Semantics for probabilistic programming: higher-order functions, continuous distributions, and soft constraints

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Abstract

We study the semantic foundation of expressive probabilistic programming languages, that support higher-order functions, continuous distributions, and soft constraints (such as Anglican, Church, and Venture). We define a metalanguage (an idealised version of Anglican) for probabilistic computation with the above features, develop both operational and denotational semantics, and prove soundness, adequacy, and termination. They involve measure theory, stochastic labelled transition systems, and functor categories, but admit intuitive computational readings, one of which views sampled random variables as dynamically allocated read-only variables. We apply our semantics to validate nontrivial equations underlying the correctness of certain compiler optimisations and inference algorithms such as sequential Monte Carlo simulation. The language enables defining probability distributions on higher-order functions, and we study their properties.

1. Introduction

Probabilistic programming is the idea to use programs to specify probabilistic models; probabilistic programming languages blend programming constructs with probabilistic primitives. This helps scientists express complicated models succinctly. Moreover, such languages come with generic inference algorithms, relieving the programmers of the nontrivial task of (algorithmically) answering queries about their probabilistic models. This is useful in e.g. machine learning.

Several higher-order probabilistic programming languages have recently attracted a substantial user base. Some languages (such as Infer.net [21], PyMC [26], and Stan [33]) are less expressive but provide powerful inference algorithms, while others (such as Anglican [34], Church [12], and Venture [20]) have less efficient inference algorithms but more expressive power. We consider the more expressive languages, that support higher-order functions, continuous distributions, and soft constraints. More precisely, we consider a programming language (§3) with higher-order functions (§6) as well as the following probabilistic primitives.

Sampling The command sample(t) draws a sample from a distribution described by t, which may range over the real numbers.

Soft constraints The command score(t) puts a score t (a positive real number) on the current execution trace. This is typically used to record that some particular datum was observed as being drawn from a particular distribution; the score describes how surprising the observation is.

Normalization The command norm(u) runs a simulation algorithm over the program fragment u. This takes the scores into account and returns a new, normalized probability distribution. The argument to sample might be a primitive distribution, or a distribution defined by normalizing another program. This is called a nested query, by analogy with database programming.

Here is a simple example of a program. We write gauss(μ, σ) for the Gaussian probability distribution whose density function is density_gauss(a, (μ, σ)) = \frac{1}{\sqrt{2\pi} \sigma} \exp\left(-\frac{(a-\mu)^2}{2\sigma^2}\right).

1  norm()
2  let x = sample(gauss(0.0, 3.0)) in
3  score(density_gauss(5.0, (x, 1.0)));
4  return(x < 4.5))

Line 2 samples x from a prior Gaussian distribution. The soft constraint on Line 3 expresses the likelihood of the observed data, 5.0, coming from a Gaussian given the prior x. Line 4 says that what we are actually interested in is a boolean random variable over the sample space. Line 1 calculates a posterior distribution for the return value, using the prior and the likelihood. In this example we can precisely calculate that the posterior distribution on \{true, false\} has \(p(\text{true}) = 0.5\).

Languages like this currently lack formal exact semantics. The aim of this paper is to provide just such a foundation as a basis for formal reasoning. Most expressive probabilistic programming languages are explained in terms of their Monte Carlo simulation algorithms. The simplest such algorithm, using importance and rejection sampling, is the de facto semantics against which other algorithms are ‘proved approximately correct’. Such ‘semantics’ are hard to handle and extend.

We provide two styles of semantics, operational and denotational. For first-order probabilistic programs, the denotational semantics is straightforward: types are interpreted as measurable spaces, and terms are interpreted as measurable functions (§4). Operational semantics is more complicated. For discrete distributions, an operational semantics might be a probabilistic transition system, but for continuous distributions, it must be a stochastic relation (labelled Markov process). We resolve this by equipping the set of configurations with the structure of a measurable space (§5).

The advantage to the operational semantics is that it is easily extended to higher-order programs (§7). Denotational semantics for higher-order programs poses a problem, because measurable spaces do not support the usual \(\beta/\eta\) theory of functions; they do not form a Cartesian closed category (indeed, \(\mathbb{R}^k\) does not exist as a measurable space [3]). Earlier semantics deal with this by either excluding higher-order functions or considering only discrete distributions. We resolve this by moving from the category of measurable spaces, where standard probability theory takes place, to a functor category based on it (§8). The former embeds in the latter, so we can still interpret first-order concepts. But the functor category does have well-behaved function spaces, so we can also interpret higher-order concepts. Moreover, by lifting the monad of probability distribu-
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...
In particular, all the usual distributions are in the language, including the Dirac distribution \(\text{dirac}(x)\) concentrated on outcome \(x\), the Gaussian distribution \(\text{gauss}(\mu, \sigma)\) with mean \(\mu\) and standard deviation \(\sigma\), the Bernoulli distribution \(\text{bern}(p)\) with success probability \(p\), the exponential distribution \(\text{exp}(r)\) with rate \(r\), and the Beta distribution \(\text{beta}(\alpha, \beta)\) with parameters \(\alpha, \beta\). For example, from the measurable functions \(\text{42.0} : 1 \to \mathbb{R}, e^{-\cdot} : \mathbb{R} \to \mathbb{R}, \text{gauss} : \mathbb{R} \times \mathbb{R} \to P(\mathbb{R})\) and \(\epsilon : \mathbb{R} \times \mathbb{R} \to 1 + 1\) we can derive:

\[
\Gamma \vdash \text{42.0} : \mathbb{R} \\
\Gamma \vdash e^{-\cdot} : \mathbb{R} \\
\Gamma \vdash \text{gauss}(\mu, \sigma) : P(\mathbb{R}) \\
\Gamma \vdash \epsilon : \mathbb{R} \times \mathbb{R} \to 1 + 1
\]

The following terms form the core of our language.

\[
\Gamma \vdash t : \text{P}(A) \\
\Gamma \vdash \text{sample}(t) : A \\
\Gamma \vdash \text{score}(t) : 1
\]

The first term samples a value from a distribution \(t\). The second multiplies the score of the current trace with \(t\). Since both of these terms express effects, they are typed under \(\Gamma\) instead of \(\text{P}\).

