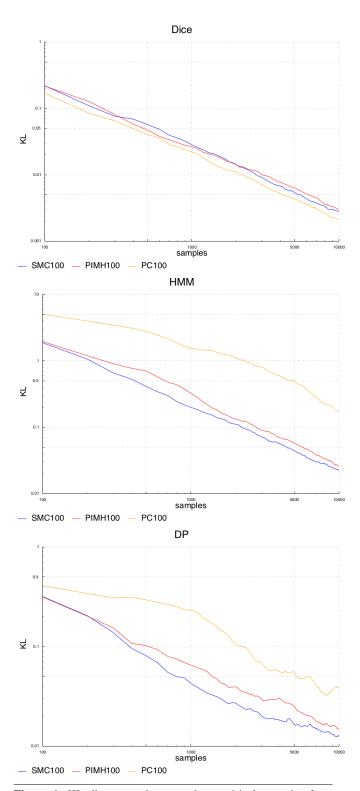


Figure 1. KL divergence between the empirical posterior from samples and the exact posterior as a function of the number of samples drawn for the HMM model. The lines drawn are mean values of KL taken across 20 independent runs. We compare three algorithms: SMC, PIMH, PC, each using 100 particles. SMC and PIMH converge to the correct posterior relatively fast. PC is less efficient per sample drawn, but still displays correct behaviour. The models are described in detail in section 2.

¹ https://bitbucket.org/dtolpin/anglican

exact marginal distribution for each latent state using the forwardbackward algorithm. The KL divergence reported is actually a sum of KL divergences between exact and empirical marginal posteriors for each latent state. We only include KLs for the latent variables that have corresponding observations, that is we exclude the initial state.

5.3 DP mixture of Gaussians

Our final test is the DP mixture model from 2.6. We report the KL divergence between posteriors over the total number of clusters for the data points presented in 2.6. The exact posterior was computed by exploiting the conjugate Normal-Inverse-Gamma prior, the exact values of the Chinese Restaurant Process prior, and an enumeration of all possible partitions.

6. Formal semantics

In this section we formally define the semantics of Dist. Two major technical difficulties involved are defining and conditioning probability distributions over uncountable sets. We turn to measure theory for a solution to those problems. Measure theory is a vast subject and rather than trying to review it here, we refer the readers to general texts such as (Rosenthal 2006).

We only define semantics for distributions over sufficiently simple types and under certain simplifying assumptions. Specifically, we require that all the functions involved always terminate, so we can treat Haskell functions as total. We also require that there is only a finite number of Conditional points in the GADT and that all the scoring functions are bounded. Relaxing those requirements is an important goal, but it is outside the scope of this paper.

Let us consider Dist to be a function from a suitable source of randomness to a pair consisting of a value and a weight. For this purpose we define Haskell functions semantics, value, and weight

```
type P a = [Double] -> Maybe (a, Prob, [Double])
semantics :: Dist a -> P a
semantics (Return x) tape = Just (x,1,tape)
semantics (Bind d f) tape = do
   (x,p,t ) <- semantics d tape
   (y,q,t') <- semantics (f x) t
  return (y,p*q,t')
semantics Primitive []
                         = Nothing
semantics Primitive (r:rs) = Just (r,1,rs)
semantics (Conditional c d) tape = do
    (x,p,t) <- semantics d tape
    return (x, p * c x, t)
weight :: Dist a -> [Double] -> Prob
weight d t = fromMaybe 0 $ fmap ((x,y,z) \rightarrow y) (
    semantics d t)
value :: Dist a -> [Double] -> Maybe a
value d t = fmap ((x,y,z) \rightarrow x) (semantics d t)
member :: Dist a -> [Double] -> (a -> Bool) -> Bool
member d t i = fromMaybe False $ fmap i $ value d t
```

We choose a source of randomness to be a finite list of real numbers from the [0, 1] interval. This means the source may sometimes be insufficient, which is why the result is wrapped in a Maybe. On the other hand, semantics always terminates on Dists that consume randomness indefinitely. The function member tests if the result belongs to a set defined by an indicator function.

Theorem 1. Dist is a monad up to equivalence defined by semantics.

Proof. In order to be a monad, Dist needs to satisfy the three monad laws. Since semantics is defined in a compositional way by recursion on the structure of Dist, we only need to consider direct application of semantics to Dists that should be equivalent by the monad laws.

left identity: return a >>= f = f a

```
semantics (Bind (Return a) f) tape =
do
  (x,p,t) <- semantics (Return a) tape
  (y,q,t') <- semantics (f x) t
  return (y,p*q,t') =
do
  (x,p,t) <- Just (a,1,tape)
  (y,q,t') <- semantics (f x) t
  return (y,p*q,t') =
do
  (y,q,t') <- semantics (f a) tape
  return (y,1*q,t') =
semantics (f a) tape</pre>
```

• right identity: m >>= return = m

```
semantics (Bind m Return) tape =
do
  (x,p,t) <- semantics m tape
  (y,q,t') <- semantics (Return x) t
  return (y,p*q,t') =
do
  (x,p,t) <- semantics m tape
  (y,q,t') <- Just (x,1,t)
  return (y,p*q,t') =
do
  (x,p,t) <- semantics m tape
  return (x,p*1,t) =
semantics m tape</pre>
```

• associativity: $m \rightarrow f \rightarrow g = m \rightarrow (x \rightarrow f x \rightarrow g)$

```
semantics (Bind (Bind m f) g) tape =
do
  (x,p,t) <- semantics (Bind m f) tape</pre>
  (y,q,t') <- semantics (g x) t
 return (y,p*q,t') =
do
  (x,p,t) <- do
      (z,r,t'') <- semantics m tape</pre>
      (w,s,t''') <- semantics (f z) t''
      return (w,r*s,t'')
  (y,q,t') <- semantics (g x) t
 return (y,p*q,t') =
do
  (z,r,t'') <- semantics m tape</pre>
  (w,s,t''') <- semantics (f z) t''
 let (x,p,t) = (w,r*s,t'')
 (y,q,t') <- semantics (g x) t
 return (y,p*q,t') =
do
  (z,r,t'') <- semantics m tape</pre>
  (w,s,t''') <- semantics (f z) t''
  (y,q,t') <- semantics (g w) t'''
 return (y,r*s*q,t') =
  (z,r,t'') <- semantics m tape
  (x,p,t) <- do
   (w,s,t''') <- semantics (f z) t''
    (y,q,t') <- semantics (g w) t'''
   return (y,s*q,t')
 return (x,r*p,t) =
do
 (z,r,t'') <- semantics m tape</pre>
```

In order to simplify the task of deriving measures from Dists we restrict the type T in Dist T not to contain any function types. This restriction only applies to the type of the final expression we wish to give semantics to and not to any intermediate components used for its construction. We do it solely to avoid technical difficulties associated with defining measures on function spaces and in principle this restriction could be lifted, at least to some degree. Formally, we require T to be either an integer, a real, or constructed by any finite sums and products of the two.

Definition 1. We define the set of simple types S to be the smallest set containing int and real and closed under binary sums and products. A type T is simple if $T \in S$, or equivalently if it is generated by the following grammar:

$$T ::= int|real|T + T|T \times T$$

Our examples in section 2 either define distributions over simple types, or lists of statically known length, which could be easily encoded as a simple type.

Definition 2. For any simple type T we define [T] to be the set of all possible values of this type. This is defined recursively as follows:

$$\llbracket int \rrbracket = \mathbb{Z} \tag{1}$$

$$\llbracket real \rrbracket = \mathbb{R} \tag{2}$$

$$[\![T_1 + T_2]\!] = [\![T_1]\!] \sqcup [\![T_2]\!]$$
(3)

 $[\![T_1 \times T_2]\!] = [\![T_1]\!] \times [\![T_2]\!]$ (4)

where \sqcup is a disjoint union and \times is a Cartesian product.