The reader may think of the score of the current execution trace as a state, but it cannot be read, nor changed arbitrarily: it can only be multiplied by another score. The argument \(t\) in \(\text{score}(t)\) is usually the density of a probability distribution at an observed data point. For instance, recall the example (1) from the Introduction:

\[
\text{norm}(\text{let } x = \text{sample}(\text{gauss}(0.0, 3.0)) \text{ in } \text{score}(\text{density}_\text{gauss}(5.0, (x, 1.0))); \text{return}(x < 4.5))
\]

An execution trace is scored higher when \(x\) is closer to the datum 5. When the argument \(t\) in \(\text{score}(t)\) is 0, this is called a hard constraint, meaning ‘reject this trace’: otherwise it is called a soft constraint. In the discrete setting, hard constraints are more-or-less sufficient, but even then, soft constraints tend to be more efficient.

**Normalization**

Two representative tasks of Bayesian inference are to calculate the so-called posterior distribution and model evidence from a prior distribution and likelihood. Programs built from sample and score can be thought of as setting up a prior and a likelihood. Consider the following program:

\[
\text{let } x = \text{sample}(\text{bern}(0.25)) \text{ in } y = (\text{if } x \text{ then return } 5.0 \text{ else return } 2.0) \text{ in } \text{score}(\text{density}_\text{exp}(0.0, y)); \text{return}(x)
\]

Here the prior \(y\) comes from the Bernoulli distribution, and the likelihood concerns datum 0.0 coming from an exponential distribution with rate \(y\). Recall that \(\text{density}_\text{exp}(0.0, y) = y\). So there are two execution traces, returning either true, with probability 0.25 and score 5.0, or false, with probability 0.75 and score 2.0.

The product of the prior and likelihood gives an unnormalized posterior distribution on the return value: \((\text{true} \mapsto 0.25 \cdot 5.125, \text{false} \mapsto 0.75 \cdot 2 = 1.5)\). The normalizing constant is the average score: \((0.25 \cdot 5.125 + 0.75 \cdot 2) = 2.75\), so the posterior is \((\text{true} \mapsto \frac{5.125}{2.75} \approx 0.45, \text{false} \mapsto \frac{2}{2.75} \approx 0.75)\). The average score is called the model evidence. It is a measure of how well the model encoded by the program matches the observation.

Note that the sample \(x = \text{true}\) matches the datum better, so the probability of true goes up from 0.25 to 0.45 in the posterior.

In our language we have a term \(\text{norm}(t)\) that will usually convert a probabilistic term \(t\) into a deterministic value, which is its posterior distribution together with the model evidence.

\[
\Gamma \vdash t : A \\
\Gamma \vdash \text{norm}(t) : (\mathbb{R} \times \text{P}(A)) + 1 + 1
\]

If the model evidence is 0 or \(\infty\), the conversion fails, and this is tracked by the ‘+1+1’.

### 4. Denotational semantics

This section discusses the natural denotational semantics of the first-order language. The basic idea can be traced back a long way (e.g. [17]) but our treatment of score and norm appear to be novel. As described, types \(\mathcal{A}\) are interpreted as measurable spaces \([\mathcal{A}]\). A context \(\Gamma = (x_1 : \mathcal{A}_1, \ldots, x_n : \mathcal{A}_n)\) is interpreted as the measurable space \([\Gamma] = \prod_{i=1}^n [\mathcal{A}_i]\) of its valuations.

- **Deterministic terms** \(\Gamma \vdash t : A\) are interpreted as measurable functions \([t] : [\Gamma] \to [A]\), providing a result for each valuation of the context.
- **Probabilistic terms** \(\Gamma \vdash t : A\) are interpreted as measurable functions \([t] : [\Gamma] \to P([\mathbb{R}_{\geq 0} \times [A]])\), providing a probability measure on \((\text{score}, \text{result})\) pairs for each valuation of the context.

In Informally, if \((\Omega, p : \Omega \to [0, 1])\) is the prior sample space of the program (specified by sample), and \(t : \Omega \to [A]\) is the likelihood (specified by score), and \(r : \Omega \to [A]\) is the return value, then a measure in \(P([\mathbb{R}_{\geq 0} \times [A]])\) is found by pushing forward \(p\) against \(r\).

**Sums and products**

The interpretation of deterministic terms follows the usual pattern of the internal language of a distributive category (e.g. [27]). For instance, \([\Gamma, x : \mathcal{A}, \text{let } y = x \text{ in } \mathcal{A}(\gamma, \alpha, \gamma, \gamma) \cong a\), and \([\Gamma \vdash f(t) : \mathcal{A}(\gamma, \alpha, \gamma, \gamma) \cong f([t](\gamma))\) for measurable \(f : [\mathcal{A}] \to [\mathcal{B}]\). This interpretation is actually the same as the usual set-theoretic semantics of the calculus, as one can show by induction that the induced functions \([\Gamma] \to [A]\) are measurable.

**Sequencing**

For probabilistic terms, we proceed as follows.

\[
[\text{return}(t)]([\gamma](U)) \cong ([1, [t](\gamma))] \in U,
\]

which denotes a Dirac distribution, and \([\text{let } x = t \text{ in } u](\gamma)(V)\) is

\[
\int_{\mathbb{R}_{\geq 0} \times [A]} \left[\left[\left[[u](\gamma, x) \{\{s, b\} \to (r \cdot s, b) \in V\}\right]\right](\gamma)(d(r, x))\right].
\]

As we will explain shortly, these interpretations come from treating \(P([\mathbb{R}_{\geq 0} \times (-)]\) as a commutative monad, which essentially means the following program equations hold.

\[
\begin{align*}
\text{let } x &= \text{return}(x) \text{ in } u = [u] & \text{let } x &= \text{return}(x) \text{ in } [t] \\
\text{let } y &= \text{let } x = t \text{ in } u \text{ in } v = \text{let } x = t \text{ in } \text{let } y = u \text{ in } v & \text{let } x &= \text{let } x = t \text{ in } y \text{ in } (x, y) \text{ in } \text{let } x &= \text{let } x = t \text{ in } y = u \text{ in } (x, y)
\end{align*}
\]

The last two equestions assume the standard conditions on free variables of \(u, v\) and \(t\). The last equation justifies a useful program optimisation technique [34, §5.5].