Definition 3. For any simple type T we define a σ -algebra Σ_T recursively as follows:

$$\Sigma_{int} = \sigma_{\mathbb{Z}}(\mathbb{Z}) \tag{5}$$

$$\Sigma_{real} = \sigma_{\mathbb{R}}(\{[a, b] | a, b \in \mathbb{R}\})$$
(6)

$$\Sigma_{T_1+T_2} = \sigma_{\llbracket T_1+T_2 \rrbracket}(\{A \sqcup B | A \in \Sigma_{T_1}, B \in \Sigma_{T_2}\})$$
(7)

$$\Sigma_{T_1 \times T_2} = \sigma_{\llbracket T_1 \times T_2 \rrbracket}(\{A \times B | A \in \Sigma_{T_1}, B \in \Sigma_{T_2}\})$$
(8)

where $\sigma_X(S)$ is the smallest σ -algebra over the set X that is a superset of S.

Together a pair $(\llbracket T \rrbracket, \Sigma_T)$ forms a measurable space and we interpret values of type Dist T to be measures over this space.

With the above definitions in place, we proceed to define the semantics in terms of a uniform probability measure on the space of sources of randomness. Since we can not construct a uniform measure on $[0, 1]^{\infty}$, we resort to a limit construction involving Borel measures on $[0, 1]^n$ for each finite n.

Definition 4. For any simple type T and any expression M :: Dist T, we define its semantics $[\![M]\!]$ to be a measure μ on $([\![T]\!], \Sigma_T)$. For any $A \in \Sigma_T$, $\mu(A)$ is defined using a limit of Lebesgue integrals. Specifically, for any $n \in \mathbb{N}$, let ν_n be a Borel measure on the set $[0, 1]^n$ representing random sources of fixed length n. Then

$$\mu(A) = \lim_{n \to \infty} \mu_n(A) \tag{9}$$

$$u_n(A) = \frac{1}{Z_n} \int \left(\lambda v.member \ M \ v \ I_A \ * \ weight \ M \ v\right) d\nu_n$$
(10)

$$Z_n = \int \left(weight \ M \right) d\nu_n \tag{11}$$

The normalising constant Z_n always exists and is finite, as we require that the number of conditioning points is fixed and that the scoring function at each of the points is bounded, which implies that the integrand in equation 11 is bounded. Similarly $\mu_n(A)$ always exists. For any A, the sequence $\{\mu_n(A)\}$ is non-decreasing, as we take the integrand to be 0 where we run out of randomness, and upper-bounded by 1. It follows that $\mu(A)$ exists for any A. It remains to show that μ is a probability measure. We use the fact that μ_n is a finite measure for any n, which follows from it being an integral of a measurable function with respect to a finite measure.

Lemma 1. Let a_{nk} be a sequence indexed by two natural numbers. Assume the sequence is bounded from above and non-decreasing in both n and k, that is $\forall_{n,k\in\mathbb{N}}a_{n+1k} \ge a_{nk} \land a_{nk+1} \ge a_{nk}$. Then $\lim_{n\to\infty} \lim_{k\to\infty} a_{nk} = \lim_{k\to\infty} \lim_{n\to\infty} a_{nk}$.

Proof. Let $b_n = \lim_{k \to \infty} a_{nk}$ and $c_k = \lim_{n \to \infty} a_{nk}$. Both b_n and c_k are bounded and non-decreasing, so they converge. Let $b = \lim_{n \to \infty} b_n$, so $b = \lim_{n \to \infty} \lim_{k \to \infty} a_{nk}$, and let $c = \lim_{k \to \infty} c_k$, so $c = \lim_{k \to \infty} \lim_{n \to \infty} a_{nk}$.

We have $a_{nk} \leq c_k$ and taking limits as $k \to \infty$ from both sides we get $b_n \leq c$ and so $b \leq c$. Similarly from $a_{nk} \leq b_n$ we obtain $c_k \leq b$ and so $c \leq b$. It follows that $\lim_{n\to\infty} \lim_{k\to\infty} a_{nk} = b = c = \lim_{k\to\infty} \lim_{n\to\infty} a_{nk}$.

Theorem 2. The semantics $\llbracket M \rrbracket = \mu$ from definition 4 is a probability measure.

Proof. To be a probability measure, μ needs to satisfy three conditions:

- $\mu(\emptyset) = 0$, which follows from the fact that for every *n* we have $\mu_n(\emptyset) = 0$, as I_{\emptyset} is always false
- countable additivity $\mu(\bigcup_k A_k) = \sum_k \mu(A_k)$, where $A_i \cap A_j = \emptyset$ for $i \neq j$ We have

$$\mu(\bigcup_{k} A_k) = \tag{12}$$

$$\lim_{n \to \infty} \mu_n(\bigcup_k A_k) =$$
(13)

$$\lim_{n \to \infty} \sum_{k=0}^{\infty} \mu_n(A_k) =$$
(14)

$$\lim_{n \to \infty} \lim_{K \to \infty} \sum_{k=0}^{K} \mu_n(A_k) =$$
(15)

$$\lim_{K \to \infty} \lim_{n \to \infty} \sum_{k=0}^{K} \mu_n(A_k) =$$
(16)

$$\lim_{K \to \infty} \sum_{k=0}^{K} \lim_{n \to \infty} \mu_n(A_k) =$$
(17)

(18)

9

$$\sum_{k=0}^{\infty} \lim_{n \to \infty} \mu_n(A_k) =$$
(19)

$$\sum_{k=0}^{\infty} \mu(A_k) \tag{20}$$

where we use the fact that μ_n is a measure to go from 13 to 14, we use lemma 1 to go from 15 to 16, and we are allowed push the limit inside a sum going from 16 to 17 because the sum is finite.

• $\mu(\llbracket T \rrbracket) = 1$, which follows from the assumption that semantics always terminates after consuming only a finite amount of randomness, as $I_{\llbracket T \rrbracket}$ is always true

There are two important aspects of the semantics that we leave for future work. One is the possibility of non-termination, including both the programs that terminate with probability 1 and those that do not. The other is allowing for more sophisticated types to be used at top level. This includes recursive types, such as lists with potentially infinite, lazily evaluated values, and function types, including higher-order functions.

7. Related Work

The work on semantics of probabilistic programming languages dates back to Dexter Kozen (1981, 1985).

We believe that our formal semantics is the first rigorous semantics for a higher-order probabilistic programming language with conditioning, an essential ingredient of Bayesian modelling. Ramsey and Pfeffer (2002) propose formal semantics of a stochastic λ -calculus in terms of probability monads and measure terms, but without considering conditioning. Borgström et al. (2013) develop a compositional semantics of first-order functional programs, including conditioning on zero-probability events, based on measure transformers, but they do not consider the higher-order case. In recent work, van de Meent et al. (2015) provide a formal operational semantics for a Church-like language to associate expressions with execution traces, so as to explain an inference method, Particle Gibbs with Ancestor Sampling, as opposed to the semantics of the Bayesian model. Instead, we have expressed various inference methods as executable Haskell code, and our formal semantics captures the meaning of a Bayesian model directly as a probability distribution. Some recent works develop operational equivalence for probabilistic λ -calculus but without considering continuous distributions, or constructs for conditioning. Dal Lago et al. (2014) develop a bisimulation theory for an untyped calculus, while Bizjak and Birkedal (2015) investigate operational equivalence and stepindexed logical relations for a typed probabilistic λ -calculus. Gretz et al. (2015) consider the semantics of conditioning in probabilistic while-programs, together with transformations to eliminate conditioning, but without higher-order functions.

A monadic Haskell library for probabilistic programming programming was first introduced by Erwig and Kollmansberger (2006). Later Larsen (2011) suggested using GADTs to improve performance of such a library. Both of these approaches, however, were limited to problems that can be solved by exhaustively enumerating all possible outcomes.

Many different probabilistic programming systems were proposed as practical tools for Bayesian modelling and inference and it is not possible to list them all here. Perhaps the first widely influential one was BUGS (Gilks et al. 1994), which performs Gibbs sampling on finite graphical models. Restricting models to those that can be represented by finite graphs allows for implementation of efficient inference algorithms and was successfully leveraged by systems such as Infer.NET (Minka et al. 2009) and Stan (Stan Development Team 2014). Those tools are fast and practical, but they do not target as wide a range of models as our approach.