**Language-specific constructs**

We use the monad:

\[
\begin{align*}
\text{score}(7.0); \text{score}(6.1) &= \text{score}(42.7) \\
\text{let } x &= \text{sample}(\text{gauss}(0.0, 1.0)) \text{ in } \text{score}(x > 0) \text{ in } \text{returnsample}(\text{bern}(0.5)) \\
\text{let } x &= \text{sample}(\text{gauss}(0.0, 1.0)) \text{ in } \text{returnsample}(\text{bern}(0.5)) \\
\end{align*}
\]

**Normalization**

We interpret \(\text{norm}(t)\) as follows. Each probability measure \(p\) on \([0, \infty)\) induces an unnormalized posterior measure \(\tilde{p}\) on \(X\): \(\tilde{p}(U) = \int_{0 \times U} d(p(d(r, x)))\). As long as the average score \(\tilde{p}(X)\) is not 0 or \(\infty\), we can normalize \(\tilde{p}\) to build
a posteriori probability measure on \( X \). This construction forms a natural transformation \( \tau_X : P(\mathbb{R}_{\geq 0} \times X) \to (\mathbb{R} \times P(X)) + 1 + 1 \)

\[
\tau_X(p) = \begin{cases} 
(1, \ast) & \text{if } \hat{p}(X) = 0 \\
(2, \ast) & \text{if } \hat{p}(X) = \infty \\
0, (\hat{p}(X), \lambda u. \; \frac{\exp(u)}{1+\exp(u)}) & \text{otherwise}
\end{cases}
\] (3)

Let \( \|\text{norm}(t)\|_\gamma \overset{\text{df}}{=} \|\text{I}(t)\|_\gamma \). Here are some examples:

\[
\begin{align*}
\text{norm(let } x = \text{ sample(gauss(0.0, 3.0))) in } & \text{\quad score(density_gauss(5.0, (x, 1.0)); return } x < 4.5) \text{\) = } (0, (xxx, bern(0.5))) \\
\text{norm(let } x = \text{ sample(bern(0.25)) in } & \text{\quad (if } x \text{ then score(5.0) else score(2.0)); return } x \text{\) = } (0, (2.75, bern(\frac{1}{10}))) \\
\text{norm(let } x = \text{ sample(exp(1.0)) in score(e^x))\} = (2, \ast) \\
\text{\quad in score(x); return } x \text{\) = [\text{norm(score(\frac{1}{2})); \\
\text{\quad sample(beta(2, 3)))}}\]
\end{align*}
\]

The fourth equation shows how infinite model evidence errors can arise when working with infinite distributions. In the last equation, the parameter \( x \) of \( \text{score} \) represents the probability of true under \( \text{bern}(x) \). The equation expresses the so-called conjugate-prior relationship between Beta and Bernoulli distributions, which has been used to optimise probabilistic programs [35].

### 5. Operational semantics

In this section we develop an operational semantics for the first-order language. There are several reasons to consider this, even though the denotational semantics is arguably straightforward. First, extension to higher-order functions is easier in operational semantics than in denotational semantics. Second, operational semantics conveys computational intuitions that are obscured in the denotational semantics. We expect these computational intuitions to play an important role in studying approximate techniques for performing posterior inference, such as sequential Monte Carlo, in the future.

Sampling from probability distributions complicates operational semantics. Sampling from a discrete distribution can immediately affect control flow. For example, in the term

\[
\text{let } x = \text{ sample(bern(0.5)) in if } x \text{ then return}(1.1) \text{ else return}(8.0)
\]

the resampled value in the continuation \( v \). Line 3 propagates the error of \( 0: w \) is a deterministic term of the right type whose choice does not matter. Finally, line 4 detects an infinite evidence error, and undoes the transformation. This error does not arise in most applications of sequential Monte Carlo simulation.

### 4.1 Sequential Monte Carlo simulation

The program equations above justify some simple program transformations. For a more sophisticated one, consider *sequential Monte Carlo simulation* [7]. A key idea of its application to probabilistic programs is: ‘Whenever there is a score, it is good to renormalize and resample’. This increases efficiency by avoiding too many program executions with low scores [24, Algorithm 1].

The denotational semantics justifies the soundness of this transformation. For a term with top-level score, i.e. a term of the form (let \( x = t \in \text{score}(u); v) \) where \( u \) and \( v \) may have free \( x \):

\[
\text{norm(let } x = t \in \text{score}(u); v))\]

\[
\begin{align*}
\text{norm(case(} \text{norm(let } x = t \in \text{score}(u); \text{return}(x)) \text{) of } 1 & \quad \text{\( 0, (e, d) \) \quad \text{\( \Rightarrow \) \( \text{score}(e); \text{let } x = \text{ sample}(d) \text{ in } v)\)}}
| \quad 2 & \quad \text{\( \Rightarrow \) \( \text{score}(0); \text{return}(w)\)}
| \quad 3 & \quad \text{\( \Rightarrow \) \( \text{let } x = t \in \text{score}(u); v)\)}
\end{align*}
\]

Let us explain the right hand side. Line 1 renormalizes the program after the score, and in non-exceptional return the model evidence \( e \) and a new normalized distribution \( d \). Line 2 immediately records the evidence \( e \) as a score, and then resamples \( d \) using the resampled value in the continuation \( v \). Line 3 propagates the error of \( 0: w \) is a deterministic term of the right type whose choice does not matter. Finally, line 4 detects an infinite evidence error, and undoes the transformation. This error does not arise in most applications of sequential Monte Carlo simulation.
Values $v$ in a canonical context $\Gamma$ are well-typed deterministic terms of the form

$$v, w ::= x_i \ | \ \ast \ | \ (v, w) \ | \ (i, v) \tag{5}$$

where $x_i$ is a variable in $\Gamma$. Similarly, a probabilistic term $t$ in context $\Gamma$ is called probabilistic value or $p$-value if $t \equiv \text{return}(v_0)$ for some value $v_0$. Remember from Section 4 that the denotational semantics of values is simple and straightforward.