A lot of work has been put into combining graphical models with first-order logic (Getoor and Taskar 2007), which extends the set of representable models. Some of the languages in this category include BLOG (Milch et al. 2005), Markov Logic Networks (Domingos and Richardson 2004), ProbLog (Kimmig et al. 2011), and IBAL (Pfeffer 2001). Those languages are more expressive than graphical models, but they still can not express models such as the Dirichlet Process. An approach similar to ours was taken by Kiselyov and Shan (2009) in HANSEI, which embeds a probabilistic programming language in OCaml. However, even though it can compose distributions in arbitrary ways, it is still limited to discrete distributions.

The idea of a universal probabilistic programming language, which can handle both discrete and continuous distributions and compose them in arbitrary ways, was pioneered by Goodman et al. (2008) in Church. Even though very expressive, Church struggles with making inference efficient. Several Church-inspired languages were invented in an attempt to make inference faster, such as Venture (Mansinghka et al. 2014), Anglican (Wood et al. 2014), and Probabilistic C (Paige and Wood 2014). Anglican was first to implement, in the context of probabilistic programming, the SMCbased inference methods used in this paper. Our work differs from Anglican by embedding a probabilistic programming language in Haskell and implementing inference as a deterministic data structure transformation.

Fun (Gordon et al. 2013; Bhat et al. 2013) is an embedding of probabilistic programming in F#. Probabilistic models are quoted F# expressions, instead of being of monadic type. Inference is achieved by parsing the quoted expressions and translating to engines such as Infer.NET.

Pfeffer (2009) describes a probabilistic object-oriented programming language called Figaro, which builds probabilistic programs as data structures in Scala. It targets Metropolis-Hastings with custom proposals, rather than SMC, as the primary inference methods. Another probabilistic programming language embedded in Scala is WOLFE (Riedel et al. 2014). WOLFE goes beyond stating models via generative processes (as in our work), and allows the programmer to compose a model in terms of scalar objectives or scoring functions, and operations such as maximization and summation. WOLFE can express conditional random fields, Markov logic networks, and matrix factorization, but has not been applied to sequential Monte Carlo methods.

8. Conclusion and Future Work

The main focus of this work was on making probabilistic programming with monads practical by implementing powerful approximate inference algorithms. We accomplished this goal by defining a GADT Dist representing probability distributions and implementing Sequential Monte Carlo and Particle Markov Chain Monte Carlo algorithms to perform inference on it. We showed that our implementation is competitive with Anglican, the original implementation of those algorithms in a non-monadic probabilistic programming setting. All of our code is freely available as a Haskell library ².

Apart from using monads, a distinctive feature of our framework is that randomised inference algorithms can be implemented as deterministic transformations on a data structure representing a distribution. This approach makes the implementation clean and

² The source code will be released upon publication

convenient and sometimes makes it possible to compose inference algorithms by simply composing the functions implementing them. In particular we obtained Particle Independent Metropolis Hastings by composing Sequential Monte Carlo with Metropolis Hastings. In order to have a notion of correctness of inference algorithms defined this way we defined formal semantics for Dist using measure theory.

We identify three directions for future work. The most straightforward one is to parallelise the implementation. Because we implement inference as a function from Dist to Dist, we could at the same time parallelise inference and sampling from a model. The main obstacle is that currently we are only using monads to build Dists and monads are inherently sequential. From the probabilistic point of view, two random variables can be sampled in parallel if they are independent conditionally on what was sampled earlier. We may enable parallel sampling if we introduce additional Dist constructors that make conditional independence explicit, such as Independent :: Dist a -> Dist b -> Dist (a,b).

Another direction is extending the formal semantics defined in section 6. It would be desirable to extend the definitions to cover recursive types and function types, as well as expressions that may not terminate. In the long run, having Dists with formally defined semantics and inference algorithms that manipulate Dist s deterministically, we might hope to formally prove correctness of inference algorithm.

Finally, we plan to investigate the idea of composing inference algorithms in probabilistic programming. The crucial requirement for making such composition really useful is finding more generalpurpose inference algorithms that can be composed.

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