Write $\text{Con}_d(\lambda)$ and $\text{Con}_p(\lambda)$ for the sets of deterministic and probabilistic configurations of type $\lambda$, and make them into measurable spaces by declaring $U \subseteq \text{Con}_d(\lambda)$ to be measurable if the set $\{\gamma \in \Gamma \mid \langle t, \gamma \rangle \in U\}$ is measurable for all judgements $\Gamma \vdash t : \lambda$.

$$\text{Con}_d(\lambda) = \sum_{(t, i) \in \text{ΓCanonical}} [\Gamma] \tag{6}$$

Further partition $\text{Con}_d(\lambda)$ into $\text{Con}_V(\lambda)$ and $\text{Con}_N(\lambda)$ based on whether a term in a configuration is a value or not:

- $\text{Con}_V(\lambda) = \{\Gamma, t, \gamma \in \text{Con}_d(\lambda) \mid t$ is a value$\}$
- $\text{Con}_N(\lambda) = \{\Gamma, t, \gamma \in \text{Con}_d(\lambda) \mid t$ is not a value$\}$
- $\text{Con}_N(\lambda) = \{\Gamma, t, \gamma \in \text{Con}_d(\lambda) \mid t$ is a p-value$\}$
- $\text{Con}_N(\lambda) = \{\Gamma, t, \gamma \in \text{Con}_d(\lambda) \mid t$ is not a p-value$\}$

Particularly well-behaved values are the ordered values $\Gamma \vdash v : \lambda$, where each variable appears exactly once, and in the same order as in $\Gamma$.

**Lemma 5.1.** Consider a canonical context $\Gamma$, a type $\lambda$, an ordered value $\Gamma \vdash v : \lambda$, and the induced measurable function $\nu_v : \text{Con}_p(\lambda) \to (\mathbb{R}_{\geq 0} \times P([\lambda])) + 1 + 1 \tag{8}$

indexed by types $\lambda$.

**Reduction of deterministic terms** Define a type-indexed family of relations $\to \subseteq \text{Con}_d(\lambda) \times \text{Con}_d(\lambda)$ as the least one that is closed under the following rules.

$$\langle \Gamma, \pi_j(v_0, v_1), \gamma \rangle \to \langle \Gamma, v_j, \gamma \rangle \tag{9}$$

$$\langle \Gamma, \text{case} (i', v) \mid \{ (i, x) : t_i \}, \gamma \rangle \to \langle \Gamma, t_v[v/x], \gamma \rangle \tag{10}$$

$$\langle \Gamma, f(w), \gamma \rangle \to \langle (\Gamma', \gamma), v, (\gamma', \gamma') \rangle \tag{11}$$

$$\langle w \text{ a value $\Gamma' \vdash v : \lambda$ an ordered value $\wedge f([w]([\gamma])) = [v]([\gamma'])\rangle \tag{12}$$

$$\langle \Gamma, \text{norm}(t), \gamma \rangle \to \langle \Gamma, xx: \mathbb{R}, y: \mathbb{P}(\mathbb{B}), (0, (x, y)), \gamma[x \to r, y \to p] \rangle \tag{13}$$

$$\langle A = \mathbb{P}(\mathbb{B}) \wedge \nu_b(\Gamma, t, \gamma) = (0, (r, p)) \wedge x, y \notin \text{dom}(\Gamma) \rangle \tag{14}$$

$$\langle \Gamma, \text{norm}(t), \gamma \rangle \to \langle \Gamma, (i, \ast), \gamma \rangle \tag{15}$$

$$\langle A = \mathbb{P}(\mathbb{B}) \wedge \nu_b(\Gamma, t, \gamma) = (i, \ast), i \in \{1, 2\} \rangle \tag{16}$$

$$\langle \Gamma, t, \gamma \rangle \to \langle \Gamma', t', \gamma' \rangle \tag{17}$$

$$\langle \Gamma, C[t], \gamma \rangle \to \langle \Gamma', C'[t'], \gamma' \rangle \tag{18}$$

where $\langle [\cdot] \rangle$ is not $(\cdot)$.

The rule for $f(w)$ keeps the original context $\Gamma$ and the closure $\gamma$ because they might be used in the continuation, even though they are not used in $v$. The rules obey the following invariant.

**Lemma 5.2.** If $\langle \Gamma, t, \gamma \rangle \to \langle \Gamma', t', \gamma' \rangle$, then $\Gamma' = \langle \Gamma, \Gamma' \rangle$ and $\gamma' = \langle \gamma, \gamma' \rangle$ for some $\Gamma''$ and $\gamma'' \in \Gamma''$.

**Proof.** By induction on the structure of derivations. □

This lemma allows us to confirm that our specification of a relation $\to \subseteq \text{Con}_d(\lambda) \times \text{Con}_d(\lambda)$ is well-formed (‘type preservation’).

**Proposition 5.3.** The induced relation is a measurable function.

**Proof.** There are three things to show: that the relation is entire (‘progress’); that the relation is single-valued (‘determinism’); and that the induced function is measurable. All three are shown by induction on the structure of the terms. The case of application of measurable functions crucially uses Lemma 5.1. □

**Reduction of probabilistic terms** Next, we define the stochastic relation $\to$ for probabilistic terms, combining two standard approaches: for indecomposable types, which are uncountable, use labelled Markov configurations, i.e., give a distribution on the measurable set of resulting configurations; for decomposable types (sums, products etc.), probabilistic branching is discrete and so a transition system labelled by probabilities suffices.

**Proposition 5.4.** Let $(X_i)_{i \in I}$ be an indexed family of measurable spaces. Suppose we are given:

- a function $q : I \to [0, 1]$ that is only nonzero on a countable subset $I_0 \subseteq I$, and such that $\sum_{i \in I} q(i) = 1$;
- a probability measure $q_i$ on $X_i$ for each $i \in I_0$.

This determines a probability measure $p$ on $\sum_{i \in I} X_i$ by

$$p(U) = \sum_{i \in I} q(i) q_i((a \mid (i, a) \in U))$$

for $U$ a measurable subset of $\sum_{i \in I} X_i$.

We will use three entities to define the desired stochastic relation $\to : \text{Con}_p(\lambda) \times \sum_{i \in I} \text{Con}(\lambda) \to [0, 1].$
Pr(⟨Γ, E[⟨t⟩], γ⟩) = Pr(Γ, t, γ) → (Γ′, E[⟨t′⟩])

Pr(⟨Γ, D[⟨t⟩], γ⟩) = Pr(⟨Γ, t, γ⟩) → (Γ′, D[⟨t′⟩])

Pr(Γ, let x = return(v) in t, γ) → (Γ, t[v/x])

Pr(⟨Γ, case j, v⟩ of {⟨i, x, t⟩ ∈ Γ, t} → (Γ, t[j/x])

Pr(⟨Γ, score(v), γ⟩) → (Γ, return(v))

Pr(⟨Γ, sample(v), γ⟩) → (Γ, Γ′, return(v′))

Sc(⟨Γ, E[⟨t⟩], γ⟩) = 1

Sc(⟨Γ, D[⟨t⟩], γ⟩) = 1

Sc((Γ, let x = return(v) in t, γ)) = 1

Sc(⟨Γ, case j, v⟩ of {⟨i, x, t⟩ ∈ Γ, t} → (Γ, t[j/x])

5.2 Termination

To see that the redcution process terminates, we first define the transitive closure. This is subtle, as sampling can introduce countably infinite branching; although each branch will terminate, the expected number of steps to termination can be infinite.

We use the deterministic transition relation to define an evaluation relation ʃ ⊆ Con(A) × ConVa(A), by setting ʃ ʃ ⊆ D if ʃ ʃ D, where

\[ C ʃ ʃ ʃ \]

To define evaluation for probabilistic configurations, we need sub-stochastic relations: functions \( f: X \times \Sigma^* \to [0, 1] \) that are measurable in \( X \), satisfy \( f(x, Y) \leq 1 \) for every \( x \in X \), and are countably additive in \( Y \), i.e. \( f(x, \bigcup_{E \in \Sigma} U) = \sum_{E \in \Sigma} f(x, U) \) for a sequence \( U_1, U_2, \ldots \) of disjoint measurable sets. Thus a stochastic relation (as in Definition 2.3) is a sub-stochastic relation with \( f(x, Y) = 1 \). Define a sub-stochastic relation

\[ Pr(ʃ−−→) : Con(A) \times \Sigma_{k≥2} \times ConVa(A) \to [0, 1] \]

by \( Pr(ʃ−−→ C) = \sum_{\gamma \in \Gamma} Pr(ʃ−−→ C) \), where \( Pr(ʃ−−→ C) \) is given by \( [(1, C) \in U] \), and \( Pr(ʃ−−→ C) \) is

\[ \int_{r(\cdot D)} Pr(D ʃ−−→ (s, E) \mid \cdot )\) Pr( C −−→ d(r, D)).

Proposition 5.5 (Termination). Evaluation of deterministic terms is a function: \( ∀C, \exists D. C ʃ−−→ D \). Evaluation of probabilistic terms is a stochastic relation: \( ∀C, Pr(C ʃ−−→ (R_{k≥0} \times ConVa(A))) = 1 \).


5.3 Soundness

Termination comes from the omission of recursion in our language. We do so now, because our semantic model does not yet handle higher-order recursion, and probabilistic while-languages are already well-understood (e.g. [17]). (See also the discussion about domain theory in §8.)
Lemma 5.8 (Context extension). Let $z \in \{d, p\}$. Suppose that $(\Gamma, t, \gamma)$ and $(\Gamma', t, (\gamma, \gamma'))$ are configurations in $\text{Con}_f(A)$. Then $s_z((\Gamma, t, \gamma)) = s_z((\Gamma', t, (\gamma, \gamma')))$.  

Proposition 5.9 (Soundness). The following diagrams commute (in the category of measurable functions, and stochastic relations, respectively).

\[
\begin{array}{c}
\text{Con}_n(A) \xrightarrow{\text{one-step reduction}} [A] \\
\text{Con}_p(A) \xrightarrow{\text{one-step reduction}} \mathbb{R}_{\geq 0} \times [A]
\end{array}
\]

\[
\begin{array}{c}
\text{Con}_n(A) \xrightarrow{\text{multiplication}} \mathbb{R}_{\geq 0} \times \text{Con}_p(A) \\
\text{Con}_p(A) \xrightarrow{\text{one-step reduction}} \mathbb{R}_{\geq 0} \times \mathbb{R}_{\geq 0} \times [A]
\end{array}
\]

Proof. By induction on the structure of syntax. The inductive steps with evaluation contexts use the extension Lemma 5.8, which applies by the invariant Lemma 5.2. \qed

Adequacy The denotational semantics is adequate, in the sense:

\[
[t](\ast) = P(R_{\geq 0} \times s_{vp})(Pr(\langle \emptyset, t, \ast \rangle \Downarrow (-)))
\]

for all $\ast : A$. That is, the denotation $[t](\ast)$ is nothing but pushing forward the probability measure $Pr(\langle \emptyset, t, \ast \rangle \Downarrow (-))$ from the operational semantics along the function $s_{vp}$. This adequacy condition holds because Proposition 5.9 ensures that

\[
\sum_{k \leq n} Pr(\langle \emptyset, t, \ast \rangle \Downarrow k \{ \langle r, C \rangle | \langle r, s_{vp}(C) \rangle \in U \}) \leq \sum_{k \leq n} [t](\ast)(U)
\]

for all $n$ and $U$, and Proposition 5.6 then guarantees that the left-hand side of this inequality converges to the right-hand side as $n$ tends to infinity.

6. A higher-order language

This short section extends the first-order language with functions and thunks [18], allowing variables to stand for program fragments. In other words, 'programmes are first-class citizens'.

Types Extend the grammar for types with two new constructors.

\[
\begin{align*}
A, B &::= R | P(A) | 1 | A \times B | \sum_{i \in I} A_i | A \Rightarrow B | T(A)
\end{align*}
\]

Informally, $A \Rightarrow B$ contains deterministic functions, and $T(A)$ contains thunks (i.e., suspended) probabilistic programs. Then $A \Rightarrow T(B)$ contains probabilistic functions. A type is measurable if it does not involve $\Rightarrow$ or $T$, i.e., if it is in the grammar of Section 3.

Terms Extend the term language with the following rules. First, the usual abstraction and application of deterministic functions:

\[
\begin{align*}
\Gamma, x : A \vdash t : B &\quad \Gamma \vdash \lambda x. t : A \Rightarrow B &\quad \Gamma \vdash t u : A
\end{align*}
\]

Second, we have syntax for thunking and forcing (e.g. [18, 22, 25]).

\[
\begin{align*}
\Gamma \vdash t : A &\quad \Gamma \vdash \text{thunk}(t) : T(A) &\quad \Gamma \vdash \text{force}(t) : A
\end{align*}
\]

All the rules from Section 3 are also still in force. For rule (2) to still make sense, we only include constant terms for measurable functions $f : [A] \rightarrow [B]$ between measurable types $A$ and $B$.

Examples One reason for higher types is to support code restructuring. The separate function types and thunk types allow us to be flexible about calling conventions. For example, sampling can be reified as the ground term

\[
\lambda x. \text{thunk(sample}(x)) : P(A) \Rightarrow T(A),
\]

which takes a probability measure and returns a suspended program that will sample from it. On the other hand, to reify the normalization construction, we use a different calling convention.

\[
\lambda x. \text{norm(force}(x)) : T(A) \Rightarrow \mathbb{R} \times P(A) + 1 + 1
\]

This function takes a suspended program and returns the result of normalizing it.

Example: higher-order expectation Higher types also allow us to consider probability distributions over programs. For an example, consider this term.

\[
E_h \equiv \lambda d, f : T(A) \times (A \Rightarrow R). \\
\text{case } (\text{norm(let } a = \text{force}(d) \text{ in score(f(a)))) of }
\]

\[
\begin{align*}
(0, (e, y)) &\Rightarrow e &\quad | (1, *) &\Rightarrow 0.0 &\quad | (2, *) &\Rightarrow 0.0
\end{align*}
\]

It has type $T(A) \times (A \Rightarrow R) \Rightarrow R$. Intuitively, given a thunked probabilistic term $t$ and a function $f$ that is nonnegative, $E_h$ forces $t$ as a probability distribution on $A$, and computes the expectation of $f$ on this distribution. Notice that $\lambda$ can be a higher type, so $E_h$ generalises the usual notion of expectation, which has not been defined for higher types because the category of measurable spaces is not Cartesian closed.

7. Higher-order operational semantics

In this section we consider operational semantics for the higher-order extension of the language. In an operational intuition, $\text{force}(t)$ forces a suspended computation $t$ to run. For example,

\[
\lambda \text{thunk(sample(gauss(0.0, 1.0))} : T(\mathbb{R})
\]

is a suspended computation that, when forced, will sample the normal distribution.

Assumption 7.1. From the operational perspective it is unclear how to deal with sampling from a distribution over functions. For this reason, in this section, we only allow the type $P(\lambda A)$ when $A$ is a measurable type. We still allow probabilistic terms to have higher-order types, and we still allow $T(A)$ wherever $A$ is higher-order.

7.1 Reduction

We now extend the operational semantics from Section 5 with higher types. Values (5) are extended as follows.

\[
v ::= \ldots | \lambda x. t | \text{thunk}(t)
\]

Evaluation contexts (7) are extended as follows.

\[
\text{C}[-] ::= \ldots | C[-] t | v \text{C}[-] | E[-] ::= \ldots | D[\text{force}][-]
\]

There are two additional redexes: $(\lambda x. t) v$ and $\text{force}(\text{thunk}(t))$. The deterministic transition relation is extended with this $\beta$-rule:

\[
(\Gamma, (\lambda x. t) v, \gamma) \rightarrow (\Gamma, t[v/x], \gamma)
\]

Extend the probabilistic transition relation with the following rules.

\[
\begin{align*}
\text{Pr}(\langle \Gamma, \text{force}(\text{thunk}(t)), \gamma \rangle) &\rightarrow (\Gamma, t) = 1 \\
\text{Pr}(\langle \Gamma, \text{force}(\text{thunk}(t)), \gamma \rangle) &\rightarrow (\Gamma, t, V) = [\gamma \in U] \\
\text{Sc}(\langle \Gamma, \text{force}(\text{thunk}(t)), \gamma \rangle) &\rightarrow 1
\end{align*}
\]

7.2 Termination

The evaluation relations for deterministic and probabilistic configurations of the higher-order language are defined as in Subsection 5.2. The resulting rewriting system still terminates, even though configurations may now include higher-order terms.

Proposition 7.2 (Termination). Evaluation of deterministic terms is a function: $\forall C, D. C \Downarrow D$. Evaluation of probabilistic terms is a stochastic relation: $\forall C. \text{Pr}(C \Downarrow (R_{\geq 0} \times \text{Con}_p(A))) = 1$. 

7
8. Higher-order denotational semantics

This section gives denotational semantics for the higher-order language, without using Assumption 7.1. We are to interpret the new constructs $T(A)$, thunk, and force. We will interpret probabilistic judgements as Kleisli morphisms $[\Gamma] \rightarrow T([\Lambda])$ for a certain monad $T$, and set $[T(A)] = T([A])$, so thunk and force embody the correspondence of maps $[\Gamma] \rightarrow T([\Lambda])$ and $[\Gamma] \rightarrow T([A])$.

On which category can the monad $T$ live? Interpreting $\lambda$-abstraction and application needs a natural ‘currying’ bijection between morphisms $[\Gamma] \times R \rightarrow R$ and morphisms $[\Gamma] \rightarrow [R \Rightarrow R]$. But measurable functions cannot do this: it is known that no measurable space $[R \Rightarrow R]$ can support such a bijection [3].

We resolve the problem of function spaces by embedding the category of measurable spaces in a larger one, where currying is possible, and that still has the structure to interpret the first order language as before. As the larger category we will take a category of functions $Meas^{op} \rightarrow \text{Set}$ from a category $\text{Meas}$ of measurable spaces and measurable functions to the category $\text{Set}$ of sets and functions. This idea arises from two traditions. First, we can think of a variable of type $R$ as a channel to a node in a random memory cell, as in the operational semantics, and functor categories have long been used to model local memory (e.g. [23]). Second, the standard construction for building a Cartesian closed category out of a distributive one is based on functor categories (e.g. [28]).

Other models of higher-order programs

Semantics of higher-order languages with discrete probability are understood well. For terminating programs, there are set-theoretic models based on a distributive monad, and for full recursion one can use probabilistic powerdomains [14] or coherence spaces [9]; our higher-order denotational semantics could be enriched in domains to support recursion. It is also plausible one could model continuous distributions in domain theory, since it supports computable real analysis (e.g. [8]); this could be interesting because computability is subtle for probabilistic programming (e.g. [1]). Nonetheless, we contend it is often helpful to abstract away computability issues when studying probabilistic programming languages, to have access to standard theorems of probability theory to justify program transformations.

8.1 Semantic model

Fix a category $\text{Meas}$ of measurable spaces and measurable functions that is essentially small but large enough for the purposes of Section 4. For example, $\text{Meas}$ could be the category of standard Borel spaces [4, 32]; one can show that $[A]$ is standard Borel by induction on $A$, and the class of all standard Borel spaces is countable up to measurable isomorphism.

In Section 4 we interpreted first-order types $A$ as measurable spaces $[A]$. We will interpret higher-order types $A$ as functors $[\Lambda] : \text{Meas}^{op} \rightarrow \text{Set}$. Informally, when $A$ is a first-order type and $\Gamma$ is a first-order context, we will have $[\Lambda][\Gamma] \simeq \text{Meas}([\Gamma], [\Lambda]) \simeq \{t : \Gamma \vdash A : t : A\}$. For a second order type $\Lambda \Rightarrow \beta$, we will have $[\Lambda](\beta) \simeq \text{Meas}([\Gamma] \times [\Lambda], [\beta]) \simeq \{t : \Gamma, x : A \vdash t : \beta\}$ so that $\beta/\eta$ equality is built in. To put it another way, $[\Lambda](\beta^n)$ models terms of type $\Lambda$ having $n$ read-only real-valued memory cells.

Lemma 8.1. For a small category $C$ with countable sums, consider the category $\mathcal{C}$ of countable-product-preserving functors $\text{C}^{op} \rightarrow \text{Set}$, and natural transformations between them.

- $\mathcal{C}$ has all colimits;
- $\mathcal{C}$ is Cartesian closed if $C$ has products that distribute over sums;
- There is a full and faithful embedding $\gamma : \mathcal{C} \rightarrow \mathcal{C}$, given by $y(c) \cong \mathcal{C}(-, c)$, which preserves limits and countable sums.

Proof. See e.g. [28, §7], or [15, Theorems 5.56 and 6.25]. The embedding $\gamma$ is called the Yoneda embedding.

For a simple example, consider the category $\mathcal{C} \text{Set}$ of countable sets and functions. It has countable sums and finite products, but is not Cartesian closed. Because every countable set is a countable sum of singletons, the category $\mathcal{C} \text{Set}$ is equivalent to $\text{Set}$.

Our semantics for the higher-order language will take place in the category $\text{Meas}$. Note that products in $\text{Meas}$ are pointwise, e.g. $(F \times G)(X) = F(X) \times G(X)$ for all $F, G \in \text{Meas}$ and all $X \in \text{Meas}$, but sums are not pointwise, e.g. $(i + 1) \in \text{Meas}$ is the functor that assigns a measurable space $X$ to the set of its measurable subsets. This is essential for $y$ to preserve sums.

Distribution types

We have to interpret distribution types $P(A)$ in our functor category $\text{Meas}$. How can we interpret a probability distribution on the type $\mathbb{R} \Rightarrow \mathbb{R}$? We can answer this pragmatically, without putting $\sigma$-algebra structure on the set of all functions. If $[\mathbb{R} \Rightarrow \mathbb{R}]$ were a measurable space, a random variable valued in $[\mathbb{R} \Rightarrow \mathbb{R}]$ would be given by a measurable space $(X, \Sigma_X)$, a probability distribution on it, and a measurable function $X \rightarrow [\mathbb{R} \Rightarrow \mathbb{R}]$. Despite there being no such measurable space $[\mathbb{R} \Rightarrow \mathbb{R}]$, we can speak of uncurried measurable functions $X \times \mathbb{R} \rightarrow \mathbb{R}$. Thus we might define a probability distribution on $[\mathbb{R} \Rightarrow \mathbb{R}]$ to be a triple $((X, \Sigma_X), f : X \times \mathbb{R} \rightarrow \mathbb{R}, p : \Sigma_X \rightarrow [0, 1])$ of a measurable space $(X, \Sigma_X)$ of ‘codes’, a measurable function $f$ where we think of $f(x, r)$ as ‘the function coded $x$ evaluated at $r$’, and a probability distribution $p$ on the codes. These triples should be considered modulo renaming the codes. This is exactly the notion of probability distribution that arises in our functor category.

Lemma 8.2. For a small category $C$ with countable sums:

- any functor $F : C \rightarrow C$ extends to a functor $F : \mathcal{C} \rightarrow \mathcal{C}$ satisfying $F \circ y \cong y \circ F$, given by $F(G)(b) = \left( \sum_a G(a) \times \mathcal{C}(b, F(a)) \right) / \sim$.
where the equivalence relation \( \sim \) is the least one satisfying
\[
(a', x, F g o f) \sim (a, G g(x), f);
\]
- similarly, any functor \( F : C \times C \to C \) in two arguments extends to a functor \( \mathcal{T} : C \times C \to C \), with \( \mathcal{T}(\omega \times y) \sim y o F \):
\[
\mathcal{T}(G, H)(c) = \left( \sum_{a \in A} G(a) \times H(b) \times C(c, F(a, b)) \right) / \sim
\]
- any natural transformation \( \alpha : F \to G \) between functors \( F, G : C \to C \) lifts to a natural transformation \( \alpha : \mathcal{T} \to \mathcal{T} \), and similarly for functors \( C \times C \to C \);
- and this is functorial, i.e. \( G \circ \mathcal{T} \cong G \circ \mathcal{T} \) and \( \mathcal{T} \circ \alpha = \mathcal{T} \circ \alpha \).

**Proof.** \( \mathcal{T}(G) \) is the left Kan extension of \( G \) along \( F \), see e.g. [15].

Direct calculation shows \( \mathcal{T}(G) \) preserves products if \( G \) does. \( \square \)

Thus the commutative monads \( P \) and \( T = P((\mathbb{R}_{\geq 0} \times (-))) \) on \( \text{Meas} \) lift to commutative monads \( P \) and \( T \cong \mathcal{T}(\mathbb{R}_{\geq 0} \times (-)) \) on \( \text{Meas} \). The latter monad captures the informal importance-sampling semantics advocated by the designers of Anglican [34].

8.2 Conservativity

We interpret the types of the higher order language as objects in \( \text{Meas} \) using its categorical structure.
\[
\begin{align*}
\langle \sum_{i \in I} A_i \rangle & \cong \prod_{i \in I} \langle A_i \rangle \quad \langle \mathbb{R} \rangle \cong \mathbb{R} \quad \langle \mathbb{P}(A) \rangle \cong \mathcal{T}(\langle A \rangle) \\
\langle A \times B \rangle & \cong \langle A \rangle \times \langle B \rangle \\
\langle A \Rightarrow B \rangle & \cong \langle A \rangle \Rightarrow \langle B \rangle
\end{align*}
\]

We extend this interpretation to contexts.
\[
\langle x_1 : A_1, \ldots, x_n : A_n \rangle \cong \prod_{i=1}^n \langle A_i \rangle
\]

Deterministic terms \( \Gamma \vdash t : A \) are interpreted as natural transformations \( \langle \Gamma \rangle \to \langle A \rangle \) in \( \text{Meas} \), and probabilistic terms \( \Gamma \vdash t : A \) as natural transformations \( \langle \Gamma \rangle \to T(\langle A \rangle) \), by induction on the structure of terms as in Section 4. Application and \( \lambda \)-abstraction are interpreted as usual in Cartesian closed categories [27]. Thunk and force are trivial from the perspective of the denotational semantics, because \( T(\langle \Gamma \rangle) = T(\langle A \rangle) \).

9. Continuous densities

In most examples, the argument \( t \) to \( \text{score}(t) \) is a density function for a probability distribution. When scores are based on density functions, this makes the relationship between score and sample tighter than we have expressed so far. Our language easily extends to accommodate such distributions. We just add a collection of density types to the syntax.
\[
\text{D ::= } \text{R} \mid \text{bool} \mid \text{N} \mid \text{D} \times \text{D} \quad A ::= \cdots \mid \text{D}(\text{D})
\]

The \( D \) in this grammar denotes a measurable space that: (i) carries a separable metrisable topology that generates the \( \sigma \)-algebra; and that (ii) comes with a chosen \( \sigma \)-finite measure \( \mu_0 \). An example is \( \text{R} \) with its usual Euclidean topology and the Lebesgue measure (which maps each interval to its size).

The type \( \text{D}(\text{D}) \) denotes a measurable space \( \text{D}(\text{D}) \) of continuous functions \( f : \text{D} \to \mathbb{R}_{\geq 0} \) with \( \int f \; d\mu_0 = 1 \). The \( \sigma \)-algebra of \( \text{D}(\text{D}) \) is the least one making \( \{ f \mid f(x) \leq r \} \) measurable for all \( (x, r) \in \text{D} \times \mathbb{R}_{\geq 0} \).
A density type $D(\mathbb{D})$ comes with two measurable functions

$$ev : [D(\mathbb{D})] \times [\mathbb{D}] \rightarrow \mathbb{R}_{\geq 0} \quad ev(f, x) = f(x)$$

$$dist : [D(\mathbb{D})] \rightarrow [P(\mathbb{D})] \quad dist(f)(U) = \int_U f \, d\mu$$

Note that measurability of $ev$ relies on continuity of the densities [3]. The usual way of imposing a soft constraint based on a likelihood can be encoded in our first-order language as score$(ev(f, x))$, where the datum $x$ is observed with a probability distribution with density $f$. Thus, the categorical machinery used to interpret higher-order functions is not needed for such soft constraints.

There is a limit to this use of continuity: probability measures produced by norm$(t)$ need not have continuous density. For example, norm$(\text{return}(42.0))$ produces a discontinuous Dirac measure.

Probability densities are often used by importance samplers. The importance sampler generates samples of $f \in [D(\mathbb{R})]$ by first sampling from a proposal distribution $g$ where sampling is easy, and then normalizing those samples $x$ from $g$ according to their importance weight $f(x)/g(x)$. This works provided the support of $g$ is $\mathbb{R}$, e.g. $g = \text{density}\_\text{gauss}(x, (0.0, 1.0))$.

$$\text{norm}(\text{sample}(dist(f))) = \left[ \text{norm}(let\ x = \text{sample}(dist(g)) \text{ in } \text{score}(ev(f, x)/ev(g, x); \text{return}(x)) \right]$$

Density types can be incorporated into the higher order language straightforwardly. The only subtlety is that denotational semantics now needs the base category to contain $[D(\mathbb{D})]$.

10. Conclusion and future work

We have defined a metalanguage for higher-order probabilistic programs with continuous distributions and soft constraints, and presented operational and denotational semantics, together with useful program equations justified by the semantics. One interesting next step is to use these tools to study other old or new language features and concepts (such as recursion, function memoisation [30], measure-zero conditioning [5], disintegration [2, 31], and exchangeability [10, 20, 34]) that have been experimented with in the context of probabilistic programming. Another future direction is to formulate and prove the correctness of inference algorithms, especially those based on Monte Carlo simulation, following [13].

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